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# Sistemas Fracamente Ligados de Três Corpos: Moléculas e Núcleos Exóticos Leves

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*Aos meus pais, Tomie e Takeshi,*

*aos quais nunca será demais agradecer,*
*e à minha companheira Raquel.*

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*"Observo-me a escrever como nunca me observei a pintar, e descubro o que há de fascinante neste acto: na pintura, vem sempre o momento em que o quadro não suporta nem mais uma pincelada (mau ou bom, ela irá torná-lo pior), ao passo que estas linhas podem prolongar-se infinitamente, alinhando parcelas de uma soma que nunca será começada, mas que é, nesse alinhamento, já trabalho perfeito, já obra definitiva porque conhecida. É sobretudo a ideia do prolongamento infinito que me fascina. Poderei escrever sempre, até o fim da vida, ao passo que os quadros, fechados em si mesmos, repelem, são eles próprios isolados na sua pele, autoritários, e, também eles, insolentes."*

José Saramago, Manual de Pintura e Caligrafia

# Resumo

Um potencial de dois corpos do tipo $\delta$-Dirac foi utilizado para descrever sistemas fracamente ligados de três corpos. A trajetória completa dos estados Efimov em função da energia ligação de dois corpos foi calculada para o caso de três bosons idênticos: se o subsistema de dois corpos é ligado, conforme a razão entre a energia de ligação de dois e três corpos aumenta, o estado excitado desaparece e um estado virtual correspondente aparece quando a energia do estado fundamental atinge o limiar dado por $6.9\hbar^2/(ma^2)$ ($a$ - comprimento de espalhamento, $m$ - massa do bóson). Quando o subsistema de dois corpos é virtual, o aumento da razão entre as energias faz com que o estado excitado se transforme em uma ressonância quando a energia do estado fundamental é $1.1\hbar^2/(ma^2)$. Neste último caso as condições para a formação de moléculas triatômicas no interior de condensados é favorecida, pois a competição com dímeros fracamente ligados está ausente. A energia de ligação de trímeros com momento angular total nulo em condensados atômicos foi estimada através da correlação desta com o coeficiente de recombinação e com a energia do dímero, ambos conhecidos experimentalmente em alguns casos. Os tamanhos de moléculas fracamente ligadas ($^4He_2$-X; X$\equiv^4$He, $^6$Li, $^7$Li e $^{23}$Na) e de núcleos exóticos leves ($^6$He, $^{11}$Li, $^{14}$Be e $^{20}$C) também foram calculados juntamente com um estudo sistemático do comportamento dos raios quadráticos médios conforme a interação dos subsistemas de dois corpos é variada. Neste último caso a classificação de um sistema de três corpos (tipo AAB) foi completada denominando de *Samba* a configuração formada por dois subsistemas de dois corpos ligados e um virtual. As equações subtraídas para os estados ligados de quatro bosons também foram deduzidas.

# Abstract

A pairwise Dirac-$\delta$ interaction was used to describe weakly bound three-body systems. The complete trajectory of an Efimov state as a function of the two-body energy was calculated for three identical bosons: if the two-body subsystem is bound, as the ratio of the two- and three-body binding energy grows up, the excited state disappears and a corresponding virtual state appears when the ground state energy hits the threshold given by $6.9\hbar^2/(ma^2)$ ($a$ - scattering length, $m$ - mass of the boson). When the two-body subsystem is virtual, the increase of the ratio between the energies turns an excited state into a resonance for a ground state energy greater than $1.1\hbar^2/(ma^2)$. This last case may be more favorable for the formation of condensed trimers in trapped ultracold monoatomic gases as the competition with the weakly bound dimers is absent. The energy of triatomic molecules with total angular momentum zero inside a condensate was estimated using its correlation with the three-body recombination coefficient and scattering length, both are known experimentally for some cases. The sizes of the weakly bound molecules ($^4He_2$-X; X$\equiv^4$He, $^6$Li, $^7$Li e $^{23}$Na) and the light exotic nuclei ($^6$He, $^{11}$Li, $^{14}$Be e $^{20}$C) were also calculated and together with a systematic study of the behavior of the root-mean-square distances as the two-body interaction is changed. In this last case the classification of a three-body system (AAB type) was completed denoting by *Samba* the configuration formed by two two-body subsystems bound and one virtual. The subtracted equations for the four-boson bound states were also deduced.

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# Capítulo 1

# Introdução

Sistemas fracamente ligados formados por três bosons com momento angular nulo exibem infinitos estados ligados conforme a energia de dois corpos tende a zero. Esses estados são chamados de estados Efimov [1, 2, 3]. Os estados Efimov, fracamente ligados, possuem uma função de onda que se estende muito além do alcance efetivo do potencial ($r_0$), ou em outras palavras, o comprimento de espalhamento de dois corpos, $a$, é muito maior que $r_0$, $\frac{a}{r_0} \gg 1$, justificando a utilização de potenciais do tipo $\delta$-Dirac para a descrição de propriedades desses sistemas. A interação de contato, ou alcance-zero, é o limite de potenciais de curto alcance e os observáveis dos sistemas físicos nos quais as partículas apresentam este tipo de interação dependem principalmente das escalas físicas que determinam os comportamentos assintóticos da função de onda. Nesta situação, aparecem no sistema de três corpos correlações entre os observáveis que independem do modelo do potencial e, portanto, apresentam uma universalidade nas predições quando as escalas físicas de dois e três corpos são mantidas fixas. O estudo dos estados Efimov aparece em vários artigos teóricos [4, 5, 6, 7, 8, 9, 10] tanto no campo da física atômica como nuclear, porém ainda não se tem uma evidência muita clara de seu aparecimento em trabalhos experimentais [3, 11, 12, 13, 14, 15, 16, 17].

A necessidade da adição de uma escala de três corpos independente da escala de dois corpos [18, 19] para descrever um observável deste sistema está relacio-

nada fisicamente com a possibilidade de colapso do sistema de três bosons na onda-$S$ em três dimensões conforme $r_0 \to 0$ mantendo-se a energia de dois corpos fixa. Isto é conhecido como colapso Thomas [20]. Uma questão que ainda continua em aberto seria se a cada bóson adicionado ao sistema haveria também a adição de uma nova escala física independente das outras escalas [18, 19]. No capítulo 2 nós mostraremos que fisicamente os efeitos Efimov e Thomas são equivalentes [21].

A existência do colapso Thomas introduz ainda, uma divergência nas equações para as componentes de Faddeev quando consideramos grandes momentos. Esse problema pode ser contornado com a introdução de um corte para momentos elevados [22, 23, 24] ou através da utilização das equações subtraídas cujo formalismo será discutido no capítulo 2. No capítulo 3 porém, onde estudamos a trajetória completa destes estados conforme variamos a energia de dois corpos, ficará claro que ambos os métodos são equivalentes e produzem o mesmo resultado numérico quando a energia de dois corpos vai para zero (ou o parâmetro de regularização vai para infinito). Ainda nesse capítulo nós analisamos a possibilidade de um estado excitado do trímero tornar-se um estado virtual conforme variamos as escalas físicas do sistema. Esses resultados vão além daqueles calculados na Ref. [15] onde a função de escala foi introduzida somente no contexto dos estados ligados, agora nós estendemos essa função para a segunda folha de Riemann no plano de energia para incluir os estados virtuais que aparecem conforme a razão entre as energias de ligação de dois e três corpos cresce. De forma a tornarmos completo o estudo da "trajetória"dos estados Efimov consideramos nesse capítulo a situação onde a energia de dois corpos é virtual, neste caso vemos que o estado ligado torna-se uma ressonância conforme a energia de dois corpos aumenta em módulo. A função de escala também é estendida para essa região.

Atualmente tem se estudado bastante os efeitos de grandes variações do comprimento de espalhamento de dois corpos no interior de armadilhas atômicas devido às mudanças de campos magnéticos externos próximos à ressonância de Feshbach do sistema átomo-átomo [25, 26, 27, 28, 29, 30]. Essa variação permite o estudo das correlações entre os observáveis do sistema de três átomos neutros e a verificação da universalidade à qual nos referimos no primeiro parágrafo. Embora ainda não

se tenha notícia da formação de moléculas triatômicas no interior de condensados, a formação de algumas moléculas diatômicas como $^{87}Rb_2$ [31] e $^{23}Na_2$ [32] já foi comprovada experimentalmente, todavia a dificuldade para a obtenção de trímeros é apenas experimental já que teoricamente não existe nenhum impedimento para a formação destas moléculas. No capítulo 4, através da correlação do coeficiente de recombinação de três corpos com as energias de dois e três corpos fazemos uma previsão das energias dos trímeros no interior dos condensados. A recombinação de três corpos é o processo pelo qual dois átomos livres no interior de armadilhas se combinam para formar um estado ligado (este processo necessita obviamente da participação de um terceiro átomo para que o momento total e a energia sejam conservados). Este processo contribui para a destruição de condensados e pode ser medido pelas perdas dos átomos da armadilha. O comprimento de espalhamento de dois corpos em átomos aprisionados também é conhecido na maioria dos experimentos e está diretamente relacionado à energia de ligação de dois corpos. Estas duas informações são suficientes para estimar a energia dos trímeros. Para interações de curto alcance a magnitude do coeficiente de recombinação é determinada principalmente pelo comprimento de espalhamento de dois corpos, porém todos os trabalhos nos quais aparece o coeficiente de recombinação também é apresentada a sua dependência com um parâmetro de três corpos [33, 34, 35], ou seja, a dependência de uma escala típica de três corpos ainda continua [18, 19, 25]. A validade da nossa aproximação é restrita a gases suficientemente diluídos, pois nossas relações de escala são derivadas de três partículas isoladas. A obtenção de moléculas triatômicas no interior de condensados pode ainda ser favorecida no contexto das ressonâncias ($a < 0$) calculadas no capítulo 3. Neste caso, os principais competidores das moléculas triatômicas - as moléculas diatômicas - estão ausentes.

Fora dos condensados a existência de moléculas fracamente ligadas é bem ilustrada pelo dímero de $^4$He [36, 37] que possui um tamanho $\sqrt{\langle r^2 \rangle} = 52 \pm 4$ Å e energia de ligação $E_2 = 1.1 + 0.3/ - 0.2$ mK [38]. Estudos teóricos mostram a possibilidade da existência de moléculas triatômicas fracamente ligadas para momento angular igual a zero, como, por exemplo, o trímero de $^4$He [39, 40]. Os cálculos para essa molécula [39] mostram que a distância entre um átomo de $^4$He e o centro-de-

massa (C.M.) do trímero varia de 6.4 a 6.5 Å para o estado fundamental e de 42.9 a 58.8 Å para o estado excitado. A distância entre dois átomos de $^4$He varia de 11.0 a 11.1 Å para o estado fundamental e de 74.8 a 102.0 Å para o estado excitado. Esses sistemas se estendem para regiões que estão bastante fora do alcance do potencial e são essencialmente uma solução da equação de Schrödinger livre, justificando a utilização de um potencial de curto-alcance e, conforme veremos no capítulo 5 - onde também calculamos os raios quadráticos médios para moléculas do tipo $^4$He-X, onde X $\equiv$ $^4$He, $^6$Li, $^7$Li e $^{23}$Na - o sistema de três corpos fica completamente definido por apenas duas escalas físicas, neste caso as energias de dois e três corpos.

Uma outra aplicação bastante interessante do potencial de alcance-zero pode ser verificada em núcleos exóticos. Estes núcleos, com elevado número de protons ou neutrons, localizam-se próximos das linhas de estabilidade e em alguns casos podem ser aproximados por um sistema de três corpos composto por um caroço e dois nucleons fracamente ligados [14, 25, 41, 42]. No capítulo 5 vamos considerar o caso de um núcleo composto por um caroço pontual ($C$) e dois neutrons ($n$). Nesta situação podemos ter quatro tipos de sistemas conforme modificamos a interação dos subsistemas de dois corpos: *Borromean* (os pares são completamente desligados), *All-Bound* (os pares são completamente ligados), *Tango* [43] (um par é ligado e dois pares são desligados) e *Samba* (dois pares são ligados e um par é desligado). Faremos cálculos para o $^6$He (*Borromean*), $^{11}$Li (*Borromean*), $^{14}$Be (*Borromean*) e $^{20}$C (*Samba*), veremos que os raios destes sistemas também podem ser representados como funções de escala universais escritas em termos de produtos adimensionais. Utilizando essas funções de escala nós podemos seguir o comportamento dos diferentes raios conforme acontece a transição entre as diversas possibilidades: iniciando de um sistema *Borromean* nós podemos ir para o tipo *Samba* aumentando a energia de ligação do par $nC$ mantendo $nn$ desligado, ou então para um sistema *Tango* aumentando a energia de ligação de $nn$ mantendo $nC$ desligado. Como os nossos cálculos restringem-se à onda-$S$ eles apresentam algumas limitações principalmente nos casos onde a interação do sistema de dois corpos na onda-$P$ poderia ser considerada importante para a energia de ligação de três corpos (por exemplo, $^5$He [44] e $^{10}$Li [45]). Todavia essa limitação é reduzida levando-se em conta que estamos considerando nos nossos cálculos as energias

de ligação medidas experimentalmente, as quais devem carregar o efeito das ondas parciais mais elevadas.

Os estudos feitos no contexto de três bosons podem também ser estendidos para quatro bosons. A questão levantada no primeiro parágrafo sobre a existência de novas escalas físicas adicionadas devido ao aumento do número de bosons pode ser estudada no contexto de quatro corpos. Isto pode ser evidenciado calculando-se a dependência da energia do estado ligado de quatro bosons com a respectiva escala introduzida nas equações para as amplitudes de Faddeev-Yakubovsky [46] através da subtração no propagador de quatro corpos (de forma análoga às equações subtraídas de três corpos). No capítulo 6 nós apresentamos essa formulação.

Em alguns artigos [47] a definição do sinal dos estados ligados e virtuais aparece diferente da nossa. Em unidades de $\hbar = m = 1$, onde $m$ é a massa de um dos constituintes do sistema de três corpos, temos que a amplitude de espalhamento de dois corpos na onda-$S$ em termos do momento $k$ é dada por: $f_0(k) = \frac{1}{k\cot\delta_0 - ik}$. Para baixas energias a expansão de alcance efetivo $k\cot\delta_0 = -a^{-1} + \frac{1}{2}r_0k^2 + ...$, fica igual a $k\cot\delta_0 = -a^{-1}$. Assim, $f_0(k) = \frac{1}{-a^{-1}-ik}$ e $a^{-1} = \pm\sqrt{E_2}$. O estado ligado é dado pelo sinal positivo e o virtual pelo sinal negativo. Adotamos essa convenção para o sinal do comprimento de espalhamento em analogia com o caso de um espalhamento em baixas energias ($k \approx 0$) por um poço quadrado (ver, por exemplo, Ref. [48]). Conforme vamos aumentando a profundidade do poço ocorre o aparecimento de um estado ligado e o comprimento de espalhamento que era negativo (na ausência do estado ligado) torna-se positivo.

Sumarizando: no capítulo 2 nós mostramos uma das formas de tratar a divergência nas equações de Faddeev para momentos grandes. Neste capítulo deduzimos as equações subtraídas onde são introduzidas as escalas físicas através do propagador de três corpos, veremos que os resultados são independentes do ponto de subtração como conseqüência da matriz-$T$ satisfazer uma equação do tipo Callan-Symanzik. No capítulo 3 nós estudamos os estados Efimov. Discutimos a equivalência entre os efeitos Efimov e Thomas. Fazemos um estudo sistemático das trajetórias desses estados conforme variamos a energia de ligação de dois corpos ($E_2$). Veremos que um

estado Efimov iniciado em um estado virtual para um valor elevado de $E_2$ (ligado), passa para um estado ligado conforme diminuímos $E_2$ [7], até "virar" finalmente uma ressonância conforme aumentamos em módulo o valor de $E_2$ (virtual) [49]. Ficará claro neste capítulo que os métodos utilizados para a regularização da equação da função espectadora - corte e subtração - são equivalentes [7]. No capítulo 4 relacionamos o coeficiente de recombinação de três corpos com as energias de dois e três corpos, mostramos que ele obedece a uma função de escala universal e conseguimos prever a energia de moléculas triatômicas no interior de condensados [8]. No capítulo 5 calculamos os tamanhos de algumas moléculas fracamente ligadas [9] e estendemos o estudo para o caso de núcleos exóticos [10]. Fazemos neste capítulo um estudo sistemático dos tamanhos de um sistema de três corpos genérico fracamente ligado conforme mudamos o tipo de interação de dois corpos [10]. No capítulo 6 nós apresentamos a dedução das equações para as amplitudes de Faddeev-Yakubovsky na forma subtraída. No capítulo 7 são apresentadas as conclusões.

# Capítulo 2

# Equações subtraídas - Formalismo

Neste capítulo descreveremos como são introduzidas as escalas físicas nas equações de Faddeev para a matriz de transição, $T$. Essas escalas aparecem na forma de uma subtração no propagador de três corpos e excluem a necessidade do uso de um corte para grandes momentos [18, 19].

O problema da não unicidade da solução da equação de Lippmann-Schwinger quando consideramos um sistema de três ou mais corpos foi solucionado em 1960 por L. D. Faddeev [50]. Uma revisão das equações de Faddeev para o caso de três partículas será feita a seguir.

## 2.1 Revisão das equações de Faddeev e notação

Consideremos a equação de Schrödinger para uma certa função de onda espalhada $\Psi^{(+)}$ (o sinal (+) indica uma função de onda esférica emergente):

$$(E - H_0)\Psi^{(+)} = (v_i + v_j + v_k)\Psi^{(+)}, \tag{2.1}$$

onde $v_i$, $v_j$ e $v_k$ são, respectivamente, os potenciais de interação entre as partículas $(j,k)$, $(i,k)$ e $(i,j)$. O hamiltoniano livre,

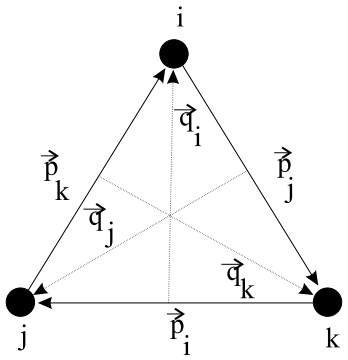


Figura 2.1: Coordenadas de Jacobi

$$H_0 = \sum_{\alpha=i,j,k} \frac{p_\alpha^2}{2m_\alpha}, \tag{2.2}$$

dado pela soma das energias cinéticas das partículas $i$, $j$ e $k$ ($p_\alpha$ e $m_\alpha$ são, respectivamente, o momento e a massa associados à partícula $\alpha = i, j, k$) escrito em termos das coordenadas de Jacobi da figura (2.1) (ver também apêndice A) no centro de massa é escrito como:

$$H_0 = \frac{p_\alpha^2}{2m_{\beta\gamma}} + \frac{q_\alpha^2}{2m_{\beta\gamma,\alpha}}, \tag{2.3}$$

onde $\beta, \gamma = i, j, k$ com $\alpha \neq \beta \neq \gamma$. As massas reduzidas $m_{\beta\gamma}$ e $m_{\beta\gamma,\alpha}$ são dadas por:

$$m_{\beta\gamma} = \frac{m_\beta m_\gamma}{(m_\beta + m_\gamma)};$$
$$m_{\beta\gamma,\alpha} = \frac{m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}.$$

As componentes de Faddeev para a função de onda de espalhamento correspondente a um estado inicial onde um par é ligado são dadas por:

$$\begin{aligned}\Psi^{(+)} &= G_0^{(+)}(E)(v_i+v_j+v_k)\Psi^{(+)} \\ &= \Psi_i^{(+)}+\Psi_j^{(+)}+\Psi_k^{(+)}, \end{aligned} \tag{2.4}$$

onde $G_0^{(+)} = \frac{1}{E-H_0+i\epsilon}$ é o propagador livre de três corpos e $\Psi_\alpha^{(+)} = G_0^{(+)}(E)v_\alpha\Psi^{(+)}$, $\alpha = i,j,k$. A função $\Psi_i^{(+)}$, por exemplo, pode ser escrita como:

$$\Psi_i^{(+)} = G_0^{(+)}(E)v_i\Psi^{(+)}, \tag{2.5}$$

e substituindo $\Psi^{(+)}$, temos que:

$$\Psi_i^{(+)} = G_0^{(+)}(E)v_i(\Psi_i^{(+)}+\Psi_j^{(+)}+\Psi_k^{(+)}); \tag{2.6}$$

$$(1-G_0^{(+)}(E)v_i)\Psi_i^{(+)} = G_0^{(+)}(E)v_i(\Psi_j^{(+)}+\Psi_k^{(+)}). \tag{2.7}$$

A função de onda de espalhamento para a partícula $i$ é dada somando-se o termo referente à onda plana:

$$\Psi_i^{(+)} = \Phi_i + (1-G_0^{(+)}(E)v_i)^{-1}G_0^{(+)}(E)v_i(\Psi_j^{(+)}+\Psi_k^{(+)}), \tag{2.8}$$

onde $\Phi_i$ é a "função de onda do estado ligado $jk \otimes$ onda plana i" e é solução da equação homogênea:

$$\begin{aligned}&(1-G_0^{(+)}(E)v_i)\Phi_i = 0; \\ &E = \frac{k_i^2}{2m_i}+E_{jk}^{lig},\end{aligned}$$

onde $E_{jk}^{lig}$ é a energia do estado ligado $jk$ e $\vec{k}_i$ é o momento associado à partícula $i$.

O operador que multiplica as componentes de Faddeev $j$ e $k$ na eq. (2.8) pode ainda ser escrito de outra forma, fazendo uso da matriz de transição de dois corpos do subsistema $j$ e $k$ ($t_i$):

$$\begin{aligned}
&t_i(E) = v_i + t_i(E)G_0^{(+)}(E)v_i = v_i + v_i G_0^{(+)}(E)t_i(E);\\
&G_0^{(+)}(E)t_i(E) = G_0^{(+)}(E)v_i + G_0^{(+)}(E)v_i G_0^{(+)}(E)t_i(E);\\
&(1 - G_0^{(+)}(E)v_i)G_0^{(+)}(E)t_i(E) = G_0^{(+)}(E)v_i;\\
&G_0^{(+)}(E)t_i(E) = (1 - G_0^{(+)}(E)v_i)^{-1}G_0^{(+)}(E)v_i. \qquad (2.9)
\end{aligned}$$

O lado direito de (2.9) é exatamente o operador aplicado a $\Psi_j^{(+)}$ e $\Psi_k^{(+)}$ na eq. (2.8). Substituindo (2.9) em (2.8) e escrevendo as componentes $j$ e $k$ que, obviamente, não possuem o termo não homogêneo, temos que:

$$\begin{cases}
\Psi_i^{(+)} = \Phi_i + G_0^{(+)}(E)t_i(E)[\Psi_j^{(+)} + \Psi_k^{(+)}];\\
\Psi_j^{(+)} = G_0^{(+)}(E)t_j(E)[\Psi_i^{(+)} + \Psi_k^{(+)}]; \qquad (2.10)\\
\Psi_k^{(+)} = G_0^{(+)}(E)t_k(E)[\Psi_i^{(+)} + \Psi_j^{(+)}].
\end{cases}$$

Na forma matricial a eq. (2.10) é escrita como:

$$\begin{pmatrix} \Psi_i^{(+)} \\ \Psi_j^{(+)} \\ \Psi_k^{(+)} \end{pmatrix} = \begin{pmatrix} \Phi_i \\ 0 \\ 0 \end{pmatrix} + G_0^{(+)}(E) \begin{pmatrix} 0 & t_i & t_i \\ t_j & 0 & t_j \\ t_k & t_k & 0 \end{pmatrix} \begin{pmatrix} \Psi_i^{(+)} \\ \Psi_j^{(+)} \\ \Psi_k^{(+)} \end{pmatrix}, \qquad (2.11)$$

cuja solução é dada por:

$$\begin{pmatrix} \Psi_i^{(+)} \\ \Psi_j^{(+)} \\ \Psi_k^{(+)} \end{pmatrix} = \left( 1 - G_0^{(+)}(E) \begin{bmatrix} 0 & t_i & t_i \\ t_j & 0 & t_j \\ t_k & t_k & 0 \end{bmatrix} \right)^{-1} \begin{pmatrix} \Phi_i \\ 0 \\ 0 \end{pmatrix}. \qquad (2.12)$$

Desta forma a não unicidade das soluções da equação de Lippmann-Schwinger para três corpos é eliminada na eq. (2.12) onde os termos homogêneos são distintos

para cada componente de Faddeev da função de onda $\Psi$. Da mesma forma que escrevemos as equações para as componentes de Faddeev da função de onda, também podemos escrever as componentes de Faddeev para a matriz de transição $T$ de três corpos, dada pela eq. (2.13):

$$T(z) = V + VG(z)V, \tag{2.13}$$

onde $G(z) = G_0(z) + G_0(z)T(z)G_0(z) = \frac{1}{z-H}$ e $H$ são, respectivamente, o propagador e o hamiltoniano completo de três corpos. $V = v_i + v_j + v_k$ é o somatório dos potenciais de dois corpos (a notação utilizada aqui é a mesma da dedução da função de onda). Separando a eq. (2.13) em três equações ($\alpha = i, j, k$):

$$T_\alpha = v_\alpha + v_\alpha G_0 T, \tag{2.14}$$

ou ainda na forma matricial:

$$\begin{pmatrix} T_i \\ T_j \\ T_k \end{pmatrix} = \begin{pmatrix} v_i \\ v_j \\ v_k \end{pmatrix} + \begin{pmatrix} v_i & v_i & v_i \\ v_j & v_j & v_j \\ v_k & v_k & v_k \end{pmatrix} G_0 \begin{pmatrix} T_i \\ T_j \\ T_k \end{pmatrix}. \tag{2.15}$$

Isolando $T_i$ da eq. (2.15)

$$(1 - v_i G_0)T_i = v_i + v_i G_0 (T_j + T_k), \tag{2.16}$$

e multiplicando por $(1 - v_i G_0)^{-1}$ pela esquerda chegamos à equação para $T_i$:

$$T_i = t_i + t_i G_0 (T_j + T_k), \tag{2.17}$$

onde $t_i = (1 - v_i G_0)^{-1} v_i$ é a matriz-$T$ de dois corpos para a componente de Faddeev $i$ (veja eq. (2.9)).

Escrevendo a eq. (2.17) para as outras componentes $T_j$ e $T_k$ temos finalmente as equações de Faddeev para a matriz-$T$:

$$\begin{pmatrix} T_i \\ T_j \\ T_k \end{pmatrix} = \begin{pmatrix} t_i \\ t_j \\ t_k \end{pmatrix} + \begin{pmatrix} 0 & t_i & t_i \\ t_j & 0 & t_j \\ t_k & t_k & 0 \end{pmatrix} G_0 \begin{pmatrix} T_i \\ T_j \\ T_k \end{pmatrix}. \tag{2.18}$$

Uma vez introduzidas as equações de Faddeev para a matriz-$T$ de três corpos, iremos agora escrevê-la na sua forma subtraída. Para isto precisamos da matriz-T para o potencial $\delta$-Dirac, a qual será deduzida na seção seguinte.

## 2.2 Matriz-$T$ para o potencial $\delta$-Dirac

Inicialmente vamos considerar o caso de dois corpos com um potencial separável $V$ singular. Escrevendo o potencial separável na forma de um operador

$$V = \lambda|\chi\rangle\langle\chi| \tag{2.19}$$

com $\langle\chi|\vec{p}\rangle = \langle\vec{p}|\chi\rangle = g(p)$ sendo o fator de forma do potencial (o fator de forma possui simetria esférica e para o caso do potencial $\delta$-Dirac $g(p) = 1$ (apêndice B)).

Substituindo $G(E)V$ por $G_0(E)T$ na equação (2.13) da matriz-$T$ e inserindo o potencial dado pela eq. (2.19) temos que:

$$T(E) = V + VG_0(E)T(E), \tag{2.20}$$

$$T(E) = \lambda|\chi\rangle\langle\chi| + \lambda|\chi\rangle\langle\chi|G_0(E)T(E), \tag{2.21}$$

multiplicando por $\langle\chi|G_0(E)$ pela esquerda e isolando-se $\langle\chi|G_0(E)T(E)$ chegamos a:

$$\langle\chi|G_0(E)T(E) = \lambda\langle\chi|G_0(E)|\chi\rangle\langle\chi| + \lambda\langle\chi|G_0(E)|\chi\rangle\langle\chi|G_0(E)T(E),$$

$$(1 - \lambda\langle\chi|G_0(E)|\chi\rangle)\langle\chi|G_0(E)T(E) = \lambda\langle\chi|G_0(E)|\chi\rangle\langle\chi|,$$

$$\langle\chi|G_0(E)T(E) = \frac{\lambda\langle\chi|G_0(E)|\chi\rangle\langle\chi|}{1 - \lambda\langle\chi|G_0(E)|\chi\rangle}. \tag{2.22}$$

Substituindo a eq. (2.22) em (2.20) temos a equação da matriz-$T$ de dois corpos:

$$T(E) = \lambda|\chi\rangle\langle\chi| + \frac{\lambda^2|\chi\rangle\langle\chi|G_0(E)|\chi\rangle\langle\chi|}{1 - \lambda\langle\chi|G_0(E)|\chi\rangle},$$

$$T(E) = \lambda|\chi\rangle\left(1 + \frac{\lambda\langle\chi|G_0(E)|\chi\rangle}{1 - \lambda\langle\chi|G_0(E)|\chi\rangle}\right)\langle\chi|. \tag{2.23}$$

A matriz-$T$ de dois corpos pode ainda ser escrita como:

$$T(E) = |\chi\rangle\tau(E)\langle\chi|, \tag{2.24}$$

onde $\tau$ é dada por:

$$\tau(E) = \frac{1}{\lambda^{-1} - \langle\chi|G_0(E)|\chi\rangle}. \tag{2.25}$$

Escrevendo explicitamente o elemento de matriz da eq. (2.24) temos que:

$$\tau(E) = \left(\lambda^{-1} - \int d^3p \frac{g(p)^2}{E - \frac{p^2}{2m_{red}} + i\epsilon}\right)^{-1}, \tag{2.26}$$

onde $m_{red}$ é a massa reduzida dos dois corpos. No caso do potencial $\delta$-Dirac o fator de forma do potencial $g(p)$ é igual a 1 e neste caso a integral que aparece na eq. (2.26) é divergente para grandes momentos. A divergência pode ser eliminada utilizando-se

um corte ou através da introdução de uma escala física (no capítulo seguinte será mostrado que os dois métodos são equivalentes). A informação física é introduzida atribuindo-se um valor físico, $\lambda_R$, para a matriz-$T$ num ponto de subtração de energia $E = -\mu_{(2)}^2$ (o índice entre parênteses subscrito em $\mu^2$ indica que estamos considerando a escala de 2-corpos), ou seja,

$$\tau_R(-\mu_{(2)}^2) = \lambda_R(-\mu_{(2)}^2). \tag{2.27}$$

o índice subscrito $R$ significa renormalizado.

Introduzindo a informação física na eq. (2.26) com o fator de forma do potencial já colocado igual a 1, temos que:

$$\tau_R(-\mu_{(2)}^2) = \left[\lambda^{-1} - \int d^3p \frac{1}{-\mu_{(2)}^2 - \frac{p^2}{2m_{red}}}\right]^{-1} = \lambda_R(-\mu_{(2)}^2),$$

$$\lambda^{-1} - \int d^3p \frac{1}{-\mu_{(2)}^2 - \frac{p^2}{2m_{red}}} = {\lambda_R}^{-1}(-\mu_{(2)}^2),$$

$$\lambda^{-1} = {\lambda_R}^{-1}(-\mu_{(2)}^2) + \int d^3p \frac{1}{-\mu_{(2)}^2 - \frac{p^2}{2m_{red}}}. \tag{2.28}$$

Substituindo agora o resultado de $\lambda^{-1}$ em (2.26) chegamos na forma da equação subtraída:

$$\tau_R^{-1}(E) = {\lambda_R}^{-1}(-\mu_{(2)}^2) + \int d^3p \left[\frac{1}{-\mu_{(2)}^2 - \frac{p^2}{2m_{red}}} - \frac{1}{E - \frac{p^2}{2m_{red}} + i\epsilon}\right],$$

$$\tau_R^{-1}(E) = {\lambda_R}^{-1}(-\mu_{(2)}^2) + (E + \mu_{(2)}^2) \int d^3p \frac{1}{\left(-\mu_{(2)}^2 - \frac{p^2}{2m_{red}}\right)\left(E - \frac{p^2}{2m_{red}} + i\epsilon\right)}. \tag{2.29}$$

Agora a integral que aparece em (2.29) é finita. Calculando a integral utilizando o método dos resíduos, substituindo a massa dos dois corpos e substituindo $E = k^2$

(em unidades de $\hbar = m = 1$), chegamos na forma final da equação da matriz-$T$ renormalizada para dois corpos idênticos:

$$\tau_R^{-1}(E) = \lambda_R^{-1}(-\mu_{(2)}^2) + 2\pi^2(\mu_{(2)} + ik). \tag{2.30}$$

Agora a eq. (2.30) pode ser interpretada em termos da amplitude de espalhamento, $f_0 \approx \frac{1}{-\frac{1}{a}-ik}$ (para $k$ tendendo a zero):

$$\begin{aligned} f_0 &= -2\pi^2\tau_R(E) \\ &= \frac{1}{-\frac{\lambda_R^{-1}(-\mu_{(2)}^2)}{2\pi^2} - \mu_{(2)} - ik}, \end{aligned}$$

assim para $\mu_{(2)} = 0$ temos que o comprimento de espalhamento é dado por $a = 2\pi^2\lambda_R(0)$.

## 2.3 Equação subtraída para a matriz-$T$

Para deduzirmos a equação subtraída para a matriz-$T$ de três corpos iremos substituir diretamente na equação da matriz-$T$ o potencial escrito em termos da matriz-$T$ definida no ponto de subtração. Veremos que esse método é geral, aplicando-se, também, ao caso de dois corpos. A seguir descreveremos o método das eqs. subtraídas [51, 52, 53].

Colocando o potencial $V$ em evidência na eq. (2.20) podemos escrever a eq. para a matriz-$T$ como:

$$T(E) = (1 + T(E)G_0^{(+)}(E))V,$$

calculando a matriz-$T$ no ponto de subtração de energia $E = -\mu^2$ podemos escrever V em termos da matriz-$T$ renormalizada $T_R(-\mu^2)$ como:

$$T(-\mu^2) = (1 + T(-\mu^2)G_0(-\mu^2))V,$$
$$V = (1 + T(-\mu^2)G_0(-\mu^2))^{-1}T(-\mu^2). \tag{2.31}$$

Substituindo V em $T(E) = V + VG_0^{(+)}(E)T(E)$ chegamos na equação para a matriz-$T$ na forma subtraída:

$$T_R(E) = T_R(-\mu^2) + T_R(-\mu^2)\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(E). \tag{2.32}$$

A eq. (2.32) deduzida no contexto de três corpos é geral, isto é, também podemos a partir dela chegar facilmente à equação para a matriz-$T$ de dois corpos na forma subtraída, eq. (2.30), apenas substituindo $T_R(-\mu^2)$ por $\lambda_R(-\mu^2)|\chi\rangle\langle\chi|$ (ver apêndice C). Iterando-se a eq. (2.32)

$$T_R^{(m)}(E) = T_R(-\mu^2)\sum_{n=0}^{m-1}\left[\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(-\mu^2)\right]^n, \tag{2.33}$$

e truncando a série no elemento $m+1$ referente ao termo que contém $T(E)$, vemos imediatamente que a subtração do kernel aparece em todas as propagações intermediárias até a ordem $m-1$. Devemos ressaltar que os resultados obtidos independem da escolha do ponto de subtração, ou seja, a princípio eles podem ser modificados desde que conheçamos o valor da matriz-$T$ no novo ponto de subtração. A independência da matriz-$T$ renormalizada em relação ao ponto de subtração pode ser demonstrada derivando-se a eq. (2.33) em relação a $\mu^2$ para $m \to \infty$:

$$\frac{d}{d\mu^2}T_R(E) = \frac{d}{d\mu^2}\left\{T_R(-\mu^2)\sum_{n=0}^{\infty}\left[\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(-\mu^2)\right]^n\right\}$$
$$= \frac{d}{d\mu^2}T_R(-\mu^2) + \frac{d}{d\mu^2}T_R(-\mu^2)\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(-\mu^2)$$
$$-T_R(-\mu^2)\frac{d}{d\mu^2}G_0(-\mu^2)T(-\mu^2) + T_R(-\mu^2)\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)\frac{d}{d\mu^2}T_R(-\mu^2) + ...$$
$$= \frac{1}{1 - T_R(-\mu^2)\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)}\left\{\frac{d}{d\mu^2}T_R(-\mu^2) - T_R(-\mu^2)\frac{1}{(\mu^2+H_0)^2}T_R(-\mu^2)\right\}$$
$$\times\frac{1}{1 - \left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(-\mu^2)}, \tag{2.34}$$

o termo que aparece entre chaves na eq. (2.34) é obtido substituindo-se $E$ por $-\mu'^2$ na eq. (2.32) e depois derivando-a em relação a $\mu^2$ no limite de $\mu' \to \mu$:

$$\frac{d}{d\mu^2}T_R(-\mu^2) - T_R(-\mu^2)\frac{1}{(\mu^2+H_0)^2}T_R(-\mu^2) = 0, \tag{2.35}$$

Assim demonstramos que:

$$\frac{d}{d\mu^2}T_R(E) = 0. \tag{2.36}$$

Podemos ainda reescrever a eq. (2.36) como:

$$\mu\frac{d}{d\mu}T_R(E) = 0, \tag{2.37}$$

que é uma equação do tipo Callan-Symanzik. Desta forma, podemos dizer que a invariância da matriz-$T$ renormalizada, $T_R(E)$, em relação ao ponto de subtração é conseqüência dela satisfazer a uma equação do tipo Callan-Symanzik [54].

## 2.4 Equações de Faddeev subtraídas

Para escrevermos as componentes de Faddeev da matriz-$T$ devemos retornar à eq. (2.32) escrita agora no contexto de 3-corpos [18, 19]:

$$T_R^{(3)}(E) = T_R^{(3)}(-\mu_{(3)}^2) + T_R^{(3)}(-\mu_{(3)}^2)\left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)T_R^{(3)}(E), \tag{2.38}$$

e definir a matriz-$T$ de três corpos no ponto de subtração como sendo a soma de todos os pares $(i,j)$ das matrizes-$T$ renormalizadas de dois corpos ($t_R$):

$$T_R(-\mu_{(3)}^2) = \sum_{\alpha=i,j,k} t_{R_\alpha}\left(-\mu_{(3)}^2 - \frac{q_\alpha^2}{2m_{\beta\gamma,\alpha}}\right), \tag{2.39}$$

onde $\alpha,\beta,\gamma = i,j,k$ com $\alpha \neq \beta \neq \gamma$ e $m_{\beta\gamma,\alpha}$ é a massa reduzida do par $\beta\gamma$ em relação à partícula espectadora $\alpha$. O elemento de matriz no espaço dos momentos relativos de $t_R(E)$ é $\langle\vec{p}\,'|t_R(E)|\vec{p}\rangle = \tau_R(E)$, com $\tau_R(E)$ dado pela eq. (2.30). O argumento da matriz-$T$ de dois corpos é a energia do centro de massa do par $(\beta\gamma)$, sendo que $q_\alpha$ é o momento relativo de Jacobi canonicamente conjugado à coordenada relativa da partícula $\alpha$ ao centro de massa de $(\beta\gamma)$ (vide fig. (2.1)). Daqui para frente a matriz-$T$ de dois corpos será representada por uma letra minúscula $t$ e a de três corpos por uma letra maiúscula $T$. O índice entre parênteses subscrito em $\mu^2$ indica se estamos considerando a escala de dois ou três corpos (note que para um potencial regular de alcance finito, a matriz-$T$ calculada em um ponto de subtração de energia finita $-\mu_{(3)}^2$ não pode ser definida como a soma dada pela eq. (2.39). Essa soma só é possível no limite $-\mu_{(3)}^2 \to \infty$. Assim a eq. (2.39) não se aplica no caso de $\mu$ finito e um potencial regular de dois corpos).

Substituindo a eq. (2.39) em (2.38) temos que:

$$T_R(E) = \sum_{\alpha=i,j,k} t_{R_\alpha}\left(-\mu_{(3)}^2 - \frac{q_\alpha^2}{2m_{\beta\gamma,\alpha}}\right)\left[1 + \left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)T_R(E)\right]. \tag{2.40}$$

A componente de Faddeev $k$ da matriz-$T$ de três corpos é escrita como:

$$T_{R_k}(E) = t_{R_k}\left(-\mu^2_{(3)} - \frac{q_k^2}{2m_{ij,k}}\right)\left[1 + \left(G_0^{(+)}(E) - G_0(-\mu^2_{(3)})\right)T_R(E)\right]. \qquad (2.41)$$

Escrevendo a matriz-$T$ de três corpos como sendo a soma de três matrizes $T_{R_\alpha}(E)$ $(\alpha = i, j, k)$ cada uma correspondente a um par interagente:

$$T_R(E) = \sum_{\alpha=i,j,k} T_{R_\alpha}(E), \qquad (2.42)$$

e finalmente substituindo-se a eq. (2.42) na eq. (2.41) podemos escrever a componente de Faddeev $k$ da matriz-$T$ em função das outras duas componentes $i$ e $j$:

$$T_{R_k}(E) = t_{R_k}\left(E - \frac{q_k^2}{2m_{ij,k}}\right)\left[1 + \left(G_0^{(+)}(E) - G_0(-\mu^2_{(3)})\right)\left(T_{R_i}(E) + T_{R_j}(E)\right)\right], \qquad (2.43)$$

onde foi utilizada a seguinte relação:

$$\begin{aligned} t_{R_k}\left(E - \frac{q_k^2}{2m_{ij,k}}\right) &= \left[1 - t_{R_k}\left(-\mu^2_{(3)} - \frac{q_k^2}{2m_{ij,k}}\right)\left(G_0^{(+)}(E) - G_0(-\mu^2_{(3)})\right)\right]^{-1} \\ &\quad \times t_{R_k}\left(-\mu^2_{(3)} - \frac{q_k^2}{2m_{ij,k}}\right), \end{aligned} \qquad (2.44)$$

obtida isolando-se $T_R(E)$ na eq. (2.32).

# Capítulo 3

# Os estados Efimov - Estados ligados, virtuais e ressonâncias

Partindo da equação subtraída para a matriz-$T$ de três corpos obtida na seção anterior, podemos deduzir a equação homogênea para os estados ligados e virtuais de três corpos idênticos. Nesta seção iremos também calcular as energias das ressonâncias no sistema de três corpos. Mostraremos que partindo-se de uma certa energia para o estado ligado de dois corpos e diminuindo o seu módulo, um estado virtual de três corpos torna-se ligado [7], esse estado ligado torna-se por sua vez uma ressonância quando a energia de dois corpos torna-se virtual [49].

Partindo-se da equação para a matriz-$T$ podemos inserir nela a seguinte relação de completeza:

$$\mathbf{1} = \sum_{L} |\Phi_L\rangle\langle\Phi_L| + \int d^3k |\Psi_k^{(+)}\rangle\langle\Psi_k^{(+)}|, \tag{3.1}$$

onde $|\Phi_L\rangle$ e $|\Psi_k^{(+)}\rangle$ são, respectivamente, a função de onda dos estados ligados e a função de onda de espalhamento das partículas de momento inicial igual a $\vec{k}$. Assim, inserindo a eq. (3.1) na equação da matriz-$T$, eq. (2.13) com $z = E$, temos que:

$$T(E) = V + \sum_L VG^{(+)}(E)|\Phi_L\rangle\langle\Phi_L|V + \int d^3k VG^{(+)}(E)|\Psi_k^{(+)}\rangle\langle\Psi_k^{(+)}|V;$$

$$T(E) = V + \sum_L \frac{V|\Phi_L\rangle\langle\Phi_L|V}{E - E_L + i\epsilon} + \int d^3k \frac{V|\Psi_k^{(+)}\rangle\langle\Psi_k^{(+)}|V}{E - \bar{E}_k + i\epsilon}, \tag{3.2}$$

onde o propagador completo, $G^{(+)}(E)$, foi escrito explicitamente em termos dos autovalores dos estados ligados, $E_L$, e dos estados de espalhamento, $\bar{E}_k$. A equação da matriz-$T$ escrita na forma da eq. (3.2) é chamada de equação de Low [55].

Para uma energia próxima a um estado ligado ($E \approx E_L$) temos que a segunda parcela é dominante (devido ao pólo correspondente ao estado ligado), assim:

$$T(E) \approx \frac{|\Gamma_L\rangle\langle\Gamma_L|}{E - E_L} = \frac{|\Gamma_L\rangle\langle\Gamma_L|}{E + |E_L|}, \tag{3.3}$$

onde a função de vértice para o estado ligado é definida por $|\Gamma_L\rangle = V|\Phi_L\rangle$. Observando a equação da matriz-$T$ para uma componente de Faddeev, eq. (2.14), vemos que neste caso a eq. (3.3) é escrita como:

$$T_\alpha(E) \approx \frac{|\Gamma_\alpha\rangle\langle\Gamma|}{E + |E_\alpha|}, \tag{3.4}$$

com $\alpha = i, j, k$, $|\Gamma_\alpha\rangle = v_\alpha|\Phi_\alpha\rangle$ e $\langle\Gamma| = \langle\Phi_\alpha|V$. Assim, substituindo a eq. (3.4) na eq. (2.43), temos que:

$$\frac{|\Gamma_k\rangle\langle\Gamma|}{E + |E_k|} \approx t_{R_k}\left(E - \frac{q_k^2}{2m_{ij,k}}\right)\left(1 + (G_0^{(+)}(E) - G_0(-\mu_{(3)}^2))\right.$$

$$\left.\times\left(\frac{|\Gamma_i\rangle\langle\Gamma|}{E + |E_k|} + \frac{|\Gamma_j\rangle\langle\Gamma|}{E + |E_k|}\right)\right), \tag{3.5}$$

onde $E_k$ é a energia do estado ligado do par $ij$. Para $E \to -|E_k|$ temos a equação homogênea:

$$|\Gamma_k\rangle = t_{R_k}\left(E - \frac{q_k^2}{2m_{ij,k}}\right)(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2))(|\Gamma_i\rangle + |\Gamma_j\rangle). \tag{3.6}$$

Escrevendo explicitamente a matriz-$T$ de dois corpos dada pela eq. (2.24) temos que:

$$|\Gamma_k\rangle = |\chi_k\rangle\tau\left(E - \frac{q_k^2}{2m_{k(ij)}}\right)\langle\chi_k|\left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)(|\Gamma_i\rangle + |\Gamma_j\rangle), \tag{3.7}$$

onde $\tau(E_2)$ é o elemento de matriz da matriz-T renormalizada dado pela eq. (2.30). A partir deste ponto usaremos a notação $\tau \equiv \tau_R$.

Multiplicando a eq. (3.7) por $\langle\vec{p}_k, \vec{q}_k|$ pela esquerda:

$$\langle\vec{p}_k, \vec{q}_k|\Gamma_k\rangle = \langle\vec{p}_k|\chi_k\rangle\tau\left(E - \frac{q_k^2}{2m_{ij,k}}\right)\langle\chi_k, \vec{q}_k|\left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)(|\Gamma_i\rangle + |\Gamma_j\rangle), \tag{3.8}$$

e utilizando que $\langle\vec{p}_k, \vec{q}_k|\Gamma_k\rangle = \langle\vec{p}_k|\chi_k\rangle\langle\vec{q}_k|f_k\rangle = f_k(\vec{q}_k)$ para o potencial $\delta$-Dirac, temos a equação homogênea do estado ligado de três corpos para a componente de Faddeev $k$:

$$f_k(\vec{q}_k) = \tau\left(E - \frac{q_k^2}{2m_{ij,k}}\right)\langle\chi_k, \vec{q}_k|\left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)(|\Gamma_i\rangle + |\Gamma_j\rangle), \tag{3.9}$$

No caso específico de três bosons idênticos, as três funções espectadoras são idênticas:

$$\langle\vec{q}_i|f_i\rangle = \langle\vec{q}_j|f_j\rangle = \langle\vec{q}_k|f_k\rangle, \tag{3.10}$$

e a eq. (3.9) fica então escrita como:

$$f_k(\vec{q}_k) = 2\tau \left( E - \frac{q_k^2}{2m_{ij,k}} \right) \langle \chi_k, \vec{q}_k | \left( G_0^{(+)}(E) - G_0(-\mu_{(3)}^2) \right) (|\chi_i\rangle |f_i\rangle) \,. \tag{3.11}$$

Calculando o elemento de matriz do lado direito da eq. (3.11) (apenas por economia de espaço no cálculo do elemento de matriz não iremos colocar a parte referente à subtração):

$$\langle \chi_k, \vec{q}_k | G_0^{(+)}(E) | \chi_i \rangle | f_i \rangle = \int d^3q_i' \langle \chi_k, \vec{q}_k | G_0^{(+)}(E) | \chi_i \rangle | \vec{q}_i\,' \rangle \langle \vec{q}_i\,' | f_i \rangle$$

$$= \int d^3q_i' d^3p_k d^3p_i \langle \chi_k, \vec{q}_k | \vec{p}_k \rangle \langle \vec{p}_k | G_0^{(+)}(E) | \vec{p}_i \rangle \langle \vec{p}_i | \chi_i, \vec{q}_i\,' \rangle f_i(\vec{q}_i\,')$$

$$= \int d^3q_i' d^3p_k d^3p_i \frac{g_k(\vec{p}_k) g_i(\vec{p}_i)}{E - \frac{q_k^2}{2m_{ij,k}} - \frac{p_k^2}{2m_{ij,k}}} \langle \vec{q}_k, \vec{p}_k | \vec{p}_i, \vec{q}_i\,' \rangle f_i(\vec{q}_i\,'). \tag{3.12}$$

Relacionando as coordenadas de Jacobi (vide figura (2.1) e apêndice A), temos que o elemento de matriz $\langle \vec{q_k}\vec{p_k} | \vec{p_i}\vec{q_i}' \rangle$ é dado por:

$$\langle \vec{q_k}\vec{p_k} | \vec{p_i}\vec{q_i}\,' \rangle = \delta(\vec{q}_k + \frac{\vec{q}_i\,'}{2} + \vec{p}_i) \delta(\vec{p}_k - \frac{\vec{q}_k}{2} - \vec{q}_i\,'), \tag{3.13}$$

substituindo também as massas, $m_i = m_j = m_k = 1$, a eq. (3.12) se reduz a:

$$\int d^3q_i' d^3p_k d^3p_i \frac{g_k(\vec{p}_k) g_i(\vec{p}_i)}{E - \frac{q_k^2}{2m_{ij,k}} - \frac{p_k^2}{2m_{ij,k}}} \langle \vec{q}_k, \vec{p}_k | \vec{p}_i, \vec{q}_i\,' \rangle f_i(\vec{q}_i\,')$$

$$= \int d^3q_i' d^3p_k d^3p_i \frac{g_k(|\vec{p}_k|) g_i(|\vec{p}_i|)}{E - \frac{3}{4}q_k^2 - p_k^2} \delta(\vec{q}_k + \frac{\vec{q}_i\,'}{2} + \vec{p}_i) \delta(\vec{p}_k - \frac{\vec{q}_k}{2} - \vec{q}_i\,') f_i(\vec{q}_i\,')$$

$$= \int d^3q_i' \frac{g_k\left( |\vec{q}_i\,' + \frac{\vec{q}_k}{2}| \right) g_i\left( |\frac{\vec{q}_i\,'}{2} + \vec{q}_k| \right)}{E - \frac{3}{4}q_k^2 - \left( \vec{q}_i\,' + \frac{\vec{q}_k}{2} \right)^2} f_i(\vec{q}_i\,')$$

$$= \int d^3q_i' \frac{1}{E - q_k^2 - q_i'^2 - \vec{q}_i\,' \cdot \vec{q}_k} f_i(\vec{q}_i\,'), \tag{3.14}$$

onde utilizamos que o fator de forma para o potencial $\delta$-Dirac $g_k = g_i = 1$. Desta forma, substituindo o elemento de matriz dado pela eq. (3.14) (note que a parte referente à subtração é idêntica à eq. (3.14) com exceção da energia $E$ que é substituída por $-\mu_{(3)}^2$) na eq. (3.12), e fazendo $q_i' \equiv q'$ e $q_k \equiv q$, temos a equação para o estado ligado de três bosons idênticos:

$$f(\vec{q}) = 2\tau\left(E - \frac{3}{4}q^2\right)\int d^3q'\left(\frac{1}{E - q^2 - q'^2 - \vec{q}'\cdot\vec{q}} - \frac{1}{-\mu_{(3)}^2 - q^2 - q'^2 - \vec{q}'\cdot\vec{q}}\right) f(\vec{q}'). \tag{3.15}$$

Introduzindo a informação física do estado ligado $\lambda_R^{-1}(-\mu_{(2)}^2) = 0$, onde $-\mu_{(2)}^2$ é a energia do estado ligado de dois corpos, na função $\tau$ dada pela eq. (2.30), temos que:

$$\tau\left(E - \frac{3}{4}q^2\right) = \frac{1/2\pi^2}{\mu_{(2)} - \sqrt{-E + \frac{3}{4}q^2}} \tag{3.16}$$

Escrevendo a eq. (3.15) para a onda-$S$, temos que:

$$f(\vec{q}) = \frac{\pi^{-2}}{\mu_{(2)} - \sqrt{-E + \frac{3}{4}q^2}}\int d^3q'\left(\frac{1}{E - q^2 - q'^2 - \vec{q}'\cdot\vec{q}} - \frac{1}{-\mu_{(3)}^2 - q^2 - q'^2 - \vec{q}'\cdot\vec{q}}\right) f(\vec{q}'). \tag{3.17}$$

Esta equação sem o segundo termo onde aparece $\mu_{(3)}$ foi obtida pela primeira vez por Skorniakov e Ter-Martirosian [56].

