

Solvable three-boson model with attractive δ -function interactions

J. G. Muga* and R. F. Snider

Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1

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A one-parameter solvable model for three bosons subject to δ -function attractive interactions in one dimension with periodic boundary conditions is studied. The energy levels and wave functions are classified and given explicitly in terms of three momenta. In particular, eigenstates and eigenvalues are described as functions of the model parameter c . Some of the states are given in terms of complex momenta and represent dimer or trimer configurations for large negative c . The asymptotic behavior for small and large values of the parameter, and at thresholds between real and complex momenta, is provided. The properties of the potential energy are also discussed. [S1050-2947(98)08905-7]

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I. INTRODUCTION

Quantum solvable models, where the wave functions, energy eigenvalues, and other quantities of physical interest can be obtained explicitly in terms of known functions or with minimum numerical effort (typically by solving a transcendental equation or by quadratures) are useful to test and refine concepts and/or numerical methods, and as first approximations to more realistic systems. Occasionally, unexpected physical phenomena are revealed [1]. In this paper we shall analyze a one-parameter model for three bosons subject to attractive δ -function pair interactions in one dimension with periodic boundary conditions (contrast this to three particles “on a ring;” see Ref. [2]). Our original motivation was to examine a system with attractive forces where single and compound particles may coexist. This is of particular interest when studying the kinetic theory of gases composed by particles that can form stable aggregates (such as dimers or trimers), especially when chemical reactions can occur [3]. This paper deals exclusively with the model itself, which has been found to be quite complex in mathematical detail. The method of analyzing for all the possible states of the system involves following the eigenvalues as a function of the coupling constant c , starting from the easily analyzed, noninteracting case, $c = 0$. It is found that certain eigenvalues are not analytic functions of the coupling constant at specific points. Such nonanalyticity of the eigenvalues has also been recently investigated [4,5] for certain polynomial potentials.

The literature on one-dimensional solvable models of three, and generally N , particles is rather extensive. These models could be primarily classified according to the type of interaction involved [6]. However, even with the same interaction but with different boundary conditions, different formal treatments are required, and very different results may be found. Periodic boundary conditions are suitable for modeling a gas or a crystal lattice in the thermodynamic limit. In contrast, in the limit where the box length becomes large, information about the corresponding scattering problem of a one-dimensional system can be extracted [7,8]. Indeed these

are the standard boundary conditions for actual calculations of time-dependent wave-function scattering [9]. The model studied here is a particular case of the “interacting Bose gas” of Lieb and Liniger [10], who examined N particles subject to two-body δ -function interactions and boson symmetry. Further analysis of this gas was carried out in several papers [11–14], but, having different objectives and applications in mind, in none of these works was the attractive case examined, except for the appendix on the $N=2$ case in Ref. [10]. Lieb and Liniger found some unexpected effects of the periodic confinement but did not investigate the analogous effects for $N>2$. In a series of papers [15–17], McGuire examined a related one-dimensional many-particle fermion system with one particle having spin-down in a sea of spin-up particles, interacting via δ -function potentials (both repulsive and attractive). For other models with periodic boundary conditions but different interactions, see Refs. [18–22].

If the particles are not confined in a box, the wave function obeys the standard vanishing boundary conditions (for bound states) or scattering boundary conditions, at infinite distances [23]. However, in most available models, rearrangement processes where a bound pair collides with a single particle to form a new pair are not allowed and cannot be examined. An exception is the work of McGuire on the attractive, two-body, δ -function interaction describing the scattering wave functions and the bound (N -body) states [24]. This model has been generalized, examined by means of several formalisms, or applied for different purposes [25–30]. As stated before, the attractive case for bosons has not been examined with periodic boundary conditions and the present work fills this lacuna for $N=3$.

II. MODEL DESCRIPTION

The stationary Schrödinger equation for three equal mass particles in one dimension with two-body δ -function interactions reads

$$-\frac{\hbar^2}{2m} \sum_{i=1}^3 \frac{\partial^2 \psi}{\partial y_i^2} + 2\tilde{c} \sum_{i<j} \delta(y_i - y_j) \psi = \tilde{E} \psi, \quad (1)$$

*Permanent address: Departamento de Física Fundamental y Experimental, Universidad de La Laguna, La Laguna, Tenerife, Spain.

where $y_i (i=1,2,3)$ are the particle coordinates. If they are enclosed in a box with length L , it is convenient to divide this equation by $\hbar^2/(2mL^2)$, and use instead

$$-\sum_{i=1}^3 \frac{\partial^2 \psi}{\partial x_i^2} + 2c \sum_{i<j} \delta(x_i - x_j) \psi = E \psi, \quad (2)$$

expressed in terms of the dimensionless quantities

$$x_i = y_i / L, \quad (3)$$

$$E = 2mL^2 \tilde{E} / \hbar^2, \quad (4)$$

$$c = 2m \tilde{c} L / \hbar^2. \quad (5)$$

Note that c is the only parameter of the model, and that, according to Eq. (5), the effect of enlarging the box or making the interaction stronger are equivalent. This work addresses the attractive case in particular, corresponding to $c \leq 0$. But the repulsive case ($c \geq 0$) is also covered, since the nature of the solutions for the repulsive case are the same as one class of solutions for the attractive case. Of particular interest is how the wave numbers associated with a wave function change, as the potential parameter c varies continuously from repulsion to attraction.

The δ -function potential produces a jump in the derivatives of the wave function where two particles meet. This jump is proportional to c and to the wave function at that point,

$$\left(\frac{\partial \psi}{\partial x_j} - \frac{\partial \psi}{\partial x_k} \right)_{x_j=x_k^+} - \left(\frac{\partial \psi}{\partial x_j} - \frac{\partial \psi}{\partial x_k} \right)_{x_j=x_k^-} = 2c \psi|_{x_j=x_k}. \quad (6)$$

Since the δ -function interaction allows the particles to cross each other, all orderings are possible, each ordering corresponding to a particular "region" of coordinate space and one of the permutations of the three particles. On the basis that the particles are bosons, it is sufficient to study the wave function in only one of these regions, specifically the "primary" region

$$R_{123}: 0 \leq x_1 \leq x_2 \leq x_3 \leq 1. \quad (7)$$

The wave function in any other region R_{ijk} of coordinate space is then simply obtained from the wave function in R_{123} by interchanging the particle labels. In region R_{123} , Eqs. (2) and (6) can be written as

$$-\sum_{i=1}^3 \frac{\partial^2 \psi}{\partial x_i^2} \psi = E \psi \quad (8)$$

for $x_1 \neq x_2 \neq x_3 \neq x_1$, and the jump conditions

$$\left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} \right) \psi \Big|_{x_{j+1}=x_j} = c \psi \Big|_{x_{j+1}=x_j}. \quad (9)$$

If periodic boundary conditions are also imposed, a displacement of 1 in any of the coordinates x_j leaves the function unchanged. In particular, in R_{123} this means that the wave function obeys

$$\psi(0, x_2, x_3) = \psi(x_2, x_3, 1). \quad (10)$$

Similarly, the derivatives satisfy

$$\frac{\partial}{\partial x} \psi(x, x_2, x_3) \Big|_{x=0} = \frac{\partial}{\partial x} \psi(x_2, x_3, x) \Big|_{x=1}. \quad (11)$$

In a two-body collision between particles of equal mass, the δ -function interaction can only interchange the momenta of the incident particles or leave them unchanged. In other words, there is no diffraction, that is, no "new" momenta, different from the initial ones, are created. For three equal mass particles with δ two-body interactions, the eigenstates can thus be written in terms of only three plane waves with (dimensionless) "momenta" $\{k_j\}$,

$$\psi(x_1 \leq x_2 \leq x_3) = \sum_P a(P) P \exp\left(i \sum_{j=1}^3 k_j x_j\right), \quad (12)$$

where the sum is over all permutations P of the $\{k_j\}$, and $a(P)$ are coefficients to be fixed by the boundary conditions determined by the periodicity [Eqs. (10) and (11)], and by the δ -function interaction [Eq. (9)]. This wave function form is known as the "Bethe ansatz," and it was first applied to spin chains [31]. In the context of the Bose gas, Yang and Yang [14] used a continuity argument to show that for positive c all states are given by Eq. (12) with real k 's, a result which was later established rigorously by Dorlas [32]. In the present work, it is shown that all states for $c \geq 0$ are continuously connected to $c \leq 0$ states in k space, so we are confident that the eigenstates discussed later form in fact a complete set. An important difference from the repulsive case is that for $c < 0$ the k 's may become complex.