Realçando a integração angular na eq. (3.17), temos que a função espectadora na onda-$S$ (que corresponde à função de onda de três bosons com momento angular orbital total nulo) fica igual a:

$$\begin{aligned} f(q) \;=\; & \frac{2/\pi}{\mu_{(2)} - \sqrt{-E + \frac{3}{4}q^2}}\int_0^\infty dq'q'^2\int_1^{-1} dz\left(\frac{1}{E - q^2 - q'^2 - q'qz}\right. \\ & \left. - \frac{1}{-\mu_{(3)}^2 - q^2 - q'^2 - q'qz}\right) f(q'). \end{aligned} \tag{3.18}$$

Reescrevendo as variáveis como $\epsilon_{3L} = \frac{-E}{\mu_{(3)}^2}$, $y = \frac{q}{\mu_{(3)}}$ e $x = \frac{q'}{\mu_{(3)}}$ e fazendo $\mu_{(3)} = 1$ temos que:

$$f(y) = \frac{-2/\pi}{\pm\sqrt{\epsilon_2} - \sqrt{\epsilon_{3L} + \frac{3}{4}y^2}} \int_0^\infty dx x^2 \int_1^{-1} dz \left[ \frac{1}{\epsilon_{3L} + y^2 + x^2 + xyz} - \frac{1}{1 + y^2 + x^2 + xyz} \right] f(x), \tag{3.19}$$

onde substituímos $\frac{\mu_{(2)}}{\mu_{(3)}}$ por $\pm\sqrt{\epsilon_2}$, sendo $\epsilon_2$ a energia de dois corpos, o sinal positivo refere-se ao estado ligado e o negativo ao estado virtual. $\epsilon_{3L}$ é a energia do estado ligado de três corpos em unidades de $\mu_{(3)}^2$.

A eq. (3.19) utilizada para calcular o estado ligado de três bosons idênticos também será utilizada para o cálculo das ressonâncias de três bosons. Neste caso, iremos considerar somente as energias dos estados virtuais de dois corpos representado pelo sinal negativo em frente a $\sqrt{\epsilon_2}$. Para calcular as ressonâncias e suas larguras iremos utilizar o método do desvio de contorno [57, 58]. Neste método a continuação analítica para a segunda folha é feita substituindo-se $x(y) \to xe^{-i\theta}(ye^{-i\theta})$, com $0 < \theta < \pi/4$. Para um ângulo $\theta$ suficientemente grande a solução da eq. (3.19) no plano complexo é encontrada para $\mathrm{tg}(2\theta) > -Im(\epsilon_3)/Re(\epsilon_3)$.

Para calcularmos a energia do estado virtual de três bosons vamos fazer a extensão analítica da eq. (3.19) para a segunda folha de Riemann passando pelo corte do espalhamento elástico (vide figura (3.1)). Na fig. (3.1) está representada esquematicamente a energia do sistema ligado de dois corpos, $-\epsilon_2$, e as energias de três corpos, $-\epsilon_{3L}$ e $-\epsilon_{3V}$, no plano de energia. Podemos ver na figura que o corte do espalhamento elástico define duas folhas de Riemann: na primeira folha está localizada a energia para o estado ligado de três corpos, $Re(\epsilon) = -\epsilon_{3L}$, e na segunda folha o estado virtual de três corpos, $Re(\epsilon) = -\epsilon_{3V}$ [59, 60]. Assim, definindo $h(\eta) \equiv \left(\epsilon_2 - \epsilon_{3L} - \frac{3}{4}y^2\right) f(\eta)$ podemos escrever a eq. (3.19) na primeira folha como:

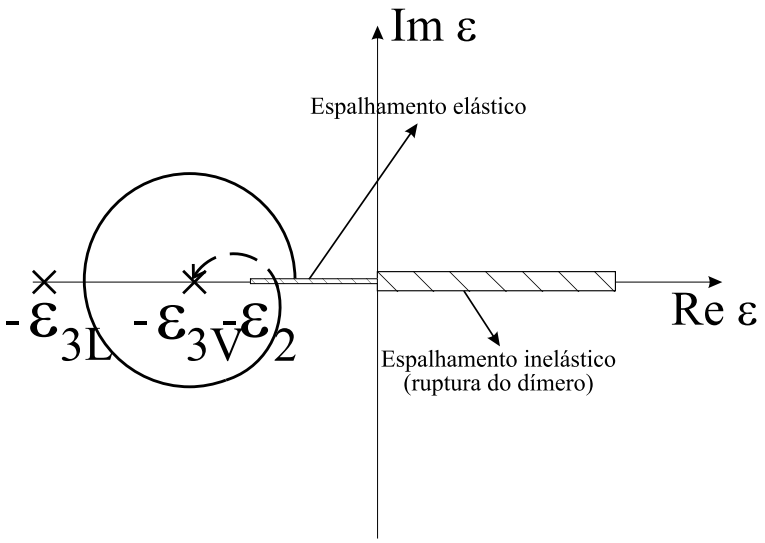


Figura 3.1: Extensão da matriz-$T$ de três corpos para a segunda folha de Riemann no plano de energia. $-\epsilon_2$ é a energia do estado ligado de dois corpos, $-\epsilon_{3L}$ é a energia do estado ligado de três corpos (localizada na primeira folha de Riemann) e $-\epsilon_{3V}$ é a energia do estado virtual (localizada na segunda folha).

$$h(y) = - \frac{2}{\pi}\left(\sqrt{\epsilon_2} + \sqrt{\epsilon_{3L} + \frac{3}{4}y^2}\right)\int_0^\infty dx x^2 \int_1^{-1} dz \left[\frac{1}{\epsilon_{3L} + y^2 + x^2 + xyz}\right.$$
$$\left. - \frac{1}{1 + y^2 + x^2 + xyz}\right]\frac{h(x)}{\epsilon_2 - \epsilon_{3L} - \frac{3}{4}x^2 + i\delta} \tag{3.20}$$

Podemos notar que o denominador $\epsilon_2 - \epsilon_{3L} - \frac{3}{4}x^2 + i\delta$ que aparece sob a função $h(x)$ pode ser interpretado como a função de Green do sistema ligado de dois corpos na presença de um terceiro corpo se aproximando do centro de massa dos dois corpos com energia cinética igual a $\frac{3}{4}x^2$, conforme mostra a figura (3.2) (obviamente essa interpretação é qualitativa tendo em vista que $\epsilon_{3L}$ e $x$ são adimensionais):

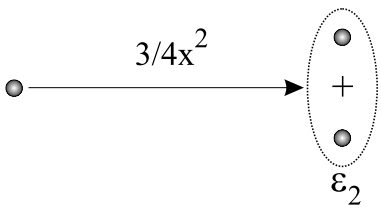


Figura 3.2: Terceira partícula se aproximando do dímero de energia de ligação $\epsilon_2$ com uma energia cinética de $\frac{3}{4}x^2$.

A extensão para segunda folha da eq. (3.20) é feita somando-se e subtraíndo-se o termo referente à descontinuidade da equação para a segunda folha (para ilustrar o método utilizado no caso de três corpos, uma dedução detalhada da extensão da equação da matriz-$T$ de dois corpos é feita no apêndice E):

$$\begin{aligned} h^{2^a}(y) &= -\frac{2}{\pi}\left(\pm\sqrt{\epsilon_2}+\sqrt{\epsilon_{3V}+\frac{3}{4}y^2}\right)\int_0^\infty dx x^2\int_1^{-1}dz\left[\frac{1}{\epsilon_{3V}+y^2+x^2+xyz}\right. \\ &- \left.\frac{1}{1+y^2+x^2+xyz}\right]\left[\frac{1}{\epsilon_2-\epsilon_{3V}-\frac{3}{4}x^2+i\delta}-\frac{1}{\epsilon_2-\epsilon_{3V}-\frac{3}{4}x^2-i\delta}\right]h(x) \\ &- \frac{2}{\pi}\left(\pm\sqrt{\epsilon_2}+\sqrt{\epsilon_{3V}+\frac{3}{4}y^2}\right)\int_0^\infty dx x^2\int_1^{-1}dz\left[\frac{1}{\epsilon_{3V}+y^2+x^2+xyz}\right. \\ &- \left.\frac{1}{1+y^2+x^2+xyz}\right]\frac{h(x)}{\epsilon_2-\epsilon_{3V}-\frac{3}{4}x^2-i\delta}. \end{aligned} \tag{3.21}$$

$\epsilon_{3L}$ foi substitído por $\epsilon_{3V}$ somente para distinguirmos as energias ligadas e virtuais de três corpos. Calculando a primeira integral utilizando o método dos resíduos (vide apêndice E) e substituindo $\epsilon_2-\epsilon_{3V}\equiv\frac{3}{4}\kappa^2$ (note que para o caso do estado virtual de três corpos $\kappa$ é definido como $\kappa\equiv -i\sqrt{\frac{4}{3}(\epsilon_{3V}-\epsilon_2)}\equiv -i\kappa_V$) chegamos na forma final para $h^{2^a}(y)$:

$$\begin{aligned} h^{2^a}(y) &= \frac{8}{3}i\kappa\left(\pm\sqrt{\epsilon_2}+\sqrt{\epsilon_{3V}+\frac{3}{4}y^2}\right) \\ &\times\int_1^{-1}dz\left[\frac{1}{\epsilon_{3V}+y^2+\kappa^2+\kappa yz}-\frac{1}{1+y^2+\kappa^2+\kappa yz}\right]h(\kappa) \\ &- \frac{2}{\pi}\left(\pm\sqrt{\epsilon_2}+\sqrt{\epsilon_{3V}+\frac{3}{4}y^2}\right)\int_0^\infty dx x^2\int_1^{-1}dz\left[\frac{1}{\epsilon_{3V}+y^2+x^2+xyz}\right. \\ &- \left.\frac{1}{1+y^2+x^2+xyz}\right]\frac{h(x)}{\epsilon_2-\epsilon_{3V}-\frac{3}{4}x^2-i\delta}. \end{aligned} \tag{3.22}$$

A energia do estado virtual de três corpos é limitada pelo corte na amplitude de espalhamento elástica que é dado pelo pólo da função de Green de três corpos

no primeiro termo da eq. (3.22),

$$\epsilon_{corte} + y^2 + x^2 + xyz = 0, \tag{3.23}$$

com $x = y = -i\kappa_{corte}$. Resolvendo a eq. (3.23) temos que o corte corresponde às energias que estão contidas no limite de

$$\frac{4}{3}|\epsilon_2| \leq |\epsilon_{corte}| \leq 4|\epsilon_2|, \tag{3.24}$$

como a energia do estado virtual deve estar fora do intervalo dado pela eq. (3.24) e obviamente deve ser maior que $|\epsilon_2|$, concluímos que a energia para o estado virtual deve ser maior que $|\epsilon_2|$ e menor que $\frac{4}{3}|\epsilon_2|$.

Os resultados para este capítulo são encontrados resolvendo-se as equações subtraídas (3.19) e (3.22). Os resultados serão comparados com cálculos realísticos e com o resultado da equação com corte para grandes momentos [21]. A equação do estado ligado utilizando o corte para grandes momentos é dada na Ref. [21] (colocaremos aqui somente a equação para o estado ligado para nortear nossa discussão sobre os estados Efimov, o colapso Thomas e a introdução da função de escala. A equação para o estado virtual com o corte nos momentos pode ser deduzida da mesma forma que foi feita a dedução no caso das equações subtraídas):

$$\chi(\vec{y}) = \frac{-\pi^{-2}}{\pm\sqrt{\epsilon_2} - \sqrt{\epsilon_3 + \frac{3}{4}y^2}} \int d^3x \frac{\theta(1-|\vec{x}|)}{\epsilon_3 + y^2 + x^2 + \vec{y}\cdot\vec{x}}\chi(\vec{x}), \tag{3.25}$$

onde o corte, $\Lambda$, foi colocado igual a 1 e os momentos e as energias de dois e três corpos foram reescalonados como $\vec{p} = \Lambda\vec{x}$, $\vec{q} = \Lambda\vec{y}$, $E_2 = \Lambda^2\epsilon_2$, e $E_3 = \Lambda^2\epsilon_3$. O número de estado ligados de três corpos $\epsilon_3 = \epsilon_3^{(N)}$ $(N = 0, 1, 2, ...)$ aumenta infinitamente conforme $\epsilon_2$ tende a zero e nesse limite satisfaz a razão $\epsilon_3^{(N)}/\epsilon_3^{(N+1)} \approx 500$ [1, 2]. Note que $\epsilon_2$ tende a zero se a energia de dois corpos, $E_2$, vai para zero (mantendo-se fixo $\Lambda$), ou se o corte $\Lambda$ vai para infinito (mantendo-se $E_2$ fixa). Este último caso equivale a

fazermos o alcance do potencial, $r_0$, tender a zero ($\Lambda \sim r_0^{-1}$), nesta situação o sistema de três corpos colapsa, $E_3^{(0)} = \Lambda^2 \epsilon_3^{(0)} \to \infty$. Esse colapso é conhecido como colapso Thomas do estado fundamental de três corpos. Assim, podemos ver claramente que os efeitos Efimov e Thomas são fisicamente equivalentes e são dados pelo mesmo limite, $\epsilon_2 \to 0$, estando relacionados apenas por uma transformação de escala [21].

O conceito de função de escala será introduzido conforme a Ref. [15] e generalizado para o caso dos estados virtuais. As soluções da eq. (3.25) são as "energias"adimensionais que são funções de $\pm\sqrt{\epsilon_2}$: $\epsilon_3^{(N)} = \epsilon_3^{(N)}(\pm\sqrt{\epsilon_2})$, assim utilizando o $N^{\text{ésimo}}$ estado da energia para obter $\Lambda$ temos que:

$$E_3^{(N+1)} = E_3^{(N)} \frac{\epsilon_3^{(N+1)}(\xi)}{\epsilon_3^{(N)}}, \tag{3.26}$$

onde $\xi \equiv \pm\sqrt{\epsilon_2} = \pm\sqrt{E_2(\epsilon_3^{(N)}/E_3^{(N)})}$. Podemos ver na eq. (3.26) que as escalas físicas de dois e três corpos determinam o estado $E_3^{(N+1)}$, o estado excitado acima de $E_3^{(N)}$. A razão entre as energias escrita conforme a eq. (3.26) não é ambígua, pois o limite:

$$\frac{E_3^{(N+1)}}{E_3^{(N)}} = \lim_{N\to\infty} \frac{\epsilon_3^{(N+1)}(\xi)}{\epsilon_3^{(N)}} = \mathcal{F}\left(\pm\sqrt{\frac{E_2}{E_3^{(N)}}}\right), \tag{3.27}$$

existe e define a função de escala $\mathcal{F}$ (um argumento qualitativo para a existência desse limite é dado na Ref. [15]. O termo "limite de escala"é o mesmo que o termo "*limit cycle*"discutido por K. Wilson na Ref. [61]). A generalização da eq. (3.27) para as energias do estado virtual de três corpos é escrita como:

$$\mathcal{K}\left(\sqrt{\frac{E_2}{E_3^{(N)}}}\right) \equiv \pm\sqrt{\frac{E_3^{(N+1)} - E_2}{E_3^{(N)}}} = \pm\sqrt{\frac{\epsilon_3^{(N+1)} - \epsilon_2}{\epsilon_3^{(N)}}}. \tag{3.28}$$

A função $\mathcal{K}$ tem os seus valores definidos nas duas folhas de Riemann no espaço dos momentos com origem no ponto onde as energias de dois e três corpos, $\epsilon_2$ e $\epsilon_3$, são iguais. A energia do subsistema de dois corpos foi colocada sempre ligada. Os sinais positivo e negativo definem, respectivamente, os estados ligados e virtuais de três

corpos.

No caso das energias das ressonâncias dos três corpos a função de escala é escrita como (a energia de dois corpos foi colocada sempre virtual):

$$\mathcal{R}\left(\sqrt{\frac{\epsilon_2}{\epsilon_{3L}}}\right) = \pm\sqrt{\frac{\epsilon_3}{\epsilon_{3L}}}, \tag{3.29}$$

O sinal $\pm$ fora dos parênteses indica se estamos considerando uma energia para uma ressonância $(+)$ ou um estado ligado $(-)$.

De forma a generalizar as funções de escala, podemos dizer que a existência de uma escala de três corpos em sistemas de três corpos em baixas energias implica na existência de uma função universal que correlaciona os observáveis de três corpos [18, 19, 62]. No limite de escala, ou *limit cycle*, ela pode ser escrita como:

$$\mathcal{O}\left(E, E_3, E_2\right) = (E_3)^{\eta}\mathcal{B}\left(\sqrt{E/E_3}, \pm\sqrt{E_2/E_3}\right) \tag{3.30}$$

onde $\mathcal{O}$ é qualquer observável do sistema de três corpos em uma energia $E$, com dimensão de energia elevada à potência $\eta$. O sinal $\pm$ indica se estamos considerando um estado ligado ou virtual de dois corpos.

A seguir serão descritos os resultados desta seção. Na fig. (3.3) mostramos o aparecimento dos estados virtuais e ligados conforme variamos a energia de ligação de dois corpos.

Nesta figura mostramos somente os três primeiros estados ligados, mas podemos ver claramente que conforme a energia de dois corpos tende a zero um número crescente de estados fracamente ligados de Efimov aparece. Na fig. (3.3) podemos, ainda, ver a natureza dos estados Efimov conforme variamos a energia de dois corpos: para uma energia $\epsilon_2$ da ordem de $10^{-1}$ vemos que existe somente o estado fundamental $\epsilon_{3L}^{(0)}$ (linha com cruzes). Neste caso, $\epsilon_2$ é muito grande para que exista o primeiro estado excitado, esse estado encontra-se na segunda folha de Riemann e corresponde a um estado virtual, representado pelos círculos. Conforme diminuímos

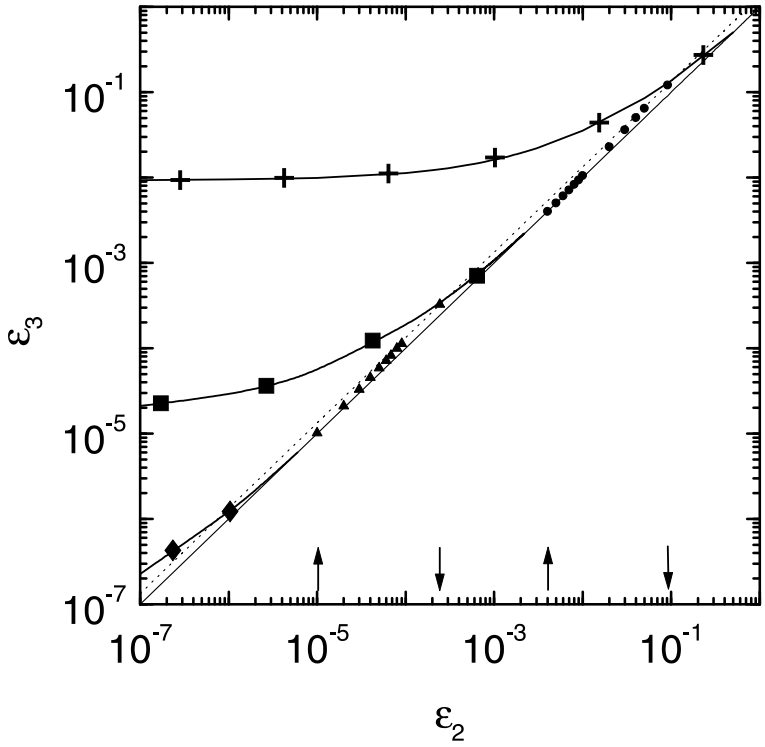


Figura 3.3: Energias dos trímeros $\epsilon_3$, em unidades de $\mu_{(3)} = 1$ em função da energia do estado ligado do dímero $\epsilon_2$. O estado fundamental, $\epsilon_{3L}^{(0)}$, está representado pela linha com cruzes, o primeiro estado excitado, $\epsilon_{3L}^{(1)}$, pela linha com quadrados e o segundo estado excitado, $\epsilon_{3L}^{(2)}$, pela linha com losangos. O estados virtuais $\epsilon_{3V}^{(1)}$ e $\epsilon_{3V}^{(2)}$ estão representados, respectivamente, pelos círculos e triângulos localizados entre os limites definidos pelas linhas pontilhada, $\epsilon_3 = \frac{4}{3}\epsilon_2$, e sólida $\epsilon_3 = \epsilon_2$.

$\epsilon_2$ o estado virtual correspondente ao primeiro estado excitado "sai"da segunda folha para tornar-se um estado ligado (linha com quadrados). Esse processo se repete conforme a energia de dois corpos tende a zero. O ponto onde o estado virtual de três corpos surge é dado pela seta para baixo, $\downarrow$, que começa no limiar do corte do espalhamento elástico, $\epsilon_3 = (4/3)\epsilon_2$, dado pela linha pontilhada. A seta para cima, $\uparrow$, indica o ponto onde o estado virtual torna-se um estado excitado, este emerge da segunda folha para a primeira em $\epsilon_3 = \epsilon_2$ (linha contínua).

Na fig. (3.4) a transição de um estado virtual para um estado ligado pode ser vista claramente. Esta figura foi construída utilizando-se o primeiro e o segundo estado Efimov. Este resultado praticamente não difere daquele obtido com o segundo e o terceiro estado Efimov (não colocamos na figura).

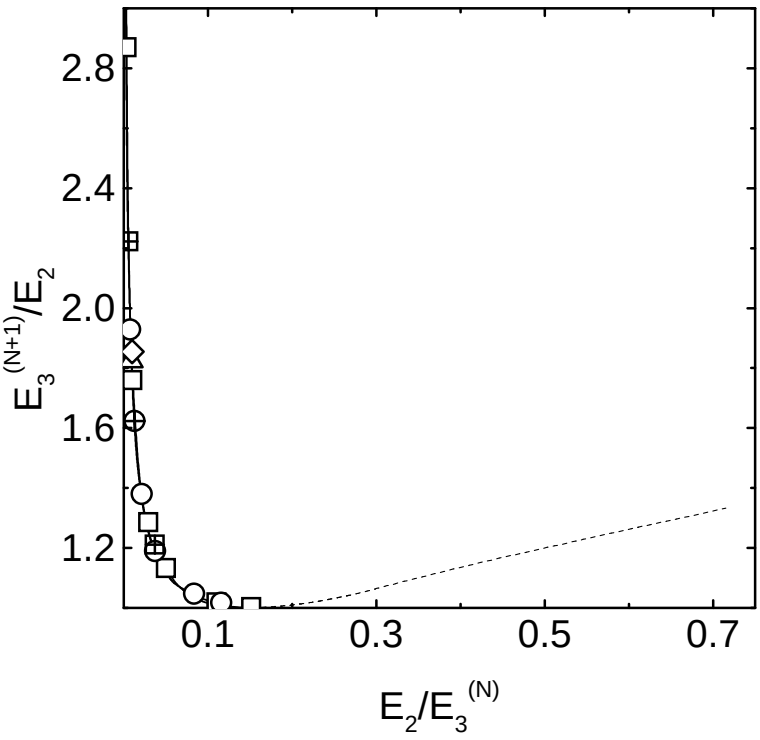


Figura 3.4: Razão da energia do $(N+1)^{\text{ésimo}}$ estado ligado ou virtual do trímero, $E_3^{(N+1)}$, e da energia do dímero, $E_2$, em função da razão da energia do dímero e do $N^{\text{ésimo}}$ estado ligado do trímero. Os estados ligados estão representados pela linha contínua e os virtuais pela linha tracejada. Resultados para $N = 0$. Os símbolos são resultados de outros cálculos para o trímero de $^4$He: quadrados vazios (onda-$S$) e círculos vazios (ondas-$S + D$) são da Ref. [63] ($N = 0$), quadrados com cruzes são da Ref. [64], círculos com cruzes são da Ref. [39], triângulos são da Ref. [65] e os losangos são da Ref. [66].

A transição de um estado ligado (linha contínua) para um estado virtual (linha tracejada) se dá para um valor crítico de $\epsilon_2$ dado pela razão $(E_2/E_3^{(N)}) = 0.145$ (correspondente ao ponto indicado pela $\uparrow$ na fig. (3.3)). Essa figura sugere fortemente que os estados Efimov não devem ser analisados somente em termos dos valores absolutos de $E_2$ porque o valor crítico para o aparecimento do estado excitado $(N+1)$ depende somente da razão $(\epsilon_2/\epsilon_3^{(N)}) = E_2/E_3^{(N)}$ que é independente da escala absoluta. O estado virtual atinge o limite superior, $(4/3)\epsilon_2$, em $(E_2/E_3^{(N)}) = 0.71$. A fig. (3.4) mostra ainda resultados de outros artigos para o caso do trímero de $^4$He (embora o nosso resultado se aplique a qualquer sistema de três bosons idênticos que seja fracamente ligado). Podemos ver que todos os pontos coincidem com os

nossos cálculos. Nenhum resultado foi encontrado na região dos estados virtuais. Enfatizamos que a função da fig. (3.4) é universal e no limite de escala, todos os estados Efimov devem obedecer a essa mesma função.

Na fig. (3.5) os resultados são apresentados de outra maneira. Nesta figura reproduzimos a curva da Ref. [15] e a estendemos para a região do estado virtual. Esta figura também compara os resultados obtidos com o método das equações subtraídas, linha pontilhada, e com o método de corte para momentos grandes, eq. (3.25), linha contínua.

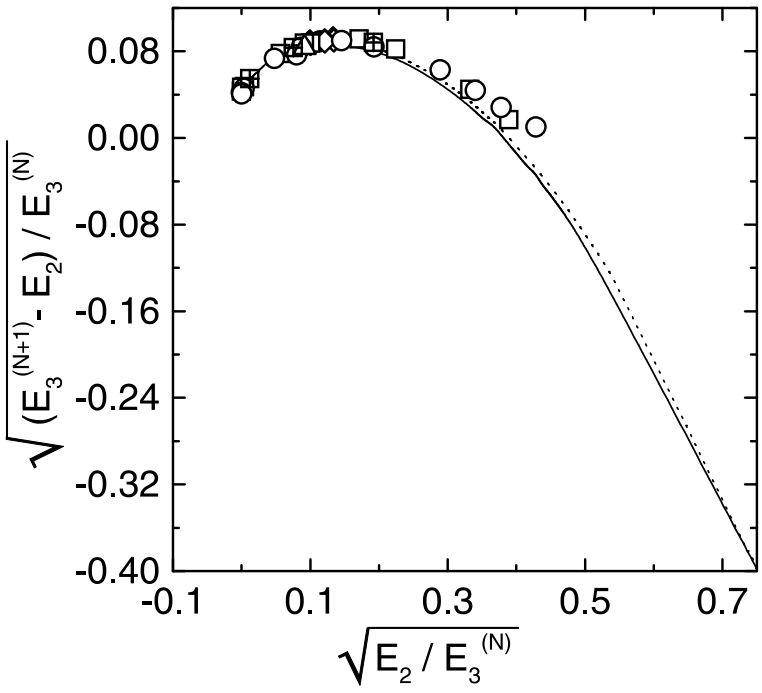


Figura 3.5: Energias dos estados ligados e virtuais de três bosons idênticos. As linhas pontilhada (subtração) e contínua (corte) mostram dois métodos para a regularização. Os símbolos obedecem às mesmas convenções da fig. (3.4). Na figura mostramos somente os resultados para $N = 0$.

A partir de $\sqrt{E_2/E_3^{(N)}} \approx 0.4$ podemos notar que os cálculos realísticos começam a se distanciar dos nossos cálculos devido aos efeitos de alcance do potencial. A partir de $\sqrt{E_2/E_3^{(N)}} = 0.38$ o estado excitado $(N+1)$ torna-se virtual, este limite confirma o resultado apresentado nas Refs. [14, 15] e mais recentemente na Ref. [67].

A trajetória completa dos estado Efimov é descrita agora com os resultados

das ressonâncias. Neste caso a energia de dois corpos é sempre virtual e será escrita nos gráficos como $E_{2V}$ (ou $\epsilon_{2V}$). As energias das ressonâncias serão escritas como $E_3$ (ou $\epsilon_3$) e as energias dos estados ligados como $E_{3L}$ (ou $\epsilon_{3L}$) (o $\epsilon$ é escrito quando as energias aparecem em unidades de $\mu_{(3)} = 1$).

Na fig. (3.6) estão representadas as energias dos estados ligados e as partes reais da energia da ressonância como função da energia de dois corpos (em unidades de $\mu_{(3)} = 1$). Podemos ver na fig. (3.6) que aumentando-se o módulo da energia de dois corpos o estado ligado torna-se uma ressonância. A fig. (3.7) mostra a parte imaginária das energias da ressonância.

Os resultados para os estados ligados e ressonâncias também podem ser representados na forma de uma função de escala universal dependente somente da razão entre a energia do estado virtual de dois corpos e da energia do estado ligado de três corpos:

$$\sqrt{E_3^{(N)}/E_{3L}^{(N-1)}} = \mathcal{R}\left(\sqrt{E_{2V}/E_{3L}^{(N-1)}}\right). \tag{3.31}$$

Na fig. (3.8) está representada a parte real da energia da ressonância (parte positiva do gráfico) e os estados ligados (parte negativa). A linha contínua representa os resultados para $N = 1$ e a pontilhada para $N = 2$. Na fig. (3.9) são mostrados os resultados para a parte imaginária da energia, a convenção utilizada nesta figura é a mesma da fig. (3.8). Nestas duas figuras fica claro o limite de escala, já que, praticamente, as duas curvas não apresentam diferença. O valor crítico de $E_{2V}$ para o qual o estados ligados tornam-se ressonâncias é dado por $E_{2V} \geq 0.0009 E_{3L}$, ou em termos do comprimento de espalhamento $a^{-1} \leq -0.03\sqrt{mE_{3L}/\hbar}$, onde $m$ é a massa do bóson.

A trajetória completa dos estados Efimov conforme variamos a razão entre as energias de dois e três corpos está mostrada na fig. (3.10). De fato, podemos notar que variando a energia de dois corpos nós temos uma transição contínua da energia de três corpos: para uma energia de dois corpos ligada e relativamente grande, os três corpos formam um estado virtual; conforme a energia de dois corpos diminui (em

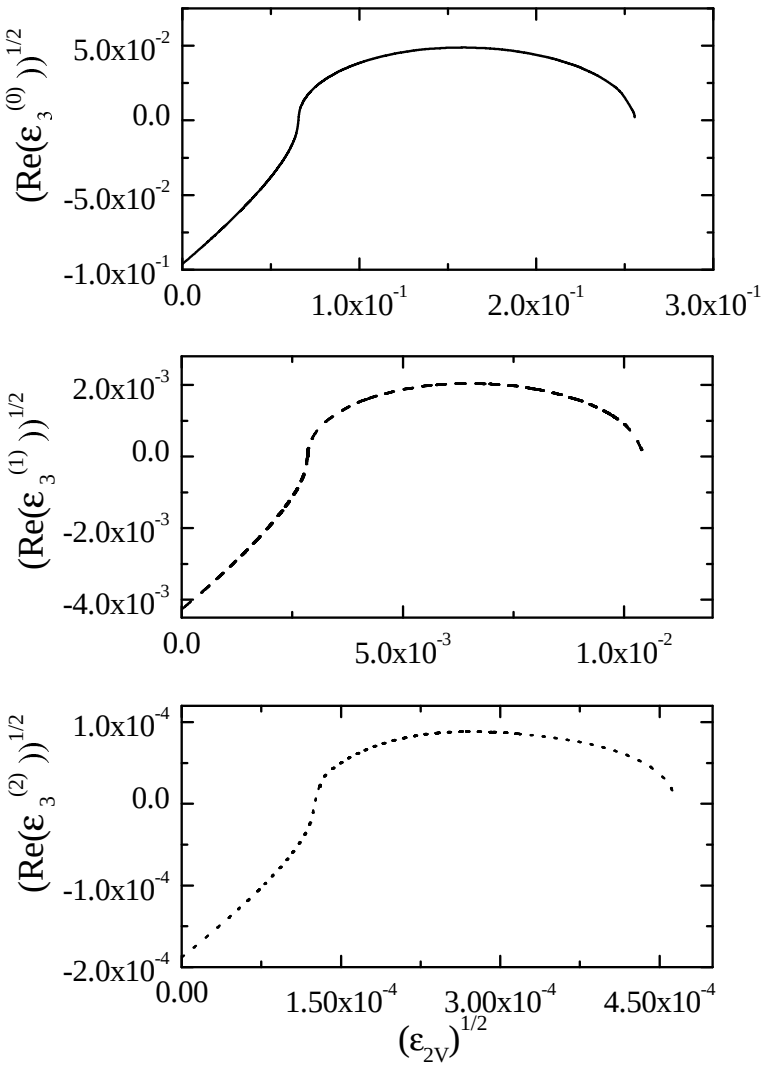


Figura 3.6: Parte real da energia de ressonância para três bosons idênticos em função da energia do estado virtual de dois corpos, em unidades de $\mu_{(3)} = 1$. Os valores negativos representam o $N^{\text{ésimo}}$ estado ligado de três corpos $\epsilon_3^{(N)}$ que se torna uma ressonância conforme aumentamos o módulo de $\epsilon_2$. Os valores positivos de $Re(\epsilon_3^{(N)})$ correspondem às ressonâncias. São mostrados os resultados para $N = 0$ (linha contínua), $N = 1$ (linha tracejada) e $N = 2$ (linha pontilhada).

módulo) o estado virtual torna-se ligado; finalmente fazendo a energia de dois corpos virtual e aumentando o seu valor, o estado ligado torna-se uma ressonância [7, 49].

No caso de átomos ultrafrios aprisionados, a existência das ressonâncias de três corpos no vácuo pode aumentar a possibilidade da existência de estados ligados de três corpos no interior de armadilhas, considerando, ainda, a inexistência de

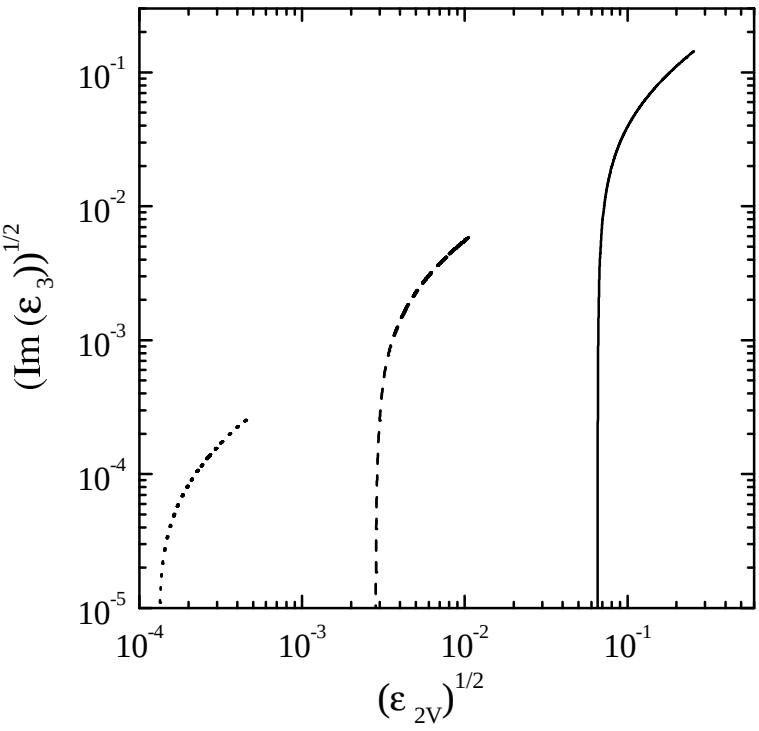


Figura 3.7: Parte imaginária da energia de ressonância para três bosons idênticos em função da energia do estado virtual de dois corpos, em unidades de $\mu_{(3)} = 1$. As curvas estão rotuladas da mesma forma que na fig. (3.6).

dímeros ligados que poderiam aparecer como concorrentes dos trímeros. Um cálculo das energias de trímeros no interior de armadilhas magneto-ópticas, quando dímeros formam um estado fracamente ligado [8], será feito no capítulo seguinte com base no coeficiente de recombinação de três corpos.

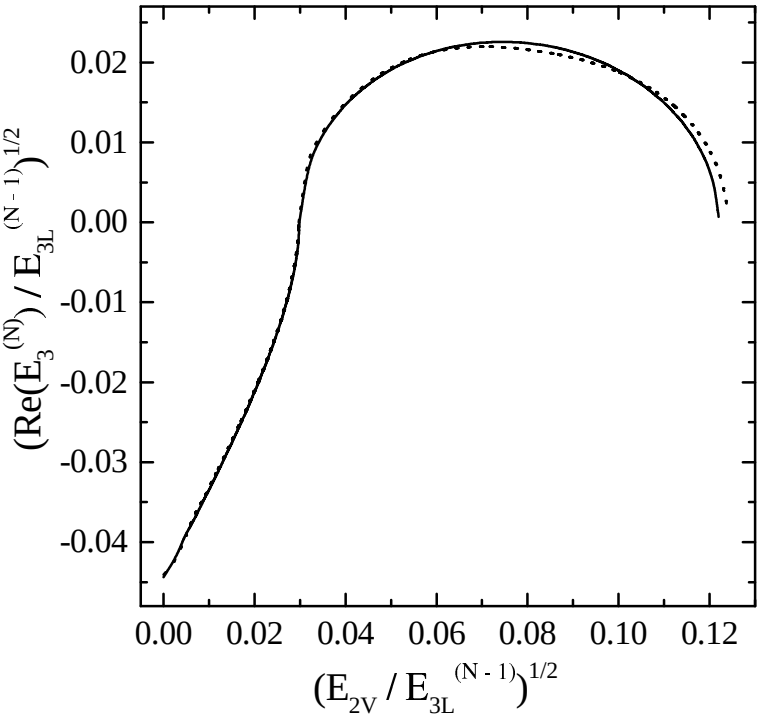


Figura 3.8: Razão da parte real da energia de ressonância (parte positiva) ou da energia do estado ligado (parte negativa), $E_3^{(N)}$, e da energia do estado ligado, $E_{3L}^{(N-1)}$ para três bosons idênticos em função da razão da energia do estado virtual de dois corpos, $E_{2V}$, e da energia do estado ligado de três corpos, $E_{3L}^{(N-1)}$. A linha contínua são os resultados para $N = 1$ e na linha pontilhada para $N = 2$.

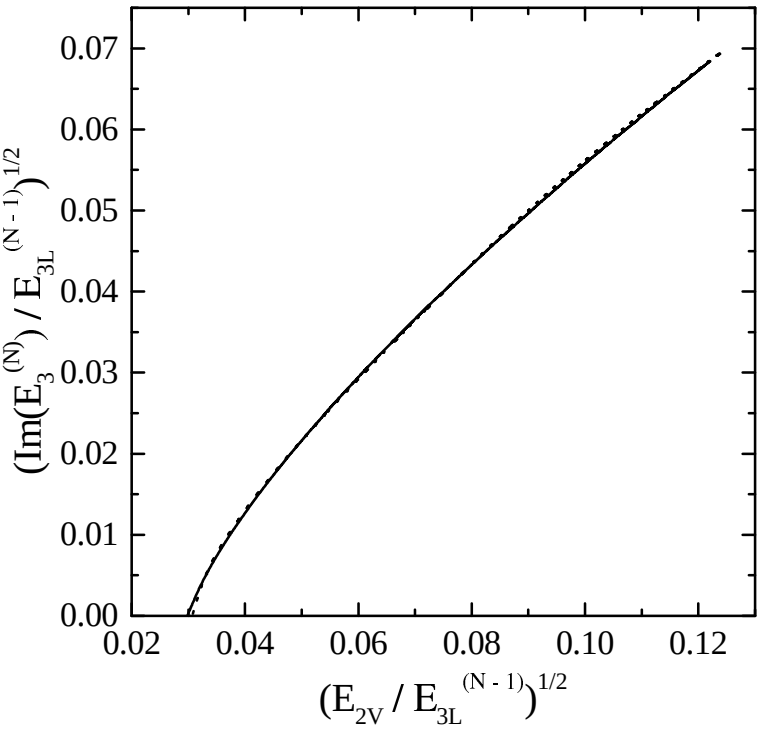


Figura 3.9: Razão da parte imaginária da energia de ressonância, $E_3^{(N)}$, e da energia do estado ligado, $E_{3L}^{(N-1)}$ para três bosons idênticos em função da razão da energia do estado virtual de dois corpos, $E_{2V}$, e da energia do estado ligado de três corpos, $E_{3L}^{(N-1)}$. A convenção para as linhas é a mesma da fig. (3.8).

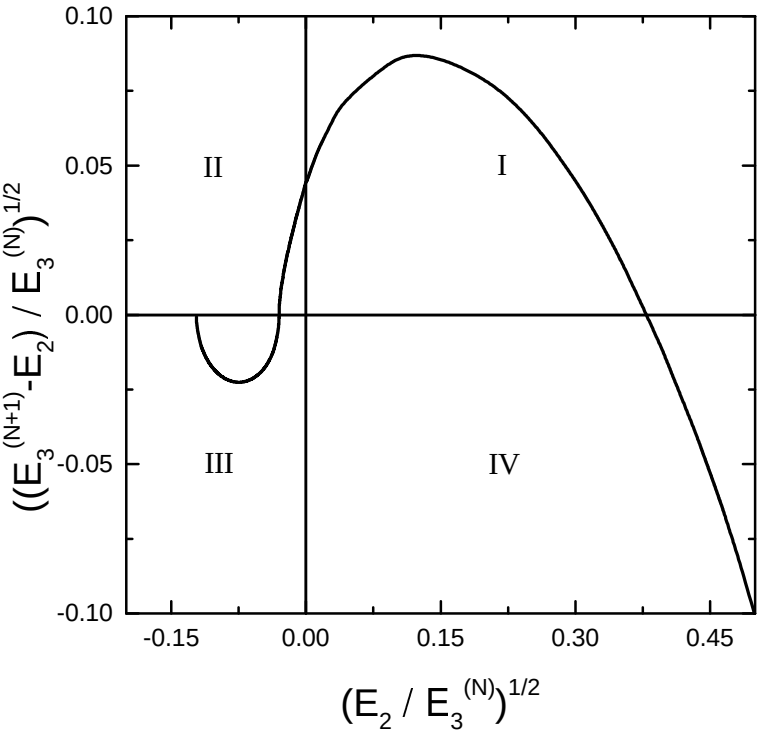


Figura 3.10: Razão da energia do $(N+1)^{\text{ésimo}}$ estado ligado, virtual ou ressonância do trímero, $E_3^{(N+1)}$, subtraída da energia do dímero, $E_2$, em função da razão da energia do dímero e do $N^{\text{ésimo}}$ estado ligado do trímero. Os quadrantes I e II referem-se, respectivamente, aos estados ligados de três corpos para $E_2$ ligado e virtual, o quadrante III corresponde às ressonâncias para $E_2$ virtual e o quadrante IV aos estados virtuais para $E_2$ ligado. Resultados para N=0.

# Capítulo 4

# Moléculas triatômicas fracamente ligadas em armadilhas magneto-ópticas

Em uma carta escrita a Ehrenfest em dezembro de 1924 Einstein comenta: "A partir de uma certa temperatura, as moléculas 'condensam-se' sem forças atrativas, isto é, acumulam-se com velocidade nula. A teoria é atraente, mas haverá nela algo de verdade?"[68]. Essa pergunta, motivada pelo sexto artigo de Bose enviado a Einstein e posteriormente publicado na revista *Zeitschrift für Physik* [69] só foi respondida aproximadamente 70 anos depois com a obtenção dos condensados de Bose-Einstein com átomos de $^{87}$Rb, em junho de 1995 pelo grupo do JILA [70], e com átomos de $^{23}$Na, obtido pelo grupo do MIT [28]. Esse trabalhos deram o Nobel a Eric Cornell, Wolfgang Ketterle e a Carl E. Wieman em 2001.

Embora a obtenção de um condensado só tenha acontecido em 1995, o confinamento de átomos em armadilhas magneto-ópticas já havia sido objeto do prêmio Nobel de 1997 (Steven Chu, Claude Cohen-Tannoudji e William D. Phillips). Esse átomos aprisionados podem ter o seu comprimento de espalhamento controlado variando-se o campo magnético [71, 72] (efeito Zeeman). O comprimento de espalhamento pode ainda tornar-se muito grande próximo a uma ressonância de Feshbach

[73]. A utilização da ressonância de Feshbach para a produção de grandes comprimentos de espalhamento foi demonstrado pela primeira vez em experimentos com átomos de $^{23}$Na [29] e $^{85}$Rb [74, 75]. Obviamente os átomos no interior das armadilhas podem se chocar e formar estados ligados. A obtenção de condensados de moléculas diatômicas já foi obtido experimentalmente, por exemplo, para os casos $^{87}Rb_2$ [31], $^{23}Na_2$ [32, 76] e $^{133}Cs_2$ [77].

Para que dois átomos em uma armadilha possam se combinar e formar um estado ligado devemos ter a participação de um terceiro átomo para que o momento e a energia sejam conservados. Esse processo é chamado de recombinação de três corpos. Utilizando o conceito de função de escala introduzido no capítulo anterior, podemos relacionar o coeficiente de recombinação com as energias dos estados ligados de dois e três corpos. Assim, conhecendo-se a energia de dois corpos e o coeficiente de recombinação (ambos já medidos experimentalmente [78, 79, 80, 81]) podemos prever a energia do estado ligado do trímero no interior de armadilhas [8].

Atualmente, já foi obtido experimentalmente condensados de moléculas formadas por átomos fermiônicos (obviamente as moléculas podem ser tratadas como bosons). Moléculas como, por exemplo, $^6Li_2$ possuem um "tempo de vida"relativamente grande (da ordem de 1 s) [82, 83, 84], outras moléculas como o $^{40}K_2$ já possuem uma "vida"menor (cerca de $10^{-3}$ s) [85]. Uma revisão bastante completa sobre a evolução da pesquisa em condensados pode ser encontrada na Ref. [86]. Nas Refs. [30, 87, 88] estão discutidos vários problemas atuais em condensados.

O nosso objetivo neste capítulo é a predição das energias de ligação de trímeros atômicos a partir dos valores experimentais dos coeficientes de recombinação de três átomos. Desta forma, iremos deduzir a seguir as equações relevantes para a obtenção do coeficiente de recombinação dentro do modelo de três corpos com força de alcance zero, formulado através das equações subtraídas. As coordenadas utilizadas estão representadas na fig. (4.1) que mostra um sistema inicialmente composto por três partículas livres de massa $m$, descritas por ondas planas de momento igual a $\vec{k}$ normalizadas para um volume de quantização $\mathcal{V}$:

$$\phi_{\vec{k}}(\vec{r}) = \frac{e^{\frac{i}{\hbar}\vec{k}\cdot\vec{r}}}{\sqrt{\mathcal{V}}}. \tag{4.1}$$

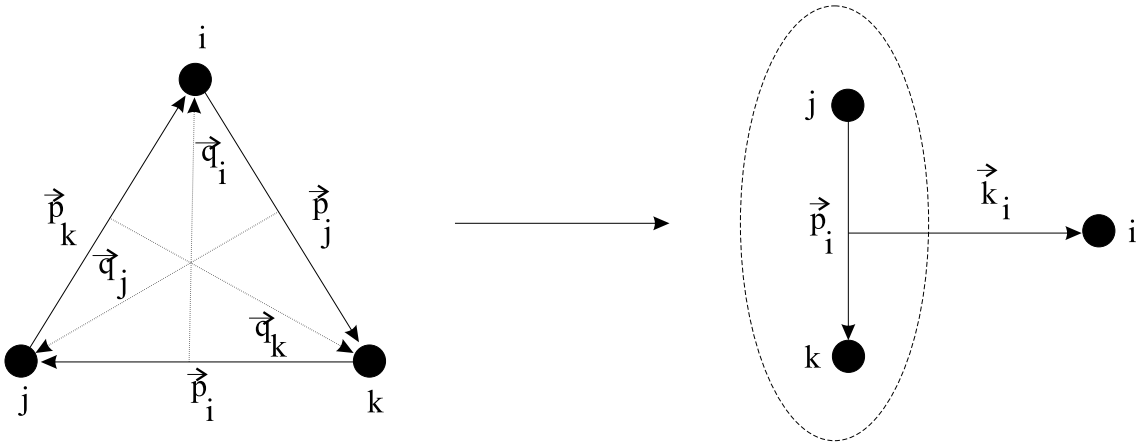


Figura 4.1: Coordenadas de Jacobi. Do lado esquerdo temos 3 partículas livres, do lado direito temos o estado ligado composto pelas partículas j e k, e a partícula livre i.

Partindo-se da "regra de ouro"de Fermi, escrevemos a taxa de transição correspondente ao processo de recombinação:

$$W = \frac{2\pi}{\hbar}\sum_{\{f\}} |\langle f|V|i\rangle|^2 \delta(E_f - E_i), \tag{4.2}$$

onde $f$ refere-se aos estados finais do sistema e $i$ ao estado inicial, com energias respectivamente iguais a $E_f$ e $E_i$. O somatório é feito sobre todos os estados finais. Substituindo-se na eq. (4.2) o estado final, composto pelo par ligado e uma partícula livre, e o estado inicial temos que a taxa de transição do processo de recombinação é dada por:

$$W = \frac{2\pi}{\hbar}\sum_{\{\vec{k}\}} |\langle \vec{k}\Phi_B^{(jk)}|V|\Psi^+\rangle|^2 \delta(E_f - E_i), \tag{4.3}$$

onde $\Phi_B$ é a função de onda do estado ligado de energia $E_{jk}$ das partículas $j$ e $k$ dada por (o cálculo da normalização da função de onda é apresentada no apêndice D):

$$\langle \vec{p}|\Phi_B^{(jk)}\rangle = \frac{E_{jk}^{\frac{1}{4}}}{\pi}\frac{1}{E_{jk}+p^2}, \tag{4.4}$$

e $\Psi^+$ é a função de onda de espalhamento completamente simétrica para o estado inicial de três bósons livres. A soma da eq. (4.3) pode ser transformada em uma integral utilizando a forma usual

$$\sum_{\{\vec{k}\}} \rightarrow \frac{\mathcal{V}}{(2\pi\hbar)^3}\int d^3k.$$

Assim, reescrevendo a eq. (4.3) na forma integral temos que:

$$W = \frac{2\pi}{\hbar}\frac{\mathcal{V}}{(2\pi\hbar)^3}\frac{(2\pi\hbar)^9}{\mathcal{V}^3}\int d^3k|\langle \vec{k}\Phi_B|V|\Psi^+\rangle|^2\delta(E_f-E_i), \tag{4.5}$$

onde o fator $\frac{(2\pi\hbar)^9}{\mathcal{V}^3}$ é proveniente da normalização das funções de onda livres $|\vec{k}\rangle$ ($\frac{(2\pi\hbar)^{3/2}}{\sqrt{\mathcal{V}}}$) e $|\Psi^+\rangle$ ($\frac{(2\pi\hbar)^3}{\mathcal{V}}$).

A perda do número de átomos em um condensado devido ao processo de recombinação de três corpos é dada pela seguinte equação:

$$\frac{dN}{dt} = -3\begin{pmatrix} N \\ 3 \end{pmatrix} W, \tag{4.6}$$

onde o fator 3 vem do fato de que a cada processo de recombinação temos a perda de três átomos da armadilha ou do condensado, o outro fator corresponde à combinação de N átomos 3 a 3 que aproximando para um valor grande de N dá:

$$\frac{dN}{dt} = -3\frac{N^3}{3!}W. \tag{4.7}$$

Escrevendo a eq. (4.7) em termos da densidade de átomos $\eta = \frac{N}{\mathcal{V}}$, temos que:

$$\frac{d\eta}{dt} = -3\frac{\eta^3}{3!}\mathcal{V}^2 W. \tag{4.8}$$

Finalmente substituindo-se a eq. (4.6) para W na eq. (4.8) temos a equação final para a taxa de perda de átomos no condensado:

$$\frac{d\eta}{dt} = -\frac{3}{3!}K_3\eta^3, \tag{4.9}$$

onde a equação para $K_3$ é dada por:

$$K_3 = \frac{2\pi}{\hbar}(2\pi\hbar)^9 \int \frac{d^3k}{(2\pi\hbar)^3}|T_{i\to f}|^2\delta(E_f - E_i). \tag{4.10}$$

A amplitude de transição $\langle\vec{k}\Phi_B|V|\Psi^+\rangle$ foi chamada de $T_{i\to f}$. A taxa de recombinação de três átomos no limite da energia do dímero tendendo a zero, eq. (4.9), é dada por [25, 89]

$$K_3 = \frac{\hbar}{m}a^4\alpha, \tag{4.11}$$

onde $\alpha$ é uma constante adimensional que possui um caráter oscilatório dado por [25]

$$\alpha = \alpha_{max}\sin^2(1.01\ \ln(a) + \delta), \tag{4.12}$$

sendo $\delta$ uma fase que depende da interação entre os átomos a pequenas distâncias. Para a energia do dímero tendendo a zero essa fase deve ser independente de pequenas variações do potencial desde que a escala de três corpos esteja fixa, como descrito pela eq. (3.30).

O elemento de matriz que aparece na eq. (4.10), $T_{i\to f}$, pode ser escrito em termos das ondas planas das partículas livres e das componentes de Faddeev da matriz de transição de três corpos. Escrevendo o potencial $V$ como a soma dos potenciais de interação entre os pares de partículas $ik$, $v_j$, e $ij$ , $v_k$,

$$T_{i\to f} = \langle \vec{k}_i \Phi_B^{(jk)} | v_j + v_k | \Psi^+ \rangle,$$

e substituindo $|\Psi^+\rangle = |\phi_0\rangle + G_0 T(E)|\phi_0\rangle$, onde $\phi_0$ é a função de onda dos bosons livres iniciais com momentos nulos, temos que:

$$\begin{aligned} \langle \vec{k}_i \Phi_B^{(jk)} | v_j + v_k | \Psi^+ \rangle &= \langle \vec{k}_i \Phi_B^{(jk)} | v_j + v_k (|\phi_0\rangle + G_0 T(E)|\phi_0\rangle) \\ &= \langle \vec{k}_i \Phi_B^{(jk)} | v_j + v_k | \phi_0 \rangle + \langle \vec{k}_i \Phi_B^{(jk)} | (v_j + v_k) G_0 T(E) | \phi_0 \rangle, \end{aligned}$$

como $T_\alpha = v_\alpha + v_\alpha G_0 T$, eq. (2.14), verificamos que:

$$T_{i\to f} = \langle \vec{k}_i \Phi_B^{(jk)} | v_j + v_k | \Psi^+ \rangle = \langle \vec{k}_i \Phi_B^{(jk)} | T_j(E) + T_k(E) | \phi_0 \rangle. \tag{4.13}$$

A partir deste ponto usaremos unidades tais que $\hbar = m = 1$. Partindo agora da equação para a matriz-T de três corpos na forma subtraída, eq. (2.43):

$$T_{R_i}(E) = t_{R_i}(E - \frac{3}{4} q_i^2) + t_{R_i}(E - \frac{3}{4} q_i^2)[G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)](T_{R_j}(E) + T_{R_k}(E)), \tag{4.14}$$

multiplicando por $\langle \vec{q}_i \vec{p}_i |$ pela esquerda e por $|\vec{0}\vec{0}\rangle$ pela direita o elemento de matriz $\langle \vec{q}_i \vec{p}_i | T_{R_i}(0) | \vec{0}\vec{0} \rangle$ para a componente de Faddeev $T_{R_i}(0)$ é dado por:

$$\begin{aligned} \langle \vec{q}_i \vec{p}_i | T_{R_i}(0) | \vec{0}\vec{0} \rangle &= \langle \vec{q}_i \vec{p}_i | \chi_i \rangle \tau(-\frac{3}{4} q_i^2) \langle \chi_i | \vec{0}\vec{0} \rangle \\ &+ 2 \langle \vec{q}_i \vec{p}_i | \chi_i \rangle \tau(-\frac{3}{4} q_i^2) \langle \chi_i | \left[ G_0^{(+)}(0) - G_0(-\mu^2) \right] T_{R_j}(0) | \vec{0}\vec{0} \rangle, \end{aligned} \tag{4.15}$$

onde foi utilizada a matriz-$T$ de dois corpos para $E = 0$ dada por $t_{R_i}(-\frac{3}{4} q_i^2) = |\chi_i\rangle \tau(-\frac{3}{4} q_i^2) \langle \chi_i|$, eqs. (2.24) e (3.16). O fator 2 que aparece na segunda parcela é

proveniente da igualdade das componentes $T_{R_j}$ e $T_{R_k}$. Manipulando a eq. (4.15), temos que:

$$\begin{aligned}\langle\vec{q}_i\vec{p}_i|T_{R_i}(0)|\vec{0}\vec{0}\rangle &= \langle\vec{p}_i|\chi_i\rangle\tau(-\frac{3}{4}q_i^2)\langle\chi_i|\vec{0}\rangle\langle\vec{q}_i|\vec{0}\rangle + 2\langle\vec{p}_i|\chi_i\rangle\tau(-\frac{3}{4}q_i^2) \\ &\quad \times\langle\chi_i,\vec{q}_i|\left[G_0^{(+)}(0) - G_0(-\mu^2)\right]T_{R_j}(0)|\vec{0}\vec{0}\rangle \\ &= \tau(-\frac{3}{4}q_i^2)\delta(\vec{q}_i) + 2\tau(-\frac{3}{4}q_i^2)z(\vec{q}_i), \qquad (4.16)\end{aligned}$$

onde utilizamos que o fator de forma $\langle\vec{p}_i|\chi\rangle$ do potencial $\delta$-Dirac é igual a 1. A função $z(\vec{q}_i)$ é dada por:

$$z(\vec{q}_i) = \int d^3p_i d^3p_j d^3q_j \langle\vec{p}_i\vec{q}_i|\ \left[G_0^{(+)}(0) - G_0(-\mu^2)\right]\ |\vec{p}_j\vec{q}_j\rangle\langle\vec{p}_j\vec{q}_j|T_{R_j}(0)|\vec{0}\vec{0}\rangle. \qquad (4.17)$$

Substituindo na eq. (4.17) o elemento de matriz dado pela eq. (4.16) temos que:

$$z(\vec{q}_i) = \int d^3p_i d^3p_j d^3q_j \langle\vec{p}_i\vec{q}_i|\ \left[G_0^{(+)}(0) - G_0(-\mu^2)\right]\ |\vec{p}_j\vec{q}_j\rangle\ \{\tau(-\frac{3}{4}q_j^2)\delta(\vec{q}_j)+2\tau(-\frac{3}{4}q_j^2)z(\vec{q}_j)\}. \qquad (4.18)$$

Escrevendo explicitamente os propagadores e fazendo a integração na primeira parcela da eq. (4.18) e lembrando que $\langle\vec{p}_i\vec{q}_i|\vec{p}_j\vec{q}_j\rangle = \delta(\vec{q}_i + \frac{\vec{q}_j}{2} + \vec{p}_j)\delta(\vec{p}_i - \frac{\vec{q}_i}{2} + \vec{q}_j)$, escrevemos $z(\vec{q}_i)$ como:

$$\begin{aligned}z(\vec{q}) &= -\tau(0)\frac{\mu^2}{q^2(\mu^2+q^2)} - 2\int d^3q'\tau(-\frac{3}{4}q'^2) \\ &\quad \times\left[\frac{1}{E + q^2 + q'^2 + \vec{q}\cdot\vec{q}\,'} - \frac{1}{\mu^2 + q^2 + q'^2 + \vec{q}\cdot\vec{q}\,'}\right]z(\vec{q}\,'), \qquad (4.19)\end{aligned}$$

onde $q_i$ e $q_j$ foram substituídos respectivamente por $q$ e $q'$.

Voltando agora à amplitude de transição, $T_{i\to f}$, dada pela eq. (4.13) vamos substituir a função de onda completamente simétrica do estado inicial de três bosons,

$$|\phi_0\rangle = \frac{1}{\sqrt{3}} \sum_{\alpha=i,j,k} |\vec{q}_\alpha \vec{p}_\alpha\rangle, \tag{4.20}$$

na eq. (4.13):

$$T_{i\to f} = 2\sqrt{3}\langle \vec{k}_i \Phi_B^{(jk)} | T_{R_j}(0) | \vec{0}\vec{0}\rangle. \tag{4.21}$$

Introduzindo $\int d^3p_j |\vec{p}_j\rangle\langle\vec{p}_j|$, $\int d^3q_j |\vec{q}_j\rangle\langle\vec{q}_j|$ e $\int d^3p_i |\vec{p}_i\rangle\langle\vec{p}_i|$ e notando que devemos ter $E_{jk} = \frac{3}{4}k_i^2$, podemos escrever $T_{i\to f}$ como:

$$T_{i\to f} = 2\sqrt{3}\int d^3p_j d^3q_j d^3p_i \frac{E_{jk}^{\frac{1}{4}}}{\pi} \frac{\langle \vec{k}_i \vec{p}_i | \vec{p}_j \vec{q}_j\rangle}{\frac{3}{4}k_i^2 + p_i^2} \langle \vec{p}_j \vec{q}_j | T_{R_j}(0) | \vec{0}\vec{0}\rangle, \tag{4.22}$$

escrevendo o primeiro elemento de matriz em termos das funções $\delta$-Dirac dadas pelas coordenadas de Jacobi e substituindo o segundo elemento de matriz pela eq. (4.16), podemos escrever a eq. (4.22) da seguinte forma:

$$\begin{aligned} T_{i\to f} &= 2\sqrt{3}\frac{E_{jk}^{\frac{1}{4}}}{\pi}\left\{\int d^3p_j d^3q_j d^3p_i \frac{\delta(\vec{k}_i + \frac{\vec{q}_j}{2} + \vec{p}_j)\delta(\vec{p}_i - \frac{\vec{k}_i}{2} - \vec{q}_j)}{\frac{3}{4}k_i^2 + p_i^2}\right. \\ &\times \left.\left[\tau(-\frac{3}{4}q_j^2)\delta(\vec{q}_j) + 2\tau(-\frac{3}{4}q_j^2)z(\vec{q}_j)\right]\right\}. \end{aligned} \tag{4.23}$$

Resolvendo as integrais e escrevendo explicitamente $\tau$ a eq. (4.22) fica igual a (o comprimento de espalhamento, $a$, é igual a $\frac{1}{\sqrt{E_{jk}}}$):

$$T_{i\to f} = \frac{3\sqrt{3}a^{\frac{5}{2}}}{4\pi^3} + \frac{4}{\pi^3 a^{\frac{1}{2}}}\int d^3q_j \frac{z(\vec{q}_j)}{q_j^2 + k_i^2 + \vec{k}_i\cdot\vec{q}_j} \frac{1}{k_i - q_j + i\epsilon}. \tag{4.24}$$

Substituindo a eq. (4.24) na eq. (4.10) (também em unidades de $\hbar = m = 1$) e fazendo a integração em $k$ temos que:

$$K_3 = \frac{(2\pi)^5 12\sqrt{3}}{\pi^3} a^4 |1 + \frac{32\pi}{3\sqrt{3}a^3} \int_0^\infty dq \frac{q}{k} \ln\left(\frac{k^2+q^2+qk}{k^2+q^2-qk}\right) \frac{z(q)}{k-q+i\epsilon}|^2, \qquad (4.25)$$

onde os índices de $k$ e $q$ foram suprimidos. O coeficiente adimensional de recombinação, eq. (4.11), é dado por

$$\alpha = \frac{(2\pi)^5 12\sqrt{3}}{\pi^3} |1 + \frac{32\pi}{3\sqrt{3}a^3} \int_0^\infty dq \frac{q}{k} \ln\left(\frac{k^2+q^2+qk}{k^2+q^2-qk}\right) \frac{z(q)}{k-q+i\epsilon}|^2, \qquad (4.26)$$

Os resultados numéricos para o coeficiente de recombinação são dados pela solução da eq. (4.26) e da eq. integral (4.19). Resolvemos a eq. (4.19) no plano complexo evitando as singularidades do espalhamento e, em seguida, integramos a eq. (4.23) no contorno do plano complexo escolhido (q→q$e^{i\theta}$). Este procedimento é conhecido como método do desvio de contorno [90]. Na fig. (4.2) temos os resultados teóricos de $\alpha$ em função da razão $\sqrt{E_2/E_3}$.

Na fig. (4.2) podemos notar claramente a existência do limite de escala conforme a energia do estado ligado de dois corpos diminui (e conseqüentemente o número de estados ligados de três corpos aumenta). O limite de escala já foi observado nas figuras anteriores nos casos dos estados virtuais e das ressonâncias. O valor máximo de $\alpha$ ocorre para o limiar $E_2 = E_3$ e para $(E_3/E_2)^{1/2} = 0.38$.

As linhas horizontais na figura 4.2, correspondentes aos valores experimentais centrais para o coeficiente de recombinação, interceptam a curva teórica em dois pontos indicando a possibilidade da existência de um trímero no condensado com energia, $E_3$ ou $E_3'$, referentes a um estado fracamente ligado. Somente para o caso do $^{85}Rb|2,-2\rangle$, onde o valor para o coeficiente de recombinação é menor, foi subtraído a contribuição referente ao estado profundamente ligado, $\sim 1$ de acordo com a Ref. [91]. Os valores em $mK$ para as energias dos trímeros estão contidos nas colunas 6 e 7 da tabela 4.

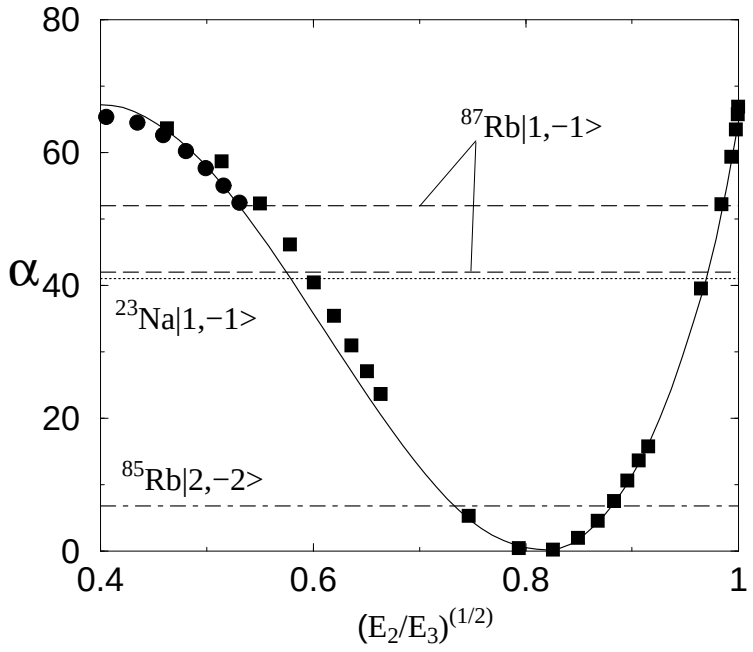


Figura 4.2: Coeficiente adimensional de recombinação, $\alpha$, como função da razão das energias de ligação das moléculas diatômicas e triatômicas. Resultados teóricos: círculos cheios (um estado ligado de três átomos), linha cheia (dois estados ligados de três átomos) e quadrados cheios (três estados ligados de três átomos). As linhas horizontais indicam os resultados experimentais (valores centrais) para o $^{23}Na$, $^{87}Rb$ e $^{85}Rb$ apresentados na tabela 4. No caso do $^{85}Rb$ foi subtraído do valor experimental de $\alpha$ a contribuição do estado profundamente ligado ($\approx 1$), conforme calculado na Ref. [91].

A hipótese de formação dos trímeros no vácuo, no interior de armadilhas, será válida somente se tivermos uma quantidade de átomos num cubo de arestas iguais ao comprimento de espalhamento muito menor do que 1. Essa quantidade é dada pelo coeficiente de diluição que aparece na coluna 3 da tabela 4. Podemos ver que exceto para o $^{85}Rb|2,-2\rangle$ onde o valor 0.5 do coeficiente de diluição pode ser considerado como o limite de nossa aproximação, os outros átomos possuem um coeficiente muito menor do que 1.

| $^A Z\|F, m_F\rangle$ | $a$(nm) | $\rho a^3$ | $\alpha_{exp}$ | $E_2$ (mK) | $S_3$(mK) | $S_3'$(mK) |
|---|---|---|---|---|---|---|
| $^{23}$Na$\|1,-1\rangle$ | 2.75 | $6\times10^{-5}$ | 42±12 [79] | 2.85 | 4.9 | 0.21 |
| $^{87}$Rb$\|1,-1\rangle$ | 5.8 | $1\times10^{-5}$ | 52±22$^*$ [78] | 0.17 | 0.39 | 0.005 |
| $^{87}$Rb$\|1,-1\rangle$ | 5.8 | $1\times10^{-4}$ | 41±17$^\dagger$ [78] | 0.17 | 0.30 | 0.013 |
| $^{87}$Rb$\|2,2\rangle$ | 5.8 | $4\times10^{-5}$ | 130±36 [80] | 0.17 | - | - |
| $^{85}$Rb$\|2,-2\rangle$ | 211.6 | 0.5 | 7.84±3.4 [92, 93] | $1.3\times10^{-4}$ | $1.14\times10^{-4}$ | $3.8\times10^{-5}$ |

Tabela 4.1: Para os átomos $^A Z|F, m_F\rangle$ ($F$ e $m_F$ são , respectivamente, o spin total e a sua projeção), dados na coluna 1, apresentamos nas colunas 6 e 7 as energias de ligação para os trímeros em relação ao limiar, $S_3 \equiv (E_3 - E_2)$ e $S_3' \equiv (E_3' - E_2)$, considerando os valores centrais para os coeficientes de recombinação adimensionais $\alpha_{expt}$ medidos experimentalmente (dados na coluna 4). O comprimento de espalhamento $a$, o coeficiente de diluição $\rho a^3$ e a energia para o estado ligado de dois corpos são dados, respectivamente, nas colunas 2, 3 e 5. O coeficiente de recombinação do $^{87}$Rb$|1,-1\rangle$ para os átomos não condensados ($^*$) e para os condensados ($^\dagger$) foi obtido da Ref. [78].

# Capítulo 5

# Limite de escala para os raios de sistemas fracamente ligados do tipo $AAB$

Neste capítulo iniciaremos o estudo dos tamanhos dos sistemas de três corpos compostos por duas partículas de massas idênticas, $A$, e uma outra partícula chamada de $B$. Calcularemos os raios quadráticos médios de separação entre $A-A$, $A-B$, $A-CM$ e $B-CM$ ($CM$ é o centro-de-massa do sistema de três corpos). Na primeira seção mostraremos o formalismo que será utilizado nas três seções seguintes. Na segunda seção faremos um estudo geral do tamanho dos diversos sistemas que podem ser formados conforme variamos a energia de dois corpos. Na terceira seção os raios serão calculados no contexto de núcleos exóticos, neste caso $A$ representará um nêutron e $B$ o caroço do núcleo [10]. Na quarta seção mostraremos que o mesmo formalismo também se aplica muito bem ao caso de moléculas fracamente ligadas, neste caso $A$ representará um átomo de $^4He$ e $B$ um outro átomo [9].

## 5.1 Formalismo

Descreveremos nosso sistema de três corpos utilizando as mesmas coordenadas de Jacobi da fig. (2.1). As posições canonicamente conjugadas ao momento relativo do centro-de-massa do par, $\vec{q}$, e do momento do par, $\vec{p}$, serão chamadas respectivamente de $\vec{R}$ e $\vec{r}$, conservando os mesmos índices dos momentos. Para as deduções consideraremos $j \equiv k \equiv A$ e $i \equiv B$. Mostraremos de forma detalhada a obtenção do raio quadrático médio de separação relativa entre as partículas $j$ e $k$, usando o fator de forma correspondente à transformada de Fourier da densidade de probabilidade como função da distância relativa. Este procedimento é conveniente, pois obtemos a função de onda diretamente no espaço dos momentos. Como as outras distâncias são obtidas mudando-se apenas as coordenadas do sistema, elas serão mostradas somente na sua forma final, sem detalhes da dedução.

O raio quadrático médio de separação relativa das partículas $j$ e $k$ é escrito da forma usual como:

$$\langle r_i^2 \rangle = \int d^3 r_i r_i^2 \rho_i(r_i), \tag{5.1}$$

onde $\rho$ é a densidade de probabilidade dada por

$$\rho_i(r_i) = \int d^3 R_i |\langle \vec{r}_i, \vec{R}_i | \Psi \rangle|^2. \tag{5.2}$$

Escrevendo a densidade em termos de uma transformada de Fourier no espaço dos momentos temos que

$$\rho_i(r_i) = \int d^3 Q F(Q^2) \frac{e^{-i\vec{Q}\cdot\vec{r}_i}}{(2\pi)^3}, \tag{5.3}$$

onde a função $F(Q^2)$ é dada pela anti-transformada de Fourier da eq. (5.3):

$$F(Q^2) = \int d^3 r_i e^{i\vec{Q}\cdot\vec{r}_i} \rho_i(r_i), \tag{5.4}$$

normalizada para $F(0) \equiv 1$. Expandindo a exponencial da eq. (5.4) em série de Taylor até segunda ordem e considerando a simetria esférica de $\rho_i$, temos que:

$$\langle r_i^2 \rangle \equiv \langle r_{AA}^2 \rangle = -6 \frac{dF_{AA}(Q^2)}{dQ^2}\bigg|_{Q^2=0}. \tag{5.5}$$

Devemos escrever agora a função $F(Q^2)$, eq. (5.4), em termos da função de onda do sistema no espaço dos momentos. Substituindo a eq. (5.2) em (5.4) temos que:

$$\begin{aligned}
F(Q^2) &= \int d^3r_i e^{i\vec{Q}\cdot\vec{r}_i} \int d^3R_i |\langle \vec{r}_i, \vec{R}_i|\Psi\rangle|^2 \\
&= \int d^3r_i d^3R_i e^{i\vec{Q}\cdot\vec{r}_i} \langle \vec{r}_i, \vec{R}_i|\Psi\rangle\langle\Psi|\vec{r}_i, \vec{R}_i\rangle \\
&= \int d^3r_i d^3R_i d^3q_i d^3q_i' d^3p_i d^3p_i' e^{i(\vec{Q}-\vec{p}_i+\vec{p}_i\,')\cdot\vec{R}_i} e^{i(\vec{q}_i-\vec{q}_i\,')\cdot\vec{r}_i} \langle \vec{q}_i, \vec{p}_i|\Psi\rangle\langle \vec{q}_i\,', \vec{p}_i\,'|\Psi\rangle \\
&= \int d^3q_i d^3q_i' d^3p_i d^3p_i' \delta(\vec{Q}-\vec{p}_i+\vec{p}_i\,')\delta(\vec{q}_i-\vec{q}_i\,')\langle \vec{q}_i, \vec{p}_i|\Psi\rangle\langle \vec{q}_i\,', \vec{p}_i\,'|\Psi\rangle \\
&= \int d^3q_i d^3p_i \langle \vec{q}_i, \vec{p}_i|\Psi\rangle\langle \vec{q}_i, \vec{p}_i+\vec{Q}|\Psi\rangle
\end{aligned}$$

Integrando a função $\delta$-Dirac escrevemos o fator de forma $F_{AA}(Q^2)$ (partícula $B$ é a espectadora) em termos das funções de onda do sistema no espaço dos momentos. Para simetrizarmos os argumentos das funções de onda vamos substituir o momento $\vec{p}_i$ por $\vec{p}_i - \frac{\vec{Q}}{2}$.

$$F_{AA}(Q^2) = \int d^3q_i d^3p_i \langle \vec{q}_i, \vec{p}_i + \frac{\vec{Q}}{2}|\Psi\rangle\langle \vec{q}_i, \vec{p}_i - \frac{\vec{Q}}{2}|\Psi\rangle. \tag{5.6}$$

A equação de Schrödinger do sistema de três corpos para um potencial separável do tipo $v_\alpha = \lambda_\alpha|\chi_\alpha\rangle\langle\chi_\alpha|$, com $\alpha = i, j, k$ ($v_i$, $v_j$ e $v_k$ são, respectivamente, os potenciais de dois corpos de $jk$, $ik$ e $ij$) pode ser escrita como:

$$(H_0 + \sum_{\alpha=i,j,k} \lambda_\alpha |\chi_\alpha\rangle\langle\chi_\alpha|)|\Psi\rangle = E|\Psi\rangle \tag{5.7}$$

$$(E - H_0)|\Psi\rangle = \sum_{\alpha=i,j,k} \lambda_\alpha |\chi_\alpha\rangle\langle\chi_\alpha|\Psi\rangle, \tag{5.8}$$

onde $H_0$ é o hamiltoniano livre do sistema.

Utilizando que o fator de forma $\langle\vec{p}_\alpha|\chi\rangle = 1$ para o potencial $\delta$-Dirac, podemos escrever a função de onda na base $|\vec{q}_i, \vec{p}_i\rangle$ e em termos das funções espectadoras $f_\alpha(\vec{q}_\alpha) = \lambda_\alpha\langle\vec{q}_\alpha\chi_\alpha|\Psi\rangle$:

$$\langle\vec{q}_i, \vec{p}_i|\Psi\rangle = \frac{f_i(|\vec{q}_i|) + f_j(|\vec{p}_i - \frac{\vec{q}_i}{2}|) + f_k(|\vec{p}_i + \frac{\vec{q}_i}{2}|)}{|E_3| + H_0}, \tag{5.9}$$

onde $f_i$, $f_j$ *e* $f_k$ *são, respectivamente, as funções espectadoras de* $B$, $A$ *e* $A$. $E_3$ é a energia do estado ligado dos três corpos. Substituindo a eq. (5.9) na eq. (5.6) temos a forma final da função $F_{AA}(Q^2)$ no espaço dos momentos:

$$\begin{aligned} F_{AA}(Q^2) &= \int d^3q_i d^3p_i \left( f_i(|\vec{q}_i|) + f_j(|\vec{p}_i + \frac{\vec{Q}}{2} - \frac{\vec{q}_i}{2}|) + f_k(|\vec{p}_i + \frac{\vec{Q}}{2} + \frac{\vec{q}_i}{2}|) \right) \\ &\times \frac{\left( f_i(|\vec{q}_i|) + f_j(|\vec{p}_i - \frac{\vec{Q}}{2} - \frac{\vec{q}_i}{2}|) + f_k(|\vec{p}_i - \frac{\vec{Q}}{2} + \frac{\vec{q}_i}{2}|) \right)}{(|E_3| + H_0)(|E_3| + H_0')}, \end{aligned} \tag{5.10}$$

onde $H_0$ e $H_0'$ são dados por:

$$H_0 = \frac{|\vec{p}_i + \frac{\vec{Q}}{2}|^2}{2m_{AA}} + \frac{q_i^2}{2m_{AA,B}}, \tag{5.11}$$

e

$$H_0' = \frac{|\vec{p}_i - \frac{\vec{Q}}{2}|^2}{2m_{AA}} + \frac{q_i^2}{2m_{AA,B}}, \tag{5.12}$$

onde $m_{AA} = \frac{m_A}{2}$ e $m_{AA,B} = \frac{2m_B m_A}{2m_A + m_B}$. De forma análoga podemos escrever as eqs. (5.5) e (5.6) para $\langle r_k^2\rangle$:

$$\langle r_k^2 \rangle \equiv \langle r_{AB}^2 \rangle = -6 \frac{dF_{AB}(Q^2)}{dQ^2}\bigg|_{Q^2=0}. \tag{5.13}$$

$$F_{AB}(Q^2) = \int d^3q_k d^3p_k \langle \vec{q}_k, \vec{p}_k + \frac{\vec{Q}}{2} | \Psi \rangle \langle \vec{q}_k, \vec{p}_k - \frac{\vec{Q}}{2} | \Psi \rangle. \tag{5.14}$$

Lembrando que $i$, $j$ e $k$ correspondem, respectivamente, às partículas espectadoras $B$, $A$, e $A$, a função de onda na base $|\vec{q}_k, \vec{p}_k\rangle$ é dada pela seguinte equação:

$$\langle \vec{q}_k, \vec{p}_k | \Psi \rangle = \frac{f_i(|\vec{p}_k - \frac{\mathcal{A}}{\mathcal{A}+1}\vec{q}_k|) + f_j(|\vec{p}_k + \frac{1}{\mathcal{A}+1}\vec{q}_k|) + f_k(|\vec{q}_k|)}{|E_3| + p_k^2 \frac{\mathcal{A}+1}{2\mathcal{A}} + q_k^2 \frac{\mathcal{A}+2}{2(\mathcal{A}+1)}}. \tag{5.15}$$

onde $\mathcal{A} = m_B/m_A$ é a razão entre as massas das partículas $A$ e $B$.

As distâncias quadráticas médias de $A$ e de $B$ ao $CM$ do sistema de três corpos são calculadas através dos respectivos fatores de forma e são dadas, respectivamente, por:

$$\begin{aligned} \langle r_A^2 \rangle &\equiv \left(\frac{m_A + m_B}{2m_A + m_B}\right)^2 \langle R_k^2 \rangle = -6 \left(\frac{m_A + m_B}{2m_A + m_B}\right)^2 \frac{dF_A(Q^2)}{dQ^2}\bigg|_{Q^2=0}, \\ F_A(Q^2) &= \int d^3q d^3p \langle \vec{q}_k + \frac{\vec{Q}}{2}, \vec{p}_k | \Psi \rangle \langle \vec{q}_k - \frac{\vec{Q}}{2}, \vec{p}_k | \Psi \rangle \end{aligned} \tag{5.16}$$

e

$$\begin{aligned} \langle r_B^2 \rangle &\equiv \left(\frac{2m_A}{2m_A + m_B}\right)^2 \langle R_i^2 \rangle = -6 \left(\frac{2m_A}{2m_A + m_B}\right)^2 \frac{dF_B(Q^2)}{dQ^2}\bigg|_{Q^2=0}, \\ F_B(Q^2) &= \int d^3q_i d^3p_i \langle \vec{q}_i + \frac{\vec{Q}}{2}, \vec{p}_i | \Psi \rangle \langle \vec{q}_i - \frac{\vec{Q}}{2}, \vec{p}_i | \Psi \rangle. \end{aligned} \tag{5.17}$$

As integrações das eqs. para os fatores de forma, $F$, podem ser reduzidas para 5 dimensões, ao invés das 6 dimensões colocando o momento $\vec{Q}$ paralelo ao eixo $z$ e $\vec{q}$ no plano $xz$, (vide fig. (5.1)):

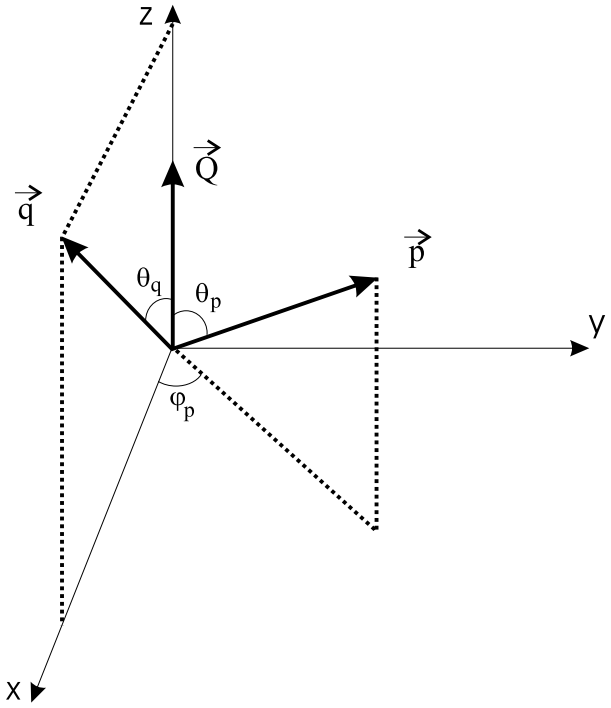


Figura 5.1: Orientação dos momentos.

Desta forma a integração dos fatores de forma é feita nas seguintes variáveis radiais e angulares com os respectivos limites:

$$\int d^3q d^3p \equiv 2\pi \int_0^\infty p^2 dp \int_0^\infty q^2 dq \int_0^\pi \mathrm{sen}\theta_p d\theta_p \int_0^\pi \mathrm{sen}\theta_q d\theta_q \int_0^{2\pi} d\varphi_p.$$

Note que as funções de onda dependem somente do ângulo relativo entre os momentos $\vec{p}$, $\vec{q}$ e $\vec{Q}$, assim, não há nenhuma perda de generalização ao fixarmos os momentos segundo a fig. (5.1).

### 5.1.1 Equações subtraídas para as funções espectadoras

A dedução das funções espectadoras para o caso onde uma das partículas é distinta das outras duas é feita da mesma forma que no capítulo 3, a mudança ocorre somente a partir da eq. (3.10), pois agora, apenas duas funções espectadoras são idênticas. Então, escrevendo a função espectadora para a componente de Faddeev $k$, temos que:

$$f_k(\vec{q}_k) = \tau\left(E - \frac{q_k^2}{2m_{ij,k}}\right)\langle\chi_k, \vec{q}_k|\left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)(|\chi_i\rangle|f_i\rangle + |\chi_j\rangle|f_j\rangle)\,, \tag{5.18}$$

a função $\tau$ é dada pela eq. (2.25), calculada agora para o caso de duas partículas de massas idênticas e uma diferente.

A função espectadora para a componente de Faddeev $i$ é escrita como (neste caso as funções espectadoras do lado direito $j$ e $k$ são idênticas, $|\chi_k\rangle|f_k\rangle \equiv |\chi_j\rangle|f_j\rangle$):

$$f_i(\vec{q}_i) = 2\tau\left(E - \frac{q_k^2}{2m_{jk,i}}\right)\langle\chi_i, \vec{q}_i|\left(G_0^{(+)}(E) - G_0(-\mu_{(3)}^2)\right)|\chi_j\rangle|f_j\rangle. \tag{5.19}$$

Os elementos de matriz $\langle\chi_k\vec{q}_k|G_0^{(+)}(E)|\chi_i\rangle|f_i\rangle$, $\langle\chi_k\vec{q}_k|G_0^{(+)}(E)|\chi_j\rangle|f_j\rangle$ que aparecem na eq. (5.18) e $\langle\chi_i\vec{q}_i|G_0^{(+)}(E)|\chi_j\rangle|f_j\rangle$ da eq. (5.19) serão calculados no apêndice F (obviamente a parte referente à subtração é idêntica a menos da energia $E$ que é substituída por $-\mu_{(3)}^2$).

Substituindo os elementos de matriz dados pelas eqs. (F.1), (F.2) e (F.3) nas eqs. (5.18) e (5.19) para as funções espectadoras, temos que:

$$\begin{aligned} f_k(\vec{q}_k) \equiv f_A(\vec{q}_k) = -\tau_A\left(E - \frac{q_k^2(\mathcal{A}+2)}{2(\mathcal{A}+1)}\right)\Bigg\{\int d^3q_i'\Bigg[\frac{1}{E - \frac{q_k^2(\mathcal{A}+2)}{2(\mathcal{A}+1)} - \frac{(\vec{q}_i\,' + \frac{\mathcal{A}}{\mathcal{A}+1}\vec{q}_k)^2(\mathcal{A}+1)}{2\mathcal{A}}} \\ - \frac{1}{-\mu_{(3)}^2 - \frac{q_k^2(\mathcal{A}+2)}{2(\mathcal{A}+1)} - \frac{(\vec{q}_i\,' + \frac{\mathcal{A}}{\mathcal{A}+1}\vec{q}_k)^2(\mathcal{A}+1)}{2\mathcal{A}}}\Bigg] f_B(\vec{q}_i\,') + \int d^3q_j\Bigg[\frac{1}{E - \frac{q_k^2(\mathcal{A}+2)}{2(\mathcal{A}+1)} - \frac{(\vec{q}_j + \frac{1}{\mathcal{A}+1}\vec{q}_k)^2(\mathcal{A}+1)}{2\mathcal{A}}} \\ - \frac{1}{-\mu_{(3)}^2 - \frac{q_k^2(\mathcal{A}+2)}{2(\mathcal{A}+1)} - \frac{(\vec{q}_j + \frac{1}{\mathcal{A}+1}\vec{q}_k)^2(\mathcal{A}+1)}{2\mathcal{A}}}\Bigg] f_A(\vec{q}_j)\Bigg\}\,, \end{aligned} \tag{5.20}$$

$$\begin{aligned} f_i(\vec{q}_i) \equiv f_B(\vec{q}_i) = -2\tau_B\left(E - \frac{q_i^2(\mathcal{A}+2)}{4\mathcal{A}}\right)\Bigg\{\int d^3q_j\Bigg[\frac{1}{E - \frac{q_i^2(\mathcal{A}+2)}{4\mathcal{A}} - (\vec{q}_j + \frac{1}{2}\vec{q}_i)^2} \\ - \frac{1}{-\mu_{(3)}^2 - \frac{q_i^2(\mathcal{A}+2)}{4\mathcal{A}} - (\vec{q}_j + \frac{1}{2}\vec{q}_i)^2}\Bigg] f_A(\vec{q}_i)\Bigg\}\,. \end{aligned} \tag{5.21}$$

As funções $\tau_A$ e $\tau_B$ são calculadas de forma análoga ao caso dos três bosons idênticos e são dadas por:

$$\tau_A^{-1}\left(E-\frac{q^2(\mathcal{A}+2)}{(\mathcal{A}+1)}\right)=\left(\frac{(\mathcal{A}+1)}{2\mathcal{A}}\right)^{(3/2)}2\pi^2\left\{\pm\sqrt{E_{AB}}-\sqrt{|E|-\frac{q^2(\mathcal{A}+2)}{\mathcal{A}+1}}\right\}, \tag{5.22}$$

$$\tau_B^{-1}\left(E-\frac{q^2(\mathcal{A}+2)}{4\mathcal{A}}\right)=2\pi^2\left\{\pm\sqrt{E_{AA}}-\sqrt{|E|+\frac{q^2(\mathcal{A}+2)}{4\mathcal{A}}}\right\}, \tag{5.23}$$

onde $E_{AB}$ e $E_{AA}$ são, respectivamente, as energias de dois corpos de $AB$ e $AA$. O sinal positivo refere-se ao estado ligado e o negativo ao virtual.

Finalmente substituindo $\tau_A$ e $\tau_B$, respectivamente, nas eqs. (5.20) e (5.21) temos a forma final das equações espectadoras em unidades de $\hbar = m_A = \mu_{(3)} = 1$ com as energias e momentos reescalonados como $\epsilon = \frac{E}{\mu_{(3)}^2}$, $\epsilon_{AA} = \frac{E_{AA}}{\mu_{(3)}^2}$, $\epsilon_{AB} = \frac{E_{AB}}{\mu_{(3)}^2}$, $\frac{\vec{q}_k}{\mu_{(3)}} \equiv \frac{\vec{q}_i}{\mu_{(3)}} \equiv \vec{q}$, $\frac{\vec{q}_i\,'}{\mu_{(3)}} \equiv \frac{\vec{q}_j}{\mu_{(3)}} \equiv \vec{k}$:

$$\begin{aligned} f_A(\vec{q}) &= \left(\frac{\mathcal{A}+1}{2\mathcal{A}}\right)^{3/2}\frac{1}{\pi}\left(\sqrt{|\epsilon|+\frac{q^2(\mathcal{A}+2)}{2(\mathcal{A}+1)}}\mp\sqrt{\epsilon_{AB}}\right)^{-1}\int_0^\infty k^2dk\int_{-1}^1 dy \\ &\times \left[\frac{1}{|\epsilon|+q^2+\frac{\mathcal{A}+1}{2\mathcal{A}}k^2+kqy}-\frac{1}{1+q^2+\frac{\mathcal{A}+1}{2\mathcal{A}}k^2+kqy}\right]f_B(\vec{k}) \\ &- \int_{-1}^1\left[\frac{1}{|\epsilon|+\frac{(\mathcal{A}+1)}{2\mathcal{A}}q^2+\frac{(\mathcal{A}+1)}{2\mathcal{A}}k^2+\frac{1}{\mathcal{A}}kqy}-\frac{1}{1+\frac{(\mathcal{A}+1)}{2\mathcal{A}}q^2+\frac{(\mathcal{A}+1)}{2\mathcal{A}}k^2+\frac{1}{\mathcal{A}}kqy}\right]f_A(\vec{k}). \end{aligned} \tag{5.24}$$

$$\begin{aligned} f_B(\vec{q}) &= \frac{2}{\pi}\left(\sqrt{|\epsilon|+\frac{(\mathcal{A}+2)}{2\mathcal{A}}q^2}\mp\sqrt{\epsilon_{AA}}\right)^{-1}\int_0^\infty k^2dk \\ &\times \int_{-1}^1 dy\left[\frac{1}{|\epsilon|+\frac{(\mathcal{A}+1)}{2\mathcal{A}}q^2+k^2+kqy}-\frac{1}{1+\frac{(\mathcal{A}+1)}{2\mathcal{A}}q^2+k^2+kqy}\right]f_A(\vec{k}). \end{aligned} \tag{5.25}$$

## 5.2 Esquema de classificação

Nesta seção faremos um estudo sistemático sobre os diferentes sistemas de três corpos (do tipo $AAB$) com momento angular orbital total nulo que podem ser formados conforme mudamos as interações entre os subsistemas de dois corpos. As diversas possibilidades de configuração são mostradas na fig. (5.2).

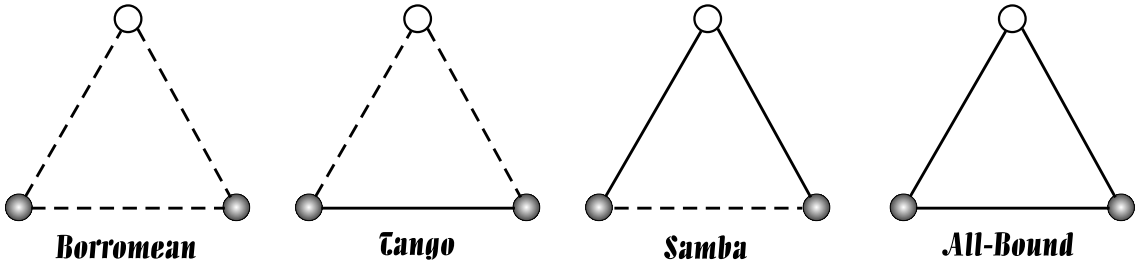


Figura 5.2: Esquema de classificação. A linha contínua representa um estado ligado e a linha tracejada um estado virtual.

Por conveniência manteremos os nomes dos sistemas conforme a Ref. [10]. O sistema onde os pares são completamente desligados é chamado de *Borromean*, pares completamente ligados *All-Bound*, um par ligado e dois pares desligados *Tango* [43] e dois pares ligados e um desligado *Samba*. O nome *Tango* foi dado ao sistema em questão porque as duas partículas ligadas devem se mexer de uma forma muito harmoniosa (como na dança que leva o mesmo nome) para que o sistema de três corpos seja ligado. No caso do sistema batizado de *Samba*, como dois subsistemas são ligados, as partículas podem se "mexer" um pouco mais e ainda assim formar um sistema ligado de três corpos.

Uma análise qualitativa das eqs. (5.24) e (5.25) nos mostra o que acontece quando passamos de um sistema para outro (note que uma maneira fácil para identificar qual sinal corresponde ao estado ligado, ou virtual, é notar que o estado ligado corresponde a um pólo na matriz-$T$ de dois corpos). Na configuração do tipo *All-Bound* os sinais na frente de $\sqrt{\epsilon_{AB}}$ e $\sqrt{\epsilon_{AA}}$ são negativos, o *Samba* possui um sinal negativo na frente de $\sqrt{\epsilon_{AB}}$ e um positivo na frente de $\sqrt{\epsilon_{AA}}$, o *Tango* possui um sinal negativo na frente de $\sqrt{\epsilon_{AA}}$ e um positivo na frente de $\sqrt{\epsilon_{AB}}$, finalmente o *Borromean* possui um sinal positivo na frente de $\sqrt{\epsilon_{AB}}$ e $\sqrt{\epsilon_{AA}}$. Assim, a seqüência das confi-

gurações de acordo com a intensidade efetiva de atração do kernel fica: *All-Bound* > *Samba* > *Tango* > *Borromean*. Essas diferenças entre os kernels se refletem nos tamanhos dos sistemas da seguinte maneira (para uma mesma energia de ligação de três corpos): no caso do kernel mais atrativo os constituintes do sistema podem ficar mais afastados e produzir um sistema ligado, já com o kernel menos atrativo as partículas devem estar mais próximas umas das outras. Obviamente poderíamos raciocinar no sentido de que quanto maior a atração mais próximas estariam as partículas, todavia veremos através dos resultados numéricos que isso não acontece. Desta forma, para uma mesma energia de ligação de três corpos o tamanho dos sistemas deve variar da seguinte maneira: *All-Bound* > *Samba* > *Tango* > *Borromean*.

De maneira análoga à eq. (3.30) podemos escrever as funções de escala para o caso de um sistema formado por duas partículas de massas idênticas, $AA$, e uma distinta, $B$. Agora o sistema depende de duas energias de dois corpos e da razão entre as massas de $A$ e de $B$. Assim, para um observável genérico $\mathcal{O}$ com dimensão de $[energia]^{\eta}$, em uma certa energia $E$, a função de escala $\mathcal{D}$ pode ser escrita como:

$$\mathcal{O}\left(E, E_3, E_{AA}, E_{AB}\right) = (E_3)^{\eta}\mathcal{D}\left(\sqrt{E/E_3}, \pm\sqrt{E_{AA}/E_3}, \pm\sqrt{E_{AB}/E_3}, \mathcal{A}\right), \quad (5.26)$$

as energias $E_{A\gamma}$ ($\gamma = A, B$) são sempre negativas. Desta forma a natureza do estado de dois corpos é dado pelo sinal $\pm$. O sinal + em frente de $\sqrt{|E_{A\gamma}|}$ indica um estado ligado e o $-$ um estado virtual.

De acordo com a eq. (5.26) as funções de escala para os raios podem ser escritas como:

$$\sqrt{\langle r^2_{A\gamma}\rangle |E_3|} = \mathcal{R}_{A\gamma}\left(\pm\sqrt{\frac{E_{AA}}{E_3}}, \pm\sqrt{\frac{E_{AB}}{E_3}}, \mathcal{A}\right), \quad (5.27)$$

$$\sqrt{\langle r^2_{\gamma}\rangle |E_3|} = \mathcal{R}^{CM}_{\gamma}\left(\pm\sqrt{\frac{E_{AA}}{E_3}}, \pm\sqrt{\frac{E_{AB}}{E_3}}, \mathcal{A}\right). \quad (5.28)$$

Os resultados das figuras (5.3) a (5.6) serão mostrados conforme a eq.

(5.27). Nessas figuras uma das energias do subsistema de dois corpos é fixada em relação à energia de três corpos, a outra energia varia. Para os cálculos nós usamos valores de $\mathcal{A}$ iguais a 0.1, 1 e 200. As energias dos subsistemas podem ser ligadas ou virtuais, desta forma conseguimos analisar as quatro configurações mostradas na fig. (5.2). Introduziremos agora as seguintes definições $K_{AA}^2 = E_{AA}/E_3$ e $K_{AB}^2 = E_{AB}/E_3$:

$$\begin{aligned} K_{AA} &= \pm\sqrt{E_{AA}/E_3} \\ K_{AB} &= \pm\sqrt{E_{AB}/E_3} \end{aligned} \tag{5.29}$$

os sinais + e − referem-se, respectivamente, aos estados ligados e virtuais dos subsistemas de dois corpos.

Nas figuras (5.3) a (5.6) os resultados são apresentados em unidades de $\hbar = m_A = 1$, assim o produto do raio quadrático médio e da energia de três corpos é um adimensional. A energia do subsistema do numerador varia e a do denominador é mantida fixa segundo uma certa razão com $E_3$.

Na fig. (5.3) superior o raio quadrático médio de $AB$ é mostrado quando o subsistema $AA$ é ligado (linha tracejada) e virtual (traço-ponto). Do lado direito da linha vertical contínua passando pelo 0, $AB$ é ligado e do lado esquerdo é virtual. Na linha tracejada podemos ver o aumento de $\sqrt{\langle r_{AB}^2\rangle|E_3|}$ conforme passamos do sistema *Tango* para o *All-Bound*. Na traço-ponto o aumento se dá quando passamos do sistema *Borromean* para o *Samba*.

Na fig. (5.3) inferior estão os resultados de $\sqrt{\langle r_{AA}^2\rangle|E_3|}$. Nessa figura, $AA$ é virtual na linha pontilhada e ligado na contínua. O aumento se dá quando passamos dos sistemas *Tango* para *All-Bound*, linha contínua, e *Borromean* para *Samba*, linha pontilhada. Nesse caso vemos uma variação muito pequena quando o subsistema $AA$ muda de virtual para ligado, essa diferença aumenta conforme aumentamos $\mathcal{A}$, como pode ser visto nas figuras (5.4) e (5.5). Isso pode ser entendido através do papel dominante da partícula mais leve, $B$, na interação de longo alcance entre as partículas

mais pesadas, $A$, conforme já foi mostrado numa aproximação adiabática do sistema de três corpos [94].

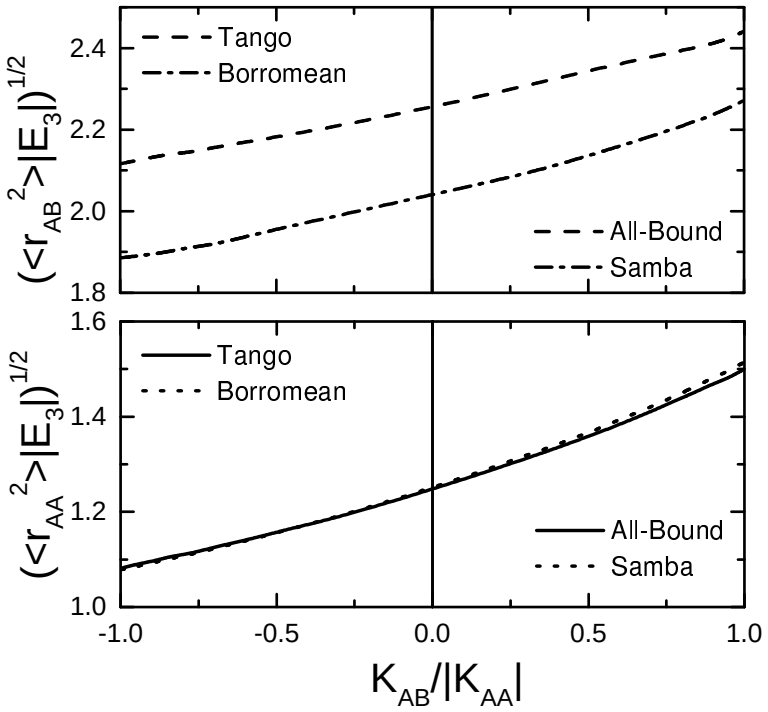


Figura 5.3: Produtos adimensionais $\sqrt{\langle r_{AB}^2\rangle|E_3|}$ (figura superior) e $\sqrt{\langle r_{AA}^2\rangle|E_3|}$ (figura inferior) para $\mathcal{A} = 0.1$ e $E_{AA}/E_3 = K_{AA}^2 = 0.1$ em função de $K_{AB}/|K_{AA}|$. Na figura superior o subsistema $AA$ ligado é representado pela linha tracejada e o virtual pela linha traço-ponto. Na figura inferior o par $AA$ ligado é representado pela linha contínua e o virtual pela pontilhada. A linha vertical passando por $K_{AB} = 0$ marca a transição entre as diferentes configurações.

Na fig. (5.4) nós mostramos os resultados de $\sqrt{\langle r_{A\gamma}^2\rangle|E_3|}$ em função de $K_{AB}/|K_{AA}|$ para três partículas de massas idênticas, $\mathcal{A} = 1$. Como na fig. (5.3) a razão $K_{AA}$ foi fixada em $K_{AA} = \pm\sqrt{0.1}$, com o sinal + para o estado ligado (linhas tracejada e contínua) e − para o virtual (linhas traço-ponto e pontilhada). Na parte superior podemos ver o resultado de $\sqrt{\langle r_{AB}^2\rangle|E_3|}$ e na parte inferior de $\sqrt{\langle r_{AA}^2\rangle|E_3|}$. O produto $\sqrt{\langle r_{A\gamma}^2\rangle|E_3|}$ aumenta conforme passamos do sistema *Tango* para *All-Bound* (linha tracejada e contínua) e do sistema *Borromean* para *Samba* (linha traço-ponto e pontilhada). Esses comportamentos se repetem quando passamos para sistemas mais pesados, $\mathcal{A} = 200$, conforme veremos nas figuras (5.5) e (5.6).

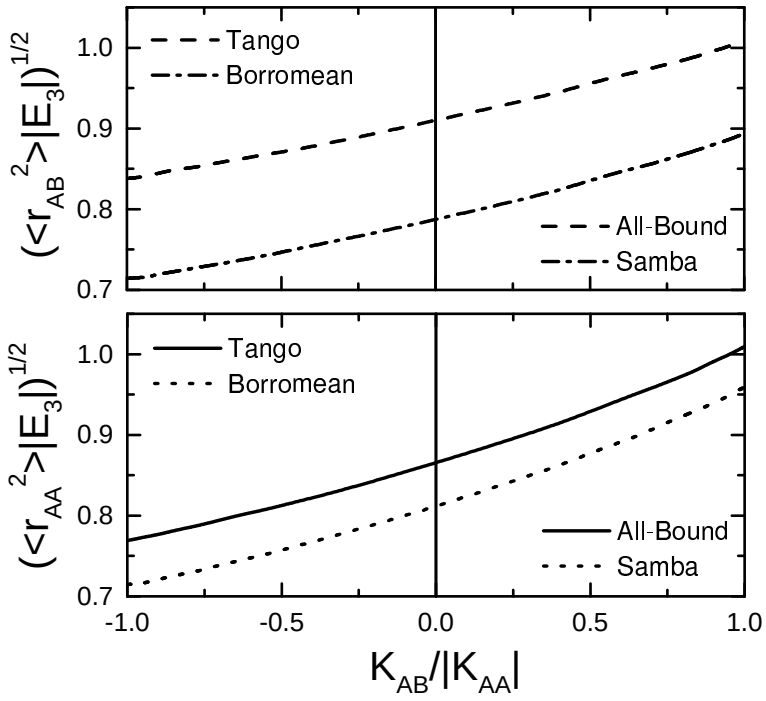


Figura 5.4: Produtos adimensionais $\sqrt{\langle r_{AB}^2\rangle|E_3|}$ (figura superior) e $\sqrt{\langle r_{AA}^2\rangle|E_3|}$ (figura inferior) para $\mathcal{A}=1$ e $K_{AA}^2=0.1$ em função de $K_{AB}/|K_{AA}|$. As convenções para as linhas são as mesmas da fig. (5.3).

Nas figuras (5.5) e (5.6) os cálculos foram feitos utilizando $\mathcal{A}=200$. Na fig. (5.5) a energia do par $AA$ foi fixada segundo a razão $K_{AA}=\pm\sqrt{0.1}$ e variamos a energia do par $AB$. Na fig. (5.6) a energia fixa foi a do par $AB$, $K_{AB}=\pm\sqrt{0.1}$, e variamos a energia do par $AA$. Podemos notar que a transição que ocorre na fig. (5.6) para $-1\leq K_{AA}/|K_{AB}|\leq 1$ é a transição vertical que se dá na fig. (5.5) quando $K_{AB}/|K_{AA}|=\pm 1$. Assim, comparando a parte superior da fig. (5.5) e a transição vertical de *All-Bound* para *Samba* para $K_{AB}/|K_{AA}|=1$ e *Tango* para *Borromean* para $K_{AB}/|K_{AA}|=-1$ vemos que elas correspondem, respectivamente, às linhas tracejada e traço-ponto na parte superior da fig. (5.6). O mesmo ocorre com as partes inferiores de ambas as figuras, a transição vertical na fig. (5.5) de *All-Bound* para *Samba* para $K_{AB}/|K_{AA}|=1$ e de *Tango* para *Borromean* para $K_{AB}/|K_{AA}|=-1$ correspondem, respectivamente, às linhas contínua e pontilhada da fig. (5.6).

Conforme havíamos antecipado, os sistema se comportam da seguinte maneira para uma mesma energia de ligação de três corpos: *All-Bound* > *Samba* > *Tango* > *Borromean*.

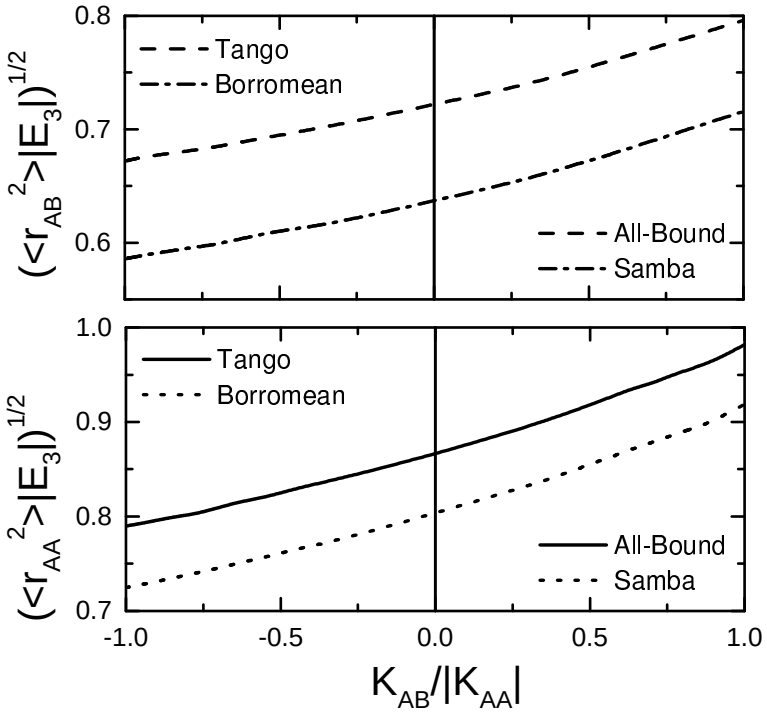


Figura 5.5: Produtos adimensionais $\sqrt{\langle r_{AB}^2\rangle|E_3|}$ (figura superior) e $\sqrt{\langle r_{AA}^2\rangle|E_3|}$ (figura inferior) para $\mathcal{A} = 200$ e $K_{AA}^2 = 0.1$ em função de $K_{AB}/|K_{AA}|$. As convenções para as linhas são as mesmas das figuras (5.3) e (5.4).

Na fig. (5.7) as energias de ligação de dois corpos foram colocadas iguais a zero e variamos a razão entre as massas, $\mathcal{A}$. Nessa figura são mostrados os resultados para $\sqrt{\langle r_{A\gamma}^2\rangle|E_3|}$ e $\sqrt{\langle r_{\gamma}^2\rangle|E_3|}$.

Na situação da fig. (5.7) como as energias de dois corpos são iguais a zero a única escala física do sistema é a energia de três corpos e as funções de escala dadas pelas eqs. (5.27) e (5.28) ficam dependentes somente da razão entre as massas das partículas e se reduzem a:

$$\sqrt{\langle r_{A\gamma}^2\rangle|E_3|} = \mathcal{R}'_{A\gamma}(\mathcal{A}), \tag{5.30}$$

$$\sqrt{\langle r_{\gamma}^2\rangle|E_3|} = \mathcal{R}'^{CM}_{\gamma}(\mathcal{A}). \tag{5.31}$$

Na fig. (5.7) vemos que as distâncias entre as partículas e das partículas ao $CM$ do sistema saturam rapidamente conforme aumentamos $\mathcal{A}$, porém elas divergem

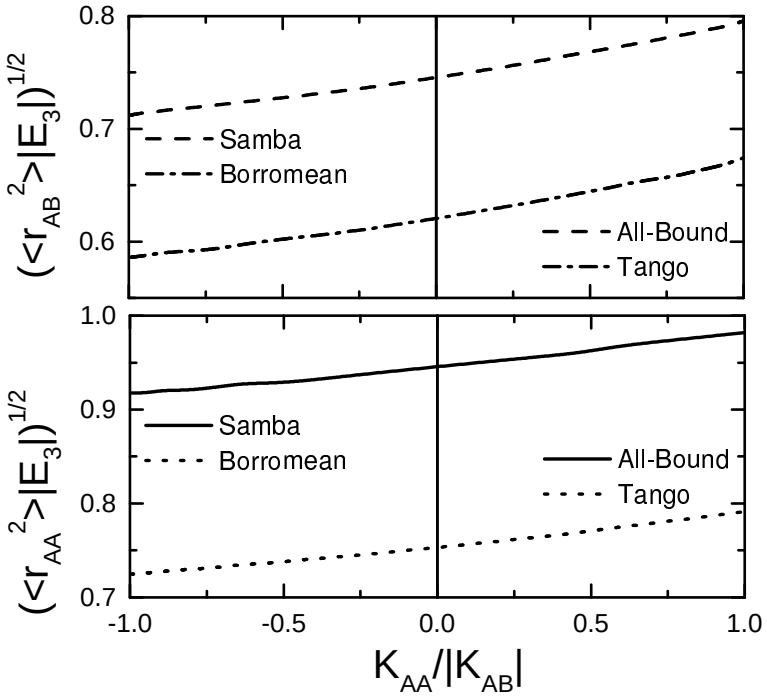


Figura 5.6: Produtos adimensionais $\sqrt{\langle r_{AB}^2\rangle|E_3|}$ (figura superior) e $\sqrt{\langle r_{AA}^2\rangle|E_3|}$ (figura inferior) para $\mathcal{A} = 200$ e $E_{AB}/E_3 = K_{AB}^2 = 0.1$ em função de $K_{AA}/|K_{AB}|$. Na figura superior o subsistema $AB$ ligado é representado pela linha tracejada e o virtual pela linha traço-ponto. Na figura inferior o par $AB$ ligado é representado pela linha contínua e o virtual pela pontilhada. A linha vertical passando por $K_{AA} = 0$ marca a transição entre as diferentes configurações. Essas linhas representam as transições verticais ($|K_{AB}| = |K_{AA}|$) nas extremidades da fig. (5.5).

conforme a razão entre as massas tende a zero. A razão para o aumento dos produtos $\sqrt{\langle r_{A\gamma}^2\rangle|E_3|}$ e $\sqrt{\langle r_{\gamma}^2\rangle|E_3|}$ é devido ao momento médio do caroço, $\sim \sqrt{\mathcal{A}|E_3|}$, que tende a zero fazendo com que o tamanho do sistema, nas unidades escolhidas, cresça infinitamente. Os resultados tendem a valores finitos após a multiplicação por $\sqrt{\mathcal{A}}$. Devemos também chamar a atenção para o fato das distâncias de $B$ ao $CM$ tender a zero e de $A$ ao $CM$ tender à distância $AB$ conforme $\mathcal{A}$ vai para infinito, como deveríamos esperar.

Nas próximas seções vamos particularizar o estudo feito sobre os tamanhos dos sistemas de três corpos para o caso de núcleos exóticos e moléculas fracamente ligadas.

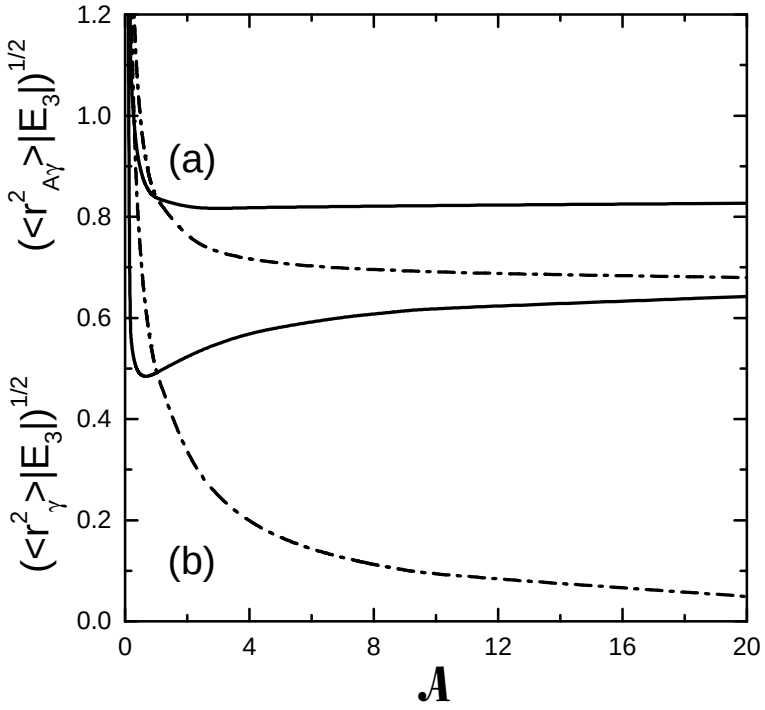


Figura 5.7: Produtos adimensionais $\sqrt{\langle r^2_{A\gamma}\rangle|E_3|}$ e $\sqrt{\langle r^2_{\gamma}\rangle|E_3|}$ ($\gamma = A, B$) em função da razão entre as massas, $\mathcal{A}$. As energias de dois corpos foram colocadas iguais a zero. A parte superior da figura, (a), mostra os resultados de $\sqrt{\langle r^2_{AA}\rangle|E_3|}$, linha contínua, e $\sqrt{\langle r^2_{AB}\rangle|E_3|}$, linha traço-ponto. A parte inferior, (b), mostra os resultados para $\sqrt{\langle r^2_{A}\rangle|E_3|}$, linha contínua, e $\sqrt{\langle r^2_{B}\rangle|E_3|}$, linha traço-ponto.

## 5.3 Núcleos exóticos leves

O estudo de núcleos que estão próximos à linha de estabilidade, mais especificamente à linha linha de estabilidade de neutrons, revelou estruturas interessantes, como por exemplo um halo formado pelos neutrons. Esses núcleos, denominados de núcleos exóticos ou núcleos-halo, tornaram-se objetos de intensas investigações da física nuclear atual. Embora a primeira observação experimental de um núcleo exótico típico tenha sido feita na segunda metade da década de 30 ($^6$He [95]) o enfoque atual dado aos núcleos próximos à fronteira de estabilidade teve início somente há 15 anos a partir da observação do aumento da seção de choque do $^{11}$Li em um experimento de medida da seção de choque de isótopos de Li colidindo com alguns alvos [96, 97] (a detecção do $^{11}$Li foi feita pela primeira vez em 1966 [98]). O aumento da seção de choque do $^{11}$Li foi interpretado como sendo uma decorrência da estrutura desse

núcleo, o qual seria formado por um caroço, $^9$Li, e dois neutrons fracamente ligados [99] (esse aumento foi verificado experimentalmente em 1989 [100]). Revisões a respeito de núcleos exóticos podem ser encontradas nas Refs. [25, 101, 102, 103, 104].

O formalismo desenvolvido no início deste capítulo que foi utilizado de uma forma genérica para um sistema de três corpos fracamente ligado e composto por duas partículas idênticas e uma diferente será utilizado nessa seção para o caso específico de núcleos exóticos leves. Os núcleos exóticos serão tratados aqui como um sistema de três corpos constituído por um caroço pontual que chamaremos de $C$ e dois neutrons fracamente ligados provenientes do halo que chamaremos de $n$. Nesta seção $\gamma = n, C$.

Nossos cálculos para os raios quadráticos médios entre os dois neutrons do halo serão comparados com os resultados experimentais de $^6$He, $^{11}$Li e $^{14}$Be provenientes das Refs. [105, 106]. A tabela 5.1 mostra esses resultados.

A fig. (5.8) reproduz os resultados já apresentados na fig. (5.7) acrescidos dos pontos experimentais para o $^6$He, $^{11}$Li e $^{14}$Be dados na tabela 5.1.

Os pontos experimentais colocados na fig. (5.8) são meramente ilustrativos considerando que os subsistemas $^5$He, $^{10}$Li e $^{13}$Be tivessem uma energia de ligação igual a zero. Conforme podemos ver na fig. (5.8) a utilização de uma energia igual a zero para o $^{10}Li$ não nos dá um resultado compatível com o resultado experimental para a distância $nn$ no halo do $^{11}Li$, tabela 5.1. Devemos ressaltar o fato de que os resultados para a energia do estado virtual do $^{10}$Li na literatura ainda são bastante controversos [108, 109, 110, 111, 112].

Podemos ver na tabela 5.1 que os resultados de $\sqrt{\langle r_{nn}^2 \rangle}$ para o $^6$He utilizando o nosso modelo indicam que o estado virtual do $^5$He deve possuir uma energia próxima de zero, ou até mesmo fracamente ligada, o que não concorda com os valores dados na literatura os quais sugerem uma energia bem maior [107, 44]. Essa discrepância é compreensível levando-se em conta que a interação para $n$-$^4$He é repulsiva na onda-$S$ e atrativa na onda $P$, produzindo, assim, um valor elevado para a energia do estado virtual do $^5$He (no nosso modelo o pólo da onda-$S$ deveria ficar próximo do

| Caroço ($C$) | $E_3$ (MeV) | $E_{nA}$ (MeV) | $\sqrt{\langle r_{nn}^2 \rangle}$ (fm) | $\sqrt{\langle r_{nn}^2 \rangle}_{exp}$ (fm) |
|---|---|---|---|---|
| $^4$He | 0.973 | 0<br>0.3(v)<br>4.0(v)[107] | 5.1<br>4.6<br>3.6 | 5.9±1.2 |
| $^9$Li | 0.32 | 0<br>0.8(v)[108] | 9.2<br>5.9 | 6.6±1.5 |
| $^9$Li | 0.29 | 0<br>0.05(v)[109, 110, 111, 112]<br>0.8(v)[108] | 9.7<br>8.5<br>6.7 | 6.6±1.5 |
| $^9$Li | 0.37 | 0<br>0.05(v)[109, 110, 111, 112]<br>0.8(v)[108] | 8.6<br>7.7<br>6.2 | 6.6±1.5 |
| $^{12}$Be | 1.337 | 0<br>0.2(v)[113] | 4.6<br>4.2 | 5.4±1.0 |
| $^{18}C$ | 3.50 | 0.16[42]<br>0.53[114] | 3.0<br>4.4 | -<br>- |

Tabela 5.1: Resultados para os raios quadráticos médios nêutron-nêutron em núcleos exóticos. Os caroços são dados na primeira coluna, os valores absolutos das energias de três corpos, $E_3$, e do subsistema nêutron-caroço, $E_{nC}$, são dados, respectivamente, na coluna dois e três. Para a energia de três corpos nós utilizamos o valor central da energia de separação de 2 neutrons, $S(2n)$, dada na Ref. [42] com exceção do caso do lítio. Neste caso nós utilizamos os valores central (0.29 MeV) e o central + 1 desvio padrão (0.32 MeV) dados na Ref. [101] e o valor central (0.37 MeV) da Ref. [115]. Para os valores de $E_{nC}$, igual à energia de separação de um nêutron $S(n)$, nós utilizamos os valores dados na literatura (as refererências aparecem na tabela), um (v) aparece na frente da energia quando esta se referir a um estado virtual. Para a energia do estado virtual $nn$ foi utilizado o valor de 143 keV. Os valores experimentais da última coluna são das Refs. [105, 106].

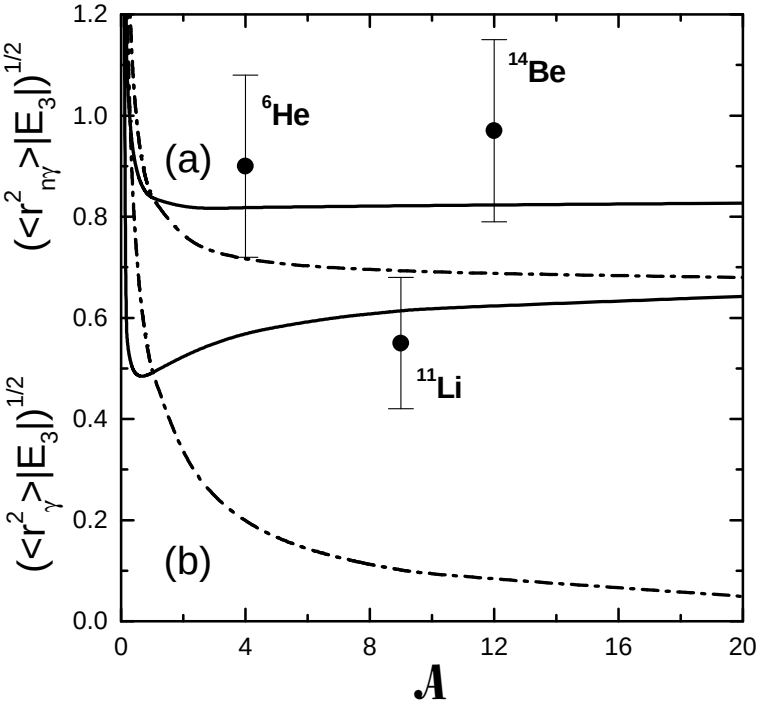


Figura 5.8: Produtos adimensionais $\sqrt{\langle r^2_{n\gamma}\rangle|E_3|}$ e $\sqrt{\langle r^2_{\gamma}\rangle|E_3|}$ ($\gamma = n, C$) em função da razão entre as massas, $\mathcal{A}$. As energias de dois corpos foram colocadas iguais a zero. A parte superior da figura, (a), mostra os resultados de $\sqrt{\langle r^2_{nn}\rangle|E_3|}$, linha contínua, e $\sqrt{\langle r^2_{nC}\rangle|E_3|}$, linha traço-ponto. A parte inferior, (b), mostra os resultados para $\sqrt{\langle r^2_{n}\rangle|E_3|}$, linha contínua, e $\sqrt{\langle r^2_{C}\rangle|E_3|}$, linha traço-ponto. Os círculos cheios são os pontos experimentais de $\sqrt{\langle r^2_{nn}\rangle|E_3|}$ para o $^6$He, $^{11}$Li e $^{14}$Be retirados da Ref. [105, 106].

limiar do espalhamento).

Para a energia de ligação do subsistema $n$-$^9$Li sabe-se que ambas as ondas, $S$ e $P$, são importantes, um dos motivos que deve explicar o desvio dos nossos resultados com os resultados experimentais. Todavia, no caso do $^{10}$Li nossa aproximação deve ser um pouco melhor já que neste caso a interação na onda-$S$ é atrativa.

Vale ressaltar também, que em todos os casos nós estamos considerando como entrada para os nossos cálculos os valores experimentais das energias dos subsistemas de dois corpos. Assim, embora o nosso modelo envolva apenas a onda-$S$, nós estamos considerando de forma indireta o efeito das ondas superiores nos nossos resultados. Os tamanhos dos sistemas também são obtidos da cauda da função de onda que é dominada pela onda-$S$. Outros fatores que poderiam melhorar os nossos

resultados seriam a inclusão no nosso modelo do princípio de Pauli e um tamanho finito para o caroço.

Os raios quadráticos médios são extraídos experimentalmente de uma função que fornece uma informação direta da função de onda do halo: a função de correlação [105, 106]. Essa função de correlação teve origem na astrofísica e foi inicialmente desenvolvida por Hanbury-Brown e Twiss na década de 50 para determinar a dimensão de objetos astronômicos distantes da Terra [116] (uma revisão sobre esse assunto pode ser encontrada na Ref. [117]), posteriormente a aplicação do método se estendeu a outras áreas da física, como, por exemplo, a física nuclear onde a função de correlação nos fornece informações sobre as dimensões nucleares.

Utilizando a mesma notação da subseção 5.1 podemos escrever a função de correlação, $C_{nn}(\vec{p}_C)$, como uma função do momento relativo dos neutrons do halo, $\vec{p}_C$, como (embora os neutrons sejam indistingüíveis entre si nós os chamaremos de $n$ e $n'$ apenas para facilitar a definição das coordenadas):

$$C_{nn}(\vec{p}_C) = \frac{\int d^3q_C |\Phi(\vec{q}_C, \vec{p}_C)|^2}{\int d^3q_C \rho(\vec{q}_{n'})\rho(\vec{q}_n)}, \qquad (5.32)$$
$$\vec{q}_{n'} \equiv \vec{p}_C - \frac{\vec{q}_C}{2} \quad \text{e} \quad \vec{q}_n \equiv -\vec{p}_C - \frac{\vec{q}_C}{2}.$$

A densidade de 1-corpo é dada por:

$$\rho(\vec{q}_{n'}) = \int d^3q_n \left| \Phi\left(-\vec{q}_{n'} - \vec{q}_n, \frac{\vec{q}_{n'} - \vec{q}_n}{2}\right)\right|^2, \qquad (5.33)$$

onde $\Phi \equiv \Phi(\vec{q}_C, \vec{p}_C)$ é a amplitude de quebra da função de onda de três corpos com a interação de estado final (FSI) entre os neutrons.

A FSI é introduzida diretamente no produto escalar $\Phi \equiv \langle \vec{q}_C; \vec{p}_C{}^{(-)} | \Psi \rangle$, onde o ket $|\vec{p}_C{}^{(-)}\rangle$ se refere à onda distorcida dos neutrons e é dada pela eq. de Lippmann-Schwinger. $\Phi$ é dada por:

$$\Phi = \Psi(\vec{q}_C, \vec{p}_C) - \frac{1/(2\pi^2)}{\sqrt{E_{nn}} + ip_C} \int d^3p \frac{\Psi(\vec{q}_C, \vec{p})}{p_C^2 - p^2 - i\epsilon}, \tag{5.34}$$

onde $E_{nn}$ é a energia do estado virtual de dois neutrons. No futuro prxímo pretendemos concluir os cálculos referentes à eq. (5.34).

## 5.4 Moléculas triatômicas fracamente ligadas

Veremos nesta seção que o formalismo também se aplica muito bem ao caso de moléculas triatômicas fracamente ligadas. Nesta seção a partícula $A$ da seção 5.1 representará um átomo de $^4$He e a partícula $B$ representará um dos seguintes átomos: $^4$He, $^6$Li, $^7$Li e $^{23}$Na.

Na fig. (5.9) são mostrados os resultados para o caso de um sistema composto por três átomos de hélio, $^4\text{He}_3$, na forma de um produto adimensional $\sqrt{\langle r^2 \rangle S_3}$, $S_3 = E_3 - E_2$, em função da razão entre as energias de dois e três corpos $\sqrt{E_2/E_3}$. Os cálculos realísticos da Ref. [39] também estão nesta figura.

Podemos ver na fig. (5.9) que os nossos resultados para o estado fundamental (linha contínua) e para o estado excitado (linha tracejada) praticamente coincidem. Isso mostra a validade do nosso limite de escala quando as energias reescalonadas com respeito a $\mu^2$ tendem a zero, neste limite os resultados devem ser os mesmos. Os cálculos realísticos mostram um desvio de aproximadamente 20% dos nossos resultados para o estado fundamental, já para o estado excitado os dois resultados mostram-se mais próximos. Esse fato pode ser compreendido levando-se em conta o tamanho dos trímeros. No caso do estado excitado o tamanho do trímero é, aproximadamente, 10 vezes maior que o estado fundamental correspondente. Desta forma, a nossa aproximação é melhor nesse caso onde o tamanho da molécula é muito maior que o alcance do potencial.

A fig. (5.10) é basicamente igual às figuras (5.7) e (5.8) com a diferença de que neste caso os cálculos são feitos para $\mathcal{A} \geq 1$ e além do estado fundamental, $N = 0$

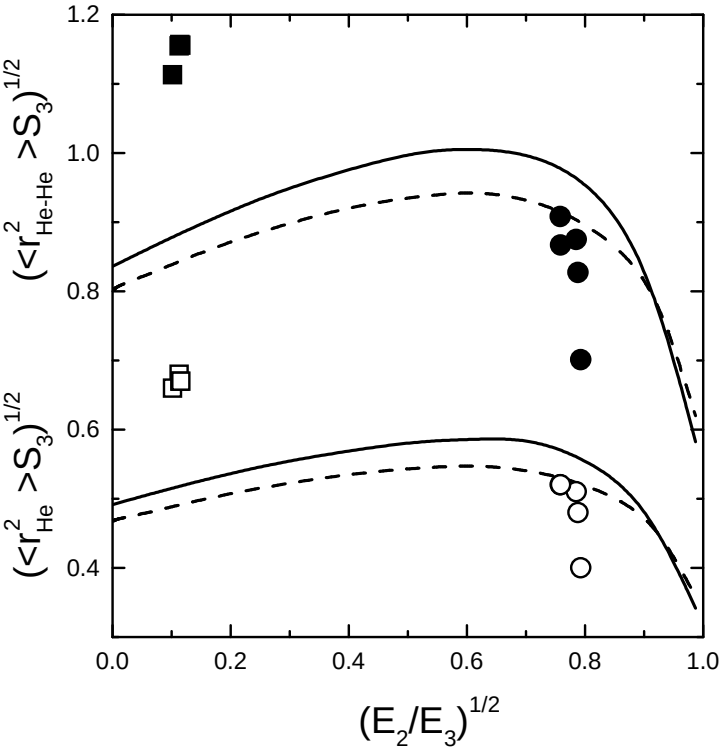


Figura 5.9: Produtos adimensionais $\sqrt{\langle r^2_{He-He}\rangle S_3}$ (curvas superiores) e $\sqrt{\langle r^2_{He}\rangle S_3}$ (curvas inferiores) em função da razão $\sqrt{E_2/E_3}$. $\langle r^2_{He-He}\rangle$ é a distância quadrática média entre dois átomos de $^4$He, $\langle r^2_{He}\rangle$ é a distância de um átomo de $^4$He ao centro-de-massa do sistema e $S_3 = E_3 - E_2$. Nossos resultados para o estado fundamental e primeiro estado excitado são dados, respectivamente, pela linha contínua e tracejada. Os cálculos realísticos retirados da Ref. [39] para $\sqrt{\langle r^2_{He-He}\rangle S_3}$ são dados pelos quadrados cheios (estado fundamental) e círculos cheios (estado excitado), e para $\sqrt{\langle r^2_{He}\rangle S_3}$ pelos quadrados vazios (estado fundamental) e círculos vazios (estado excitado).

(linha contínua), foi incluído o primeiro estado excitado, $N = 1$ (linha tracejada). Embora a fig. (5.10) esteja inserida no contexto das moléculas ela é bastante geral, por esse motivo iremos manter a notação $AAB$ para representar um sistema triatômico.

Conforme podemos ver na fig. (5.10) superior, (a), as curvas saturam rapidamente. Para $\mathcal{A} \sim 3$ as curvas assumem o mesmo valor que $\mathcal{A} \to \infty$. Fazendo $\mathcal{A} \to \infty$ os cálculos dão para $\langle r^2_{AA}\rangle$ o valor de $0.69/E_3$ para $N = 0$ e $0.61/E_3$ para $N = 1$ e para $\langle r^2_{AB}\rangle$ o valor de $0.45/E_3$ para $N = 0$ e $0.40/E_3$ para $N = 1$. A parte inferior da fig. (5.10), (b), mostra os raios quadráticos médios em relação ao $CM$ do sistema. Aumentando-se $\mathcal{A}$ vemos que $\langle r^2_A\rangle$ e $\langle r^2_B\rangle$ tendem, respectivamente, a

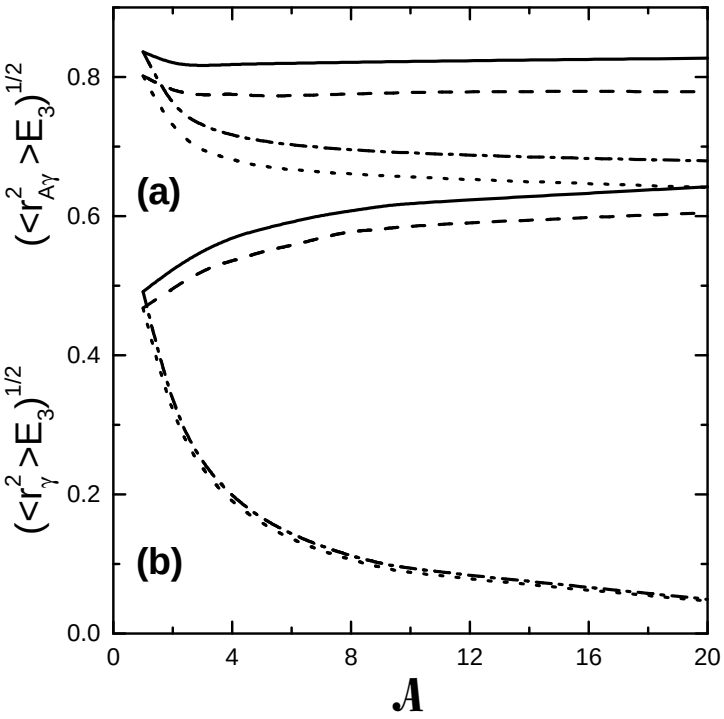


Figura 5.10: Resultados para um sistema triatômico do tipo $AAB$, com $\gamma = A, B$. Produtos adimensionais $\sqrt{\langle r^2_{A\gamma}\rangle S_3}$ (curvas superiores) e $\sqrt{\langle r^2_{\gamma}\rangle S_3}$ (curvas inferiores) em função da razão entre as massa $\mathcal{A}$. $\langle r^2_{A\gamma}\rangle$ é a distância quadrática média entre os átomos $A$ e $\gamma$, e $\langle r^2_{\gamma}\rangle$ é a distância do átomo $\gamma$ ao CM do sistema. As energias dos subsistemas de dois corpos são iguais a zero. Nossos resultados para o estado fundamental são dados pela linha contínua ($\gamma = A$) e traço-ponto ($\gamma = B$), e para o primeiro estado excitado pelas linhas tracejada ($\gamma = A$) e pontilhada ($\gamma = B$).

$\langle r^2_{AB}\rangle$ e a 0, como era esperado considerando que a partícula pesada deve estar no $CM$ do sistema para $\mathcal{A}$ muito grande. Devemos ressaltar o fato de que embora a razão entre as energias do estado fundamental, N=0, e do estado excitado, N=1, seja aproximadamente 500 para $\mathcal{A} = 1$ e 300 para $\mathcal{A} = 10$, as variações entre as duas curvas é de apenas 10%.

Na tabela (5.2) nós apresentamos os resultados do raios quadráticos médios para diferentes moléculas constituídas de dois átomos de $^4$He e um outro átomo que pode ser: $^4$He, $^6$Li, $^7$Li e $^{23}$Na. Os raios são calculados para o estado fundamental e as energias teóricas $E_3$, $E_{AA}$ e $E_{AB}$ são retiradas da Ref. [118].

Nosso resultado para $^4\mathrm{He}_3$ dá como resultado para $\sqrt{\langle r^2_{AA}\rangle}$ um valor de

| B | $E_3$ (mK) | $E_{AA}$ (mK) | $E_{AB}$ (mK) | $\sqrt{\langle r_{AA}^2\rangle}$ (Å) | $\sqrt{\langle r_{AB}^2\rangle}$ (Å) | $\sqrt{\langle r_A^2\rangle}$ (Å) | $\sqrt{\langle r_B^2\rangle}$ (Å) |
|---|---|---|---|---|---|---|---|
| $^4$He | 106.0 | 1.31 | 1.31 | 9.45 | 9.45 | 5.55 | 5.55 |
| $^6$Li | 31.4 | 1.31 | 0.12 | 16.91 | 16.38 | 10.50 | 8.14 |
| $^7$Li | 45.7 | 1.31 | 2.16 | 14.94 | 13.88 | 9.34 | 6.31 |
| $^{23}$Na | 103.1 | 1.31 | 28.98 | 11.66 | 9.54 | 8.12 | 1.94 |

Tabela 5.2: Raios quadráticos médios para moléculas do tipo $AAB$, com $A \equiv^4$He e com $B$ indicado na primeira coluna. A energia para o estado fundamental de três corpos e as energias dos subsistemas de dois corpos, obtidas da Ref. [118], estão representadas nas colunas 2, 3 e 4. $\sqrt{\langle r_{A\gamma}^2\rangle}$ e $\sqrt{\langle r_\gamma^2\rangle}$, com $\gamma = A, B$, são, respectivamente, os raios quadráticos médios entre os átomos $A$ e $\gamma$ e entre $\gamma$ e o $CM$ do sistema.

9.45 Å, que é 14 % menor que o valor de 11 Å obtido com os cálculos realísticos variacionais da Ref. [39]. Nosso resultado para $\sqrt{\langle r_A^2\rangle}$, 5.55 Å, também concorda com o valor 6.4 Å da Ref. [39]. Nossos resultados são bastante surpreendentes tendo em vista a simplicidade do cálculo onde as únicas entradas são as energias de dois e três corpos.

Utilizando as energias previstas no capítulo 3 para os trímeros no interior de condensados nós mostramos na tabela (5.3) os raios quadráticos médios dos átomos em relação ao $CM$ do trímero.

| Átomo | $E_2$ (mK) | $E_3$ (mK) | $\sqrt{\langle r_A^2 \rangle}$ (Å) | $E_3'$ (mK) | $\sqrt{\langle r_A^2 \rangle'}$ (Å) |
|---|---|---|---|---|---|
| $^{23}Na\|1,-1\rangle$ | 2.85 | 7.75 | 12 | 3.06 | 38 |
| $^{87}Rb\|1,-1\rangle^*$ | 0.17 | 0.56 | 22 | 0.175 | 114 |
| $^{87}Rb\|1,-1\rangle^\dagger$ | 0.17 | 0.47 | 25 | 0.183 | 91 |
| $^{85}Rb\|2,-2\rangle$ | $1.3 \times 10^{-4}$ | $2.4 \times 10^{-4}$ | 1293 | $1.7 \times 10^{-4}$ | 1944 |

Tabela 5.3: Resultados para o raio quadrático médio do átomo em relação ao $CM$ do sistema no interior de armadilhas magneto-ópticas utilizando as energias previstas no capítulo 3. Os átomos estão identificados na primeira coluna. Para cada energia do dímero, dada na coluna 2, nós temos duas energia para o trímero, colunas 3 e 5, com os raios correspondentes dados nas colunas 4 e 6. $^*$ átomos não condensados. $^\dagger$ átomos condensados. $|F, m_F\rangle$ são, respectivamente, o spin total e a sua projeção.

# Capítulo 6

# 4-corpos

A possibilidade de colapso de um sistema composto por três bosons quando o alcance da interação de dois corpos tende a zero (colapso Thomas) adiciona ao sistema uma nova escala - uma escala de três corpos - independente da escala de dois corpos. No contexto do problema de 4-corpos com interação de alcance zero existe portanto, a questão do aparecimento de uma nova escala física quando um bóson é adicionado ao sistema de três corpos. Neste primeiro estudo para investigar a dependência da energia do estado ligado de 4-corpos com uma escala típica de 4-corpos iremos formular as equações subtraídas de Faddeev-Yakubovsky através do propagador de 4-corpos de maneira análoga ao caso de três corpos. A escala física de 4-corpos traduz-se na energia referente ao ponto de subtração que ao ser variada, mantendo-se $\mu^2_{(3)}$ e $\tau$ fixos, poderá apresentar efeitos de reescalonamento na energia de 4-bosons, caso esta escala seja realmente necessária. A investigação numérica deste aspecto será deixada para um trabalho futuro.

## 6.1 Formalismo

A dinâmica de um sistema de 4-bosons pode ser descrita em termos das amplitudes de Faddeev-Yakubovsky (FY) [46], K e H, mostradas na figura (6.1), e definidas pelas seguintes equações:

$$|K^l_{ij,k}\rangle = G_{ij}v_{ij}G_0(v_{ik}+v_{jk})|\Psi\rangle \ (i<j), \tag{6.1}$$

$$|H_{ij,kl}\rangle = G_{ij}v_{ij}G_0v_{kl}|\Psi\rangle \ (i<j,k<l), \tag{6.2}$$

onde $G_{ij}$ é o propagador de 4-corpos dado por $G_{ij} = (E - H_0 - v_{ij})$ ($H_0$ é a energia cinética), $v_{ij}$ é o potencial de dois corpos entre as partículas $i$ e $j$ e $G_0$ é o propagador livre de 4-corpos. A função de onda total do sistema, $\Psi$, é dada pela soma das 18 amplitudes de FY, 12 delas dada pela eq. (6.1) e 6 pela eq. (6.2). As amplitudes $K^l_{ij,k}$ e $H_{ij,kl}$ descrevem, respectivamente, um sistema formado por 3 partículas ligadas, $ijk$, e uma livre, $l$, e um sistema formado pelos pares ligados, $ij$ e $kl$.

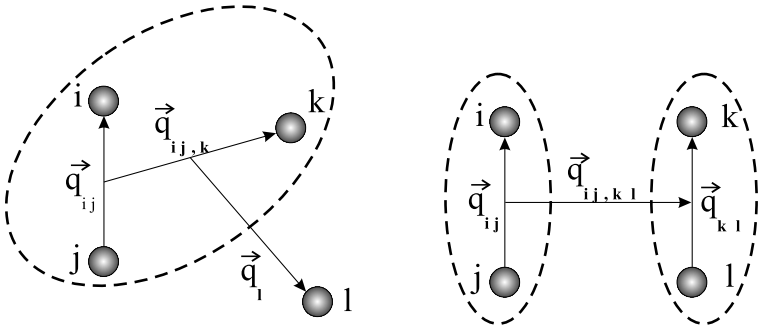


Figura 6.1: Coordenadas de Jacobi para as amplitudes de Faddeev-Yakubovsky do tipo K, lado esquerdo, e H, lado direito.

As amplitudes K e H podem ainda ser escritas em termos das amplitudes de Faddeev como:

$$|K^l_{ij,k}\rangle = G_{ij}v_{ij}(|F_{ik}\rangle + |F_{jk}\rangle)) \ (i<j), \tag{6.3}$$

$$|H_{ij,kl}\rangle = G_{ij}v_{ij}|F_{kl}\rangle \ (i<j,k<l), \tag{6.4}$$

onde $|F_{ij}\rangle = G_0v_{ij}|\Psi\rangle$ é a amplitude de Faddeev que pode também ser escrita em termos das amplitudes K e H da seguinte maneira:

$$|F_{ij}\rangle = |K^l_{ij,k}\rangle + |K^k_{ij,l}\rangle + |H_{ij,kl}\rangle, \tag{6.5}$$

desta forma substituindo a eq. (6.5) nas eqs. (6.3) e (6.4) e utilizando que $G_{ij}v_{ij} = G_0 t_{ij}$, temos que:

$$\begin{aligned}|K^l_{ij,k}\rangle &= G_0^{(3)} t_{ij}(E - E_{ij,k} - E_l)[|K^l_{ik,j}\rangle + |K^l_{jk,i}\rangle + |K^j_{ik,l}\rangle + |K^i_{jk,l}\rangle \\ &+|H_{ik,jl}\rangle + |H_{jk,il}\rangle], \qquad (6.6)\\ |H_{ij,kl}\rangle &= G_0^{(4)} t_{ij}(E - E_{ij,kl} - E_{kl})[|K^j_{kl,i}\rangle + |K^i_{kl,j}\rangle + |H_{kl,ij}\rangle], \qquad (6.7)\end{aligned}$$

onde os índices (3) e (4) sobrescritos nos $G_0$ indicam a escala que está sendo subtraída nos propagadores, isto é, $G_0^{(3)} = \frac{1}{E-H_0} - \frac{1}{\mu^2_{(3)}-H_0}$ e $G_0^{(4)} = \frac{1}{E-H_0} - \frac{1}{\mu^2_{(4)}-H_0}$, onde $\mu_{(3)}$ e $\mu_{(4)}$ são, respectivamente, as escalas de 3- e 4-corpos. Assim, substituindo as seguintes definições

$$|K^l_{ij,k}\rangle = G_0^{(3)}|\chi_{ij}\rangle\tau(E - E_{ij,k} - E_l)|k^l_{ij,k}\rangle,$$

$$|H_{ij,kl}\rangle = G_0^{(4)}|\chi_{ij}\rangle\tau(E - E_{ij,kl} - E_{kl})|h_{ij,kl}\rangle,$$

nas eqs. (6.6) e (6.7) e fazendo os devidos cancelamentos chegamos a:

$$\begin{aligned}|k^l_{ij,k}\rangle &= \langle\chi_{ij}|G_0^{(3)}|\chi_{ik}\rangle\tau(E - E_{ik,j} - E_l)|k^l_{ik,j}\rangle + \langle\chi_{ij}|G_0^{(3)}|\chi_{jk}\rangle\tau(E - E_{jk,i} - E_l)|k^l_{jk,i}\rangle \\ &+\langle\chi_{ij}|G_0^{(3)}|\chi_{ik}\rangle\tau(E - E_{ik,l} - E_j)|k^j_{ik,l}\rangle + \langle\chi_{ij}|G_0^{(3)}|\chi_{jk}\rangle\tau(E - E_{jk,l} - E_i)|k^i_{jk,l}\rangle \qquad (6.8)\\ &+\langle\chi_{ij}|G_0^{(4)}|\chi_{ik}\rangle\tau(E - E_{ik,jl} - E_{jl})|h_{ik,jl}\rangle + \langle\chi_{ij}|G_0^{(4)}|\chi_{jk}\rangle\tau(E - E_{jk,il} - E_{il})|h_{jk,il}\rangle,\end{aligned}$$

e

$$\begin{aligned}|h_{ij,kl}\rangle &= \langle\chi_{ij}|G_0^{(3)}|\chi_{kl}\rangle\tau(E - E_{kl,i} - E_j)|k^j_{kl,i}\rangle + \langle\chi_{ij}|G_0^{(3)}|\chi_{kl}\rangle\tau(E - E_{kl,j} - E_i)|k^i_{kl,j}\rangle \\ &+\langle\chi_{ij}|G_0^{(4)}|\chi_{kl}\rangle\tau(E - E_{kl,ij} - E_{ij})|h^l_{kl,ij}\rangle, \qquad (6.9)\end{aligned}$$

sendo $\langle \vec{q}_{ij}|\chi_{ij}\rangle = g(\vec{q}_{ij}) = 1$ o fator de forma para o potencial $\delta$-Dirac. Igualando os termos idênticos do lado direito da equação temos que:

$$|k^l_{ij,k}\rangle = 2\langle\chi_{ij}|G_0^{(3)}|\chi_{ik}\rangle\tau(E - E_{ik,j} - E_l)|k^l_{ik,j}\rangle + 2\langle\chi_{ij}|G_0^{(3)}|\chi_{ik}\rangle\tau(E - E_{ik,l} - E_j)|k^j_{ik,l}\rangle$$
$$+2\langle\chi_{ij}|G_0^{(4)}|\chi_{ik}\rangle\tau(E - E_{ik,jl} - E_{jl})|h_{ik,jl}\rangle, \tag{6.10}$$
$$|h_{ij,kl}\rangle = 2\langle\chi_{ij}|G_0^{(3)}|\chi_{kl}\rangle\tau(E - E_{kl,i} - E_j)|k^j_{kl,i}\rangle + \langle\chi_{ij}|G_0^{(4)}|\chi_{kl}\rangle\tau(E - E_{kl,ij} - E_{ij})|h_{kl,ij}\rangle. \tag{6.11}$$

Redefinindo $\tau(E)|k\rangle$ como $\mathcal{K}$ e $\tau(E)|h\rangle$ como $\mathcal{H}$, multiplicando as eqs. (6.10) e (6.11), respectivamente, por $\langle\vec{q}_{ij,k};\vec{q}_l|$ e $\langle\vec{q}_{ij,kl};\vec{q}_{kl}|$ pela esquerda e inserindo algumas resoluções da unidade chegamos a:

$$\begin{aligned}
&\langle\vec{q}_{ij,k};\vec{q}_l|\mathcal{K}^l_{ij,k}\rangle = 2\tau(E - E_{ij,k} - E_l)\\
&\times\left[\int d^3q_{ik,j}d^3q_l'd^3q_{ij}d^3q_{ik}\frac{\langle\vec{q}_{ij};\vec{q}_{ij,k};\vec{q}_l|\vec{q}_{ik,j};\vec{q}_l\,';\vec{q}_{ik}\rangle}{E - \frac{q^2_{ij,k}}{2m_{ij,k}} - \frac{q^2_l}{2m_l} - \frac{q^2_{ij}}{2m_{ij}}}\langle\vec{q}_{ij,k};\vec{q}_l\,'|\mathcal{K}^l_{ik,j}\rangle\right.\\
&+\int d^3q_{ik,l}d^3q_jd^3q_{ij}d^3q_{ik}\frac{\langle\vec{q}_{ij};\vec{q}_{ij,k};\vec{q}_l|\vec{q}_{ik,l};\vec{q}_j;\vec{q}_{ik}\rangle}{E - \frac{q^2_{ij,k}}{2m_{ij,k}} - \frac{q^2_l}{2m_l} - \frac{q^2_{ij}}{2m_{ij}}}\langle\vec{q}_{ik,l};\vec{q}_j|\mathcal{K}^j_{ik,l}\rangle\\
&\left.+\int d^3q_{ik,jl}d^3q_{jl}d^3q_{ij}d^3q_{ik}\frac{\langle\vec{q}_{ij};\vec{q}_{ij,k};\vec{q}_l|\vec{q}_{ik,jl};\vec{q}_{jl};\vec{q}_{ik}\rangle}{E - \frac{q^2_{ij,k}}{2m_{ij,k}} - \frac{q^2_l}{2m_l} - \frac{q^2_{ij}}{2m_{ij}}}\langle\vec{q}_{ik,jl};\vec{q}_{jl}|\mathcal{H}_{ik,jl}\rangle\right]
\end{aligned} \tag{6.12}$$

$$\begin{aligned}
&\langle\vec{q}_{ij,kl};\vec{q}_{kl}|\mathcal{H}_{ij,kl}\rangle = 2\tau(E - E_{ij,kl} - E_{kl})\\
&\times\left[\int d^3q_{kl,i}d^3q_jd^3q_{ij}d^3q_{kl}'\frac{\langle\vec{q}_{ij,kl};\vec{q}_{kl};\vec{q}_{ij}|\vec{q}_{kl,i};\vec{q}_j;\vec{q}_{kl}\,'\rangle}{E - \frac{q^2_{ij,kl}}{2m_{ij,kl}} - \frac{q^2_{kl}}{2m_{kl}} - \frac{q^2_{ij}}{2m_{ij}}}\langle\vec{q}_{kl,i};\vec{q}_j|\mathcal{K}^j_{kl,i}\rangle\right.\\
&\left.+\int d^3q_{kl,ij}d^3q_{ij}\,'d^3q_{ij}d^3q_{kl}\,'\frac{\langle\vec{q}_{ij,kl};\vec{q}_{kl};\vec{q}_{ij}|\vec{q}_{kl,ij};\vec{q}_{ij}\,';\vec{q}_{kl}\,'\rangle}{E - \frac{q^2_{ij,kl}}{2m_{ij,kl}} - \frac{q^2_{kl}}{2m_{kl}} - \frac{q^2_{ij}}{2m_{ij}}}\langle\vec{q}_{kl,ij};\vec{q}_{ij}\,'|\mathcal{H}^j_{kl,ij}\rangle\right]
\end{aligned} \tag{6.13}$$

Finalmente podemos escrever as eqs. (6.12) e (6.13) na forma de uma equação integral com os momentos orientados conforme a figura 6.2. O cálculo do elementos de matriz das eqs. (6.12) e (6.13) está no apêndice G. Os momentos que aparecem do lado esquerdo $\vec{q}_{ij,k}$ e $\vec{q}_{ij,kl}$ foram chamados de $\vec{q}$ e $\vec{q}_l$, respectivamente, e

$\vec{q}_{kl}$ foi chamado de $\vec{p}$. Do lado direito o momento que sobra após a integração dos $\delta$'s foi chamado de $\vec{k}$.

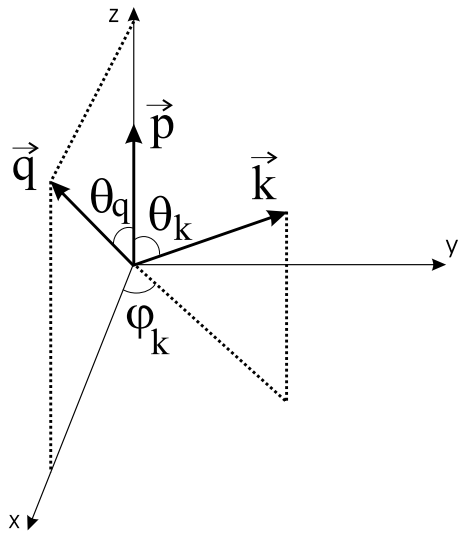


Figura 6.2: Orientação dos momentos.

$$
\begin{aligned}
\mathcal{K}(q,p) = 2\tau(E - \frac{3}{4}q^2 - \frac{2}{3}p^2) \Bigg\{ & \int d\cos\theta_k d\cos\theta_q d\phi_k k^2 dk \mathcal{K}(k,p) \\
& \left[ \frac{1}{-|E| - q^2 - k^2 - \frac{2}{3}p^2 + qkz} - \frac{1}{-1 - q^2 - k^2 - \frac{2}{3}p^2 + qkz} \right] \\
& + \int d\cos\theta_k d\cos\theta_q d\phi_k k^2 dk \mathcal{K}(k, 3\sqrt{k^2 + p^2 - 2pk\cos\theta_k}) \\
& \left[ \frac{1}{-|E| - q^2 - \frac{70}{9}p^2 - 9k^2 + 16pk\cos\theta_k + \frac{8}{3}pq\cos\theta_q - 3kqz} \right. \\
& \left. - \frac{1}{-1 - q^2 - \frac{70}{9}p^2 - 9k^2 + 16pk\cos\theta_k + \frac{8}{3}pq\cos\theta_q - 3kqz} \right] \\
& + \int d\cos\theta_k d\cos\theta_q d\phi_k k^2 dk \mathcal{H}(k, \sqrt{k^2 + \frac{16}{9}p^2 - \frac{8}{3}pk\cos\theta_k}) \\
& \left[ \frac{1}{-|E| - q^2 - \frac{10}{9}p^2 - k^2 - qkz + \frac{4}{3}pk\cos\phi_k + \frac{2}{3}pq\cos\theta_q} - \right. \\
& \left. - \frac{1}{-\mu_{(4)}^2 - q^2 - \frac{10}{9}p^2 - k^2 - qkz + \frac{4}{3}pk\cos\phi_k + \frac{2}{3}pq\cos\theta_q} \right] \Bigg\},
\end{aligned}
\tag{6.14}
$$

$$\mathcal{H}(q,p) = \tau(E - \frac{1}{2}q^2 - p^2)\left\{2\int d\cos\theta_k d\cos\theta_q d\phi_k k^2 dk \mathcal{K}(k, \sqrt{\frac{4}{9}k^2 + q^2 + \frac{4}{3}kqz})\right.$$
$$\left[\frac{1}{-|E| - \frac{3}{4}q^2 - p^2 - k^2 - qkz} - \frac{1}{-1 - \frac{3}{4}q^2 - p^2 - k^2 - qkz}\right] \qquad (6.15)$$
$$+ \int d\cos\theta_k d\cos\theta_q d\phi_k k^2 dk \mathcal{H}(q,k)$$
$$\left.\left[\frac{1}{-|E| - \frac{1}{2}q^2 - p^2 - k^2} - \frac{1}{-\mu_{(4)}^2 - \frac{1}{2}q^2 - p^2 - k^2}\right]\right\},$$

onde $z = \cos\theta_q \cos\theta_k + \text{sen}\theta_q \text{sen}\theta_k \cos\phi_k$. Os propagadores foram escritos explicitamente em termos da energia de 4-corpos, $E$, e dos demais momentos. $\mu_{(4)}^2$ é o ponto de subtração de 4-corpos que em unidades de $\hbar = m = 1$ tem dimensão de energia. A energia de subtração de 3-corpos foi colocada igual a 1.

Note que as funções espectadoras dependem somente do módulo dos momentos, uma vez que estamos interessados em estudar o estado fundamental de momento angular orbital total nulo. A energia de 4-corpos é a solução do sistema de eqs. acopladas (6.14) e (6.15).

Uma análise qualitativa das eqs. (6.10) e (6.11) nos permite tirar algumas conclusões: a amplitude do tipo $k$ "cai"com a escala de três corpos $\mu_{(3)}$ e a amplitude do tipo $h$ com a escala de quatro corpos $\mu_{(4)}$. Se fixarmos $\mu_{(3)} = 1$ e $\mu_{(4)} \gg 1$, então para momentos grandes as eqs. (6.10) e (6.11) ficariam reduzidas a

$$|k_{ij,k}^l\rangle = 2\langle\chi_{ij}|G_0^{(4)}|\chi_{ik}\rangle\tau(E - E_{ik,jl} - E_{jl})|h_{ik,jl}\rangle,$$
$$|h_{ij,kl}\rangle = \langle\chi_{ij}|G_0^{(4)}|\chi_{kl}\rangle\tau(E - E_{kl,ij} - E_{ij})|h_{kl,ij}\rangle,$$

ou seja, as equações se desacoplam e precisamos resolver somente a segunda equação que pode possuir infinitas soluções, desta forma, segundo a nossa análise qualitativa, a escala de quatro bosons seria realmente nova.

# Capítulo 7

# Conclusões e perspectivas

A utilização de um potencial tipo $\delta$-Dirac mostrou-se uma ferramenta muito útil para a descrição de propriedades de sistemas fracamente ligados de três e quatro corpos tanto no campo da física atômica como da física nuclear. Vimos que para potenciais de curto-alcance a física desses sistemas está contida nas escalas de dois e três corpos ou em outras palavras, qualquer observável desse sistema pode ser representado em termos de uma função de escala universal. Esse limite de escala é atingido quando a razão entre o comprimento de espalhamento de dois corpos e o alcance efetivo do potencial tende a infinito. Os cálculos, feitos utilizando as equações subtraídas para a matriz-T, se reduzem àqueles calculados com um corte para grandes momentos quando o ponto de subtração vai para infinito [7].

Mostramos o comportamento de um estado Thomas-Efimov excitado conforme variamos a energia do subsistema de dois corpos. De fato, se o subsistema de dois corpos é ligado, conforme aumentamos a razão entre a energia de ligação de dois e três corpos o estado excitado desaparece e um estado virtual correspondente aparece quando a energia do estado fundamental atinge o limiar dado por $6.9\hbar^2/(ma^2)$ [7]. Quando o subsistema de dois corpos é virtual, o aumento da razão entre as energias faz com que o estado excitado se transforme em uma ressonância quando a energia do estado fundamental é $1.1\hbar^2/(ma^2)$ [49]. Neste último caso as condições para a formação de moléculas triatômicas no interior de condensados é favorecida, pois a

competição com dímeros fracamente ligados está ausente.

O conceito de universalidade, i.e., o reescalonamento dos observáveis, ainda foi utilizado para escrevermos a dependência do coeficiente de recombinação de três corpos como uma função da razão entre as energias dos dímeros e trímeros atômicos. Essa função também tende a uma função de escala universal. Utilizando a função de escala e os valores experimentais conhecidos para o comprimento de espalhamento de dois átomos e o coeficiente de recombinação de três átomos, calculamos as energias de moléculas triatômicas no interior de armadilhas magneto-ópticas [8]. A formação desses trímeros poderia ainda envolver colisões de quatro corpos, tipo dímero-dímero ou um dímero e dois átomos livres.

Finalmente, as funções de escala foram utilizadas para descrever os tamanhos de moléculas triatômicas fracamente ligadas [9] e núcleos exóticos (aproximados por um caroço e dois neutrons) [10]. Neste último caso completamos a nomenclatura denominando de *Samba* a configuração de um sistema de três corpos formado por dois subsistemas de dois corpos ligados e um virtual. O tamanho desses sistemas, para uma mesma energia de três corpos, comporta-se de maneira inesperada já que o maior sistema corresponde àquele onde os pares formam estados ligados e o menor àquele onde os pares não formam estados ligados.

A questão formulada na introdução sobre o aparecimento de uma nova escala física cada vez que um bóson fosse adicionado ao sistema ainda não foi respondida apesar da formulação das equações de quatro corpos. Todavia, a análise qualitativa das eqs. (6.10) e (6.11), feita no final do capítulo referente ao problema de 4-corpos, indica a introdução de uma nova escala física a esse sistema. É claro que a simplificação feita deve, ainda, ter um suporte numérico ou uma prova matemática mais rigorosa.

Como perspectivas continuaremos estudando a dinâmica dos sistemas de três e quatro corpos utilizando interações tipo $\delta$-Dirac juntamente com a formulação das equações subtraídas de Faddeev invariantes sob transformações do grupo de renormalização. Um estudo da trajetória dos estados Efimov será feita no contexto de

sistemas de três corpos do tipo AAB. Serão feitos cálculos das energias de ligação de estados excitados, raios quadráticos médios e funções de correlação de dois corpos em função das escalas físicas de dois e três corpos no contexto de hipernúcleos do tipo Λ-hipernúcleo. Será investigada a necessidade da introdução de uma nova escala para o sistema de quatro bosons, independente das escalas de dois e três corpos, na regularização das equações de Faddeev-Yakubovsky em três dimensões.

# Apêndice A

# Coordenadas de Jacobi (3-corpos)

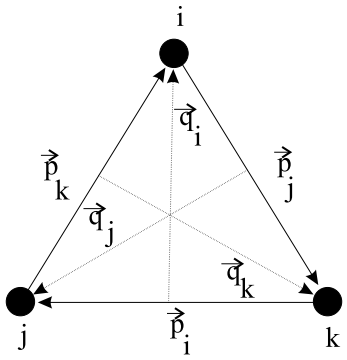


Figura A.1: Coordenadas de Jacobi

Sejam $\vec{k}_i+\vec{k}_j+\vec{k}_k=0$ os momentos das partículas em relação ao centro-de-massa (C.M.) e $m_\alpha$ e $v_\alpha$ $(\alpha=i,j,k)$ as suas massas e velocidades, respectivamente. Temos então que $\vec{p}_i$ e $\vec{q}_i$ são dados por:

$$\vec{p}_i=\frac{m_j m_k}{m_j+m_k}(\vec{v}_j-\vec{v}_k)=\frac{m_k\vec{k}_j-m_j\vec{k}_k}{m_j+m_k} \tag{A.1}$$

$$\vec{q}_i=\frac{m_i(m_j+m_k)}{m_i+m_j+m_k}\left[\vec{v}_i-\frac{m_j\vec{v}_j+m_k\vec{v}_k}{m_j+m_k}\right]=\vec{k}_i. \tag{A.2}$$

Analogamente temos que: $\vec{q}_j=\vec{k}_j$ e $\vec{q}_k=\vec{k}_k$. Assim, relacionando as

coordenadas temos que:

$$\vec{p_i} = \frac{m_k\vec{q_j} - m_j\vec{q_k}}{m_j + m_k} \tag{A.3}$$

$$\vec{p_j} = \frac{m_i\vec{q_k} - m_k\vec{q_i}}{m_i + m_k} \tag{A.4}$$

$$\vec{p_k} = \frac{m_j\vec{q_i} - m_i\vec{q_j}}{m_i + m_j} \tag{A.5}$$

# Apêndice B

# Dedução do fator de forma para o potencial $\delta$-Dirac

Demonstraremos a seguir que no caso do potencial $\delta$-Dirac temos que $\langle\chi|\vec{p}\rangle = \langle\vec{p}|\chi\rangle = g(p) = 1$. Sendo $\vec{R}$ um vetor ligando duas partículas quaisquer, temos que o elemento de matriz $\langle\vec{R}'|V|\vec{R}\rangle$ para um potencial local $V$ pode ser escrito como:

$$\langle\vec{R}'|V|\vec{R}\rangle = \delta(\vec{R}' - \vec{R})V(\vec{R}).$$

Para o potencial $\delta$-Dirac:

$$V(\vec{R}) \equiv (2\pi)^3\lambda\delta(\vec{R}),$$

desta forma substituindo o potencial $V(\vec{R})$, temos:

$$\begin{aligned}\langle\vec{R}'|V|\vec{R}\rangle &= (2\pi)^3\lambda\delta(\vec{R}' - \vec{R})\delta(\vec{R}) \\ &= (2\pi)^3\lambda\delta(\vec{R}')\delta(\vec{R}).\end{aligned}$$

Desta forma podemos notar que o potencial $\delta$-Dirac além de ser local é também um potencial separável. Escrevendo o elemento de matriz $\langle \vec{p}'|V|\vec{p}\rangle$, temos:

$$\begin{aligned}\langle \vec{p}'|V|\vec{p}\rangle &= \lambda \int d^3R\; d^3R'\; e^{i\vec{p}\cdot\vec{R}}\; e^{-i\vec{p}'\cdot\vec{R}'}\; \delta(\vec{R}')\; \delta(\vec{R}) \\ &= \lambda g^*(\vec{p}')g(\vec{p}),\end{aligned}$$

onde $g(\vec{p}) = \int d^3R\; e^{i\vec{p}\cdot\vec{R}}\; \delta(\vec{R}) = 1$.

# Apêndice C

# Dedução da matriz-$T$ de dois corpos na forma subtraída

A seguir é feita uma dedução para a matriz-$T$ de dois corpos na forma subtraída a partir da forma "geral"da equação da matriz-$T$ renormalizada. Assim, partindo-se da eq. (2.32):

$$T_R(E) = T_R(-\mu^2) + T_R(-\mu^2)\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(E),$$

e substituindo $T_R(-\mu^2)$ por $\lambda_R(-\mu^2)|\chi\rangle\langle\chi|$ temos que:

$$T_R(E) = \lambda_R(-\mu^2)|\chi\rangle\langle\chi| + \lambda_R(-\mu^2)|\chi\rangle\langle\chi|\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(E), \qquad \text{(C.1)}$$

multiplicando a eq. (C.1) por $\langle\chi|\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)$ pela esquerda e isolando $\langle\chi|\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(E)$ temos que:

$$\langle\chi|\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)T_R(E) = \frac{\lambda_R(-\mu^2)\langle\chi|\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)|\chi\rangle\langle\chi|}{1 - \lambda_R(-\mu^2)\langle\chi|\left(G_0^{(+)}(E) - G_0(-\mu^2)\right)|\chi\rangle}, \qquad \text{(C.2)}$$

substituindo a eq. (C.2) na eq. (C.1) chegamos na matriz-$T$ de dois corpos na forma subtraída:

$$T_R(E) = \lambda_R(-\mu^2)|\chi\rangle \left(1 + \frac{\lambda_R(-\mu^2)\langle\chi| \left(G_0^{(+)}(E) - G_0(-\mu^2)\right) |\chi\rangle\langle\chi|}{1 - \lambda_R(-\mu^2)\langle\chi| \left(G_0^{(+)}(E) - G_0(-\mu^2)\right) |\chi\rangle}\right) \langle\chi|, \quad \text{(C.3)}$$

que é a eq. (2.25) na forma subtraída.

# Apêndice D

# Normalização da função de onda do estado ligado de dois corpos

$$
\begin{aligned}
&\int d^3p \frac{N^2}{(E_2+p^2)^2} = 1 \\
&-4\pi \frac{\partial}{\partial\lambda} \int_0^\infty dp \frac{N^2}{E_2+\lambda p^2}\bigg|_{\lambda=1} = 1 \\
&-4\pi \frac{\partial}{\partial\lambda} \frac{1}{2\lambda} \int_{-\infty}^\infty dp \frac{N^2}{(p+i\sqrt{E_2/\lambda})(p-i\sqrt{E_2/\lambda})} = 1 \\
&-4\pi \frac{\partial}{\partial\lambda} \frac{N^2\pi}{2\sqrt{E_2}\lambda^{-1/2}} = 1 \\
&N = \frac{E_2^{1/4}}{\pi}
\end{aligned}
\tag{D.1}
$$

# Apêndice E

# Extensão da matriz-$T$ de dois corpos para a segunda folha de Riemann

A seguir faremos a extensão da equação da matriz-$T$ de dois corpos para a segunda folha de Riemann como mostra a figura (E.1).

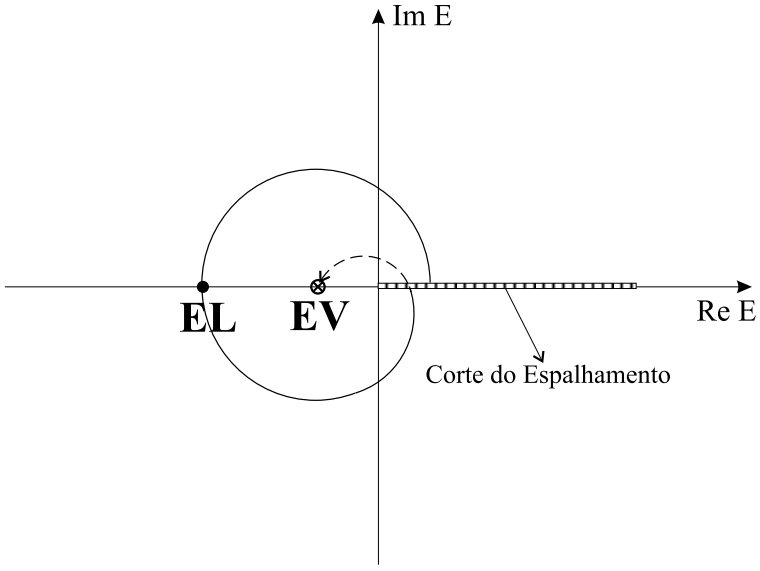


Figura E.1: Extensão da Matriz-$T$ de Dois Corpos para a Segunda Folha de Riemann. EL representa a energia do estado ligado de dois corpos e EV a energia do estado virtual.

Escrevendo o elemento de matriz de $T$ na base de momento $|\vec{k}\,\rangle$ e $|\vec{p}\rangle$, temos que:

$$\langle\vec{k}\,|T(E)|\vec{p}\rangle = \langle\vec{k}\,|V|\vec{p}\rangle + \int d^3q\langle\vec{k}\,|V|\vec{q}\rangle\langle\vec{q}|\frac{T(E)}{E-\frac{q^2}{2m}+i\delta}|\vec{p}\rangle, \tag{E.1}$$

onde $m$ é a massa reduzida dos dois corpos. A extensão da eq. (E.1) para a segunda folha de Riemann é feita somando-se e subtraindo-se a descontinuidade referente ao corte do espalhamento:

$$\begin{aligned}\langle\vec{k}\,|T(E)|\vec{p}\rangle &= \langle\vec{k}\,|V|\vec{p}\rangle + \int d^3q\langle\vec{k}\,|V|\vec{q}\rangle\left[\frac{1}{E-\frac{q^2}{2m}+i\delta}-\frac{1}{E-\frac{q^2}{2m}-i\delta}\right]\langle\vec{q}|T(E)|\vec{p}\rangle \\ &+ \int d^3q\langle\vec{k}\,|V|\vec{q}\rangle\frac{1}{E-\frac{q^2}{2m}-i\delta}\langle\vec{q}|T(E)|\vec{p}\rangle. \end{aligned}\tag{E.2}$$

Vamos agora calcular a primeira integral:

$$I = \int d^3q\; v(\vec{k},\vec{q})\left[\frac{1}{E-\frac{q^2}{2m}+i\delta}-\frac{1}{E-\frac{q^2}{2m}-i\delta}\right]t(\vec{q},\vec{p};E), \tag{E.3}$$

onde: $v(\vec{k},\vec{q}) \equiv \langle\vec{k}\,|V|\vec{q}\,\rangle$ e $t(\vec{q},\vec{p};E) \equiv \langle\vec{q}\,|T(E)|\vec{p}\rangle$.

$$\begin{aligned} I &= 2m\int d\Omega_q\int_0^\infty q^2dqv(\vec{k},\vec{q})\left[\frac{1}{k^2-q^2+i\delta}-\frac{1}{k^2-q^2-i\delta}\right]t(\vec{q},\vec{p};E) \\ &= 2m\int d\Omega_q\int_0^\infty q^2dq\frac{v(\vec{k},\vec{q})}{(k+q)}\left[\frac{1}{k-q+i\delta}-\frac{1}{k-q-i\delta}\right]t(\vec{q},\vec{p};E) \\ &= -2m\int d\Omega_q\int_0^\infty q^2dq\frac{v(\vec{k},\vec{q})}{(k+q)}\left[\frac{1}{q-k+i\delta}-\frac{1}{q-k-i\delta}\right]t(\vec{q},\vec{p};E). \end{aligned}$$

onde substituímos $k^2 = 2mE$ (em unidades de $\hbar = 1$). Utilizando o teorema dos resíduos para fazer a integração, vide figura (E.2):

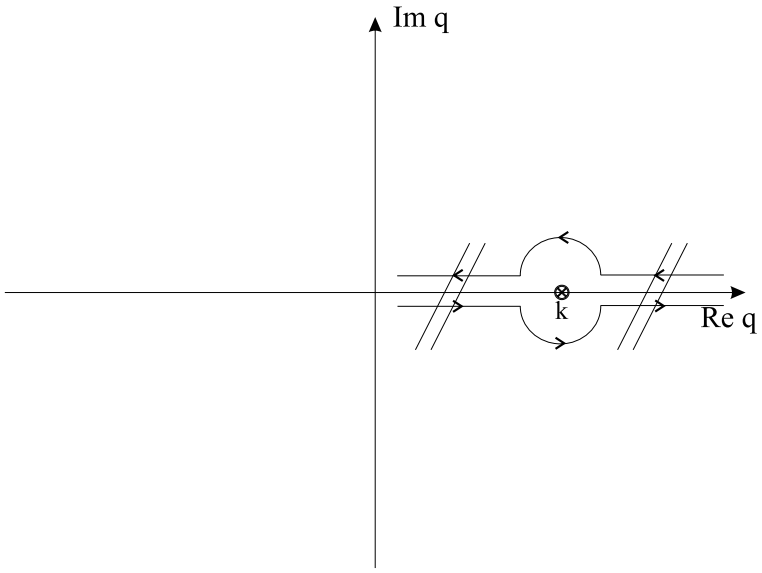


Figura E.2: Caminho da integração utilizado para calcular a eq. (E.3) utilizando o teorema dos resíduos.

$$\begin{aligned} I &= -2m(2\pi i).\frac{k^2}{k+k}\int d\Omega_q v(\vec{k},\vec{q})t(\vec{q},\vec{p};E)\Big|_{|\vec{q}|=k} \\ &= -2\pi imk\int d\Omega_q v(\vec{k},\vec{q})t(\vec{q},\vec{p};E)\Big|_{|\vec{q}|=k}. \end{aligned}$$

Voltando à eq. (E.2), temos que:

$$\begin{aligned} t(\vec{k},\vec{p};E) &= v(\vec{k},\vec{p}) - 2\pi mik\int d\Omega_q v(\vec{k},\vec{q})t(\vec{q},\vec{p};E)\Big|_{|\vec{q}|=k} + \\ &+ \int d^3q\frac{v(\vec{k},\vec{q})t(\vec{q},\vec{p};E)}{E-\frac{q^2}{2m}-i\delta}. \end{aligned} \tag{E.4}$$

A equação integral homogênea para o estado virtual deduzida a partir da Matriz-$T$ na segunda folha é análoga à equação homogênea do estado ligado. A matriz-$T$ na segunda folha para energias próximas ao estado virtual apresenta um pólo, escrito como:

$$t(\vec{k},\vec{p};E\simeq -|E_V|) = \frac{\Gamma_V(\vec{k})\Gamma_V(\vec{p})}{E+|E_V|}, \tag{E.5}$$

onde a função $\Gamma_V$ é a função de vértice do estado virtual e $E_V$ a energia do estado virtual. Assim, para $E \to -|E_V|$ podemos substituir a eq. (E.5) na eq. (E.4):

$$\frac{\Gamma_V(\vec{k})\Gamma_V(\vec{p})}{E+|E_V|} \simeq -2m\pi|k_V| \int d\Omega_q v(\vec{k},\vec{q}) \frac{\Gamma_V(\vec{q})\Gamma_V(\vec{p})}{E+|E_V|}\bigg|_{|\vec{q}|=-i|k_V|} + \int d^3q v(\vec{k},\vec{q}) \frac{1}{-|E_V|-\frac{q^2}{2m}} \frac{\Gamma_V(\vec{q})\Gamma_V(\vec{p})}{E+|E_V|}, \tag{E.6}$$

para o estado virtual de três corpos, $k = \pm i\sqrt{2m|E|}$ é definido com o sinal negativo. Assim temos $k = -i\sqrt{2m|E_V|}$ com $k_V = \sqrt{2m|E_V|}$. Cancelando o termo $\frac{\Gamma_V(\vec{p})}{E+|E_V|}$ nos dois lados da eq. (E.6) chegamos finalmente à equação integral homogênea para o vértice do EV:

$$\Gamma_V(\vec{k}\,) = -2m\pi|k_V| \int d\Omega_q v(\vec{k},\vec{q})\Gamma_V(\vec{q})\bigg|_{|\vec{q}|=-i|k_V|} + \int d^3q v(\vec{k},\vec{q}) \frac{\Gamma_V(\vec{q})}{-|E_V|-\frac{q^2}{2m}}. \tag{E.7}$$

Podemos calcular de maneira análoga a equação integral homogênea para o vértice do EL:

$$\begin{aligned} t(\vec{k},\vec{p};E) &\simeq \frac{\Gamma_L(\vec{k})\Gamma_B(\vec{p})}{E-E_L}; \\ \frac{\Gamma_L(\vec{k})\Gamma_L(\vec{p})}{E-E_L} &\simeq \int d^3q \frac{v(\vec{k},\vec{q})}{-|E_L|-\frac{q^2}{2m}} \frac{\Gamma_L(\vec{q})\Gamma(\vec{p})}{E-E_L}; \\ \Gamma_L(\vec{k}\,) &= \int d^3q \frac{v(\vec{k},\vec{q})}{-|E_L|-\frac{q^2}{2m}} \Gamma_L(\vec{q}). \end{aligned} \tag{E.8}$$

Comparando as eqs. (E.7) e (E.8) vemos que a segunda parcela da eq. (E.7) é análoga à eq. (E.7) para o vértice do estado ligado. A existência, porém, da primeira parcela na eq. (E.7) faz com que, na prática, o estado virtual "sinta"o potencial de uma forma um pouco mais atrativa que para o estado ligado (note que a primeira parcela é positiva $v < 0$).

# Apêndice F

# Cálculo dos elementos de matriz das eqs. (5.18) e (5.19)

$$\begin{aligned}
\langle\chi_k\vec{q}_k|G_0^{(+)}(E)|\chi_i\rangle|f_i\rangle &= \int d^3q_i'\langle\chi_k\vec{q}_k|G_0^{(+)}(E)|\chi_i\vec{q}_i\,'\rangle f_i(\vec{q}_i\,') \\
&= \int d^3q_i'd^3p_kd^3p_i\frac{1}{E-\frac{q_k^2}{2\mu_k}-\frac{p_k^2}{2m_{ij,k}}}\langle\vec{q}_k\vec{p}_k|\vec{q}_i\,'\vec{p}_i\rangle f_i(\vec{q}_i\,') \\
&= \int d^3q_i'd^3p_kd^3p_i\frac{\delta(\vec{p}_k-\vec{q}_i\,'-\frac{m_i}{m_i+m_j}\vec{q}_k)\delta(\vec{q}_k+\vec{p}_i+\frac{m_k}{m_j+m_k}\vec{q}_i\,')}{E-\frac{q_k^2}{2m_{ij}}-\frac{p_k^2}{2m_{ij,k}}}f_i(\vec{q}_i\,') \\
&= \int d^3q_i'\frac{1}{E-\frac{q_k^2}{2m_{ij}}-\frac{(\vec{q}_i\,'+\frac{m_i}{m_i+m_j}\vec{q}_k)^2}{2m_{ij,k}}}f_i(\vec{q}_i\,'). \qquad \text{(F.1)}
\end{aligned}$$

$$\begin{aligned}
\langle\chi_k\vec{q}_k|G_0^{(+)}(E)|\chi_j\rangle|f_j\rangle &= \int d^3q_j\langle\chi_k\vec{q}_k|G_0^{(+)}(E)|\chi_j\vec{q}_j\rangle f_j(\vec{q}_j) \\
&= \int d^3q_jd^3p_kd^3p_j\frac{1}{E-\frac{q_k^2}{2m_{ij}}-\frac{p_k^2}{2m_{ij,k}}}\langle\vec{q}_k\vec{p}_k|\vec{q}_j\vec{p}_j\rangle f_j(\vec{q}_j) \\
&= \int d^3q_jd^3p_kd^3p_j\frac{\delta(\vec{p}_k-\vec{q}_j-\frac{m_j}{m_i+m_k}\vec{q}_k)\delta(\vec{p}_j-\vec{q}_k-\frac{m_k}{m_k+m_i}\vec{q}_j)}{E-\frac{q_k^2}{2m_{ij}}-\frac{p_k^2}{2m_{ij,k}}}f_j(\vec{q}_j) \\
&= \int d^3q_j\frac{1}{E-\frac{q_k^2}{2m_{ij}}-\frac{(\vec{q}_j+\frac{m_j}{m_i+m_j}\vec{q}_k)^2}{2m_{ij,k}}}f_j(\vec{q}_j). \qquad \text{(F.2)}
\end{aligned}$$

$$
\begin{aligned}
\langle\chi_i\vec{q}_k|G_0^{(+)}(E)|\chi_j\rangle|f_j\rangle &= \int d^3q_j\langle\chi_i\vec{q}_i|G_0^{(+)}(E)|f_j\vec{q}_j\rangle f_j(\vec{q}_j) \\
&= \int d^3q_j d^3p_i d^3p_j \frac{1}{E-\frac{q_i^2}{2m_{jk}}-\frac{p_i^2}{2m_{jk,i}}}\langle\vec{q}_i\vec{p}_i|\vec{q}_j\vec{p}_j\rangle f_j(\vec{q}_j) \\
&= \int d^3q_j d^3p_i d^3p_j \frac{\delta(\vec{p}_i-\vec{q}_j-\frac{m_j}{m_j+m_k}\vec{q}_i)\delta(\vec{q}_i-\vec{p}_j-\frac{m_i}{m_k+m_i}\vec{q}_j)}{E-\frac{q_i^2}{2m_{jk}}-\frac{p_i^2}{2m_{jk,i}}} f_j(\vec{q}_j) \\
&= \int d^3q_j \frac{1}{E-\frac{q_i^2}{2m_{jk}}-\frac{(\vec{q}_j+\frac{m_j}{m_j+m_k}\vec{q}_i)^2}{2m_{jk,i}}} f_j(\vec{q}_j). \qquad \text{(F.3)}
\end{aligned}
$$

# Apêndice G

# Cálculo dos elementos de matriz das eqs. (6.12) e (6.13)

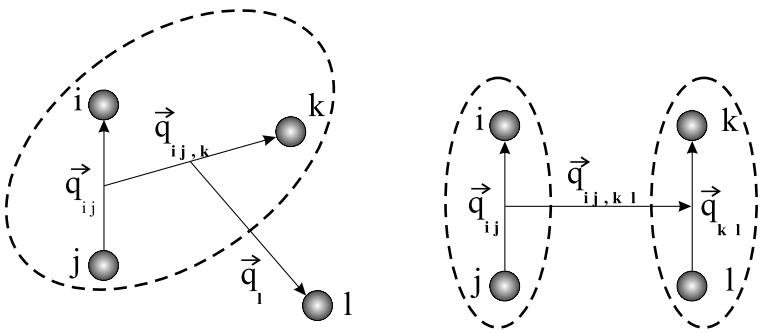


Figura G.1: Coordenadas de Jacobi para as amplitudes de Faddeev-Yakubovsky do tipo K, lado esquerdo, e H, lado direito.

Sejam $\vec{k}_i + \vec{k}_j + \vec{k}_k + \vec{k}_k = 0$ os momentos das partículas em relação ao centro-de-massa (C.M.) e $m_\alpha$ e $v_\alpha$ ($\alpha = i, j, k, l$) as suas massas e velocidades, respectivamente. Podemos escrever os momentos de Jacobi que aparecem na figura em função dos momentos $\vec{k}$ da seguinte maneira:

$$\vec{q}_l = \frac{m_l(m_i+m_j+m_k)}{m_i+m_j+m_k+m_l}\left[\vec{v}_l - \frac{m_i\vec{v}_i+m_j\vec{v}_j+m_k\vec{v}_k}{m_i+m_j+m_k}\right] = \vec{k}_l \tag{G.1}$$

$$\vec{q}_{ij,k} = \frac{m_k(m_i+m_j)}{m_i+m_j+m_k}\left[\vec{v}_k - \frac{m_i\vec{v}_i+m_j\vec{v}_j}{m_i+m_j}\right] = \vec{k}_k + \frac{m_k}{m_i+m_j+m_k}\vec{k}_l \tag{G.2}$$

$$\vec{q}_{ij} = \frac{m_im_j}{m_i+m_j}(\vec{v}_i+\vec{v}_j) = \frac{m_j\vec{k}_i - m_i\vec{k}_j}{m_i+m_j} \tag{G.3}$$

$$\vec{q}_{ij,kl} = \frac{(m_i+m_j)(m_k+m_l)}{m_i+m_j+m_k+m_l}\left[\frac{m_k\vec{v}_k+m_l\vec{v}_l}{m_k+m_l} - \frac{m_i\vec{v}_i+m_j\vec{v}_j}{m_i+m_j}\right] = \vec{k}_k+\vec{k}_l \tag{G.4}$$

Os elementos de matriz das eqs. (6.12) e (6.13) estão calculados a seguir.

$$\langle \vec{q}_{ij};\vec{q}_{ij,k};\vec{q}_l|\vec{q}_{ik,j};\vec{q}_l\,';\vec{q}_{ik}\rangle = \delta(\vec{q}_l-\vec{q}_l\,')\delta(\vec{q}_{ik}-\frac{\vec{q}_{ij}}{2}+\frac{3}{4}\vec{q}_{ij,k})\delta(\vec{q}_{ij}+\vec{q}_{ik,j}-\frac{\vec{q}_{ij,k}}{2}). \tag{G.5}$$

$$\begin{aligned}\langle \vec{q}_{ij};\vec{q}_{ij,k};\vec{q}_l|\vec{q}_{ik,l};\vec{q}_j;\vec{q}_{ik}\rangle &= \delta(\vec{q}_{ij}+\vec{q}_j+\frac{\vec{q}_{ij,k}}{2}+\frac{1}{3}\vec{q}_l)\delta(\vec{q}_{ik,l}-\frac{\vec{q}_j}{3}-\vec{q}_l)\\ &\quad\times\delta(\vec{q}_{ik}+\vec{q}_{ij,k}+\frac{\vec{q}_j}{2}+\frac{1}{6}\vec{q}_l).\end{aligned} \tag{G.6}$$

$$\begin{aligned}\langle \vec{q}_{ij};\vec{q}_{ij,k};\vec{q}_l|\vec{q}_{ik,jl};\vec{q}_{jl};\vec{q}_{ik}\rangle &= \delta(\vec{q}_{ik}+\frac{1}{2}\vec{q}_{ik,jl}+\vec{q}_{ij,k}-\frac{1}{3}\vec{q}_l)\delta(\vec{q}_{ik,jl}+\vec{q}_{ij}+\frac{1}{2}\vec{q}_{ij,k}-\frac{2}{3}\vec{q}_l)\\ &\quad\times\delta(\vec{q}_{jl}-\vec{q}_{ik,jl}+\frac{4}{3}\vec{q}_l)\end{aligned} \tag{G.7}$$

$$\langle \vec{q}_{ij,kl};\vec{q}_{kl};\vec{q}_{ij}|\vec{q}_{kl,i};\vec{q}_j;\vec{q}_{kl}\,'\rangle = \delta(\vec{q}_{kl}-\vec{q}_{kl}\,')\delta(\vec{q}_{ij}+\vec{q}_j+\frac{1}{2}\vec{q}_{ij,kl})\delta(\vec{q}_{kl,i}+\frac{2}{3}\vec{q}_j+\vec{q}_{ij,kl}). \tag{G.8}$$

$$\langle \vec{q}_{ij,kl};\vec{q}_{kl};\vec{q}_{ij}|\vec{q}_{kl,ij};\vec{q}_{ij}\,';\vec{q}_{kl}\,'\rangle = \delta(\vec{q}_{kl}-\vec{q}_{kl}\,')\delta(\vec{q}_{ij}-\vec{q}_{ij}\,')\delta(\vec{q}_{kl,ij}-\vec{q}_{ij,kl}). \tag{G.9}$$

# Apêndice H

# Anexo dos trabalhos publicados referentes à tese

Os seguintes trabalhos, colocados em ordem cronológica, referem-se aos assuntos tratados nesta tese. Eles estão anexados nas páginas seguintes.

• "Scaling limit of virtual states of triatomic systems"de autoria de M. T. Yamashita, T. Frederico, A. Delfino e Lauro Tomio, Physical Review A 66, 052702 (2002).

• "Weakly bound atomic trimers in ultracold traps"de autoria de M. T. Yamashita, T. Frederico, Lauro Tomio and A. Delfino, Physical Review A 68, 033406 (2003).

• "Scaling predictions for radii of weakly bound triatomic molecules"de autoria de M. T. Yamashita, R. S. Marques de Carvalho, Lauro Tomio e T. Frederico, Physical Review A 68, 012506 (2003).

• "Radii in weakly-bound light halo nuclei"de autoria de M. T. Yamashita, Lauro Tomio e T. Frederico, Nuclear Physics A 735, 40 (2004).

• "Triatomic continuum resonances for large negative scattering lengths"de autoria de F. Bringas, M. T. Yamashita e T. Frederico, Physical Review A 69, 040702(R) (2004).

• "Radii of weakly bound three-body systems: halo nuclei and molecules"de autoria

de M. T. Yamashita, T. Frederico, R. S. Marques de Carvalho e Lauro Tomio, Nuclear Physics A 737, S195 (2004).

• "Three-Body Recombination in Ultracold Systems: Prediction of Weakly-Bound Atomic Trimer Energies"de autoria de L. Tomio, V. S. Filho, M. T. Yamashita, A. Gammal e T. Frederico, Few-Body Systems 34, 191 (2004).

# Scaling limit of virtual states of triatomic systems

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For a system with three identical atoms, the dependence of the *s*-wave virtual state energy on the weakly bound dimer and trimer binding energies is calculated in the form of a universal scaling function. The scaling function is obtained from a renormalizable three-body model with a pairwise Dirac-$\delta$ interaction. The threshold condition for the appearance of the trimer virtual state was also discussed.

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## I. INTRODUCTION

Weakly bound three-body zero-angular-momentum states appear in a three-boson system, with the number of states growing to infinity, condensing at zero energy as the pair interactions are just about to bind two particles in the *s* wave. These three-body states are known as the Efimov states [1,2]. Their wave functions, loosely bound, extend far beyond those of normal states and dominate the low-energy scattering phenomena in these systems. The Efimov states have been studied in a number of model calculations [3–5], in atomic and nuclear systems, without yet a clear experimental signature of their occurrence [2,6–10].

Actually, the search of Efimov states in atomic systems is becoming more appealing, due to the experimental realization of Bose-Einstein condensation [11], and due to the possibility of altering the effective scattering length of the low-energy atom-atom interaction in the trap, from large negative to large positive values crossing the dimer zero-binding-energy value, by using an external magnetic field [12]. This possibility of changing the two-body scattering length to large values, as recently shown in Ref. [13], can alter in an essential way the balance between the nonlinear first few terms of the mean-field description presented in the equations that model Bose-Einstein condensed gases [14]. This can certainly open new perspectives for theoretical and experimental investigations related to the many-body behavior of condensate systems. Even in systems where the occurrence of an excited bound Efimov state has shown to be doubtful or even not possible, as for example, in the case of halo nuclei like $^{20}$C or $^{18}$C (seen as a core with a halo of two neutrons) [8], one can verify the occurrence of three-body virtual states. The physics of these three-body systems is related to the unusually large size of the wave function compared to the range of the potential. Thus, the detailed form of the short-ranged potential is not important for the three-body observables [15], which gives to the system universal properties, defined by few physical scales [8]. Strictly speaking, in the limit of a zero-range interaction, the three-body system is parametrized by the physical two- and three-body scales, which are identified with the two-body scattering lengths and one three-body binding energy [9,16]. The physical reason for the sensibility of the three-body binding energy to the interaction properties comes from the collapse of the system in the limit of a zero-range force, which is known as the Thomas effect [17].

In the present work, we analyze the possibility that an excited trimer state becomes a virtual state, when the physical scales of the system are changed. This is expected to occur, for example, near the limit when the two-body scattering length goes from large positive to large negative value; the corresponding two-body energy is close to zero and goes from a bound to a virtual state, with the appearance of many bound and virtual three-body states. The three-body virtual state energy is a pole of the *S* matrix in the second sheet of the complex energy plane. In a general case, as the strength of the two-body potential diminishes, the pole moves towards the first energy sheet to become a bound state [5]. More recently, this behavior of the Efimov state going to a virtual state with the increase of the strength of the interaction has been confirmed in realistic calculation of the helium trimer [18]. Here, we study another aspect of the emergence of the *s*-wave virtual state from an Efimov state: *it appears when the ratio between the dimer and trimer binding energies grows*. This approach goes beyond a previous analysis of excited three-body bound states with short-range interactions, that was performed in Ref. [9]. In Ref. [9], a scaling function was introduced to analyze the behavior of bound Efimov states when modifying the triatomic physical scales. Essentially, we are extending to the second sheet of the complex energy plane (to include virtual trimer states) a previous investigation on a universal scaling mechanism that was applied to two- and three-body bound states [9,10]. The extension of the scaling function to the second energy sheet is performed by following the Efimov states as they move from bound to virtual, according to the variation of the ratio of the dimer to trimer bound-state energies. On the other hand, as we present the discussion through a universal scaling mechanism with the results in dimensionless units, all the conclusions apply equally to any low-energy three-boson system. For the regularization and renormalization of the zero-range model, we compare two different approaches: by using a momentum cutoff parameter [9] and via kernel subtraction [16,19,20]. As the two-body energy goes to zero (or equiva-

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lently the regularization parameter goes to infinity), we conclude that the results of both methods do not differ.

The paper is organized as follows. In Sec. II, we generalize the scaling function defined in Ref. [9] to include virtual trimer states. In this section, we also revise the connection between the Thomas and Efimov effects, while introducing our notation and the homogeneous integral equation for the Faddeev component of the vertex of the wave function for zero-range potential. In Sec. III we present our main numerical results. In the Sec. III A, we present the subtracted homogeneous Faddeev equation that we have used for determining the trimer bound and virtual states, and we briefly explain how the renormalization method of Refs. [19,20] implies in the subtracted three-body equation first formulated in Ref. [16]. In the Sec. III B, we present our new numerical results for the virtual-state energies, including the previous bound-state results and we compare, as well, the results obtained by using the sharp-cutoff and the subtraction schemes. Comparison with other calculations are also discussed. Our conclusions are summarized in Sec. IV.

## II. THOMAS-EFIMOV EFFECT AND THE GENERALIZED SCALING FUNCTION

In this section, we introduce the generalization of the scaling function defined in Ref. [9], to be used in the second energy sheet of the trimer energy. In order clarify this extension, and to define our notation, we begin by revising the main findings of Refs. [9,21].

The two-boson system in the limit of a zero-range interaction has only one physical scale, which one can choose as the scattering length $a$ or the energy of the bound or virtual state. The two-body $s$-wave scattering amplitude in units of $\hbar=m=1$ is parametrized as a function of the momentum $k$, by $f(k)=(k\cot\delta_0-ik)^{-1}$, where the $s$-wave phase shift $\delta_0$ is given by $k\cot\delta_0=-a^{-1}+\frac{1}{2}r_0k^2+\cdots$, and $r_0$ is the effective range. For $a>0$, the two-body system is bound; otherwise, for $a<0$, it is virtual. A short-range potential is characterized by $r_0|a|^{-1}\ll 1$ and, in this case, $f(k)=(-a^{-1}-ik)^{-1}$ and $a^{-1}=\pm\sqrt{E_2}$ ($+$ for bound and $-$ for virtual state).

The three-boson system for $\ell=0$ in three dimensions collapses when $r_0\to 0$ with a fixed two-body scale, which is known as the Thomas effect [17]. Thus, the three-body system has a characteristic physical scale independent of the two-body ones [16]. In one and two space dimensions, the collapse is absent [15]. In the limit where the binding energy of the two-boson system goes to zero, the three-boson system has an infinite number of bound Efimov states [1] condensing at zero energy. The Thomas and Efimov effects were shown to be physically equivalent [21], since in both cases the ratio between the interaction range and the two-body scattering length goes to zero.

The integral equation for the Faddeev components, $\phi$, of the three-boson bound-state vertex, for $\ell=0$, with the zero-range interaction, needs a momentum cutoff $\Lambda$ of the order of $r_0^{-1}$, due to the Thomas collapse. According to Ref. [21], using units of $\Lambda=1$, we rescale the momentum variables and the two- and three-body binding energies, respectively, such that $\vec{p}=\Lambda\vec{x}$, $\vec{q}=\Lambda\vec{y}$, $E_2=\Lambda^2\epsilon_2$, and $E_3=\Lambda^2\epsilon_3$. In this dimensionless variables, after redefining $\phi$ as $\chi(\vec{x})\equiv\Lambda^{3/2}\phi(\vec{p})$, we obtain the integral equation [21,7,8]:

$$\chi(\vec{y})=\frac{-\pi^{-2}}{\pm\sqrt{\epsilon_2}-\sqrt{\epsilon_3+\frac{3}{4}\vec{y}^2}}\int d^3x\frac{\theta(1-|\vec{x}|)}{\epsilon_3+\vec{y}^2+\vec{x}^2+\vec{y}\cdot\vec{x}}\chi(\vec{x}). \tag{1}$$

The number of three-body bound states, given by the values of $\epsilon_3$ that satisfies Eq. (1), grows without limit when $\epsilon_2$ decreases to zero; $\epsilon_3=\epsilon_3^{(N)}$ $(N=0,1,2,\ldots)$, with $\epsilon_3^{(N)}/\epsilon_3^{(N+1)}\approx 500$ [1]. They are the energies of the Efimov states, in units of $\Lambda=1$. But, the limit of $\epsilon_2$ going to zero can be realized either by $E_2\to 0$ (with a fixed $\Lambda$) or by $\Lambda\sim r_0^{-1}\to\infty$ (with $E_2$ fixed). In this last case, the range of the interaction is set to zero and the system collapses; $E_3^{(0)}=\epsilon_3^{(0)}\Lambda^2\to\infty$. This is known as the Thomas collapse of the three-body ground state. Therefore, the Thomas and the Efimov states are given by the same limit $\epsilon_2\to 0$ of Eq. (1), and are related by a scale transformation [21].

Now, the concept of the scaling function is introduced according to Ref. [9]. For a nonvanishing $\epsilon_2$, the solutions of Eq. (1) defines the dimensionless three-body energies as functions of $\pm\sqrt{\epsilon_2}$; $\epsilon_3^{(N)}\equiv\epsilon_3^{(N)}(\pm\sqrt{\epsilon_2})$. Using the $N$th energy to obtain $\Lambda$, then $\Lambda^2=E_3^{(N)}/\epsilon_3^{(N)}$, and

$$E_3^{(N+1)}=E_3^{(N)}\frac{\epsilon_3^{(N+1)}(\xi)}{\epsilon_3^{(N)}}, \tag{2}$$

where $\xi\equiv\pm\sqrt{\epsilon_2}=\pm(E_2\epsilon_3^{(N)}/E_3^{(N)})^{1/2}$. In Eq. (2), the two- and three-body physical scales determine $E_3^{(N+1)}$, the next excited state above $E_3^{(N)}$. In Ref. [9], $E_3^{(N)}$ was identified with the three-body scale, as any state $N$ works equally well to set the trimer scale. However, we will be interested in the two most excited three-body states that, in practice, we are going to identify with the ground- and the first-excited-state in triatomic systems. This identification is unambiguous because, with $N$ and $N+1$ being two consecutive excited states, the limit

$$\frac{E_3^{(N+1)}}{E_3^{(N)}}=\lim_{N\to\infty}\frac{\epsilon_3^{(N+1)}(\xi)}{\epsilon_3^{(N)}}=\mathcal{F}\left(\pm\sqrt{\frac{E_2}{E_3^{(N)}}}\right) \tag{3}$$

exists and defines the scaling function $\mathcal{F}$ [8,9]. A qualitative argument to explain the scaling limit has been provided in Ref. [9] based on the notion of the long-range potential [1,2,22].

In the following, we provide the generalization of the scaling function (3), which is obtained by extending the formalism to the second sheet of the three-body complex energy plane. In the present approach, we only consider the two-body subsystem as bound. For this purpose, we define the general scaling function $\mathcal{K}$, given by

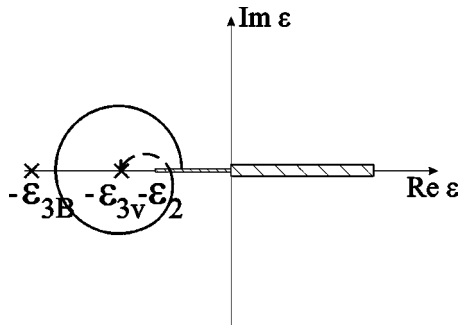


FIG. 1. Schematical representation of the complex energy plane, in our dimensionless units. $\epsilon_{3B}$ and $\epsilon_{3V}$ are, respectively, pictorial representations of the positions of the three-body bound- and virtual-state energies in the first and second three-body energy sheet. The three-body cut is shown for $\mathrm{Re}(\epsilon)>0$. The elastic cut (the narrow one) is shown with the origin at $\mathrm{Re}(\epsilon)=-\epsilon_2$, where $\epsilon_2$ is the energy of the two-body bound state.

$$\mathcal{K}\left(\sqrt{\frac{E_2}{E_3^{(N)}}}\right)\equiv\pm\sqrt{\frac{E_3^{(N+1)}-E_2}{E_3^{(N)}}}=\pm\sqrt{\frac{\epsilon_3^{(N+1)}-\epsilon_2}{\epsilon_3^{(N)}}}. \tag{4}$$

This defined function $\mathcal{K}$ has its values on the imaginary axis of a three-body momentum space; a space that is defined with origin at the point in which the energies of the three-body system and the bound two-body subsystem are equal $(E_3=E_2)$. In this respect, relative to the bound subsystem, we can define bound and virtual states for the three-body system. $\mathcal{K}$ assumes a negative value for a three-body virtual state and a positive value for a three-body bound state. Schematically, we represent in Fig. 1 the energies of the two- and three-body system in the complex energy plane. The two-body subsystem is bound and the three-body system can be bound or virtual, with the energies given, respectively, by $\epsilon_{3B}$ and $\epsilon_{3V}$. Through the elastic cut (corresponding to the atom-dimer elastic scattering), one defines two sheets; in the first sheet, we have the three-body bound-state energy at $\mathrm{Re}(\epsilon)=-\epsilon_{3B}$; in the second sheet, we have the three-body virtual-state energy at $\mathrm{Re}(\epsilon)=-\epsilon_{3V}$, as illustrated in Fig. 1.

We would like to add one more comment to this section. The existence of a three-body scale implies in the low-energy universality found in three-body systems, or correlations between three-body observables [23,16]. In the scaling limit, one has

$$O(E,E_3,E_2)=(E_3)^{\eta}\mathcal{A}(\sqrt{E/E_3},\sqrt{E_2/E_3}), \tag{5}$$

where $O$ is a general observable of the three-body system at energy $E$, with dimension of energy to the power $\eta$. The scattering amplitude of the elastic process $a+bc\rightarrow a+bc$, $f_3=\sqrt{E_3}^{-1}F(\sqrt{E/E_3},\sqrt{E_2/E_3})$ for $E=E_2$, implies that the scattering length is given by a function $a_3=\sqrt{E_3}^{-1}F(\sqrt{E_2/E_3})$. In the three-nucleon system this originates the ''Phillips plot,'' the correlation between the doublet neutron-deuteron scattering length and the triton energy [24]. The scaling functions, Eqs. (3) and (4), express the correlation between the excited- or virtual-state energies of the trimer and its ground-state energy, which can be understood as particular cases of Eq. (5).

## III. NUMERICAL RESULTS FOR VIRTUAL AND BOUND TRIMERS

In this section, we present our main results for the trimer bound and virtual states. With the sake to be complete, we first briefly sketch a new derivation of the subtracted equations that were numerically solved.

### A. Renormalization and subtracted equations

The homogeneous form of the subtracted Faddeev equation [16] for the bound three-boson system with a zero-range interaction is given by

$$\chi(\vec{y})=\frac{-\pi^{-2}}{\pm\sqrt{\epsilon_2}-\sqrt{\epsilon_3+\frac{3}{4}\vec{y}^2}}\int d^3x\left(\frac{1}{\epsilon_3+\vec{y}^2+\vec{x}^2+\vec{y}\cdot\vec{x}}-\frac{1}{1+\vec{y}^2+\vec{x}^2+\vec{y}\cdot\vec{x}}\right)\chi(\vec{x}), \tag{6}$$

which is written in units such that the three-body subtraction energy is $\mu_{(3)}^2=1$. It has a similar form as that of Eq. (1) with a different regulator, which expresses the physical condition at the subtraction point.

We briefly explain below the main physical steps to derive the three-body renormalized equation [16] used in our numerical calculation of the scaling functions through Eq. (6) for the bound state and its analytic continuation to the second energy sheet for the virtual state. We begin from the general Lippman-Schwinger equation expressed in a subtracted form [19]:

$$T_{\mathcal{R}}(E)=T_{\mathcal{R}}(-\mu^2)+T_{\mathcal{R}}(-\mu^2)[G_0^{(+)}(E)-G_0(-\mu^2)]T_{\mathcal{R}}(E), \tag{7}$$

where $T_{\mathcal{R}}(-\mu^2)$ is the $T$ matrix at a given energy scale $-\mu^2$ (negative energy, for convenience), $G_0^{(+)}(E)=[E-H_0+\mathrm{i}\delta]^{-1}$, and $H_0$ is the free Hamiltonian. Equation (7) defines the renormalized $T$ matrix in which $T_{\mathcal{R}}(-\mu^2)$ is known and replace the original ill-defined potential $V$:

$$T_{\mathcal{R}}(-\mu^2)=[1-VG_0(-\mu^2)]^{-1}V. \tag{8}$$

The renormalized $T$ matrix does not depend on the arbitrary subtraction point $-\mu^2$ (once $dV/d\mu^2=0$), which implies in a Callan-Symanzik-type [19,20] equation for $T_{\mathcal{R}}(-\mu^2)$:

$$\frac{d}{d\mu^2}T_{\mathcal{R}}(-\mu^2)=T_{\mathcal{R}}(-\mu^2)[G_0(-\mu^2)]^2T_{\mathcal{R}}(-\mu^2). \tag{9}$$

This expresses the renormalization-group invariance of the subtracted equation.

To solve Eq. (7) for the three-body $T$ matrix $T_{\mathcal{R}}^{(3)}(E)$, a dynamical assumption has to be made at a particular subtrac-

tion point $-\mu_{(3)}^2$, where we assume that the three-body $T$ matrix is equal to the driving term, which is given by the sum of the pairwise two-body $T$ matrices. Thus, at the energy $-\mu_{(3)}^2$, it is assumed that the three-body multiple-scattering series vanishes beyond the driving term. Observe that this is not true for a regular finite-range potential, only in the limit of $\mu_{(3)}\to\infty$. However, in the scaling limit, in fact, the actual value of $\mu_{(3)}$ tends to infinity such that $E_2/\mu_{(3)}^2$ goes to zero, as it be will be clear in our numerical calculations.

With our assumption, the $T$ matrix at the subtraction point $\mu_{(3)}$ is given by

$$T_{\mathcal{R}}^{(3)}(-\mu_{(3)}^2)=\sum_{(ij)} T_{\mathcal{R}(ij)}^{(2)}\left(-\mu_{(3)}^2-\frac{q_k^2}{2m_{k(ij)}}\right), \qquad (10)$$

where $(i,j,k)=(1,2,3)$, $(2,3,1)$, $(3,1,2)$. The summation is performed over all pairs and the renormalized two-body $T$-matrix elements for the pair $(ij)$ are given by $\langle\vec{P}'|T_{\mathcal{R}}^{(2)}(E)|\vec{P}\rangle=1/[2\pi^2(\pm\sqrt{E_2}+i\sqrt{E})]$. The argument of the two-body $T$ matrix is the center-of-mass pair energy, where $q_k$ is the Jacobi relative momentum canonically conjugated to the relative coordinate of the particle $k$ to the center of mass of the pair $(ij)$, and $m_{k(ij)}$ is the reduced mass.

Using Eqs. (7) and (10) and after some straightforward manipulations, the equations for the Faddeev components of the $T$ matrix at the bound-state pole give Eq. (6), which has a natural momentum scale given by $\mu_{(3)}^2$. In principle, $\mu_{(3)}^2$ can be varied without changing the content of the theory as long as the three-body $T$ matrix at the new subtraction energy $\mu_{(3)}^2$ is found from the solution of Eq. (9) with the boundary condition Eq. (10); and consequently, Eq. (6) should be conveniently rewritten. In the scaling limit, Eqs. (1) and (6) produce the same results (as we are going to illustrate numerically), since they are solved for $\epsilon_2$ going to zero, and the detailed form of the regularization implied in both equations is not important anymore. However, Eq. (6) has conceptual and practical advantages over Eq. (1), namely, it is explicitly renormalization-group invariant and also regularized.

To simplify the notation of Eq. (6), we introduce another definition related to the two-body energy; $\kappa_2\equiv\pm\sqrt{\epsilon_2}$, where $+$ refers to bound and $-$ to virtual two-body-state energies. After partial-wave projection of Eq. (6), the $s$-wave integral equation for the three-boson system is

$$\chi_s(y)=\tau(y;\epsilon_3;\kappa_2)\int_0^\infty dx\,x^2 G(y,x;\epsilon_3)\chi_s(x), \qquad (11)$$

where

$$\tau(y;\epsilon_3;\kappa_2)=-\frac{2}{\pi}\left[\sqrt{\epsilon_3+\frac{3}{4}y^2}-\kappa_2\right]^{-1}, \qquad (12)$$

$$G(y,x;\epsilon_3)=(\epsilon_3-1)\times\int_{-1}^{1}dz\,\frac{1}{(\epsilon_3+y^2+x^2+yxz)(1+y^2+x^2+yxz)}. \qquad (13)$$

For the $\ell$th angular-momentum three-body state, the Thomas collapse is forbidden if $\ell>0$; consequently, no regularization is required and the integration over momentum can be extended to infinity even in the limit $\mu_{(3)}\to\infty$. For $\ell>0$, the original Skornyakov and Ter-Martirosian equation [25] is well defined, and the three-body observables are completely determined by the two-body physical scale corresponding to $E_2$. One finds examples of the disappearance of the dependence on the three-body scale in *p-wave* virtual states, for the trineutron system when $n$-$n$ is artificially bound [26,27], and in three-body halo nuclei (represented as a core with a halo of two neutrons) [28].

The analytic continuation to the second energy sheet, of the scattering equations for separable potentials, is discussed in detail by Glöckle, in Ref. [26]. The particular case of the zero-range three-body model [25] is also given in Ref. [29]. On the second energy sheet, the integral equations are obtained by the analytical continuation through the two-body elastic scattering cut corresponding to the atom-dimer scattering. The elastic scattering cut comes through the pole of the atom-atom elastic scattering amplitude in Eq. (12). We perform the analytic continuation of Eq. (11) to the second energy sheet. By substituting the spectator function $\chi_s(y)$ by $\overline{\chi_s}(y)\equiv(\epsilon_{3v}-\epsilon_2+\frac{3}{4}y^2)\chi_s(y)$, where $\epsilon_{3v}$ is the modulus of the virtual-state energy, the resulting equation in the second energy sheet is given by

$$\overline{\chi_s}(y)=\overline{\tau}(y;\epsilon_{3v};\kappa_2)\frac{4\pi\kappa_{3v}}{3}G(y,-i\kappa_{3v};\epsilon_{3v})\overline{\chi_s}(-i\kappa_{3v}) + \overline{\tau}(y;\epsilon_{3v};\kappa_2)\int_0^\infty dx\,x^2\frac{G(y,x;\epsilon_{3v})\overline{\chi_s}(x)}{\epsilon_{3v}-\epsilon_2+\frac{3}{4}x^2}, \qquad (14)$$

where the on-energy-shell momentum at the virtual state is $\kappa_{3v}\equiv\sqrt{\frac{4}{3}(\epsilon_{3v}-\epsilon_2)}$, and

$$\overline{\tau}(y;\epsilon_{3v};\kappa_2)\equiv-\frac{2}{\pi}\left[\sqrt{\epsilon_{3v}+\frac{3}{4}y^2}+\kappa_2\right]. \qquad (15)$$

The cut of the elastic amplitude given by the exchange of one atom between the different possibilities of the bound dimer subsystems is near the physical region due to the small value of $\epsilon_2$. This cut is given by the values of imaginary $x$ between the extreme poles of the free three-body Green's function $G(y,x;\epsilon_{3v})$, given by Eq. (13), which appears in the right-hand side of Eq. (14),

$$\epsilon_{3cut}+y^2+x^2+xyz=0, \qquad (16)$$

with $-1<z<1$, $y=x=-i\kappa_{cut}$, and $\epsilon_{3cut}=\frac{3}{4}\kappa_{cut}^2+\epsilon_2$. With the above, the cut satisfies

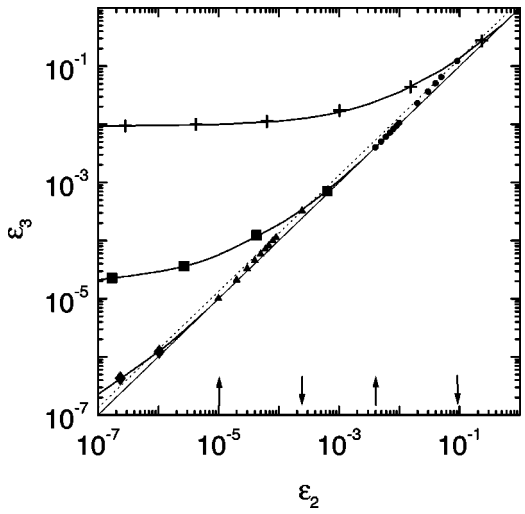


FIG. 2. Trimer energies $\epsilon_3$ as functions of the dimer bound-state energy $\epsilon_2$. The trimer ground-state energy ($\epsilon_3^{(0)}$) is shown by the curve with crosses; the first excited bound state ($\epsilon_3^{(1)}$) is shown by the curve with squares; and the second excited bound state ($\epsilon_3^{(2)}$) by the curve with diamonds. The behavior of two trimer virtual-state energies, $\epsilon_{3v}^{(1)}$ (small circles) and $\epsilon_{3v}^{(2)}$ (small triangles), are also shown as functions of the two-body energy, varying from the threshold $\epsilon_3=\epsilon_2$ (solid line) to the threshold for the one-particle-exchange cut $\epsilon_3=\frac{4}{3}\epsilon_2$ (dotted line). All the energies are given in arbitrary units.

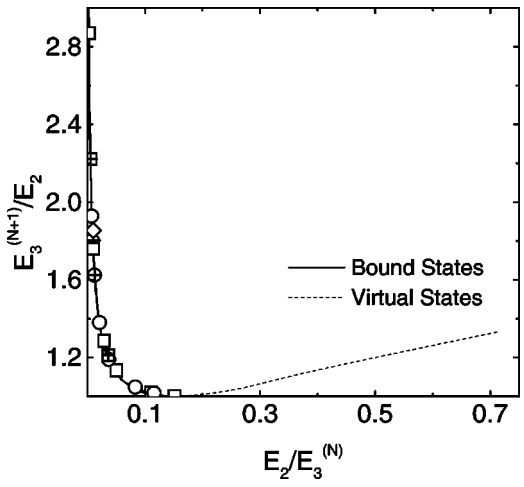


FIG. 3. Ratio of the trimer excited or virtual $(N+1)$th state energy as a function of the ratio of the dimer energy and trimer $N$th bound-state energy. The results for the trimer excited bound-state energies are shown by the solid curve, and the virtual-state energies are shown by the dotted curves. Our calculations show that the results for $N=0$ and $N=1$ practically coincide. The symbols represent results from other calculations: empty squares ($s$ wave) and empty circles ($s+d$ waves) are from Ref. [30] (for $N=0$); crossed squares are from Ref. [31]; the crossed circle is from Ref. [32]; the triangle is from Ref. [33]; and the lozenge is from Ref. [34].

$$4\epsilon_2 > \epsilon_{3cut} > \tfrac{4}{3}\,\epsilon_2\,. \tag{17}$$

The virtual-state energy $\epsilon_{3v}$ in the second energy sheet is found between the scattering threshold and the cut, $\epsilon_2 < \epsilon_{3v} < \frac{4}{3}\epsilon_2$.

### B. Scaling plots

It is usual to analyze how the Efimov states arise by varying the strength of the interaction to change the value of the two-body binding energy. In our case, instead of this procedure, we change directly the value of the energies in units of $\mu=1$, and by doing this we calculate the $s$-wave three-body energy evolution in the complex energy plane, corresponding to the bound and virtual triatomic states from Eqs. (11) and (14), respectively. As $\epsilon_2$ goes to zero, a crescent number of weakly bound (in units of $\mu=1$) Efimov states appear. The Thomas-Efimov limit for $\epsilon_2$ going to zero is clearly seen in Fig. 2, where we plot $\epsilon_3^{(N)}$ as a function of $\epsilon_2$. In this figure we display only the energies of the first three states. The main purpose of Fig. 2 is to show the real nature of the energies of the Thomas-Efimov states. The small circles and triangles correspond, respectively, to the first and second excited virtual-state energies, which begin at the cut from the one-particle exchange mechanism that gives $\epsilon_{3v}=(4/3)\epsilon_2$ (shown in the figure by the dotted line). The threshold, from which the virtual three-body states arise, are exhibited by down arrows ($\downarrow$). When the two-body energy is enough for a trimer bound state to exist, then a decrease in $\epsilon_2$ allows the virtual state to appear from the one-particle-exchange cut. Further decrease in $\epsilon_2$ favors the appearance of the excited state, which emerges from the second energy sheet to the first one at the threshold value $\epsilon_3=\epsilon_2$ (solid line), indicated by the up arrow ($\uparrow$). The critical value of $\epsilon_2$ is given by the ratio $(\epsilon_2/\epsilon_3^{(N)})^{1/2}=0.38$ where the excited state is labeled by $N+1$, and in the figure is indicated by the up arrow. This figure also strongly suggests that the Thomas-Efimov states cannot be completely understood only through the absolute value of $E_2$ itself, because the critical value for the appearance of the $(N+1)$ excited state depends only on the ratio $E_2/E_3^{(N)}=\epsilon_2/\epsilon_3^{(N)}$, which is independent of the absolute scale. Therefore, to show that this argument is universal, we study the function $E_3^{(N+1)}/E_2=\epsilon_3^{(N+1)}/\epsilon_2$ as a function of $E_2/E_3^{(N)}=\epsilon_2/\epsilon_3^{(N)}$, where the $(N+1)$ state can be virtual or bound. This study is presented in Fig. 3.

The plot of Fig. 3 is constructed with the results for the first and second Thomas-Efimov states. This plot practically coincides with the corresponding one obtained from the second and third states (not shown). Figure 3 shows a universal route for the energy of the $(N+1)$ trimer state in the complex energy plane, from the second energy sheet to the first one, as the ratio $E_2/E_3^{(N)}=\epsilon_2/\epsilon_3^{(N)}$ decreases. The three-body virtual-state energy reaches $4E_2/3$ at $E_2/E_3^{(N)}=0.71$. Also realistic calculations for the helium trimer are available and are displayed in this figure. The agreement between our calculations and the realistic ones, shows the significance of our scaling picture. Unfortunately, there is not yet, to our knowledge, realistic calculations of the virtual state in helium trimer or even in any other weakly bound three-boson

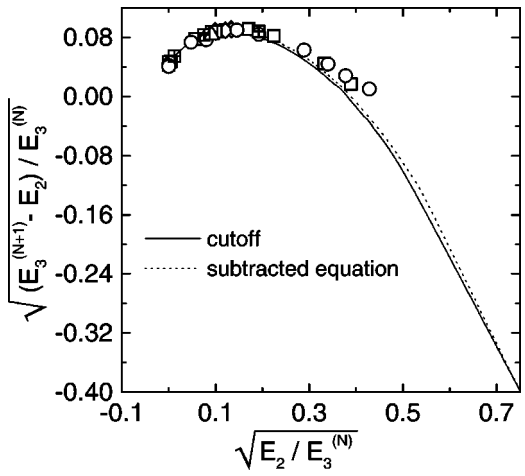


FIG. 4. Results for the trimer bound and virtual excited $(N+1)$th state energies, scaled by the $N$th bound-state energy. A comparison between calculations performed with cutoff and subtraction methods for the regularizations is given for $N=0$. We also present results from other calculations, as described in Fig. 3.

system, in which our route should also apply. We emphasize that although we have presented results only for the second and third Thomas-Efimov states, the scaling limit is practically approached as we see in Fig. 3. We expect that going further in diminishing the absolute value of $E_2$, the new excited states will also follow the same route. The claim is, of course, that the route is universal for all states in the scaling limit.

The results for the energy of the excited Efimov state in $^4He_3$ molecule given by $\mathcal{K}(z)$ $(z=[E_2/E_3^{(N)}]^{1/2})$, obtained by solving Eqs. (1), (11), and (14) in the scaling limit, are compared to the realistic model calculations also presented in Fig. 4. The homogeneous integral equation with the sharp cutoff momentum regulator, which generalizes Eq. (1) for the virtual trimer state, is not written explicitly in the text as it can be easily derived. We observe the ratio $[(E_3^{(N+1)} - E_2)/E_3^{(N)}]^{1/2}$ depends on $z$ for realistic models as well. In this plot we only show results for a bound dimer and $N=0$. The extreme limit of $z$ allowing the excited state are given by $\mathcal{K}(z)=0$, which gives $z=0.38$. The solution of Eqs. (1) and (11) in the scaling limit qualitatively reproduces the results for several interatomic potentials. A deviation is seen for $z\approx 0.4$, which is due to corrections from the finite range of the potential. The excited $(N+1)$ three-body state becomes virtual for $E_2/E_3^{(N)} > 0.145$ (as seen in Fig. 3), implying that $E_3^{(N)} < 6.9\hbar^2/(ma^2)$ in this case. This threshold value agrees with the value previously found in Refs. [8,9], recently confirmed in Ref. [35], for the condition of the disappearance of the excited trimer state in the limit of a zero-range interaction. Let us stress that the regularization schemes used in Eqs. (1) and (11) are consistent not only for the calculation of the bound excited trimer energies but also for the virtual trimer energies, as shown in Fig. 4. The small difference between the two regularization schemes tends to vanish fast for higher values of $N$.

## IV. CONCLUSIONS

Natural scales determine the physics of quantum few-body systems with short-range interactions. The physical scales of three interacting particles, in the state of zero total angular momentum, are identified with the bound or virtual subsystem energy and the ground-state three-body binding energy. The scaling limit is found when the ratio between the scattering length and the interaction range tends to infinity, while the ratio between the physical scales are kept fixed. This defines a scaling function for a given observable. From the formal point of view, we showed the relation of the scaling limit and the renormalization aspects of a few-body model with a zero-range interaction, through the derivation of subtracted three-body $T$-matrix equations that are renormalization-group invariant.

In the present work, we investigate the behavior of an excited Thomas-Efimov state as the binding energy of the subsystem increases with respect to the energy of the next lower bound three-body state. As shown, by allowing the two-body binding energy to increase in respect to the three-particle ground-state energy, the excited three-body state disappears, and a corresponding three-body virtual state emerges. The threshold for the three-body virtual state was found to be at the energy of the weakly bound trimer equal to $6.9\hbar^2/(ma^2)$ for large positive scattering lengths $a$. The dependence of the $s$-wave virtual-state three-body energy on the two- and three-atom ground-state binding energies is calculated in the limit of a zero-range potential in a form of an universal scaling function. The scaling plots are an useful tool to classify observables and provide first guess to guide realistic calculations, as well as for planning experiments, with the aim of looking for weakly bound excited state of triatomic molecules.

The results of the present study can also be particularly relevant to the interpretation of experiments in atomic condensation, in which the effective atom-atom scattering length can be altered from negative to positive, in a wide range of values crossing zero-energy bound dimer [12]. For large positive scattering lengths, our estimate gives the threshold for the zero-binding trimer state, which allows to settle the experimental conditions for an investigation of the Efimov effect, and search for their influence on the observables of condensed systems. On the other hand, large negative two-body scattering lengths have been recently investigated in Ref. [13]. There is the possibility that the observed discrepancy related with previous theoretical predictions can have their explanations in three-body effects as well, because large two-body scattering lengths give the conditions where three-body (bound or virtual) Efimov states are likely to occur.

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# Weakly bound atomic trimers in ultracold traps

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The experimental three-atom recombination coefficients of the atomic states $^{23}\mathrm{Na}|F=1,m_F=-1\rangle$, $^{87}\mathrm{Rb}|F=1,m_F=-1\rangle$, and $^{85}\mathrm{Rb}|F=2,m_F=-2\rangle$, together with the corresponding two-body scattering lengths, allow predictions of the trimer bound-state energies for such systems in a trap. The recombination parameter is given as a function of the weakly bound trimer energies, which are in the interval $1<m(a/\hbar)^2E_3<6.9$ for large positive scattering lengths $a$. The contribution of a deep-bound state to our prediction, in the case of $^{85}\mathrm{Rb}|F=2,m_F=-2\rangle$, for a particular trap, is shown to be relatively small.

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The formation of molecules in ultracold atomic traps offers new and exciting possibilities to study the dynamics of condensates [1]. The formation of rubidium molecules $^{87}\mathrm{Rb}_2$ in a bosonic condensate was reported, which allowed to measure its binding energy with unprecedented accuracy [2]. Ultracold sodium molecules $^{23}\mathrm{Na}_2$ have also been formed through photoassociation [3]. However, nothing has been reported till now about the formation of molecular trimers in cold traps. The first information, one is led to ask, is about the magnitude of the binding energy of trimers in a cold trap. Two-body scattering lengths of trapped atoms are well known in several cases, as well as their closely related dimer binding energy. In the limit of large scattering lengths, it is necessary to know in addition one low-energy three-body observable to predict any other one. In this case, the detailed form of the two-body interaction is not important [4,5]. The recombination rate of three atoms in the ultracold limit, measured by atomic losses in trapped condensed systems, can supply the necessary information to estimate the trimer binding energy. For short-range interactions, the magnitude of the recombination rate of three atoms is mainly determined by the two-body scattering length $a$ [6]. However, it is important to remark that a dependence on one typical low-energy three-body scale [4,5] still remains. Indeed, it is gratifying to note that all the works on three-body recombination, consistently, present a dependence on a three-body parameter in addition to the scattering length [7–9].

The aim of the present work is to report on how one can obtain the trimer binding energy of a trapped atomic system, from the three-body recombination rate and the corresponding two-body scattering length. For this purpose, we use a scale independent approach valid in the limit of large positive scattering lengths (or when the interaction range goes to zero), obtained from a renormalized zero-range three-body theory [4], which relates the recombination rate, the scattering length, and the trimer binding energy. Considering the experimental values of the recombination rates and scattering lengths given in Refs. [10–13], the method is applied to predict the trimer binding energies of $^{23}\mathrm{Na}|F=1,m_F=-1\rangle$, $^{87}\mathrm{Rb}|F=1,m_F=-1\rangle$, and $^{85}\mathrm{Rb}|F=2,m_F=-2\rangle$, where $|F,m_F\rangle$ is the respective hyperfine states of the total spin $F$. We note that the bound states considered here are in fact high-lying resonances, not true bound states, as they can decay into lower-lying channels.

The validity of our approach is restricted to sufficiently diluted gases, because all the scaling relations are derived for three isolated particles. Also, when the scattering length is tuned via external field in a trap, the parameters are different from the vacuum values, and consequently, our predictions only apply to that particular experimental conditions. For the trapped gases that we are analyzing, the diluteness parameter $\rho a^3$ (where $\rho$ is the gas density) should not be much larger than one, otherwise one needs to consider higher-order correlations between the particles. Indeed, we observe that, in general, for the analyzed condensed systems, the diluteness parameter is much smaller than one. Even in the case of $^{85}\mathrm{Rb}$, where the considered scattering length is obtained via Feshbach resonance techniques [13], the diluteness parameter is about 1/2.

Another relevant remark, pointed out in Ref. [14], is that the recombination into deep-bound states can affect the theoretical results that are based on calculation of this rate into shallow states alone. This additive contribution depends on one more constant, beyond the three-body scale. However, the fitted contribution of the recombination into deep-bound states is fortunately much smaller than the contribution of the shallow bound state, as found in the case of $^{85}\mathrm{Rb}$ [14]. Such an evidence supports our estimation of trimer energies, when $a>0$, that are obtained by only considering the contribution of recombination rates into the shallow state.

The values of $a$ are usually defined as large with respect to the effective range $r_0$, such that $a/r_0\gg 1$. The low-energy three-boson system presents, in this limit, the Efimov effect [15], where an infinite number of weakly bound three-body states appears. The size of such states are much larger than the effective range. The limit $a/r_0\to\infty$ can be realized either by $a\to\infty$ with $r_0$ kept constant or by $r_0\to 0$ with $a$ constant. In the last case, the limit of a zero-range interaction corresponds to the Thomas bound-state collapse [16]. In this respect, the Efimov and Thomas limits are equivalent or different aspects of the same physics [17]. The Thomas-Efimov connection is also reviewed in Ref. [5]. In the limit $a/r_0$

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$\rightarrow\infty$, the details of the interaction for the low-energy three-body system are contained in one typical three-body scale and the two-body scattering length (or the dimer bound-state energy $E_2$); they are enough to determine all three-body observables [4]. Considering, for example, the trimer binding energy $E_3$ as the three-body scale, any three-body observable $O_3$ that has dimension of $(\text{energy})^\beta$, in the limit of $r_0 \rightarrow 0$, can be expressed as

$$O_3 = E_2^\beta \mathcal{F}_2(E_2/E_3) = E_3^\beta \mathcal{F}_3(E_2/E_3). \tag{1}$$

The dimensional factor in the above equation is chosen for convenience as $E_2$ or $E_3$. The scaling function in each case is $\mathcal{F}_2$ or $\mathcal{F}_3$. The existence of the scaling limit for zero-range interactions was verified in Refs. [18,19]. In practice, such a limit is approached by the excited state of the atomic trimer obtained in realistic calculations, allowing as well the theoretical interpretation of those excited states as Efimov states [19]. Here, we observe that the binding energy $E_3$ refers to the magnitude of the total energy of the bound system; the binding energy with respect to the two-body threshold is defined as $S_3 \equiv E_3 - E_2$.

The rate of three free bosons to recombine, forming a dimer and one remaining particle, is given in the limit of zero energy, by the recombination coefficient [5,6]

$$K_3 = \frac{\hbar}{m} a^4 \alpha, \tag{2}$$

where $\alpha$ is a dimensionless parameter and $m$ is the mass of the atom. When $a > 0$, the recombination parameter $\alpha$ oscillates between zero and a maximum value, which is a function of $a$, as shown in Refs. [7] ($\alpha \leqslant 68.4$), [8] ($\alpha \leqslant 65$), and [9] ($\alpha \leqslant 67.9$). With amplitude $\alpha_{\max}$ and phase $\delta$, we can write it as [5]

$$\alpha = \alpha_{\max} \sin^2[1.01 \ln(a) + \delta], \tag{3}$$

where $\delta$ depends on the interaction at short distances. The physics at short distances, in the three-boson system, is parametrized by one typical three-body scale, which we have chosen as the unknown trimer binding energy. So, by using the general scaling given by Eq. (1), one can explicitly express the functional dependence of $\alpha$ as $\alpha \equiv \alpha(\sqrt{E_2/E_3})$, considering that for large scattering lengths we have $1/a = \sqrt{mE_2/\hbar^2}$. To exemplify the scaling form of $\alpha$, we can rewrite Eq. (3) such that the $\sqrt{E_2/E_3}$ dependence is explicit. Therefore,

$$\alpha = \alpha_{\max} \sin^2\left[ -1.01 \ln \sqrt{\frac{E_2}{E_3}} + \Delta\left( \sqrt{\frac{E_2}{E_3}} \right) \right], \tag{4}$$

where $\Delta(\sqrt{E_2/E_3}) = \delta - 1.01 \ln(\sqrt{mE_3/\hbar^2})$. Our next task is the calculation of the scaling function by using the renormalized subtracted Faddeev equations [4].

The three-boson recombination coefficient at zero energy is derived from the Fermi's golden rule as

$$K_3 = \frac{2\pi}{\hbar} (2\pi\hbar)^9 \int \frac{d^3p}{(2\pi\hbar)^3} |\mathcal{T}_{\text{i}\to\text{f}}|^2 \delta\left( \frac{3}{4m} p^2 - E_2 \right), \tag{5}$$

where $\mathcal{T}_{\text{i}\to\text{f}}$ is the transition amplitude between the initial ($i$) and final ($f$) momentum states, which are normalized as plane waves: $\langle \vec{r} | \vec{p} \rangle = \exp[-i(\vec{p}/\hbar)\cdot\vec{r}]/(2\pi\hbar)^{3/2}$. The number of atoms $N$ in the condensed state decreases, due to the recombination process, as

$$\frac{1}{N}\frac{dN}{dt} = -\frac{3}{3!} K_3 \rho^2. \tag{6}$$

For each recombination process three atoms are lost, justifying the factor 3 in the numerator. The factor 3! in the denominator appears only in case of condensed systems; it counts for the number of triples in such a state [11].

Considering the symmetrized scattering wave function for the initial state of three free particles, $|\Phi_0\rangle = (1/\sqrt{3}) \Sigma_{i=1}^3 |\vec{q}_i, \vec{p}_i\rangle$, we obtain the transition amplitude, in terms of the Faddeev components of the three-body $T$ matrix $T_i(E)$, as

$$\mathcal{T}_{\text{i}\to\text{f}} = \langle \vec{k}_i \Phi_b^{(jk)} | [T_j(E) + T_k(E)] | \Phi_0 \rangle, \tag{7}$$

where $(i,j,k) = (1,2,3)$ are cyclic permutations, and $E$ $[= 3q_i^2/(4m) + p_i^2/m = 3k_i^2/(4m) - E_2]$ is the energy of the scattering state. $\vec{q}_i$ is the Jacobi relative momentum of the particle $i$ with respect to the center of mass of particles $j$ and $k$, $\vec{p}_i$ is the relative momentum of $j$ with respect to $k$, and $\vec{k}_i$ is the relative momentum of the free particle $i$ in the final state. $|\Phi_b^{(jk)}\rangle$ is the normalized two-body bound-state wave function of the pair $jk$. The calculation of the Faddeev components is performed with the use of the subtracted approach given in Ref. [4], such that

$$T_i(E) = t_i\left( E - \frac{3q_i^2}{4m} \right) \{ 1 + [G_0^+(E) - G_0(E_\mu)] \times [T_j(E) + T_k(E)] \}, \tag{8}$$

where $E_\mu \equiv -\mu^2/m$ is the subtraction energy scale with $\mu$ a constant in momentum units. It is possible to vary $\mu$ without changing the physics of the theory as long as the inhomogeneous term of Eq. (8) is modified according to the renormalization group equations [20]. $t_i$ is the two-body $t$ matrix for the subsystem of particles $(jk)$. For $E = 0$ and zero-range potential the corresponding matrix elements are given by [4]

$$\left\langle \vec{p}\,' \middle| t\left( \frac{-3q^2}{4m} \right) \middle| \vec{p} \right\rangle = \tau\left( \frac{-3q^2}{4m} \right) = \frac{1}{m\sqrt{3}\pi^2} \frac{1}{k - q + i\epsilon}, \tag{9}$$

where $k \equiv \sqrt{4mE_2/3}$. From Eqs. (8) and (9), and for $E = 0$, the matrix elements of $T_i$ are given by

$$\langle \vec{q}_i \vec{p}_i | T_i(0) | \vec{0}\vec{0} \rangle = \tau(0)\delta(\vec{q}_i) + 2\tau[-3q_i^2/(4m)] h(q_i), \tag{10}$$

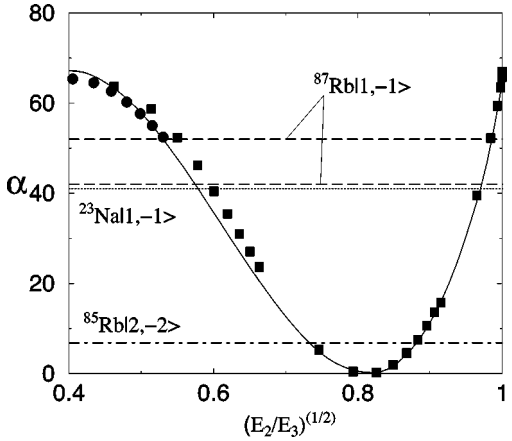


FIG. 1. The dimensionless recombination parameter $\alpha$ as a function of the ratio between the binding energies of the diatomic and triatomic molecules. Theoretical results: full circles (one triatomic bound state), solid line (two triatomic bound states), and full squares (three triatomic states). The lines indicate the center of experimental data, given in Table I, for $^{23}$Na, $^{87}$Rb, and $^{85}$Rb. In case of $^{85}$Rb we subtracted the contribution of the deep-bound state, which was reported in Ref. [14].

where the $s$ wave function $h(q)$ is the solution of

$$h(q)=-\frac{\mu^2}{\sqrt{3}\pi^2 k q^2(\mu^2+q^2)}-\frac{4}{\sqrt{3}\pi}\int_0^\infty \frac{dq'}{q}\,\frac{q' h(q')}{k-q'+i\epsilon}\times\ln\left(\frac{q^2+q'^2+qq'}{q^2+q'^2-qq'}\,\frac{\mu^2+q^2+q'^2-qq'}{\mu^2+q^2+q'^2+qq'}\right). \quad (11)$$

The normalized two-body bound-state wave function, in the zero-range model, to be introduced in Eq. (7), is given by

$$\langle \vec{p}|\Phi_b\rangle=\frac{1}{\pi}\sqrt{\frac{\hbar}{a}}\frac{1}{(\hbar/a)^2+p^2}. \quad (12)$$

By considering the above equations, we obtain the final form of the recombination parameter:

$$\alpha=\frac{8(2\pi)^8 m^2}{3\sqrt{3}}\left(\frac{\hbar}{a}\right)^5|\mathcal{T}_{i\to f}|^2=6\sqrt{3}(8\pi)^2\left|1+\frac{16\pi\hbar^2}{3a^2}\int_0^\infty dq\,\frac{q\,h(q)}{k-q+i\epsilon}\times\ln\left(\frac{k^2+q^2+qk}{k^2+q^2-qk}\right)\right|^2. \quad (13)$$

The numerical results for the recombination parameter are obtained from the solution of Eq. (11), for different values of $\mu$. When $\mu\to\infty$, the results approach the scaling limit [18,19]. Therefore, the theoretical results for $\alpha$ are shown in Fig. 1 as a function of the ratio $\sqrt{E_2/E_3}$. The calculations were performed in dimensionless units, such that all the momentum variables were rescaled in units of $\mu$ (in other words, $\mu=1$ in our calculations). So, the two-atom binding energy is decreased with respect to this scale. In that sense, the Thomas-Efimov states appear for $E_2/E_\mu$ going towards zero, which is equivalent of having $E_2$ fixed and $\mu\to\infty$. The parameter $\alpha$, shown in Fig. 1, is obtained as a function of the most excited trimer state. We have performed numerical calculations with at most three Efimov states. The full circles show the results when only one bound state exists. When $E_2/E_\mu$ allows two Efimov states, the results are represented by the solid curve, which is plotted against the energy of the excited state. With full squares we represent the results when $E_2/E_\mu$ allows three Efimov states. The scaling limit is well approached in our calculations. The maximum $\alpha$ occurs at the threshold ($E_3=E_2$) and when $(E_3/E_2)^{1/2}=0.38$ [19]. So, according to this figure one obtains that $1<m(a/\hbar)^2E_3<6.9$, a range consistent with Refs. [18,19,21]. The scaling limit for $\alpha$ has been obtained in Refs. [7,9], but without reference to the weakly bound triatomic molecular state.

In Fig. 1, we represent with horizontal lines the center of experimental values of $\alpha$, as given in Table I, for the hyperfine states $^{23}$Na$|1,-1\rangle$, $^{87}$Rb$|1,-1\rangle$, and $^{85}$Rb$|2,-2\rangle$. Using the measured values of $\alpha_{expt}$ one obtains, from the universal scaling plot, two weakly bound triatomic molecular states, denoted by $E_3$ and $E_3'$, consistent with these values.

TABLE I. For the atomic species $^AZ|F,m_F\rangle$, given in the first column, we present in the sixth and seventh columns our predicted trimer binding energies, with respect to the threshold, $S_3\equiv(E_3-E_2)$ and $S_3'\equiv(E_3'-E_2)$, considering the central values of the experimental dimensionless recombination parameters $\alpha_{expt}$ (given in the fourth column). It is also shown that the corresponding two-body scattering lengths $a$ (second column), the diluteness parameters $\rho a^3$ (third column), and the dimer binding energies $E_2$ (fifth column). For $^{87}$Rb$|1,-1\rangle$, the recombination process was obtained in Ref. [11] for noncondensed (*) and condensed ($^\dagger$) trapped atoms.

| $^AZ\|F,m_F\rangle$ | $a$ (nm) | $\rho a^3$ | $\alpha_{expt}$ | $E_2$ (mK) | $S_3$ (mK) | $S_3'$ (mK) |
|---|---|---|---|---|---|---|
| $^{23}$Na$\|1,-1\rangle$ | 2.75 | $6\times10^{-5}$ | $42\pm12$ [10] | 2.85 | 4.9 | 0.21 |
| $^{87}$Rb$\|1,-1\rangle$ | 5.8 | $1\times10^{-5}$ | $52\pm22^*$ [11] | 0.17 | 0.39 | 0.005 |
| $^{87}$Rb$\|1,-1\rangle$ | 5.8 | $1\times10^{-4}$ | $41\pm17^\dagger$ [11] | 0.17 | 0.30 | 0.013 |
| $^{87}$Rb$\|2,2\rangle$ | 5.8 | $4\times10^{-5}$ | $130\pm36$ [12] | 0.17 | | |
| $^{85}$Rb$\|2,-2\rangle$ | 211.6 | 0.5 | $7.84\pm3.4$ [1,13] | $1.3\times10^{-4}$ | $1.14\times10^{-4}$ | $3.8\times10^{-5}$ |

Considering the center of experimental values of $\alpha$, our predicted values for $E_3$ and $E_3'$ are given in Table I in millikelvin. We are also giving in the table the corresponding known values of the scattering lengths. The range for the predicted values can be easily estimated from Fig. 1, considering the corresponding errorbars in $\alpha_{expt}$. See also Ref. [22], for a recent experiment with ultracold thermal gas of $^{133}$Cs$|3,3\rangle$, where the obtained values of $\alpha_{max}$, considering their systematic error limits, are in good agreement with theory.

One observe that the trap diluteness parameter is smaller than one in all the cases. For $^{85}$Rb$|2,-2\rangle$, we study a case corresponding to $K_3 \approx 3.5 \pm 1.5 \times 10^{-23}$ cm$^6$/s, extracted from Fig. 2(c) of Ref. [13], measured in an ultracold noncondensed gas with external field $B=156$ G. This value of $B$ corresponds to $a=4000a_0$ ($a_0$ is the Bohr radius) (see Claussen *et al.* [1]). As the resulting value of $\alpha$ is quite small for $^{85}$Rb$|2,-2\rangle$, one should expect a more significant contribution from the deep-bound state. Thus, we found instructive to subtract such a contribution from $\alpha_{expt}$, which is about 1 $\mu$, as found in Ref. [14]. However, the resulting effect in the determination of the trimer energy is not so dramatic, as seen in Fig. 1. The experimental value of $\alpha$ for $^{87}$Rb$|2,2\rangle$ does not appear in the figure, as it is well above the maximum. By increasing the value of $a$ from 5.8 nm to 6.8 nm we can make the experimental value consistent with our scaling limit approach. We also point out that the trimer can only support $E_3$ or $E_3'$, not both simultaneously [19].

In our predictions for the trimer's energies, except for $^{85}$Rb, we have disregarded the possible much smaller contribution of the recombination rate into deep-bound states for $a>0$, considering only recombinations into shallow states. When the recombination into deep-bound states is taken into account, the curve in Fig. 1 is moved upward by an unknown amount. But, using the value found in Ref. [14], this contribution is hardly going to affect the extracted values for the trimer's binding energies, given in Table I. It seems natural that if one were to measure the recombination rate as a function of an applied magnetic field, leading to a Feshbach resonance, one perhaps could be able to fix this additional contribution and determine the trimer binding energy. This additional contribution may help to explain part of the measured value of $\alpha$ for $^{87}$Rb$|2,2\rangle$.

In summary, in the present work, we derived the scaling dependence of the recombination parameter as a function of the ratio between the energies of the atomic dimer and the most excited trimer states. The scaling function tends to a universal function in the limit of zero-range interaction or infinite scattering length. The maximum of the recombination rate comes at the threshold for the appearance of a bound triatomic molecule. In the cases of diluted gases of $^{23}$Na$|1,-1\rangle$, $^{87}$Rb$|1,-1\rangle$, and $^{85}$Rb$|2,-2\rangle$, we use the scaling function, with the corresponding known experimental values of the recombination rates and two-atom scattering lengths, to predict the binding energies of weakly bound trimers in ultracold traps. We stress that the possible contribution of a deep-bound state in our predictions is expected to be relatively small, as verified for $^{85}$Rb$|2,-2\rangle$, in a particular trap. We also note that for $^{85}$Rb$|2,-2\rangle$ the diluteness parameter is about 0.5, a value that may be considered near the limit of validity of the present approach, which does not include higher-order correlations between the particles.

Finally, we would like to remark that, at a first sight, one could think that formation of trimers requires four-body collisions, which are very unlikely unless the density is high. However, the recent experimental results given in Ref. [1] indicate formation of molecules in the trap, as also discussed in Ref. [23]. Therefore, other collision processes such as dimer-dimer or dimer and two atoms could also lead to trimer formations, enhancing the possibility of producing trimers in a trapped ultracold gas.

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# Scaling predictions for radii of weakly bound triatomic molecules

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The mean-square radii of the molecules $^4He_3$, $^4He_2-^6Li$, $^4He_2-^7Li$, and $^4He_2-^{23}Na$ are calculated using a three-body model with contact interactions. They are obtained from a universal scaling function calculated within a renormalized scheme for three particles interacting through pairwise Dirac-$\delta$ interaction. The root-mean-square distance between two atoms of mass $m_A$ in a triatomic molecule are estimated to be of the order of $\mathcal{C}\sqrt{\hbar^2/[m_A(E_3-E_2)]}$, where $E_2$ is the dimer and $E_3$ is the trimer binding energies, and $\mathcal{C}$ is a constant (varying from $\sim 0.6$ to $\sim 1$), which depends on the ratio between $E_2$ and $E_3$. Considering previous estimates for the trimer energies, we also predict the sizes of rubidium and sodium trimers in atomic traps.

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## I. INTRODUCTION

Weakly bound molecules are large size quantum systems in which the atoms have an appreciable probability to be found much beyond the interaction range, and at the same time tiny changes in the potential parameters can produce huge effects in the properties of these states [1]. The best illustration of such systems is the experimentally found $^4He_2$ dimer [2], with $\sqrt{\langle r^2\rangle}=52\pm 4$ Å and binding energy $E_2=1.1+0.3/-0.2$ mK [3]. Other examples of weakly bound molecules are found through the experimental realization of Bose-Einstein condensation (BEC) [4], where the possibility to change the effective scattering length of the low-energy atom-atom interaction in the trap to large positive values by using an external magnetic field [4,5] can produce very large dimers. In fact, weakly bound molecules in ultracold atomic traps were reported in Ref. [6]. The binding energy of the $^{87}Rb_2$ dimer formed in a Bose-Einstein condensate was measured with unprecedented accuracy [7]. Ultracold $Na_2$ molecules have also been formed through photoassociation [8]. One should note that in the limit of an infinite atom-atom scattering length tuned by the Feshbach resonances in the trap, in principle the Efimov condition [9] can be achieved, in which an infinite number of weakly bound trimers exist. The formation of weakly bound trimers in ultracold atomic systems have not been reported till now, but recently the recombination coefficient rate was used to predict trimer binding energies of some specific atomic species that are being studied in atomic traps [10].

Theoretically it is possible to exist weakly bound molecules of zero-angular momentum states in triatomic systems, as for example, in the extensively studied $^4He$ trimer system (see, e.g., Ref. [11] and therein). These molecules are special due to the large spatial size, which spreads out much beyond the potential range [11,12]. In such trimer, the calculations of the mean-square distance of each $^4He$ atom to the corresponding center of mass (c.m.) have been performed for the ground and excited states [11,12], and also for the mean-square interatomic distance [11]. These sizes are of the order of 5–10 Å for the ground state of the $^4He_3$ molecule, and of about 50–90 Å for the excited Efimov state [11]. Therefore, the system heals through the regions that are well outside of the potential range, in which the wave function is essentially a solution of the free Schrödinger equation, and where the physical properties of the bound system is defined by a few physical scales. For example, the dimensionless product of the mean-square interatom distance with the separation energy of one atom from the trimer is not far from the unity [11] in the ground and also in the excited states, despite the large difference between such energies $E_3^{(0)}/E_3^{(1)}\approx 50$ ($E_3^{(n)}$ is the binding energy of the $n$th trimer state). So, as already discussed in Refs. [13–16], we should note that quite naturally the binding energy is the scale that dominates the physics of the trimer. One should remember as well that the collapse of the three-body system in the limit of a zero-range force [17] makes the three-body energy one of the scales of the system, beyond the two-body energy [13].

The calculation of the low-energy properties of the three-body system can be performed with a renormalization scheme applied to three-body equations with $s$ wave zero-range pairwise potential [13,18]. In this approach, one can fix the three-body ground-state (the three-body physical scale) and the two-body scattering lengths [13]. Consequently, all the detailed information about the short-range force, beyond the low-energy two-body observables, are retained in only one three-body physical information in the limit of zero-range interaction.

In the present work, we first study the mean-square distances of one atom to the c.m. system and between two atoms in the ground and excited states of triatomic molecules of type $^4He_2-X$, where $X\equiv$ $^4He$, $^6Li$, $^7Li$, and $^{23}Na$. Next, using trimer energies derived from the recombination

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coefficient rates [10], we make estimates of the corresponding sizes of rubidium and sodium trimers. We introduce and calculate scaling functions that describe the different radii as functions of the physical scales of the triatomic system obtained in the limit of a zero-range interaction. In this way, we are generalizing the concept of scaling function, which was previously introduced in Refs. [15] and [18] to study the behavior of bound and excited virtual Efimov states [9] in terms of triatomic physical scales.

The scaling function depends only on dimensionless ratios of the binding energies of two and three atoms, and the ratio of masses of the different atoms. In that sense our conclusions apply equally well to any other low-energy triatomic system. The validity condition for the scaling relations is that the interaction range must be small compared to particle distances, which is the case for weakly bound three-body systems.

The paper is organized as follows. In Sec. II, we present the Faddeev equations for the spectator functions for a triatomic system with two equal particles $\alpha$ and a third one $\beta$, and the form factors from which the different mean-square radii are obtained. Also in this section we discuss the generalization of the scaling function defined in Refs. [15,18] to describe the different radii. In Sec. III, we present our numerical results for the mean-square distances of one atom with respect to the c.m. system and between two atoms in the ground and excited states of triatomic molecules. Our conclusions are summarized in Sec. IV.

## II. RENORMALIZED THREE-BODY MODEL AND FORM FACTORS

In this section, we introduce the generalization of the scaling function defined in Refs. [15] and [18], to be used to obtain the different radii. We write down the coupled renormalized equations for the spectator functions and the expressions for the form factors, which allow the calculation of the different mean-square distances.

### A. Subtracted Faddeev equations

Throughout this paper we use units such that $\hbar = m_\alpha = 1$. For $\alpha = {}^4$He, $\hbar^2/m_{^4\mathrm{He}} = 12.12$ K Å$^2$. After partial wave projection, the $s$-wave coupled subtracted integral equations, for two identical particles $\alpha$ and a third one $\beta$, are given by

$$\chi_{\alpha\alpha}(y) = 2\,\tau_{\alpha\alpha}(y;\epsilon_3)\int_0^\infty dx\,\frac{x}{y}G_1(y,x;\epsilon_3)\chi_{\alpha\beta}(x), \quad (1)$$

$$\chi_{\alpha\beta}(y) = \tau_{\alpha\beta}(y;\epsilon_3)\int_0^\infty dx\,\frac{x}{y}[G_1(x,y;\epsilon_3)\chi_{\alpha\alpha}(x) + AG_2(y,x;\epsilon_3)\chi_{\alpha\beta}(x)], \quad (2)$$

$$\tau_{\alpha\alpha}(y;\epsilon_3) \equiv \frac{1}{\pi}\left[\sqrt{\epsilon_3 + \frac{A+2}{4A}y^2} \mp \sqrt{\epsilon_{\alpha\alpha}}\right]^{-1}, \quad (3)$$

$$\tau_{\alpha\beta}(y;\epsilon_3) \equiv \frac{1}{\pi}\left(\frac{A+1}{2A}\right)^{3/2}\left[\sqrt{\epsilon_3 + \frac{A+2}{2(A+1)}y^2} \mp \sqrt{\epsilon_{\alpha\beta}}\right]^{-1}, \quad (4)$$

$$G_1(y,x;\epsilon_3) \equiv \log\frac{2A(\epsilon_3+x^2+xy)+y^2(A+1)}{2A(\epsilon_3+x^2-xy)+y^2(A+1)} - \log\frac{2A(1+x^2+xy)+y^2(A+1)}{2A(1+x^2-xy)+y^2(A+1)}, \quad (5)$$

$$G_2(y,x;\epsilon_3) \equiv \log\frac{2(A\epsilon_3+xy)+(y^2+x^2)(A+1)}{2(A\epsilon_3-xy)+(y^2+x^2)(A+1)} - \log\frac{2(A+xy)+(y^2+x^2)(A+1)}{2(A-xy)+(y^2+x^2)(A+1)}. \quad (6)$$

The mass number $A$ is given by the ratio $m_\beta/m_\alpha$. The plus and minus signs in Eq. (3) and (4) refer to virtual and bound two-body subsystems, respectively.

In the present context that we have three particle systems with two identical ones, it is worthwhile to call the attention to two particular definitions of three-body quantum halo states: the *Borromean* states [19], where all the two-body subsystems are virtual $(\alpha-\alpha-\beta)$, and the *tango* states [20], where the $\alpha-\beta$ subsystems are virtual and $\alpha\alpha$ is bound $(\alpha\alpha-\beta)$. Note that the virtual pair of particles is denoted with a dash between the symbols. The Borromean case corresponds to positive signs in front of the square-root energy of the subsystems in both Eqs. (3) and (4), implying in the weakest attractive kernel of Eqs. (1) and (2) among all the possibilities of signs in the two-body scattering amplitude, and, for the tango three-body system, we have negative sign only in front of $\sqrt{\epsilon_{\alpha\alpha}}$ in Eq. (3), with positive sign in front of $\sqrt{\epsilon_{\alpha\beta}}$ in Eq. (4). So, a more effective attraction occurs in a tango state than in a Borromean case. Of course, if all the two-body subsystems are bound, the effective attraction is maximized, and, if all such subsystems are unbound (virtual), the effective attraction is minimized.

One can extend the classification scheme of three-body quantum halo states of the type $\alpha\alpha\beta$ [21], considering the four possibilities, for increasing values of the magnitude of the effective attraction in Eqs. (1) and (2). The weakest attractive situation corresponds to the previous defined Borromean-type (only virtual subsystems) $(\alpha-\alpha-\beta)$. The tango situation $(\alpha\alpha-\beta)$ is followed by a three-body system with $\alpha-\alpha$ virtual and $\alpha\beta$ bound, which we represent by $(\alpha\beta\alpha)$ halo system. Three-body system with the strongest effective attraction has all the subsystems bound and is represented by $(\alpha\alpha\beta)$.

We solve Eqs. (1)–(6) in units such that the three-body subtraction point $\mu_{(3)}$ is equal to 1 [18]. The corresponding dimensionless quantities are $\epsilon_3 \equiv E_3/\mu_{(3)}^2$, $\epsilon_{\alpha\alpha} \equiv E_{\alpha\alpha}/\mu_{(3)}^2$, $\epsilon_{\alpha\beta} \equiv E_{\alpha\beta}/\mu_{(3)}^2$. The three-body physical quantities can be written in terms of the three-body binding energy $E_3$ when first the value of $\mu_{(3)}^2$ is determined from the known value of $E_3$. Therefore, the results for the renormalized model appear

when the subtraction point energy is written as a function of $E_3$ and, consequently, the three-body quantities naturally scale with $E_3$. Finally, the scaling functions are obtained when the dimensionless product of physical quantities are written as a function of the ratios between two-body energies and $E_3$.

### B. Scaling functions for the radii

The existence of a three-body scale implies in the low-energy universality found in three-body systems, or correlations between three-body observables [13,22]. In the scaling limit [14,18], one has

$$\mathcal{O}(E,E_3,E_{\alpha\alpha},E_{\alpha\beta})(E_3)^{-\eta} = \mathcal{A}(\sqrt{E/E_3},\sqrt{E_{\alpha\alpha}/E_3},\sqrt{E_{\alpha\beta}/E_3},A), \quad (7)$$

where $\mathcal{O}$ is a general observable of the three-body system at energy $E$, with dimension of energy to the power $\eta$. In the present paper we discuss only the situation that we have only bound subsystems $(\alpha\alpha\beta)$; however, the analysis could be easily extended to other three-body halo systems such as the Borromean, tango, and $(\alpha\beta\alpha)$ systems.

In the case of the mean-square separation distances, $\langle r_\gamma^2\rangle$ with $\gamma=\alpha$ or $\beta$, i.e, the distance of the atom $\gamma$ to the c.m., and $\langle r_{\alpha\gamma}^2\rangle$, i.e, the distance between the atoms $\alpha$ and $\gamma$, the scaling functions are of the form

$$\sqrt{\langle r_\gamma^2\rangle S_3}=\mathcal{R}_\gamma(\sqrt{\epsilon_{\alpha\alpha}/\epsilon_3},\sqrt{\epsilon_{\alpha\beta}/\epsilon_3},A) \quad (8)$$

and

$$\sqrt{\langle r_{\alpha\gamma}^2\rangle S_3}=\mathcal{R}_{\alpha\gamma}(\sqrt{\epsilon_{\alpha\alpha}/\epsilon_3},\sqrt{\epsilon_{\alpha\beta}/\epsilon_3},A), \quad (9)$$

where $S_3$ is the smallest separation energy of the three-body system, i.e., $S_3=\min(E_3-E_{\alpha\alpha},E_3-E_{\alpha\beta})$. Two particular situations are worth mentioning, one is the case of trimer systems $(A=1)$, where the above scaling functions above reduce to

$$\sqrt{\langle r_\gamma^2\rangle S_3}=\mathcal{R}_\gamma(\sqrt{\epsilon_2/\epsilon_3}) \quad (10)$$

and

$$\sqrt{\langle r_{\alpha\alpha}^2\rangle S_3}=\mathcal{R}_{\alpha\gamma}(\sqrt{\epsilon_2/\epsilon_3}). \quad (11)$$

The other special situation is found for $\epsilon_{\alpha\gamma}=0$ where the dimensionless product of the square radii and triatomic binding energy depend only on the mass ratio:

$$\sqrt{\langle r_\gamma^2\rangle E_3}=\mathcal{R}_\gamma(A) \quad (12)$$

and

$$\sqrt{\langle r_{\alpha\gamma}^2\rangle E_3}=\mathcal{R}_{\alpha\gamma}(A). \quad (13)$$

### C. Form factors

The mean-square radii are calculated from the derivative of the Fourier transform of the respective matter density with respect to the square of the momentum transfer. The Fourier transform of the one- and two-body densities define the respective form factors, $F_\beta(q^2)$ and $F_{\alpha\gamma}(q^2)$, as a function of the dimensionless momentum transfer $\vec{q}$. For the mean-square radius of the particle $\gamma$ $(=\alpha$ or $\beta)$ to c.m., we have

$$\langle r_\gamma^2\rangle=-6\left(1-\frac{m_\gamma}{2m_\alpha+m_\beta}\right)^2\left|\frac{dF_\gamma(q^2)}{dq^2}\right|_{q^2=0}, \quad (14)$$

where

$$F_\alpha(q^2)=\int d^3y\,d^3z\,\Psi_{\alpha\beta}\left(\vec{y}+\frac{\vec{q}}{2},\vec{z}\right)\Psi_{\alpha\beta}\left(\vec{y}-\frac{\vec{q}}{2},\vec{z}\right),$$
$$F_\beta(q^2)=\int d^3y\,d^3z\,\Psi_{\alpha\alpha}\left(\vec{y}+\frac{\vec{q}}{2},\vec{z}\right)\Psi_{\alpha\alpha}\left(\vec{y}-\frac{\vec{q}}{2},\vec{z}\right). \quad (15)$$

For the mean-square distance between the particles $\alpha$ and $\gamma$, we have

$$\langle r_{\alpha\gamma}^2\rangle=-6\left|\frac{dF_{\alpha\gamma}(q^2)}{dq^2}\right|_{q^2=0}, \quad (16)$$

where

$$F_{\alpha\gamma}(q^2)=\int d^3y\,d^3z\,\Psi_{\alpha\gamma}\left(\vec{y},\vec{z}+\frac{\vec{q}}{2}\right)\Psi_{\alpha\gamma}\left(\vec{y},\vec{z}-\frac{\vec{q}}{2}\right). \quad (17)$$

The above triatomic wave functions in momentum space are given in terms of the spectator functions $\chi_{\alpha\gamma}$:

$$\Psi_{\alpha\alpha}(\vec{y},\vec{z})=\left(\frac{1}{\epsilon_3+\frac{A+2}{4A}\vec{y}^2+\vec{z}^2}-\frac{1}{1+\frac{A+2}{4A}\vec{y}^2+\vec{z}^2}\right)\times\left[\chi_{\alpha\alpha}(|\vec{y}|)+\chi_{\alpha\beta}\left(\left|\vec{z}-\frac{\vec{y}}{2}\right|\right)+\chi_{\alpha\beta}\left(\left|\vec{z}+\frac{\vec{y}}{2}\right|\right)\right], \quad (18)$$

$$\Psi_{\alpha\beta}(\vec{y},\vec{z})=\left(\frac{1}{\epsilon_3+\frac{A+1}{2A}\vec{z}^2+\frac{A+2}{2(A+1)}\vec{y}^2}-\frac{1}{1+\frac{A+1}{2A}\vec{z}^2+\frac{A+2}{2(A+1)}\vec{y}^2}\right)\times\left[\chi_{\alpha\alpha}\left(\left|\vec{z}-\frac{A\vec{y}}{A+1}\right|\right)+\chi_{\alpha\beta}(|\vec{y}|)+\chi_{\alpha\beta}\left(\left|\vec{z}+\frac{\vec{y}}{A+1}\right|\right)\right],$$

where $\vec{z}$ is the relative momentum of the pair and $\vec{y}$ is the relative momentum of the spectator particle to the pair in units of $\mu_{(3)}=1$. Note that the subindices of $\Psi$ in Eq. (18)

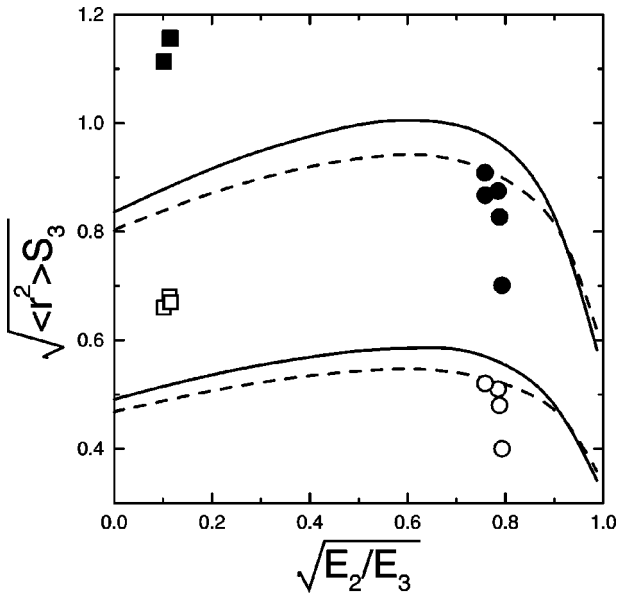


FIG. 1. The dimensionless products $\sqrt{\langle r_\alpha^2\rangle S_3}$ (lower curves) and $\sqrt{\langle r_{\alpha\alpha}^2\rangle S_3}$ (upper curves) as functions of $\sqrt{E_2/E_3}$. Our results for the ground state and first excited state are shown, respectively, by solid and dashed lines. Realistic calculations from Ref. [11], for $\sqrt{\langle r_\alpha^2\rangle S_3}$, are given by empty squares (ground state) and empty circles (excited state), and, for $\sqrt{\langle r_{\alpha\alpha}^2\rangle S_3}$, by full squares (ground state) and full circles (excited state).

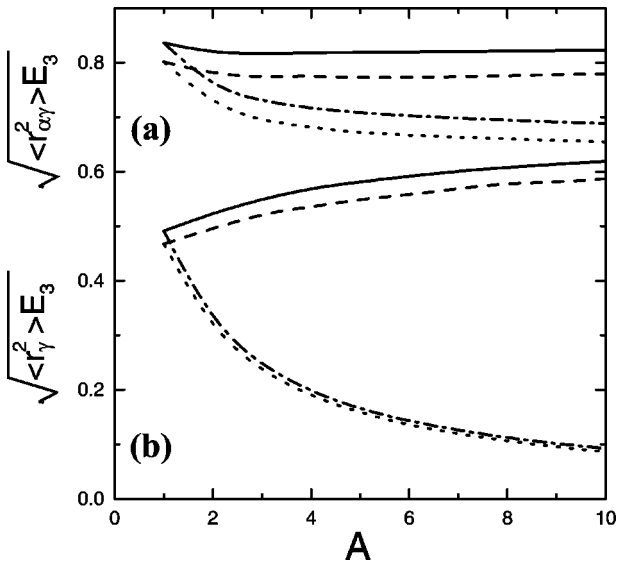


FIG. 2. For the triatomic $\alpha\alpha\beta$ system, with $\gamma\equiv\alpha$, $\beta$, it is shown the dimensionless products $\sqrt{\langle r_{\alpha\gamma}^2\rangle E_3}$ [upper (a) plots] and $\sqrt{\langle r_\gamma^2\rangle E_3}$ [lower (b) plots], as functions of $A\equiv m_\beta/m_\alpha$, in the limit $E_{\alpha\alpha}=E_{\alpha\beta}=0$. $\sqrt{\langle r_\gamma^2\rangle}$ is the root-mean-square distance of particle $\gamma$ from the center of mass, and $\sqrt{\langle r_{\alpha\gamma}^2\rangle}$ is the root-mean-square distance between the particles $\alpha$ and $\gamma$. The results for the ground state ($N=0$) are shown by the solid line ($\gamma=\alpha$) and dot-dashed line ($\gamma=\beta$), and, for the excited state ($N=1$), by the dashed line ($\gamma=\alpha$) and dotted line ($\gamma=\beta$).

just denote the pair of Jacobi relative momenta used to evaluate the wave function. For $\alpha\gamma$ with $\gamma=\alpha$ or $\beta$, one has the relative momentum between $\alpha$ and $\gamma$ and the relative momentum of the third particle to the center of mass of the system $\alpha\gamma$.

### III. RESULTS FOR TRIATOMIC RADII

Our analysis has considered some particular three-body molecular systems, in which the three-body ground-state energy and the corresponding energies of the two-body subsystem are known theoretically for $^4$He trimer [11], $^4$He$_2-^6$Li, $^4$He$_2-^7$Li, and $^4$He$_2-^{23}$Na [23]. In Ref. [11], the authors have considered realistic two-body interactions; their results for the ground and excited state radii are appropriate for our purpose of comparing with the present scaling approach.

The ground and excited Efimov state energies of the $^4$He$_3$ molecule were extensively studied in the scaling approach of Refs. [15,18], with the results that are in very good agreement with realistic calculations. This leads us to conclude that other details (beyond the dimer and trimer ground-state energies) presented in the realistic interactions, which have been used, are quite irrelevant to the existence of Efimov states. These features validates a universal scaling function, relating the trimer ground state, the dimer, and the weakly bound excited three-body energy state. Realistic calculations for the excited states of $^4$He trimer approaches reasonably well the scaling limit [15,18], which suggests to investigate the scaling limit of other observables such as the different radii defined in Eqs. (14) and (16). The conditions for the validity of the present approach are that the atoms should have a very shallow and short-ranged two-body interaction and the binding energy close to 0, i.e., the ratio between the interaction range and dimer size should be much smaller than 1. These are indeed the cases we are considering.

The results for the radii of $^4$He$_3$ molecule in the ground and excited states are shown in Fig. 1, in the form of a scaling plot. The dimensionless products $\sqrt{\langle r_\alpha^2\rangle S_3}$ and $\sqrt{\langle r_{\alpha\alpha}^2\rangle S_3}$ as functions of $\sqrt{E_2/E_3}$ are shown in the figure and compared to the realistic calculations, obtained from Ref. [11]. Our calculations for the ground and excited states are practically the same, which would be the case if the energies with respect to $\mu^2$ are, in fact, going to 0, i.e., the scaling limit. The results for $\sqrt{\langle r_\alpha^2\rangle S_3}$ and $\sqrt{\langle r_{\alpha\alpha}^2\rangle S_3}$ for the excited state are in good agreement with the realistic result. However, for the ground state the results show a deviation of about 20%. The excited state size is about ten times larger than the corresponding size of the ground state. Therefore, the scaling limit is better approached in the excited state, which is much larger than the interaction range, which is not strictly valid for the ground state, and consequently deviations in the scaling plot are stronger for this state.

In Fig. 2, the results for the dimensionless products $\sqrt{\langle r_{\alpha\alpha}^2\rangle E_3}$, $\sqrt{\langle r_{\alpha\beta}^2\rangle E_3}$, and $\sqrt{\langle r_\gamma^2\rangle E_3}$, as functions of $A=m_\beta/m_\alpha$, for $E_{\alpha\alpha}=E_{\alpha\beta}=0$ are shown. We perform calculations for the ground ($N=0$) and excited ($N=1$) states, as indicated in the figure. One observes in the upper frame of Fig. 2 that the results almost saturate above $A\approx 3$ to the values found in the limit of $A=\infty$. The calculations for $A=\infty$ give for $\langle r_{\alpha\alpha}^2\rangle$ the values of $0.69/E_3$ for $N=0$ and

TABLE I. Results for different radii of the molecular systems $\alpha\alpha\beta$, where $\alpha \equiv {}^4$He and $\beta$ is identified in the first column. The ground-state energies of the triatomic molecules and the corresponding energies of the diatomic subsystems, obtained from Ref. [23], are given in the second, third, and fourth columns. $\langle r_{\alpha\gamma}^2 \rangle$ is the corresponding mean-square distance between the particles $\alpha$ and $\gamma$ $(=\alpha,\beta)$. $\langle r_\gamma^2 \rangle$ is the mean-square distance of $\gamma$ from the trimer center of mass.

| $\beta$ | $E_3^{(0)}$ (mK) | $E_{\alpha\alpha}$ (mK) | $E_{\alpha\beta}$ (mK) | $\sqrt{\langle r_{\alpha\alpha}^2 \rangle}$ (Å) | $\sqrt{\langle r_{\alpha\beta}^2 \rangle}$ (Å) | $\sqrt{\langle r_\alpha^2 \rangle}$ (Å) | $\sqrt{\langle r_\beta^2 \rangle}$ (Å) |
|---|---|---|---|---|---|---|---|
| $^4$He | 106.0 | 1.31 | 1.31 | 9.45 | 9.45 | 5.55 | 5.55 |
| $^6$Li | 31.4 | 1.31 | 0.12 | 16.91 | 16.38 | 10.50 | 8.14 |
| $^7$Li | 45.7 | 1.31 | 2.16 | 14.94 | 13.88 | 9.34 | 6.31 |
| $^{23}$Na | 103.1 | 1.31 | 28.98 | 11.66 | 9.54 | 8.12 | 1.94 |

$0.61/E_3$ for $N=1$. Therefore, for the ground state, the root-mean-square distance between two $^4$He in the triatomic molecules can be estimated by $0.83\sqrt{\hbar^2/(E_3 m_{^4\mathrm{He}})}$, in the limit of zero pairwise binding energy. Our results for $\langle r_{\alpha\beta}^2 \rangle$ are $0.45/E_3$ for $N=0$ and $0.40/E_3$ for $N=1$. The saturation value for $\sqrt{\langle r_{\alpha\alpha}^2 \rangle E_3}$ is achieved fast with increasing $A$ than for $\sqrt{\langle r_{\alpha\beta}^2 \rangle E_3}$, which depends on the difference in the masses of the atomic pair. The mean-square distance of one of the atoms $\gamma$ $(=\alpha$ or $\beta)$ to the center of mass of the molecule can be obtained from the lower frame of Fig. 2, where we plot $\sqrt{\langle r_\gamma^2 \rangle E_3}$ as a function of $A$. One sees that, for the infinitely heavy $\beta$ atom, the results for $\langle r_\alpha^2 \rangle$ are the same as for $\langle r_{\alpha\beta}^2 \rangle$, while $\sqrt{\langle r_\beta^2 \rangle E_3}=0$, as the heavy particle should rest in the c.m. of the molecule in this limit. We remind the reader that the ratio between the binding energies for $N=0$ and $N=1$ is about 500 for $A=1$ [9] and 300 for $A=10$, while the dimensionless products of square radius and energy change only around 10%.

In the above, we have considered examples of molecules with two helium atoms. However, our results presented in Figs. 1 and 2 are more general, such that we can extend the estimates to other atomic systems. Of particular interest is the analysis of possible formation of molecular systems in experiments with ultracold trapped gases. By considering, for example, the estimates of trimer energies obtained from the recombination coefficient, given in Ref. [10], within our approach we can predict the corresponding trimer sizes. In this case, we have $\alpha=\beta$ and $A=1$ in the previous equations and in the figures. However, our unit for a specific trimer of an atom with $A$ nucleons will be $\hbar^2/m_A=(48.48/A)$ K Å$^2$.

In Table I, we present our results for the different radii of the ground state $(N=0)$ of the weakly bound molecular systems $\alpha\alpha\beta$, where $\alpha \equiv {}^4$He and $\beta={}^4$He, $^6$Li, $^7$Li, and $^{23}$Na, obtained from the known theoretical values of $E_3^{(0)}$, $E_{\alpha\alpha}$, and $E_{\alpha\beta}$ [23]. Our calculation for $^4\mathrm{He}_3$ of $\sqrt{\langle r_{\alpha\alpha}^2 \rangle}$ gives 9.45 Å, which is 14% of the value 11 Å obtained in the realistic variational calculations of Ref. [11]. The same quality of agreement is found for $\sqrt{\langle r_\alpha^2 \rangle}$, which in our calculation is 5.55 Å compared to 6.4 Å of Ref. [11]. The quality of the reproduction of the realistic results by our calculations are quite surprising in view of the simplicity of the present approach, where the only physical inputs are the values of the dimer and trimer binding energies. The several different radii of the molecules $^4\mathrm{He}_2$-$^6$Li, $^4\mathrm{He}_2$-$^7$Li, and $^4\mathrm{He}_2$-$^{23}$Na have values larger than those found in the $^4\mathrm{He}_3$, which makes plausible that our predictions are even better in quality.

TABLE II. Results for the size of trimer systems predicted in Ref. [10]. The sizes are given by $\sqrt{\langle r_\alpha^2 \rangle}$, the root-mean-square distance between the atom $\alpha$ and the center of mass of the trimer system. The atoms of the trimer are identified in the first column. For each dimer energy, given in the second column, we have two possible trimer energies (columns 3 and 5), with the corresponding radii given in columns 4 and 6.

| Atom | $E_2$ (mK) | $E_3$ (mK) | $\sqrt{\langle r_\alpha^2 \rangle}$ (Å) | $E_3'$ (mK) | $\sqrt{\langle r_\alpha^2 \rangle'}$ (Å) |
|---|---|---|---|---|---|
| $^{23}$Na$\vert 1,-1\rangle$ | 2.85 | 7.75 | 12 | 3.06 | 38 |
| $^{87}$Rb$\vert 1,-1\rangle$ [a] | 0.17 | 0.56 | 22 | 0.175 | 114 |
| $^{87}$Rb$\vert 1,-1\rangle$ [b] | 0.17 | 0.47 | 25 | 0.183 | 91 |
| $^{85}$Rb$\vert 2,-2\rangle$ | $1.3\times10^{-4}$ | $2.4\times10^{-4}$ | 1293 | $1.7\times10^{-4}$ | 1944 |

[a]The trimer estimates, given in Ref. [10], for $^{87}$Rb$\vert 1,-1\rangle$, are for noncondensed trapped atoms.

[b]The trimer estimates, given in Ref. [10], for $^{87}$Rb$\vert 1,-1\rangle$, are for condensed trapped atoms.

We point out that the results in Table I for the $^4$He dimer sizes inside the molecules shrink with respect to the free value of 52 Å, due to the large values of the trimer binding energies. Qualitatively this is explained just by considering that the dimer size scales roughly with the inverse of the square-root of its binding energy inside the molecule, which can be estimated to be two-thirds of the molecule binding, from which one finds for that the dimer has sizes around 10 Å, close to that we have found in Table I.

In Table II, we are also presenting results for different radii of the trimers predicted in Ref. [10], from where we obtain the energy of the dimer and the most weakly bound trimer energies of $^{23}$Na$\vert F=1,m_F=-1\rangle$, $^{87}$Rb$\vert F=1,m_F=-1\rangle$, and $^{85}$Rb$\vert F=2,m_F=-2\rangle$, where $\vert F,m_F\rangle$ is the respective hyperfine states of the total spin $F$. We are presenting the mean-square distance from each atom to the center of mass of the corresponding trimer. From Fig. 1, one can also obtain the corresponding mean-square distance between the atoms. We observe that one value of the recombination rate is consistent with two values of the most weakly bound trimer energy, as discussed in Ref. [10]. Therefore, we present two possible values for the radii that are consistent with the corresponding weakly bound trimer energies. Actually, we should also mention that, in a trap, one can achieve dimer and trimer molecules with very large sizes, following the possibility to alter the corresponding two-body scattering length [5].

Finally, it is interesting to recall the results for the hyperradius calculations obtained by Jensen and collaborators [21]. From their scaling plot, one can observe that the hyperradius of a tango system is bigger than the hyperradius of a Borromean system, for the same three-body energy. This point can become very clear, for instance, if we take as an example the results shown for the ${}^3_\Lambda H$ (filled circles in Fig. 2

of Ref. [21]) and estimate the dimensionless product of observables, $\langle \rho^2 \rangle mB/\hbar^2$ (product of the $x$ axis and $y$ axis in Fig. 2 of Ref. [21], where $\rho$ is the hyperradius and $B$ is the three-body binding energy). When going from the tango to the Borromean configuration, this product will decrease. Therefore, if one keeps the same binding energy, the Borromean system would be more compact than the tango system. Extending this analysis to $(\alpha\beta\alpha)$ halos, where $(\alpha - \alpha)$ is virtual and $(\alpha\beta)$ is bound, and also to all-bound pairs $(\alpha\alpha\beta)$, one should expect that the sizes increase when going from the Borromean states to halos with all-bound subsystems, while keeping the three-body energy fixed. Within our approach, the scaling relations are expected to be followed in all the cases, in the limit of a zero-range interaction. The Borromean halo (the less attractive system), in order to have the same three-body energy as a tango state, should be more compact in agreement with the scaling plot of Ref. [21]. In a realistic case, our scheme is expected to produce better results in the all-bound case, when comparing systems with the same three-body energies. This occurs because the all-bound case would have the most extended wave function; consequently, the range of the potential, in relation to the size, would have the smallest value, satisfying better the validity condition for the scaling relations, which is that the interaction range must be small compared to particle distances.

## IV. CONCLUSIONS

The mean-square radii of the triatomic molecules $^4He_3$, $^4He_2-^6Li$, $^4He_2-^7Li$, and $^4He_2-^{23}Na$ are calculated using a renormalized three-body model with a pairwise Dirac-$\delta$ interaction, having as physical inputs only the values of the binding energies of the diatomic and triatomic molecules. Presently, we have considered molecular three-body systems with bound subsystems, due to the available data. The renormalized zero-range model can also be applied to the cases where at least one of the subsystems is virtual. When comparing systems with the same three-body energies and potential ranges, the validity of the renormalized zero-range model is expected to be better in the all-bound case, because this case corresponds to the most extended wave function.

The validity of the present framework is substantiated by the agreement of our results for the different radii with the realistic potential model calculations of Ref. [11] for $^4He_3$ ground and excited states, which are within about 14%. These results are quite surprising in view of the simplicity of the approach, where only the physical inputs are the values of diatomic and triatomic binding energies. We predicted for the first time, as far as we know, the values of several different radii for $^4He_2-^6Li$, $^4He_2-^7Li$, and $^4He_2-^{23}Na$ molecules, from the theoretical values of the binding energies calculated in Ref. [23]. These other molecules are, in general, larger than the $^4$He-trimer, indicating that our radii predictions for these triatomic ground states can be even better in quality than those found for $^4He_3$.

In view of the actual relevance of ultracold atomic systems that are being experimentally studied, and the possibility to observe the formation of molecular systems in trapped condensates, we also present results for the sizes of rubidium and sodium trimers, considering the binding energies that were recently estimated [10] from the analysis of the corresponding three-body recombination coefficients.

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# Radii in weakly-bound light halo nuclei

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**Abstract**

A systematic study of the root-mean-square distance between the constituents of weakly-bound nuclei consisting of two halo neutrons and a core is performed using a renormalized zero-range model. The radii are obtained from a universal scaling function that depends on the mass ratio of the neutron and the core, as well as on the nature of the subsystems, bound or virtual. Our calculations are qualitatively consistent with recent data for the neutron–neutron root-mean-square distance in the halo of $^{11}$Li and $^{14}$Be nuclei.
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## 1. Introduction

Light exotic-nuclei with one or two weakly bound neutrons in their halo offer the opportunity to study large systems at small nuclear density. (A review on the theoretical approaches and characteristics of halo nuclei can be found in Ref. [1].) The constituents of the halo have a high probability to be found much beyond the interaction range. Then, the concept of a short-range interaction between the particles and its implications are useful in understanding the few-body physics of the halo. The quantum description of such large and weakly bound systems are universal and can be defined by few physical scales despite the range and details of the pairwise interaction [2]. The particular halo-nuclei, with a

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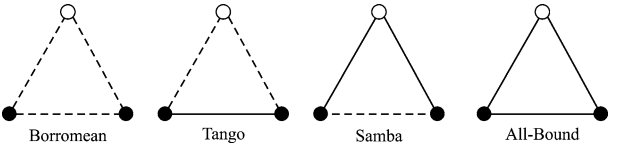


Fig. 1. Diagrammatical representation of the classification scheme for weakly-bound three-body systems. Two-body bound state are represented with solid line, and virtual state with dashed line.

neutron–neutron–core ($n$–$n$–$c$) structure, like $^{6}$He, $^{11}$Li, $^{14}$Be and $^{20}$C, are examples of weakly-bound three-body systems [3], where the above universal aspects can be explored theoretically [4].

In weakly bound three-body systems, when the two-particle $s$-wave scattering lengths have large magnitudes, it is possible the occurrence of excited $s$-wave Efimov states [5]. It was suggested in Ref. [6] that these states could be present in some halo nuclei. This possibility was further investigated and refined in Ref. [4]. A parametric region was determined in which Efimov states can exist. Such region, for a bound three-body system, was defined in a plane given by the two possible (bound or virtual) subsystem energies. The promising candidate to exhibit an excited Efimov state was found to be $^{20}$C [4,7].

A few-body system interacting through a short range force can be parameterized by few physical scales [8]. For a zero-range force in three-space dimensions, it is expected a new physical scale for each new particle added to the system, unless symmetry and/or angular momentum forbids the particles to be near each other. The three-body system in the state of zero total angular momentum, has the bound or virtual subsystems energies and the ground state three-body energy as the dominating physical scales. Any observable can be expressed in terms of the ratios between the physical scales, given by a scaling function, when the scattering length goes to infinity, or the interaction range tends to zero (scaling limit) [9,10]. In that sense the scaling function is an useful tool to study three-body observables and provides a zero order approximation to guide realistic calculations with short-range interactions.

The scaling functions allow one to easily perform systematic studies of various three-body halo-nuclei properties with different types of two-body subsystems as, for example, $^{6}$He, $^{11}$Li, $^{14}$Be and $^{20}$C [11]. A classification scheme proposed for a bound three-body system [12], can be investigated in terms of a scaling function for the different average distances between the constituents of a neutron–neutron–core halo nucleus. The classification of the three-body halo system depends on the kind of the two-body subsystems, bound or virtual.

For the case of two identical particles in the three-body system, we have to consider four possibilities for the two-body subsystems (see Fig. 1): all unbound (*Borromean*); all bound (*All-Bound*); one bound and two unbound (*Tango* [13] configuration); and one unbound with two bound (we suggest a name *Samba* for this configuration). One natural example of halo-nuclei *Samba* system is the $^{20}$C nucleus, which is composed by two-neutrons and a $^{18}$C core. The neutron and $^{18}$C forms the weakly bound state of $^{19}$C [3,14].

In the present work, we study the root-mean-square distances between the constituents of a bound three-body system, where we have two identical particles $n$ and a core named $A$. By $n$ we mean neutron in halo nuclei, but we allow the pair neutron–neutron ($nn$) to be

bound in order to cover all the configurations presented above. We represent the radii in a scaling plot in terms of a dimensionless product, extending to halo nuclei a previous application that was done for molecules [15]. Using these scaling plots we can follow the behavior of the different radii when it happens a transition between one kind of system to another one. Starting from the *Borromean* case (all unbound), we can go to the *Samba* case by increasing the binding energy of the pair $nA$ (keeping $nn$ unbound); and to the *Tango* case by increasing the binding energy of the pair $nn$ (keeping $nA$ unbound). In particular, we calculate the mean square distance between the two neutrons in $^{6}$He, $^{11}$Li and $^{14}$Be (which have been measured recently [16]) from the known bound or virtual energies of the subsystems and the two-neutron separation energy.

The calculation of the scaling function for the different radii of the three-body system is performed with a renormalization scheme applied to three-body equations with $s$-wave zero-range pairwise potential, which makes use of subtracted equations [8,17].

As our approach is restricted to $s$-wave two-body interactions, some limitations in the application of our analysis are expected. The argument has the origin in the fact that, in some cases, the two-body subsystem interaction in $p$-wave is considered to be important for the three-body binding. The examples are $^{6}$He [18], known to be bound by the $p$-wave interaction in $n$–$^{4}$He; and $^{11}$Li, where both $p$- and $s$-waves might be relevant to describe the ground state of the unbound subsystem $^{10}$Li (see discussion and references in [19]). However, as pointed out in Ref. [20] (in a discussion related to $^{11}$Li), one should also noticed that even the three-body wave function with $s$-wave $nn$ correlation produces a ground state of the halo nuclei with two or more shell-model configurations. The effect of the above $s$-wave restriction is also reduced due to the fact that we are considering the experimental energies in our approach, which implicitly are carrying the effect of higher partial waves in the interaction. Another aspect is that the radius are obtained from the tail of the wave-function, which is dominated by the $s$-wave.

The paper is organized as follows. In Section 2, we present our formalism, which contains the subtracted method to treat the Faddeev equations with two identical particles, leading to the form factors from which we obtain the different mean-square radii. We also give a brief discussion of the scaling functions to describe the radii. In Section 3, we discuss the classification scheme. In Section 4, we present our numerical results for the root-mean-square distances between the particles. Our conclusions are summarized in Section 5.

## 2. Formalism

In the next subsection, we consider the formalism given in Refs. [15,17] for coupled channels to calculate the three-body wave functions and the possible different radii with a zero-range pairwise interaction. We solve the homogeneous three-body Faddeev equations for a system with two identical particles $\alpha$ and a third one $\beta$ in a renormalized subtracted form, which allows one to obtain the observables as a function of the two and three-body scales of the system. The corresponding masses of the particles $\alpha$ and $\beta$ are $m_\alpha$ and $m_\beta$.

### 2.1. Subtracted Faddeev equations

Next, we follow the model presented in Refs. [15,17] for the subtracted Faddeev equations, and consider units such that $\hbar = 1$ and $m_\alpha = 1$. For the subtraction energy that is required in the model, we choose $\mu^2_{(3)}$. In this case, all the energies and momentum variables are rescaled to dimensionless variables considering this subtraction energy. After partial wave projection, the $s$-wave coupled subtracted integral equations for the Faddeev spectator functions $\chi_{\alpha\alpha}$ and $\chi_{\alpha\beta}$, are given by:

$$\chi_{\alpha\alpha}(y) = 2\tau_{\alpha\alpha}(y;\epsilon_3)\int_0^\infty dx\frac{x}{y}G_1(y,x;\epsilon_3)\chi_{\alpha\beta}(x), \tag{1}$$

$$\chi_{\alpha\beta}(y) = \tau_{\alpha\beta}(y;\epsilon_3)\int_0^\infty dx\frac{x}{y}\big[G_1(x,y;\epsilon_3)\chi_{\alpha\alpha}(x) + AG_2(y,x;\epsilon_3)\chi_{\alpha\beta}(x)\big], \tag{2}$$

$$\tau_{\alpha\alpha}(y;\epsilon_3) \equiv \frac{1}{\pi}\big[\sqrt{\epsilon_3 + \mathcal{C}_1^A y^2} \mp \sqrt{\epsilon_{\alpha\alpha}}\,\big]^{-1}, \tag{3}$$

$$\tau_{\alpha\beta}(y;\epsilon_3) \equiv \frac{1}{\pi}\frac{(\mathcal{C}_2^A)^{3/2}}{[\sqrt{\epsilon_3 + \mathcal{C}_2^{(A+1)} y^2} \mp \sqrt{\epsilon_{\alpha\beta}}]}, \tag{4}$$

$$G_1(y,x;\epsilon_3) \equiv \log\frac{(\epsilon_3 + x^2 + xy) + \mathcal{C}_2^A y^2}{(\epsilon_3 + x^2 - xy) + \mathcal{C}_2^A y^2} - \log\frac{(1 + x^2 + xy) + \mathcal{C}_2^A y^2}{(1 + x^2 - xy) + \mathcal{C}_2^A y^2}, \tag{5}$$

$$G_2(y,x;\epsilon_3) \equiv \log\frac{(\epsilon_3 + xy/A) + \mathcal{C}_2^A (y^2 + x^2)}{(\epsilon_3 - xy/A) + \mathcal{C}_2^A (y^2 + x^2)} - \log\frac{(1 + xy/A) + \mathcal{C}_2^A (y^2 + x^2)}{(1 - xy/A) + \mathcal{C}_2^A (y^2 + x^2)}, \tag{6}$$

where we are defining the mass ratio and the constant mass factors by

$$A \equiv \frac{m_\beta}{m_\alpha}, \quad \mathcal{C}^A_{j=1,2} \equiv \left(\frac{j}{4} + \frac{1}{2A}\right). \tag{7}$$

The plus and minus signs in Eqs. (3) and (4) refer to virtual and bound two-body subsystems, respectively. In the equations above, the dimensionless three-body energy $\epsilon_3$ and the two-body energies ($\epsilon_{\alpha\alpha}$ and $\epsilon_{\alpha\beta}$), are related to the corresponding physical quantities by $\epsilon_3 \equiv -E_3/\mu^2_{(3)}$, $\epsilon_{\alpha\alpha} \equiv -E_{\alpha\alpha}/\mu^2_{(3)}$, and $\epsilon_{\alpha\beta} \equiv -E_{\alpha\beta}/\mu^2_{(3)}$. The three-body physical quantities can be written in terms of a scaling function, i.e., the dimensionless product of the observable and some power of the three-body binding energy $E_3$, when the value of $\mu^2_{(3)}$ is determined from the known value of $E_3$ and consequently the three-body quantities are naturally a function of $E_3$ and the ratios $E_{\alpha\alpha}/E_3$ and $E_{\alpha\beta}/E_3$. Note that we are using the same symbol $A$ for the mass ratio as well as for the core label, considering that, in a $n$–$n$–core nucleus we have the core consisting of $A$ nucleons and $A$ can also be identified with the mass ratio ($m_\beta = Am_n$, $m_\alpha = m_n$). However, our expression can be generally applied for non-integer values of $A$.

For large scattering lengths, the details of the interaction are unimportant to describe few-body systems, as the short-range informations, beyond the two-body scattering

lengths, are carried out by one typical three-body scale. Therefore, the low-energy observables present a scaling behavior quite universal with the three-body binding energy [8,21]. In the limit of infinite scattering lengths or zero range interactions, the function which represents a given correlation between two three-body observables, written in terms of scaled variables, converges to a single curve, despite the existence of many other Efimov states.

For a three-body system with binding energy $E_3$, in the *scaling limit* [4,17], one general three-body physical observable $\mathcal{O}$, with dimension of energy to the power $\eta$, at a particular energy $E$, can be written as a function $\mathcal{F}$ of the ratios between the two and three-body energies, such that

$$\mathcal{O}(E, E_3, E_{\alpha\alpha}, E_{\alpha\beta}) = (E_3)^{\eta}\mathcal{F}\left(\sqrt{\frac{E}{E_3}}, \pm\sqrt{\frac{E_{\alpha\alpha}}{E_3}}, \pm\sqrt{\frac{E_{\alpha\beta}}{E_3}}, A\right). \tag{8}$$

The two-body energies $E_{\alpha\gamma}$ ($\gamma = \alpha, \beta$), are negative quantities, corresponding to bound or virtual states. The nature of such two-body state, bound or virtual, is revealed in the momentum space, such that we have a bound state when $\sqrt{|E_{\alpha\beta}|}$ is positive and a virtual state when $\sqrt{|E_{\alpha\beta}|}$ is negative. So, in Eq. (8), the signs $+$ or $-$ mean a bound or virtual two-body subsystem, respectively. The different radii of the bound $\alpha\alpha\beta$ system are functions defined from the Eq. (8) with $E = E_3$, which depend on the mass ratio, $A$, the ratios of the two and three-body energies and the kind of subsystem interactions (bound or virtual).

### 2.2. Radii calculation

The Faddeev components of the wave-function for the $\alpha\alpha\beta$ system are written in terms of the spectator functions, obtained from the solution of Eqs. (1) and (2) in momentum space:

$$\begin{aligned}
\Psi_{\alpha\alpha}(\vec{y},\vec{z}) &= \left(\frac{1}{\epsilon_3 + \mathcal{C}_1^A\vec{y}^2 + \vec{z}^2} - \frac{1}{1 + \mathcal{C}_1^A\vec{y}^2 + \vec{z}^2}\right) \\
&\quad\times\left[\chi_{\alpha\alpha}\left(|\vec{y}|\right) + \chi_{\alpha\beta}\left(\left|\vec{z} - \frac{\vec{y}}{2}\right|\right) + \chi_{\alpha\beta}\left(\left|\vec{z} + \frac{\vec{y}}{2}\right|\right)\right], \\
\Psi_{\alpha\beta}(\vec{y},\vec{z}) &= \left(\frac{1}{\epsilon_3 + \mathcal{C}_2^A\vec{z}^2 + \mathcal{C}_2^{A+1}\vec{y}^2} - \frac{1}{1 + \mathcal{C}_2^A\vec{z}^2 + \mathcal{C}_2^{A+1}\vec{y}^2}\right) \\
&\quad\times\left[\chi_{\alpha\alpha}\left(\left|\vec{z} - \frac{A\vec{y}}{A+1}\right|\right) + \chi_{\alpha\beta}\left(|\vec{y}|\right) + \chi_{\alpha\beta}\left(\left|\vec{z} + \frac{\vec{y}}{A+1}\right|\right)\right],
\end{aligned} \tag{9}$$

where $\mathcal{C}_j^A$ is defined in Eq. (7). The Faddeev components are denoted by the sub-indices of the interacting pair. Representing the pair by $\alpha\gamma$ with $\gamma = \alpha$ or $\beta$, one has that $\vec{z}$ is the relative momentum between $\alpha$ and $\gamma$ and $\vec{y}$ is the relative momentum of the third particle to the center-of-mass of the system $\alpha\gamma$. For the halo nuclei the notation is $\alpha = n$ and $\beta$ is the core represented by $A$.

The momentum component of the total wave-function,

$$\Psi_{Ann'} = \Psi_{nn'} + \Psi_{An} + \Psi_{An'}, \tag{10}$$

is symmetrical by the exchange between the neutrons, $n$ and $n'$, while the antisymmetry is given by the singlet spin-component (not explicitly shown). The different mean-square radii are calculated from the derivative of the Fourier transform of the respective matter density in respect to the square of the momentum transfer. The relative mean-square distances between the halo neutrons and between the neutron and the core ($\gamma = n, A$) are obtained from the expression

$$\langle r^2_{n\gamma}\rangle = -6\frac{dF_{n\gamma}(q^2)}{dq^2}\bigg|_{q^2=0}, \tag{11}$$

where

$$F_{n\gamma}(q^2) = \int d^3y\, d^3z\, \Psi_{Ann'}\left(\vec{y}, \vec{z} + \frac{\vec{q}}{2}\right)\Psi_{Ann'}\left(\vec{y}, \vec{z} - \frac{\vec{q}}{2}\right) \tag{12}$$

is the Fourier transform of the two-body densities, which is a function of the momentum transfer $\vec{q}$ (given in units of $\mu_{(3)}$). The relative momentum between $n$ and $\gamma$ is $\vec{z} \pm \vec{q}/2$ and the relative momentum of the third particle to the center-of-mass of $n\gamma$ is $\vec{y}$.

Analogous equations can be found for the mean square distances of the neutron and the core to the center-of-mass system ($\langle r^2\rangle_\gamma$), in terms of the Fourier transform of the one-body density.

### *2.3. Scaling functions for the radii*

The scaling functions for the mean-square separation distances between the particles in the three-body system can be written according to Eq. (8) with $E \equiv E_3$. The scaling functions for the radii are written as:

$$\sqrt{\langle r^2_{n\gamma}\rangle |E_3|} = \mathcal{R}_{n\gamma}\left(\pm\sqrt{\frac{E_{nn}}{E_3}}, \pm\sqrt{\frac{E_{nA}}{E_3}}, A\right), \tag{13}$$

$$\sqrt{\langle r^2_{\gamma}\rangle |E_3|} = \mathcal{R}^{cm}_{\gamma}\left(\pm\sqrt{\frac{E_{nn}}{E_3}}, \pm\sqrt{\frac{E_{nA}}{E_3}}, A\right). \tag{14}$$

To study the different types of three-body systems, the general scaling function for the radii given by Eqs. (13) and (14) will be studied in the configurations of Fig. 1. However, one noticeable situation occurs when the Efimov limit is reached, for which the subsystems energies vanishes, and

$$\sqrt{\langle r^2_{n\gamma}\rangle |E_3|} = \mathcal{R}_{n\gamma}(A), \qquad \sqrt{\langle r^2_{\gamma}\rangle |E_3|} = \mathcal{R}^{cm}_{\gamma}(A), \tag{15}$$

depends only on the mass ratio $A$ ($\gamma = n, A$). Curiously, this configuration contains simultaneously all types shown in Fig. 1.

## 3. Classification scheme: qualitative properties

A discussion of a classification scheme for a bound three-body system, with two identical particles, is given in Ref. [12], according to the nature of the subsystem interactions, which can present a bound or virtual state, as depicted diagrammatically in Fig. 1.

The different possibilities of three-body systems are reflected in the qualitative properties of the dynamics as given by the coupled equations (1) and (2) in terms of the strength of the attractive kernel of these equations. Let us describe all these possibilities. The *Borromean* case corresponds to positive signs in front of the square-root of the energies of the subsystems in both Eqs. (3) and (4). A *Tango* three-body system has a negative sign only in front of $\sqrt{\epsilon_{\alpha\alpha}}$ in Eq. (3), with positive sign in front of $\sqrt{\epsilon_{\alpha\beta}}$ in Eq. (4). For a *Samba* configuration of the three-body system, a minus sign appears multiplying $\sqrt{\epsilon_{\alpha\beta}}$ in Eq. (4), while a plus sign multiplies $\sqrt{\epsilon_{\alpha\alpha}}$ in Eq. (3). The All-Bound system has negative signs in Eqs. (3) and (4). As a consequence of the differences in Eqs. (3) and (4), the weakest attractive kernel in Eqs. (1) and (2) is given by a *Borromean* three-body system, followed by the *Tango*, *Samba* and *All-Bound* systems. Therefore, once fixed a three-body binding energy, the system for which the kernel presents the weakest attraction will have the smallest configuration. So, the size of the corresponding system will increase in the following order: *Borromean*, *Tango*, *Samba* and *All-Bound*. The *All-Bound* configuration has the biggest size among all, for a given three-body binding energy. One of course has to remind that the sizes are expected to increase when the binding energy hits one scattering threshold. Therefore, for nonvanishing three-body binding energy this situation does not happen only in the *Borromean* case. In this sense, it is physically sensible that the *Borromean* case corresponds to the smallest configuration size. This observation will be explored in our numerical calculations. In this respect, we are showing the quantitative detailed implication to the different radii of weakly-bound three-body systems of the classification scheme proposed in Ref. [12].

## 4. Numerical results for the radii: scaling plots

We present numerical results for the different possible radii for *Borromean*, *Tango*, *Samba* and *All-Bound* three-body configurations obtained from the wave-function, Eq. (10) derived from the solution of Eqs. (1) and (2). In particular, we give results for the neutron–neutron ($nn$) average distance in the three-body halo nuclei, $^{6}$He, $^{11}$Li, $^{14}$Be, $^{20}$C.

It is interesting to present results in a general scaled form in terms of scaled two-body binding energies and mass ratio, as given by Eqs. (13) and (14), which turns to be useful for the prediction of the several radii in different situations for weakly bound molecules up to light halo-nuclei. Our calculations present results independent on the detailed form of the interactions in a weakly bound three-body system. It means that they apply very well to halo nuclei and weakly bound molecules. The present approach is valid as long as the interactions within the three-body system are of short range while the two-body energies are close to zero, i.e., the ratio between the interaction range and the modulus of the scattering lengths should be somewhat less than 1. These are indeed the cases we are

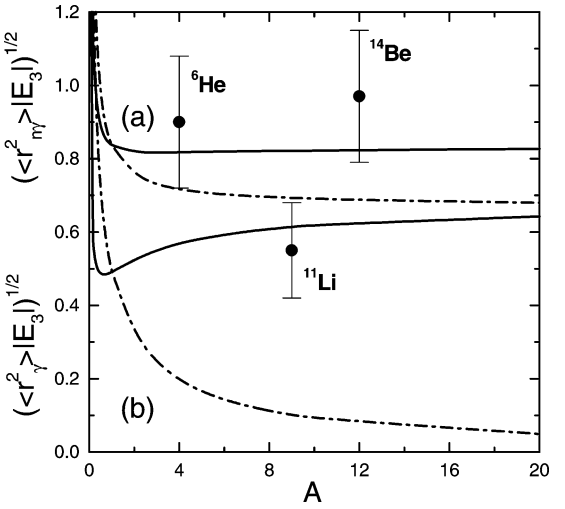


Fig. 2. Dimensionless products $\sqrt{\langle r^2_{n\gamma}\rangle|E_3|}$ and $\sqrt{\langle r^2_{\gamma}\rangle|E_3|}$ ($\gamma = n, A$) as a function of $A$ for zero two-body energies. Results for: (a) $\sqrt{\langle r^2_{nn}\rangle|E_3|}$ (upper solid line) and $\sqrt{\langle r^2_{nA}\rangle|E_3|}$ (upper dot-dashed line); (b) $\sqrt{\langle r^2_{n}\rangle|E_3|}$ (lower solid curve) and $\sqrt{\langle r^2_{A}\rangle|E_3|}$ (lower dot-dashed curve). The experimental data, obtained from [16], are for $\sqrt{\langle r^2_{nn}\rangle|E_3|}$.

considering. We present results only for the ground state of the three-body system. We have shown that the scaling function for the radii is indeed approached even for a calculation of the ground state in our subtraction scheme [15], which will be enough for our purpose.

In Fig. 2, we show the results of the scaling function for the mean square distances, $\sqrt{\langle r^2_{n\gamma}\rangle}$ and $\sqrt{\langle r^2_{\gamma}\rangle}$ with $\gamma = n$ or $A$ (see Eq. (15)) which are shown as a function of $A$ for $E_{n\gamma} = 0$. The comparison with experimental results of $\sqrt{\langle r^2_{nn}\rangle}$ [16], for the $^{6}$He, $^{14}$Be and $^{11}$Li is just for illustrative purpose, considering the hypothetical cases that $^{5}$He, $^{13}$Be and $^{10}$Li would have virtual states close to zero energy. Such hypothesis is more realistic in case of $^{14}$Be, while for the $^{6}$He and $^{11}$Li are not so. As shown by our results for $^{11}$Li, given in Table 1, the assumption of a virtual state with energy close to zero ($|E_{nA}| \lesssim 0.05$ MeV [20]) for $^{10}$Li lead to an average $nn$ separation distance (in the halo of $^{11}$Li) not compatible with the corresponding experimental result. Given that it is well documented the difficulty in studying the $^{10}$Li [19], we can consider $\sqrt{\langle r^2_{nn}\rangle}$ [16] as one of our inputs to predict the virtual state of the $n$–$^{9}$Li system. In this case, we conclude that it cannot be smaller than $\sim 0.1$ MeV.

In this case ($E_{n\gamma} = 0$) the only physical scale is $E_3$ and the scaling plots will depend solely on $A$. The average separation distance between the neutrons and the neutron–core tends naturally to a constant for large $A$, while it diverges for $A$ tending towards zero. The reason for the unbound increase of the products $\langle r^2_{nn}\rangle|E_3|$ and $\langle r^2_{nA}\rangle|E_3|$ for small $A$ is due to the average momentum of the core which tends to zero ($\sim \sqrt{A|E_3|}$) extending the

Table 1
Results of the neutron–neutron root-mean-square radii in halo nuclei. The cores ($A$) are given in the first column, the absolute values of the three-body ground state energies $E_3$ are given in the second column. For $-E_3$, which is equal to the two-neutron separation energy $S(2n)$, we consider the center value of the corresponding energies given in Ref. [3], except for lithium. In case of lithium we consider for $-E_3$ the maximum (0.32 MeV) and the center value (0.29 MeV) given in Ref. [22]. In the third column we give our input values for $-E_{nA}$, considering several values, covering the values suggested in the literature (the references are given together with the corresponding number). For bound two-body subsystem $nA$, we have $-E_{nA}$ equal to the one-neutron separation energy $S(n)$. The virtual states are indicated by (v), and the $nn$ virtual state energy is taken as $-143$ keV. The experimental values, in the last column, are obtained from Marqués et al. (2000) [16].

| Core ($A$) | $-E_3$ (MeV) | $-E_{nA}$ (MeV) | $\sqrt{\langle r_{nn}^2\rangle}$ (fm) | $\sqrt{\langle r_{nn}^2\rangle}_{\rm exp}$ (fm) |
|---|---|---|---|---|
| $^4$He | 0.973 | 0 (v) | 5.1 | |
| | | 0.3 (v) | 4.6 | 5.9±1.2 |
| | | 4.0 [23] (v) | 3.6 | |
| $^9$Li | 0.32 | 0 (v) | 9.2 | 6.6±1.5 |
| | | 0.8 [24] (v) | 5.9 | |
| $^9$Li | 0.29 | 0 (v) | 9.7 | |
| | | 0.05 [20,25,26] (v) | 8.5 | 6.6±1.5 |
| | | 0.8 [24] (v) | 6.7 | |
| $^{12}$Be | 1.337 | 0 (v) | 4.6 | 5.4±1.0 |
| | | 0.2[27] (v) | 4.2 | |
| $^{18}$C | 3.50 | 0.16 [3] | 3.0 | – |
| | | 0.53 [14] | 4.4 | – |

system to infinity. We have checked that the results shown in Fig. 2 tends to finite values after multiplication by $\sqrt{A}$ (one has to remember that we are using units of $m_n = 1$).

The average distance of the neutron to the center of mass system tends to become the relative distance to the core, when the core mass grows to infinity. This fact is clearly seen in Fig. 2 with the lower solid line approaching the upper dot-dashed one when $A \gtrsim 10$. Also, one sees that the core distance to the center of mass vanishes with growing $A$ as it should be.

In Figs. 3–6, we show results for $\sqrt{\langle r_{nn}^2\rangle |E_3|}$ and $\sqrt{\langle r_{nA}^2\rangle |E_3|}$, when one of the subsystem energies is fixed in respect to the three-body binding energy, while the other one varies. We use values of $A$ equal to 0.1, 1 and 200. The subsystems can be bound or virtual and therefore all configurations are covered, i.e., we show results for *Borromean*, *Tango*, *Samba* and *All-Bound*-type systems. Anticipating the presentation of these figures, in general we find that, the radii increase in the following order *Borromean*, *Tango*, *Samba* and *All-Bound* for a given three-body energy and fixed $A$. In our analysis below, we fix either $E_{nn}/E_3 = 0.1$ or $E_{nA}/E_3 = 0.1$ which can correspond to bound or virtual subsystem energies. In the next, we also consider the definitions $E_{nA}/E_3 \equiv K_{nA}^2$ and $E_{nn}/E_3 \equiv K_{nn}^2$ (for both bound or virtual-state energies), such that

$$K_{nA} = \pm\sqrt{E_{nA}/E_3} \quad \text{and} \quad K_{nn} = \pm\sqrt{E_{nn}/E_3}. \tag{16}$$

The $+$ $(-)$ sign refers to bound (virtual) state. One should also note that, the dimensionless quantities $K_{nn}$ and $K_{nA}$ are directly related to poles in the imaginary axis of the respective two-body momentum space.

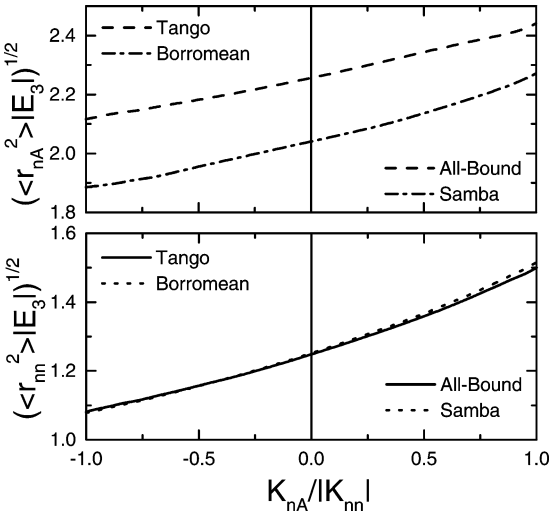


Fig. 3. Dimensionless products $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ (upper frame) and $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ (lower frame) for $A = 0.1$ and $E_{nn}/E_3 = K_{nn}^2 = 0.1$ as a function of $K_{nA}/|K_{nn}|$. In the upper frame, a bound $nn$ pair is represented with dashed line; and a virtual $nn$ pair with dot-dashed line. In the lower frame, a bound $nn$ pair is represented with solid line; and a virtual $nn$ pair with dotted line. The transition between the configurations occurs when $K_{nA} = 0$ (represented by the vertical line).

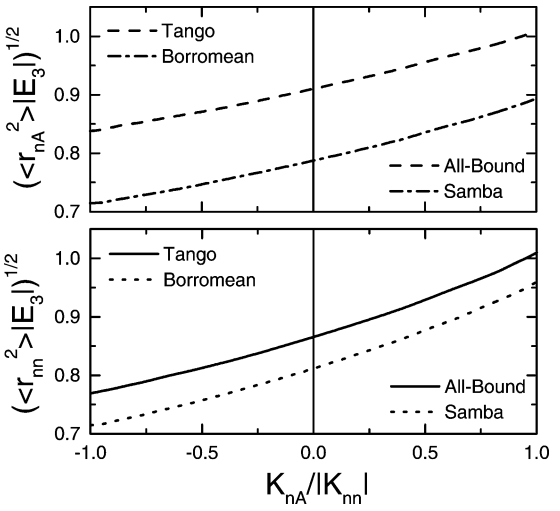


Fig. 4. Dimensionless products $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ (upper frame) and $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ (lower frame) for $A = 1$ and $K_{nn}^2 = 0.1$ as a function of $K_{nA}/|K_{nn}|$. The convention of the lines is the same as given in Fig. 3.

In Fig. 3, we present calculations of the $nA$ and $nn$ root-mean-square radius as functions of $K_{nA}/|K_{nn}|$. Such average radius, multiplied by $\sqrt{|E_3|}$, are scaled to dimensionless quantities. We consider $A = 0.1$ and $E_{nn}/E_3 = 0.1$ fixed, corresponding to bound ($K_{nn} =$

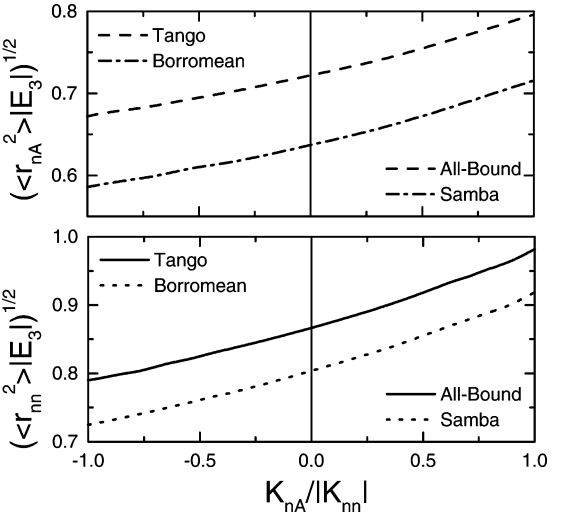


Fig. 5. Dimensionless products $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ (upper frame) and $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ (lower frame) for $A = 200$ and $E_{nn}/E_3 = 0.1$ as a function of $K_{nA}/|K_{nn}|$. The convention of the lines is the same as given in Figs. 3 and 4.

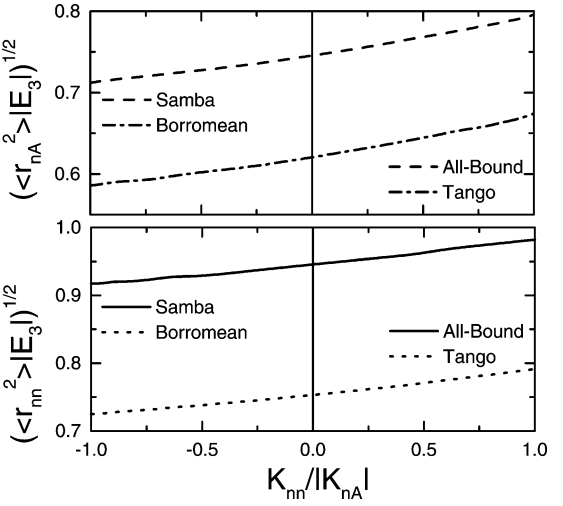


Fig. 6. Dimensionless products $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ (upper frame) and $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ (lower frame) for $A = 200$ and $E_{nA}/E_3 = 0.1$ as a function of $K_{nn}/|K_{nA}|$. In the upper we represent the case of a bound $nA$ pair with dashed line; and the case of a virtual $nA$ pair with dot-dashed line. In the lower frame we represent the bound $nA$ pair with solid line and the virtual $nA$ pair with dotted line. The lines of this figure correspond to the vertical transitions represented in Fig. 5 in both extreme sides where $|K_{nA}| = |K_{nn}|$.

$\sqrt{0.1}$) or virtual ($K_{nn} = -\sqrt{0.1}$) subsystems. In this case, the mass of the particle $n$ is much heavier than the "core", which does not happen in halo nuclei. However, we consider this case for the sake of general interest. In the $x$-axis, the positive (negative) values of

$K_{nA}/|K_{nn}|$ correspond to bound (virtual) $nA$ states. In the upper frame, the average $nA$ radius is shown for a bound $nn$ pair (dashed line) and for a virtual $nn$ pair (dot-dashed line). So, the dashed line shows that the value of $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ increases with the transition from *Tango* to *All-Bound* configuration. In the other possibility, represented by the dot-dashed line ($nn$ in a virtual state), the value of $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ increases from the most compact *Borromean* configuration ($K_{nA}$ negative) to the *Samba*-type configuration ($K_{nA}$ positive).

In the lower frame of Fig. 3, we also show that $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ increases with the transition from *Tango* to *All-Bound* and *Borromean* to *Samba* configurations. We observe, in this case, a small sensitivity on $K_{nn}$, when going from $-\sqrt{0.1}$ (dotted line) to $\sqrt{0.1}$ (solid line), with $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ having practically the same value for the All-Bound and Samba configurations; and also for the Tango and Borromean configurations. As we increase $A$, this sensitivity increases, as one can see in Figs. 4 and 5. We interpret this as the dominant role played by a light particle in the long-range interaction between two heavy particles, $n$, as already shown in an adiabatical approximation of the three-body system [28].

In Fig. 4, we show the radii for the ground state of the three-body system with the mass ratio $A = 1$. As in Fig. 3, we fixed $K_{nn} = \pm\sqrt{0.1}$, corresponding to bound (+) or virtual (−) subsystems. The same behavior found in Fig. 3 for $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ is found in the upper frame of Fig. 4 for $A = 1$, i.e., the configurations for which the $nn$ pair is virtual (dot-dashed line) are smaller than the ones that have the $nn$ pair bound (dashed line). Besides that, the configuration increases in size when the system changes from a *Borromean* to a *Samba* type and when it changes from a *Tango* to an *All-Bound* type. For $A = 1$, the mean square distance between the two-neutrons (lower frame of Fig. 4) exhibits the same qualitative behavior as found for $\sqrt{\langle r_{nA}^2\rangle|E_3|}$ when the configuration type is modified for a fixed three-body energy. These conclusions are still valid for a heavy core particle with $A = 200$, as one can verify in Fig. 5. It is worthwhile to mention that $\sqrt{\langle r_{nn}^2\rangle|E_3|}$ attains its asymptotic value fast with the increase of $A$ consistently with the calculations presented in Fig. 2 for $E_{nn} = E_{nA} = 0$. (Compare the results for $A = 1$ and $A = 200$ in the lower frames of Figs. 4 and 5.)

In correspondence with Fig. 5, for the same mass ratio $A = 200$, in the last set of systematic calculations we consider in Fig. 6 the energy of the subsystem $nA$ fixed in relation to $E_3$, with $K_{nA} = \pm\sqrt{0.1}$, corresponding to bound (+) or virtual (−) $nA$ subsystem. In this case, the ratio $K_{nn}/|K_{nA}|$ is changed from $-1$ to $+1$, such that the transitions of configurations from the left side to the right side of this figure correspond to the vertical transitions in the extreme side of Fig. 5 (when $|K_{nA}| = |K_{nn}| = \sqrt{0.1}$). So, comparing the upper frames of Figs. 5 and 6, we observe that the vertical transition from *All-Bound* to *Samba* configuration in Fig. 5 corresponds to the dashed line of Fig. 6; and, the vertical transition from *Tango* to *Borromean* configuration in Fig. 5 corresponds to the dot-dashed line of Fig. 6. In the lower frames of both figures, similarly we observe that the vertical transitions of Fig. 5 correspond to the lines represented in Fig. 6: the transition from *Samba* to *All-Bound* configuration is given by the solid line; and the transition from *Borromean* to *Tango* configuration given by the dotted line. In general, one can observe that the three-body bound state has a smaller size when the $nA$ pair forms a virtual state

(see in each frame of Fig. 6, where the upper line is for bound and the lower line is for virtual $nA$ pair).

The calculations of the average distances of the neutrons in the halo of $^6$He, $^{11}$Li, $^{14}$Be and $^{20}$C are shown in Table 1 and compared with the available experimental data. For the input, we have considered $E_{nn} = -0.143$ MeV and the center of the available experimental values of $E_3$ and $E_{nA}$. For the cases that we have unbound virtual $nA$ systems, the $E_{nA}$ input values are taken from several recent theoretical and experimental analysis; we prefer to keep at least two possible values in order to verify the consistency of the model with the experimental data.

Within the possible limitations of our approach, by comparing our results for the $nn$ mean-square radius with the experimental ones, which are known in the cases of $^6$He, $^{11}$Li and $^{14}$Be, as given in Table 1, one can also predict the corresponding virtual energies of the $nA$ subsystem.

In the particular case of $^6$He, the comparison between the experimental $nn$ mean-square radius with our result is pointing out to a virtual energy close to zero for $n$–$^4$He, which is not supported by the quite large values given in the literature [18,23]. However, as discussed in [18,23], the interaction for $n-^4$He is attractive in $p$-wave and repulsive in $s$-wave producing a large value for the energy of the virtual state, such that a deviation of our calculation from the experimental result is expected (in our model the $s$-wave poles should be near the scattering thresholds). For the binding of $^{11}$Li, it is also known that both $p$- and $s$-waves are important in the subsystem $n$–$^9$Li. This fact can also explain some deviations of our results when compared with experimental ones. However, in this last case, our approach can be more reliable based on the fact that:

(i) the $s$-wave $n$–$^9$Li interaction is attractive and it has a virtual state near the scattering region;
(ii) we are considering the experimental energies for the inputs, such that we are partially taking into account the effect of higher partial waves in the interactions;
(iii) the radius is obtained from the tail of the wave-function, which is dominated by the $s$-wave;
(iv) as noted in Ref. [20], even the three-body wave function with $s$-wave $nn$ correlation produces a ground state of the halo nuclei with two or more shell-model configurations.

One should also expect that other effects like the finite size of the core and Pauli principle, missing in our model, could affect the average relative distances, if the three-body wave function would overlap appreciably with the core. At least for $^{11}$Li this is not expected due to the small binding. It is of notice that indeed the halo neutrons have a large probability to be in a region in which the wave function is an eigenstate of the free Hamiltonian, and thus dominated by few asymptotic scales.

## 5. Conclusions

The mean-square radii of a light halo-nuclei modelled as a three-body system (two neutrons $n$ and a core $A$) are calculated using a renormalized three-body model with

a pairwise Dirac-$\delta$ interaction, which works with a minimal number of physical inputs directly related to observables. These physical scales are the two-neutron separation energy $S(2n) = -E_3$, and the $nn$ and $n$–core $s$-wave scattering lengths.

The existent data for $^{11}$Li and $^{14}$Be compare qualitatively well with our theoretical results, which means that the neutrons of the halo have a large probability to be found outside the interaction range. Therefore the low-energy properties of these halo neutrons are, to a large extend, model independent as long as few physical input scales are fixed. The model provides a good insight into the three-body structure of halo nuclei, even considering some of its limitations. We pointed out that the model is restricted to $s$-wave subsystems, with small energies for the bound or virtual states. So, the model is not suitable for the $^6$He, since the $s$-wave virtual state energy of $^5$He is quite large ($-4$ MeV). There is no $n$–core $p$-wave interaction, although some of its physics is effectively included through the value of the two-neutron separation energy, which is an input for our radii calculations. Also the finite size of the core and consequently the antisymmetrization of the total nuclear wave function, are both missing in our model. However, as the three-body halo nuclei tend to be more and more weakly bound with subsystems that have bound or virtual states near the scattering threshold, our approach becomes adequated and the above limitations are softened. The results indicate that the model is reasonable for $^{11}$Li and $^{14}$Be.

As an example of application to other halo-nuclei system, considering the available energies, we have also estimated the $nn$ root-mean-square radius for the $n$–$n$–$^{18}$C system.

We have also studied in detail the consequences of the classification scheme proposed in Ref. [12] for weakly bound three-body systems. This study was performed analyzing the dimensionless products $\sqrt{\langle r_{nA}^2\rangle |E_3|}$ and $\sqrt{\langle r_{nn}^2\rangle |E_3|}$ in terms of scaling functions depending on the dimensionless product of the scattering lengths and the square-root of the neutron–neutron separation energy. In the cases we have addressed, there are four different types of a three-body system when we allow the neutron–neutron pair to be bound: *Borromean* (only virtual two-body subsystems), *Tango* ($nn$ bound and $nA$ virtual), *Samba* ($nn$ virtual and $nA$ bound) and *All-Bound* (only bound two-body subsystems). The name *Samba* was introduced to refer to a system quite stable because it has two bound two-body subsystem than the *Tango* type, so it can "shake" a little bit more and continue to be bound.

The qualitative properties of the different possibilities of three-body systems are easily understood in terms of the effective attraction in the model: when a pair has a virtual state the effective interaction is weaker than when the pair is bound. Thus, a three-body system has to shrink to keep the binding energy unchanged if a pair which is bound turns to be virtual. We have illustrated through several examples this property, which show that dimensionless sizes $\sqrt{\langle r_{nA}^2\rangle |E_3|}$ and $\sqrt{\langle r_{nn}^2\rangle |E_3|}$ increase from *Borromean*, *Tango*, *Samba* and to *All-Bound* configurations. Of course the size is expected to increase beyond limits when a nonvanishing three-body energy hits a scattering threshold, with the *Borromean* configuration being the only exception. In spite of that, we conclude that even far from the threshold situation, the configuration sizes increase as we pointed out.

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# Triatomic continuum resonances for large negative scattering lengths

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We study triatomic systems in the regime of large negative scattering lengths which may be more favorable for the formation of condensed trimers in trapped ultracold monoatomic gases as the competition with the weakly bound dimers is absent. The manipulation of the scattering length can turn an excited weakly bound Efimov trimer into a continuum resonance. Its energy and width are described by universal scaling functions written in terms of the scattering length and the binding energy $B_3$ of the shallowest triatomic molecule. For $a^{-1}<-0.0297\sqrt{mB_3/\hbar^2}$, the excited Efimov state turns into a continuum resonance.

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It is by now well established that shallow dimers are formed in trapped ultracold or condensed monoatomic gases, as it has been reported for $^{23}$Na [1], $^{87}$Rb [2], and $^{85}$Rb [3]. In the experiment in Ref. [3], an atom-molecule coherence in the Bose-Einstein condensate was also observed. The measured oscillation frequency of the quantum superposition of $^{85}$Rb dimers and atoms in the condensate was in agreement with the shallow $^{85}Rb_2$ binding energy over a wide range of values near a Feshbach resonance. However, the formation of triatomic molecules has not yet been observed.

Recently, the energy of the shallowest bound triatomic molecule in trapped ultracold and condensed monoatomic gases was predicted using the value of the measured recombination rate into a shallow dimer; the energies ranged from 7.75 mK down to 0.24 nK near a Feshbach resonance [4]. Condensed triatomic molecules coexisting with dimers and atoms near a Feshbach resonance would present an oscillatory dependence of observables on the trimer binding energy [5]. For negative scattering lengths and zero energy, the recombination rate into deep diatomic molecular states shows a resonant peak at values of $a$ for which the trimer Efimov state [6] hits the three-body continuum threshold [7]. If the magnitude of the large negative scattering length is decreased after an Efimov state hits the continuum, it turns into a three-body resonance, as we will show. Therefore, at nonzero energies, or temperatures, the resonant peak of the recombination rate would, in principle, appear when the resonance energy matches the energy of the continuum triatomic system.

Furthermore, the manipulation of the scattering length in monoatomic condensates in the regime of large and negative values offers an interesting possibility. No shallow dimers can exist in this case. Then, the formation of triatomic molecules may be more favorable as the main competitors are absent. If a coherent quantum superposition of atoms and trimers or resonances appears, it will present an oscillatory frequency corresponding only to the shallow three-body bound or resonant state. As we will show, this frequency scales with the scattering length and with a triatomic physical scale in the form of a universal function. Here, the binding energy of the shallowest trimer state is chosen as the three-body physical scale.

In 1970, Efimov predicted that infinitely many weakly bound three-boson states appear when the $s$-wave two-boson scattering length $a$ goes to the limit of $a\to\pm\infty$ [6]. For large scattering lengths, an attractive long-ranged effective interaction binds the three-particle system in a range of about $|a|$ (see also Ref. [8]). A new bound state appears for every increase of $|a|$ to $\sim 23|a|$. For positive $a$, at the threshold of the new state, the trimer binding energy is $6.9B_2$ [9–11] ($B_2$ is the dimer binding energy). For $a<0$, a new state becomes bound when the trimer has an energy of $\sim 1100B_2$ [9], where now $B_2$ is the energy of the virtual dimer state. Due to the large size of the system, the threshold conditions for the existence of excited Efimov trimers are universal [8,12], i.e., independent of the detailed potential shape, and exhibit a scaling form for large values of $a/r_0$ [6,9,11] (the interaction range is $r_0$). The three-body system heals through regions that are outside the potential action, where the wave function is essentially a solution of the free Schrödinger equation, and therefore the properties of the system are defined by few physical scales.

The dimer and trimer binding energies are the only physical scales that survive in the limit of $(a/r_0)\to\pm\infty$ (scaling limit), which essentially relates the Thomas collapse of the trimer state for $r_0\to 0$ [13] to the Efimov effect ($|a|\to\infty$) [14]. In the scaling limit, the three-boson observables are functions of the shallowest trimer binding energy (reference three-body energy) and $B_2$. These functions approach universal curves [6,9]. The collapse of the three-boson system in the limit of a zero-range force makes the trimer energy the three-body scale of the system beyond the two-body energy [15].

For large scattering lengths, an excited Efimov state turns into a virtual state when $a>0$ is decreased [16]. The threshold moves faster than the energy of the excited state. Therefore, with the increase of $a>0$, states pump out from the second sheet of energy to become bound states [10]. If $a<0$ is decreased in magnitude, the trimer bound states dive into the continuum [9]. It is our aim here to evaluate the scaling properties of the energy and width (for the decay into the three-body continuum) of the resonance born from an Efimov state, when a large $a<0$ is varied.

The $^4$He excited trimer state calculated also with realistic models offers a good example of an Efimov state and its

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universal scaling properties with the shallow dimer and trimer binding energies [9,11]. These molecules are special due to the large spatial size which spreads out much beyond the range of the potential [17,18]. The $^4$He-$^4$He root-mean-square distances in $^4He_3$ for the ground and excited states [17,19] are of the order of 5 to 10Å and of about 50 to 90Å, respectively. The product of the mean-square interatom distance with the separation energy of one atom from the trimer in units of $\hbar=m=1$ ($m$ is the atom mass) is about 1 in the ground and the excited states [17,19], while the ratio of the binding energies $B_3^{(0)}/B_3^{(1)}\approx 500$ [6] ($B_3^{(N)}$ is the binding energy of the $N^{th}$ trimer state).

In the present work we calculate the three-boson resonance energy and width for the decay into continuum states for large and negative scattering lengths. In this case it is justifiable to use a Dirac-$\delta$ potential. We solve subtracted homogeneous equations defined within a renormalization scheme applied to a three-body system interacting with $s$-wave zero-range pairwise potentials [10,15]. We present the results for the energies and widths in the form of a universal scaling function [9], which gives the trajectory of the three-body energy in the complex plane as a function of the shallow two-body virtual state energy. We show that a resonance becomes an excited trimer Efimov state when the large $a<0$ is decreased. We go beyond Ref. [10], where it was found the dependence of the virtual three-boson state energy on $a>0$ originated from an Efimov state which entered into the second energy sheet.

One can fix the energy of one three-body bound state (the three-body physical scale), and the two-body scattering length and get other observables. All the detailed information about the short-range force, beyond the low-energy two-body observables, is retained in only one three-body physical information in the limit of zero-range interaction. The existence of a three-body scale implies in the low energy universality found in three-body systems, or correlations between three-body observables [20,15]. In the scaling limit [9,10], one has

$$\mathcal{O}(E,B_3,B_2)(B_3)^{-\eta}=\mathcal{F}(\sqrt{E/B_3},\pm\sqrt{B_2/B_3}), \tag{1}$$

where $\mathcal{O}$ is a general observable of the three-body system at an energy $E$, with dimension of energy to the power $\eta$. This equation means that any observable of the system can be represented by a function that depends only on one three- and one two-body scales. The three-body scale is brought by the reference energy $B_3$ (binding energy) of the shallowest trimer state. The ± sign denotes positive or negative scattering lengths. In the case of the energies of a resonance, of an excited or virtual trimer state, instead of Eq. (1), the scaling function is written as

$$E_3=B_3\,\mathcal{E}(\pm\sqrt{B_2/B_3}). \tag{2}$$

(Throughout this paper, we use units such that $\hbar=m=1$, where $m$ is the mass of the atom.)

After partial-wave projection, the $s$-wave subtracted integral equation for three identical bosons is given by [10]

$$\chi(q)=4\pi\tau(\xi)\int_0^\infty dq'q'^2\int_{-1}^1 dy\chi(q')\times\left(\frac{1}{E_3-q^2-q'^2-qq'y}-\frac{1}{-\mu^2-q^2-q'^2-qq'y}\right), \tag{3}$$

where $\xi=E_3-\frac{3}{4}q^2$, $\mu$ is the subtraction point, and $\tau$ is given by

$$\tau^{-1}(\xi)=-2\pi^2\sqrt{B_2}-4\pi\xi\int_0^\infty\frac{dp}{\xi-p^2}. \tag{4}$$

Here $B_2$ is the dimer virtual state energy. [For positive values of the real part of $E_3$, Eqs. (3) and (4) are analytically extended to the second energy sheet, as we discuss below.]

Throughout this work we perform calculations only considering $a<0$ for a virtual dimer state. We use a contour deformation method to calculate the resonance energy and width [21]. The homogeneous equation (3) is analytically continued to the second sheet of energy by making $q(q')\rightarrow qe^{-i\theta}(q'e^{-i\theta})$ with $0<\theta<\pi/4$. For large enough $\theta$, the solution of Eq. (3) in the complex energy plane is found for $\tan(2\theta)>-\mathrm{Im}\,(E_3)/\mathrm{Re}\,(E_3)$.

In the limit of a virtual dimer energy tending to zero, an infinite number of Efimov states appears from the solution of Eq. (3) for negative $E_3(=-B_3)$. The $N^{th}$ Efimov state has binding energy given by $B_3^{(N)}$ with $N=0$ indicating the ground state obtained from Eq. (3). When the $N^{th}$ Efimov state turns into a resonance its complex energy is denoted by $E_3^{(N)}$. In Fig. 1 the real part of the complex energies is shown, in units of $\mu=1$, for the first three states obtained by solving numerically Eq. (3). In the figure, the values of $[\mathrm{Re}\,(E_3)]^{1/2}$ for the first three resonances are described by the positive part of the plot. The curves represent $E_3^{(0)}$ (solid line), $E_3^{(1)}$ (dashed line), and $E_3^{(2)}$ (dotted line), i.e., the complex energies of the first three states of Eq. (3). Note that the subtraction present in Eq. (3) regularizes it, and the Thomas collapse is avoided. When $B_2$ is decreased, the resonance turns into a bound state and the negative part of the plot gives the energies of the ground ($B_3^{(0)}$), first ($B_3^{(1)}$), and second ($B_3^{(2)}$) bound trimer states. One realizes that the form of the curves is very similar which indicates that the function $\mathcal{E}$ of Eq. (2) does not depend on the state, which will be confirmed later on in the scaling plot of Fig. 3. The values of $\sqrt{B_2}$ in units of $\mu=1$ at which the Efimov state becomes unbound are 0.066, 0.0028, and 0.000 13 for the ground, first, and second states, respectively. The ratios $(0.066/0.0028)^2\approx(0.0028/0.000\,13)^2\sim 500$ are practically independent of the state, in agreement with the scaling limit implied by Eq. (2). It is curious that the real part of the resonance energy tends to zero for large enough $B_2$, while the width is nonzero.

In Fig. 2 the results for the imaginary part of the resonance complex energy are shown as a function of $B_2$ in units of $\mu=1$. The solid, dashed, and dotted lines are, respectively, the corresponding imaginary parts of $E_3^{(0)}$, $E_3^{(1)}$, and $E_3^{(2)}$. The threshold values of $B_2$ for which the resonant state becomes bound are clearly seen in the figure and the resonance width

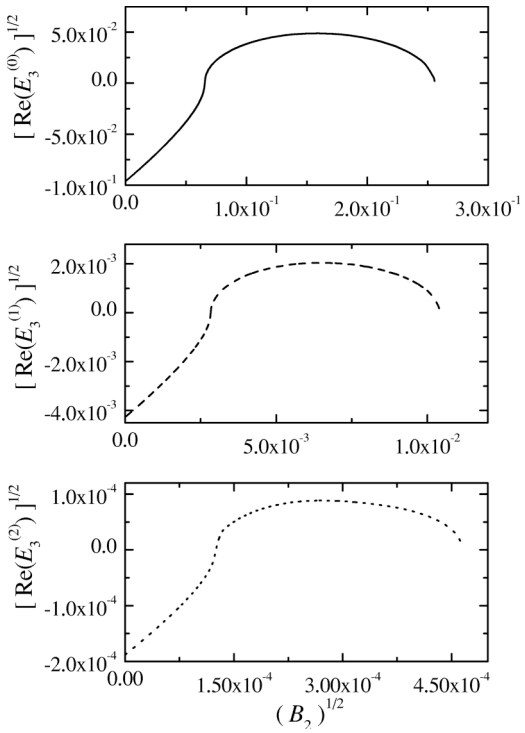


FIG. 1. Real part of the three-body resonance energy as a function of the two-body virtual state energy in units of $\mu=1$. The negative values represent the results for square root of the energy of the $N$th bound trimer state $[B_3^{(N)}]^{1/2}$, which turns into a resonance when $|B_2|$ is increased. The positive values of $[\mathrm{Re}(E_3^{(N)}]^{1/2}$ correspond to the resonance. The results are given for $N=0$ (solid line), $N=1$ (dashed line), and $N=2$ (dotted line).

$\Gamma_3^{(N)}=2|\mathrm{Im}\,[E_3^{(N)}]|$ increases with the virtual dimer energy. The results shown in Figs. 1 and 2 give the complete trajectory of a three-body Efimov state when the two-atom interaction with $a<0$ is changed, as can be done for trapped atoms near a Feshbach resonance. These results extend the findings of Ref. [10]. Now, we can give a complete picture of the route of an Efimov state when $a$ is varied passing through a Feshbach resonance. If one begins with positive $a$ and increases it, a virtual trimer state becomes bound, then crossing a Feshbach resonance and decreasing the magnitude of the large negative value of $a$, the trimer bound state becomes unbound and turns into a resonance. The results for the trimer bound state or resonance energies can be expressed in the form of a universal scaling function, Eq. (2), that depends only on the ratio of the two- and the reference three-body energies. From the calculations given in Figs. 1 and 2, we construct the scaling plots of Figs. 3 and 4, respectively. For this purpose, we use the first and second Efimov states (bound or resonant) and we numerically obtain

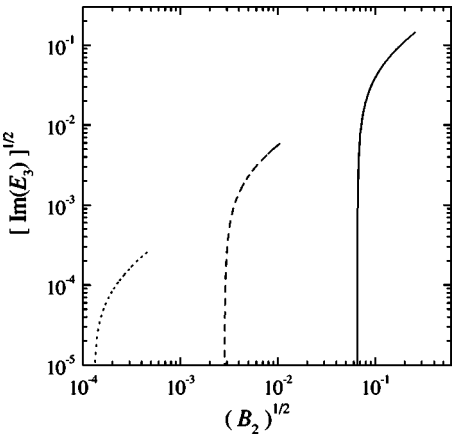


FIG. 2. Imaginary part of the three-body resonance energy as a function of the two-body virtual state energy in units of $\mu=1$. The curves are labeled as in Fig. 1.

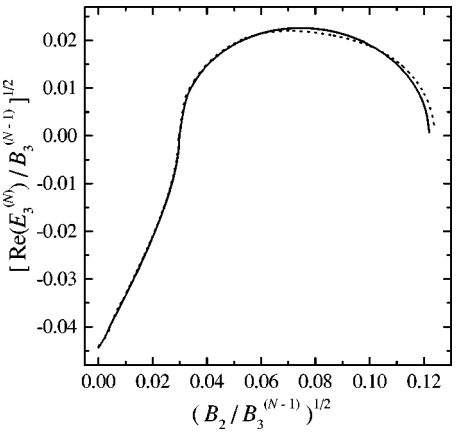


FIG. 3. Ratio of the real part of $E_3^{(N)}$ and $B_3^{(N-1)}$ as a function of $B_2/B_3^{(N-1)}$. The solid line is the results for $N=1$ and the dashed line for $N=2$.

$$E_3^{(N)} = B_3^{(N-1)}\mathcal{E}(-\sqrt{B_2/B_3^{(N-1)}}), \tag{5}$$

using $N$ equal to 1 and 2. [In Eq. (5) the states are in fact indexed, which was not explicitly shown in Eq. (2).] We show the results for the real and imaginary parts of the resonance energy in the form of scaling plots in Figs. 3 and 4, respectively. In these figures the solid line corresponds to $N=1$ and the dotted line to $N=2$. In Fig. 3, the negative values of $[\mathrm{Re}(E_3)/B_3]^{1/2}$ give the trimer bound state results, while the positive values come from the resonant state. It

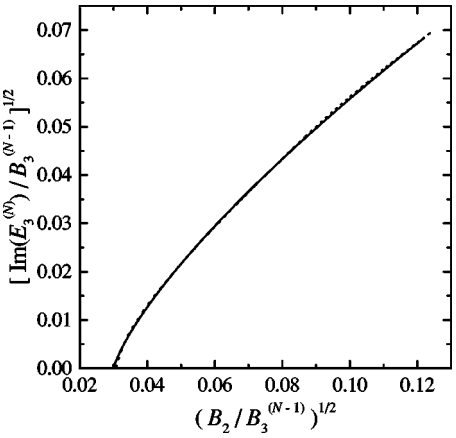


FIG. 4. Ratio of the imaginary part of $E_3^{(N)}$ and $B_3^{(N-1)}$ as a function of $B_2/B_3^{(N-1)}$. The curves are labeled as in Fig. 3.

is clear that a universal curve for the scaling function $\mathcal{E}(-\sqrt{B_2/B_3})$ is approached as the results for $N=1$ and 2 practically overlap. The imaginary part of the resonance energy in Fig. 4 appears for the dimer virtual state energy $B_2 \geqslant 0.000\,882 B_3$, where the excited Efimov bound state turns into the resonance. Our results extend the scaling function $\mathcal{E}(\sqrt{B_2/B_3})$ (bound dimer states) obtained previously in Refs. [9,10] to negative values of the argument and for the trimer resonance region.

In conclusion, we have obtained the trajectory of an Efimov state when the two-atom interaction crosses a Feshbach resonance, in the form of a scaling function. The value of the resonance energy and width depends only on the dimer bound or virtual energy and the shallowest trimer binding energy. The route of an Efimov state when $a$ is varied passing through a Feshbach resonance can be summarized as follows: beginning from a large positive $a$ and increasing it further, a virtual trimer state becomes bound and then after crossing a Feshbach resonance and decreasing the magnitude of the large negative value of $a$, the trimer bound state becomes unbound and turns into a resonance, for $a^{-1} < -0.0297\sqrt{mB_3/\hbar^2}$, where $B_3$ is the binding energy of the shallowest trimer state. In this respect, the study of trapped Bose-Einstein condensates near a Feshbach resonance can be fruitful not only to reveal the properties of an interacting coherent quantum state under extreme conditions, but could also give new insights into the few-body physics underlying the curious phenomenon of Efimov resonant states.

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# Radii of weakly bound three-body systems: halo nuclei and molecules

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A renormalized three-body model with zero-range potential is used to estimate the mean-square radii of three-body halo nuclei and molecular systems. The halo nuclei ($^6$He, $^{11}$Li, $^{14}$Be and $^{20}$C) are described as point-like inert cores and two neutrons. The molecular systems, with two helium atoms, are of the type $^4$He$_2-$X, where X=$^4$He, $^6$Li, $^7$Li, or $^{23}$Na. The estimations are compared with experimental data and realistic results.

Halo nuclei and weakly bound molecules are quantum systems with very large sizes in which the constituent particles have a large probability to be found much beyond the interaction range. Under this circumstances, the physical properties of such bound systems can be defined by few physical scales.

In the present contribution we report results obtained for the root-mean-square radii of three-body halo nuclei and molecular systems that are obtained from a *universal scaling function* calculated within a renormalized scheme for three particles interacting through pairwise Dirac-$\delta$ potential. In the case where we have the two-body scattering length, $a$, much greater than the effective range of the potential, $r_0$, ($a/r_0 \gg 1$) our zero-range approach is expected to be a good aproximation [1]. In the *scaling limit* [2,3] all the observables of the three-body system can be represented by a function that depends only on the three- and two-body scales.

Figure 1 and Table 1 show results for halo nuclei systems, where $C$ represents the core and $n$ the neutron. In Fig. 1, our results ($\hbar = m_n = 1$) are given as functions of the mass ratio $A \equiv m_C/m_n$, where $m_C$ and $m_n$ are the masses of the core and the neutron, respectively. $r_\gamma^2$ ($\gamma \equiv C,\ n$) is the mean-square distance from the particle $\gamma$ to the center-of-mass of the system. $r_{n\gamma}^2$ is the mean-square distance between the particles $n$ and $\gamma$. The results given in Fig. 1 are obtained in the limit where the two-body energies are equal to zero, such that the system have just the three-body energy as a physical scale. Our formalism is presented in detail in ref. [4], where we show that Fig. 1 applies equally well to weakly bound molecular systems, as the results are given in terms of dimensionless quantities.

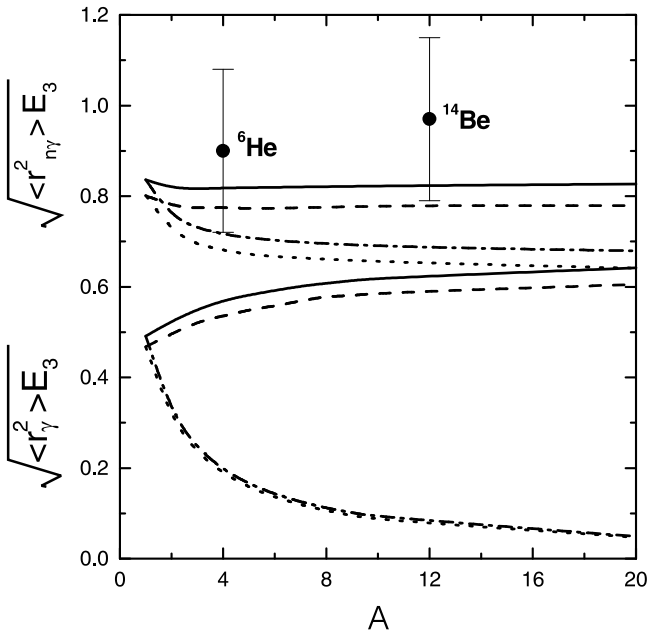


Figure 1. Dimensionless products $\sqrt{\langle r^2_{n\gamma}\rangle E_3}$ [upper (a) plots] and $\sqrt{\langle r^2_{\gamma}\rangle E_3}$ [lower (b) plots], are given as functions of $A \equiv m_C/m_n$, for $E_{nn} = E_{nC} = 0$. The results for the ground-state are shown with solid line ($\gamma = n$) and dot-dashed line ($\gamma = C$); and, for the first excited state, with dashed line ($\gamma = n$) and dotted line ($\gamma = C$).

We can see in Fig. 1 that, although the ratio between the energies of the ground and the first excited states are about few hundreds [5], we have practically no difference between our dimensionless curves, supporting the validity of our *scaling limit*. The experimental results for the halo nuclei $^6$He ($^4$He+n+n) and $^{14}$Be ($^{12}$Be+n+n) are quite consistent with our predictions based on the zero-range calculations. Therefore, our assumption that such nuclei could be represented by inert cores and two neutrons, interacting through short range forces, produces a reasonable description of the average interparticle distances.

In Table 1 we present the results of the neutron-neutron root-mean-square distances, for the halo nuclei C-n-n system $^6$He, $^{11}$Li, $^{14}$Be, and $^{20}$C. Our results are compared with experimental values, given in ref. [6]. Although the calculations are in reasonable agreement with data, they systematically underestimate the measured values. Analogously, we show in Table 2 our results, obtained in ref. [4] for weakly-bound three-body molecules. In this case, we present results for the root-mean-square distances between the particles and also the root-mean-square distances of each particle to the center-of-mass of the system. For the $^4$He$_3$ trimer, our calculations deviate only about 14% from the realistic results obtained in ref. [7].

In conclusion, the present model for the weakly bound halo nuclei and molecular systems gives a reasonable description of these systems, validated by the comparison with experimental data and realistic results.

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Table 1
Results of the neutron-neutron root-mean-square radii in halo nuclei. The core ($C$) is given in the first column, the three-body ground state energy and the corresponding two-body energy are respectively given in the second and third columns. The virtual states are indicated by (v), and the $nn$ virtual state energy is taken as 143 keV. The experimental values, in the last column, come from ref. [6].

| Core | $E_3^{(0)}$ (MeV) | $E_{nC}$ (MeV) | $\sqrt{\langle r_{nn}^2 \rangle}$ (fm) | $\sqrt{\langle r_{nn}^{2\{exp\}} \rangle}$ (fm) |
|---|---|---|---|---|
| $^4He$ | 0.97[8] | 0[9] | 5.1 | 5.9±1.2 |
| $^9Li$ | 0.32[10] | 0.8[10](v) | 5.9 | 6.6±1.5 |
| $^{12}Be$ | 1.34[8] | 0.002[11](v) | 4.4 | 5.4±1.0 |
| $^{18}C$ | 3.51[8] | 0.16[8] | 3.0 | - |

Table 2
Results for different radii of the molecular systems $\alpha\alpha\beta$, where $\alpha \equiv^4$He and $\beta$ is identified in the first column. The ground-state energies of the triatomic molecules and the corresponding energies of the diatomic subsystems, obtained from ref. [12], are given in the second, third and forth columns. $\langle r_{\alpha\gamma}^2 \rangle$ is the corresponding mean-square distance between the particles $\alpha$ and $\gamma$ $(= \alpha, \beta)$. $\langle r_\gamma^2 \rangle$ is the mean-square distance of $\gamma$ to the center-of-mass of the system.

| $\beta$ | $E_3^{(0)}$ (mK) | $E_{\alpha\alpha}$ (mK) | $E_{\alpha\beta}$ (mK) | $\sqrt{\langle r_{\alpha\alpha}^2 \rangle}$ (Å) | $\sqrt{\langle r_{\alpha\beta}^2 \rangle}$ (Å) | $\sqrt{\langle r_\alpha^2 \rangle}$ (Å) | $\sqrt{\langle r_\beta^2 \rangle}$ (Å) |
|---|---|---|---|---|---|---|---|
| $^4$He | 106.0 | 1.31 | 1.31 | 9.45 | 9.45 | 5.55 | 5.55 |
| $^6$Li | 31.4 | 1.31 | 0.12 | 16.91 | 16.38 | 10.50 | 8.14 |
| $^7$Li | 45.7 | 1.31 | 2.16 | 14.94 | 13.88 | 9.34 | 6.31 |
| $^{23}$Na | 103.1 | 1.31 | 28.98 | 11.66 | 9.54 | 8.12 | 1.94 |

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# Three-Body Recombination in Ultracold Systems: Prediction of Weakly-Bound Atomic Trimer Energies*

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**Abstract.** The three-body recombination coefficient of an ultracold atomic system, together with the corresponding two-body scattering length $a$, allow us to predict the energy $E_3$ of the shallow trimer bound state, using a universal scaling function. The production of dimers in trapped Bose-Einstein condensates, from three-body recombination processes, in the regime of short magnetic pulses near a Feshbach resonance, is also studied in line with the experimental observation.

## 1 Introduction

The interaction among neutral atoms is equivalent to a range zero in the limit of $a \to \infty$. For identical bosonic atoms, either the Efimov effect [1] or the Thomas collapse [2] can happen when the ratio between $a$ and the range goes to infinity. This is the scaling limit, where the three-boson properties can be determined just by two scales: the dimer binding energy (or virtual dimer energy) and the shallow trimer binding energy [3].

Recently, Bose-Einstein condensation (BEC) has been obtained with trapped ultra-cold atomic gases. Losses of atoms in BEC can occur due to three-atom recombination processes, which are measured in several cases: $^{23}\mathrm{Na}|F = 1, m_F = -1\rangle$

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[4], $^{87}\mathrm{Rb}|F=1,m_F=-1\rangle$ [5, 6], and $^{85}\mathrm{Rb}|F=2,m_F=-2\rangle$ [7, 8]. The value of the three-body recombination coefficient, together with the corresponding two-body scattering length, allow us to predict the energy of the shallow trimer bound state, as described in Sect. 2.

Another aspect related to the three-body recombination process, supported by experimental observations, is a possible enhancement due to quantum coherence (laser effect), which may happen in a special situation of fast changes of $a$. In Sect. 3, we discuss the dynamics of BEC related to this aspect of the three-body recombination process. Our conclusions are summarized in Sect. 4.

## 2 Weakly Bound Atomic Trimer Energies

It was shown by some of us, in ref. [9], how to obtain the trimer binding energies of an atomic system from the three-body recombination rate and the corresponding two-body scattering length. A universal scaling function which gives the dependence of the recombination parameter as a function of the weakly bound trimer energy ($E_3$) is calculated within a renormalized scheme for three particles interacting through pairwise Dirac-delta interaction [9]. For atoms with mass $m$ and for large $a$, $E_3$ is shown to be in the interval $1 < m(a/\hbar)^2 E_3 < 6.9$. The contribution of a deep-bound state to the prediction, in the case of $^{85}\mathrm{Rb}|F=2,m_F=-2\rangle$ for a particular trap, is shown to be relatively small. Also, using the predicted energies of the triatomic molecules in ultra-cold traps, the sizes of the trimers $^{23}\mathrm{Na}|1,-1\rangle$ and $^{87}\mathrm{Rb}|1,-1\rangle$ can be estimated. In this case, a scaling function gives the mean-square radii as a function of $E_3$ and $a$. The root-mean-square distance between two atoms in a triatomic molecule is estimated to be $0.8\sqrt{\hbar^2/(m(E_3-E_2))}$, where $E_2$ is the dimer binding energy [10].

The rate of three free bosons to recombine, forming a dimer and one remaining particle, is given in the limit of zero energy, by the recombination coefficient [11, 12]

$$K_3 = \kappa \frac{\hbar}{m} a^4, \tag{1}$$

where $\kappa$ is a dimensionless parameter. When $a > 0$, the recombination parameter $\kappa$ oscillates between zero and a maximum value as a function of $a$, as shown in refs. [13] ($\kappa \leq 68.4$), [14] ($\kappa \leq 65$), and [15] ($\kappa \leq 67.9$).

By using a general scaling procedure, it is shown in ref. [9] that one can express the functional dependence of $\kappa$ in terms of the two- and three-body energies, $\kappa \equiv \kappa\left(\sqrt{E_2/E_3}\right)$, considering that for large scattering lengths one has $1/a = \sqrt{mE_2/\hbar^2}$. Such scaling form of $\kappa$ is derived in detail in ref. [9], using results presented in ref. [11]. It is given by

$$\kappa = \kappa_{\max} \sin^2\left(-1.01 \ln \sqrt{\frac{E_2}{E_3}} + \Delta\left(\sqrt{\frac{E_2}{E_3}}\right)\right), \tag{2}$$

where $\Delta$, a function of the ratio $E_2/E_3$, depends on the interaction at short distances, which defines $E_3$.

**Table 1.** For the atomic species $^{A}Z|F, m_F\rangle$, the predicted trimer binding energies with respect to the atom-dimer threshold are shown in the 4th and 5th columns. $\kappa_{\text{expt}}$ and $E_2$ are, respectively, given in the 2nd and 3rd column. For $^{87}\text{Rb}|1, -1\rangle$, the recombination process was obtained in ref. [5] for noncondensed ($^*$) and condensed ($^\dagger$) trapped atoms

| $^{A}Z\|F, m_F\rangle$ | $\kappa_{\text{expt}}$ | $E_2$ (mK) | $S_3$ (mK) | $S_3'$ (mK) |
|---|---|---|---|---|
| $^{23}\text{Na}\|1, -1\rangle$ | $42 \pm 12$ [4] | 2.85 | 4.9 | 0.21 |
| $^{87}\text{Rb}\|1, -1\rangle$ | $52 \pm 22^*$ [5] | 0.17 | 0.39 | 0.005 |
| $^{87}\text{Rb}\|1, -1\rangle$ | $41 \pm 17^\dagger$ [5] | 0.17 | 0.30 | 0.013 |
| $^{87}\text{Rb}\|2, 2\rangle$ | $130 \pm 36$ [6] | 0.17 | – | – |
| $^{85}\text{Rb}\|2, -2\rangle$ | $7.84 \pm 3.4$ [7, 8] | $1.3 \times 10^{-4}$ | $1.14 \times 10^{-4}$ | $3.8 \times 10^{-5}$ |

Next, considering the calculation of the scaling function, with the subtracted form of the Faddeev equations [16], and considering the relation between the transition matrix elements and the three-body recombination coefficient at zero energy, the functional dependence of $\kappa$ was derived in terms of the ratio $E_2/E_3$ (see Fig. 1 of ref. [9]). The scaling limit is well approached in the calculations, with the maximum $\kappa$ occurring near the atom-dimer threshold ($E_3 \approx E_2$) and when $(E_3/E_2)^{1/2} \approx 0.38$ [3], such that between two consecutive maxima of $\kappa$ we have $1 < m(a/\hbar)^2 E_3 < 6.9$.

Using the experimental values $\kappa_{\text{expt}}$, for a few atomic species $^{A}Z|F, m_F\rangle$, one can obtain two possible values of the weakly bound triatomic molecular states that are consistent with the universal scaling plot that was derived. In Table 1, the predicted trimer binding energies, in respect to the threshold, $S_3 \equiv (E_3 - E_2)$ and $S_3' \equiv (E_3' - E_2)$, are given in milliKelvins. We consider the central values of the experimental dimensionless recombination parameters.

## 3 Coherent Dimer Formation

One should note that the three-body recombination coefficient was derived in the previous section considering very dilute systems and considering that the two-body interaction is kept fixed. Another interesting possibility may happen in a special situation when we have fast changes of the two-body scattering length $a$. In this case, the three-body recombination process may be enhanced due to quantum coherence. The remaining atoms and dimers are produced in a single state and, due to the symmetrization of the full wave-function, the recombination process which happens in this background is enhanced (laser effect).

Supporting this possibility, it was observed [8] an isotropic burst of relatively hot $^{85}$Rb atoms with temperature of about 150 nK, when a fast magnetic pulse near a Feshbach resonance increases the scattering length up to 4000 $a_0$. The maximum value of $a$ gives a lower bound for the temperature of the remaining atoms about 75 nK consistent with the experiment. In line with the experimental observation, we make an attempt to describe the remaining number of condensed atoms after the pulse, within a mean field description. For that, we consider that: (i) shallow dimers, with their centre-of-mass in $s$-wave, are formed (the temperature of the atoms in the burst is consistent with weakly bound dimers and not deeply bound

dimers); (ii) the recombination process shows a coherence effect, evidently for $s$-wave propagating dimers and atoms (the isotropic burst supports it); and (iii) a fitted magnitude of the parameter $\kappa$ in Eq. (1) depends on the rise time ($t_r$) of the scattering length.

One has to go beyond the mean-field model to implement the coherence effect in a defined theory. The phenomena should be described in a coupled model, with the condensed atoms, the remaining atoms and the dimers. In this respect, it was suggested recently, in a theoretical microscopic approach [17], that in a collision of two atomic condensates producing two molecular condensates in counterpropagating momentum eigenstates, there is the possibility of an atom-molecule laser fed by stimulated three-body recombination processes, where atoms and molecules produced in the same state enhance the three-body recombination rate with respect to the vacuum values.

In an effective way, i.e., using the mean-field equation, the coherence effect in a single $s$-wave state will appear as the increase of the magnitude of the recombination parameter in respect to the vacuum value. As the process becomes faster, the loss of coherence of the atoms and dimers is reduced; and, as suggested by our results, the increase in the three-body recombination rate is even higher [18].

For describing the dynamics of BEC as nonconservative systems, we can follow the extended mean field formalism developed in ref. [19], in which one considers an extended approach of the Gross-Pitaevskii formalism, by including losses of the system by three-body recombination. Here, we should also include the time variation of the relevant physical parameters.

Near a Feshbach resonance, the scattering length $a$ has been observed to vary as a function of the magnetic field $B$, according to theoretical prediction [20], as

$$a = a_b \times \left(1 - \frac{\Delta}{B - B_r}\right), \tag{3}$$

where $a_b$ is the background scattering length, $B_r$ is the resonance magnetic field and $\Delta \equiv (B_0 - B_r)$ is the resonance width, where $B_0$ is the value of $B$ at $a = 0$. For the case of $^{85}$Rb, one has $\Delta \cong 11.0\,\mathrm{G}$, $B_r \cong 154.9\,\mathrm{G}$, and $a_b \cong -450\,a_0$. We consider in our calculations the same experimental parameters used in ref. [8]: initial field $B_0 \cong 166\,\mathrm{G}$ (harmonic oscillator state), applied to an initial sample of $N_0 = 16500$ condensed atoms; spherical symmetry, with mean geometric frequency $\omega \cong 2\pi \times 12.77\,\mathrm{Hz}$, for simulating the cylindrical geometry of JILA ($\omega_r = 2\pi \times 17.5\,\mathrm{Hz}$ and $\omega_z = 2\pi \times 6.8\,\mathrm{Hz}$).

For the above conditions, the remaining number of atoms in BEC was obtained and compared with JILA experimental data. The results are given in Table 2. We note that, in order to obtain the best fit of the experimental data, we need to adjust $\kappa$ to values much higher than the vacuum values given by Eq. (2). For instance, if we

**Table 2.** Numerical values of the three-body recombination coefficient $\kappa$ as function of the rise time $t_r$ of the magnetic field pulses applied to the $^{85}$Rb BEC

| $t_r$ ($\mu$s) | 12.5 | 25.3 | 75.8 | 151.6 | 202.1 | 252.6 |
|---|---|---|---|---|---|---|
| $\kappa$ | 1800 | 1700 | 1600 | 500 | 200 | 100 |

consider the rise time of the magnetic field pulses lower than 100 μs, we have $1000 \lesssim \kappa \lesssim 2000$. However, $\kappa$ decreases while $t_r$ increases, such that $\kappa \sim 100$ for $t_r$ of the order of 250 μs. In this case, slowing the rise time, we note that $\kappa$ approaches the predicted interval $0 \leq \kappa \lesssim 68$.

The phenomenon of enhancement in the magnitude of the three-body recombination coefficient gives an indication that a laser-like effect may be occurring in the experiment of ref. [8]. Our picture suggests that for very short time scales (time ranges varying from 0 up to 100 μs) the three-body recombination processes produce shallow dimers and a third atom (burst effect) in many-boson states.

The coherent production of shallow dimers occurs for very short rise times and disappears for longer ones, producing the strange effect reported in ref. [8], of a decreasing dissipation from the condensate for long rise times. This effect is brought to the mean-field calculation by the enhanced values of $\kappa$ as a function of $t_r$, which can be approximately given by the parametrization

$$\kappa(t_r) = 2300 \exp(-0.01 \times \omega t_r). \tag{4}$$

Such parametrization is convenient to study the remaining number of atoms in $^{85}$Rb BEC as a function of the scaled rise time of the applied magnetic pulse, for fixed hold times, with the parameters considered in ref. [8] (where the magnetic field during the hold time is $B_h = 156.7$ G). The results of our model calculation describe the observed behavior of the remaining number of atoms (see Fig. 3 of ref. [18]).

## 4 Conclusions

In the present communication, we report recent results that we have obtained by considering the three-body recombination processes in ultracold or condensed atomic gases. From the experimental values of the recombination coefficient together with the corresponding two-body scattering length, we are able to predict energies of the shallow trimer bound state for a few atomic systems. To obtain the scaling function corresponding to the dependence of the dimensionless recombination parameter with the shallow trimer binding energy, we use a zero-range model which is valid for large scattering lengths. We point out that, at least, one experimental result for $^{87}$Rb$|2, 2\rangle$ is outside the interval of theoretical vacuum values of $\kappa$, which may indicate that some particular physics is present in that experiment.

We also observe that, when considering the special situation of fast variations of the two-body scattering length, near a Feshbach resonance, the experimental results can be put consistent with a mean-field description, if one allows a strong enhancement of the three-body recombination process motivated by possible quantum coherence phenomena in the production of dimers (laser effect). However, certainly one has to go beyond the mean-field description with only condensed atoms, to be able to implement the coherence effect in a defined way. Such a mean-field theory should describe simultaneously the dynamics of the condensed atoms, the remaining atoms and the dimers, which is within the scope of a future investigation.

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