From Eqs. (8) and (12), the energy is simply obtained as

$$E = \sum_{j=1}^3 k_j^2, \quad (13)$$

but this should not be interpreted as purely kinetic energy since there is generally a potential-energy contribution to E . Note that Eq. (8) is the Schrödinger equation only when the positions of the particles are all different. The true kinetic energy has to take into account the jumps in the wavefunction derivative at the region boundaries. The calculation of the potential energy is, however, somewhat involved and is discussed in the Appendix.

The structure of the coefficients $a(P)$ is imposed by the jump boundary condition (9) as explained, e.g., in Ref. [10]: The amplitudes for two permutations differing by a transposition of two particles are related by a factor $-e^{i\theta_{j\ell}}$,

$$a(123) = 1,$$

$$a(213) = -e^{i\theta_{21}}, \quad (14)$$

$$a(132) = -e^{i\theta_{32}},$$

$$\begin{aligned}
a(321) &= -e^{i(\theta_{21} + \theta_{31} + \theta_{32})}, \\
a(312) &= e^{i(\theta_{31} + \theta_{32})}, \\
a(231) &= e^{i(\theta_{21} + \theta_{31})},
\end{aligned} \tag{15}$$

where

$$e^{i\theta_{j\ell}} \equiv \frac{c - i(k_j - k_{\ell})}{c + i(k_j - k_{\ell})}. \tag{16}$$

By substituting Eqs. (12) and (14) into the periodicity conditions (10) and (11), the following set of coupled transcendental equations is found:

$$e^{-ik_j} = \exp \left[i \sum_{s=1}^3 \theta_{sj} \right], \quad j=1,2,3, \tag{17}$$

where, by convention, $\theta_{jj}=0$. Solving Eq. (17) for k_j gives

$$\begin{aligned}
k_1 &= 2\pi m_1 - \theta_{21} - \theta_{31}, \\
k_2 &= 2\pi m_2 - \theta_{12} - \theta_{32}, \\
k_3 &= 2\pi m_3 - \theta_{23} - \theta_{13},
\end{aligned} \tag{18}$$

for some set of integers $\{m_j\}$, while $\theta_{j\ell}$ is given in terms of k_j by

$$\theta_{j\ell} = i \ln \left[\frac{c + i(k_j - k_{\ell})}{c - i(k_j - k_{\ell})} \right] = -2 \arctan \left(\frac{k_j - k_{\ell}}{c} \right). \tag{19}$$

While it may appear to be natural to choose the principal branch of the logarithm and the arctangent, another choice is more appropriate. Since a state is uniquely defined by the set of numbers $\{k_j\}$, irrespective of the order, because the particles are bosons, it is convenient to order k_j 's, when they are real, according to

$$k_1 \leq k_2 \leq k_3. \tag{20}$$

Consistent with this, the ranges of θ_{21} , θ_{32} , and θ_{31} are chosen to satisfy

$$-2\pi < \text{Re}(\theta_{j\ell}) \leq 0, \tag{21}$$

on the basis that the corresponding $k_j - k_{\ell}$ are positive. In this way, solving for the set of $\{k_j\}$ is equivalent to solving for the set of $\theta_{j\ell}$, and it is noted that, for the above choice for the range of $\theta_{j\ell}$'s, $\theta_{j\ell}$'s vary continuously as c and/or the k_j 's vary continuously over their allowed ranges. This is also true if some of the k_j 's and/or $\theta_{j\ell}$'s become complex, as discussed in later sections. Thus m_j provides a unique classification of the energy levels, and for a given set of m_j , the energy eigenvalue (and eigenvector) can be followed continuously as a function of c , as c varies from ∞ to $-\infty$.

On taking the product of the three equations of the form of Eq. (17), it follows that the total momentum p is quantized,

$$p \equiv \sum_j k_j = 2\pi(m_1 + m_2 + m_3) = 2\pi n_p. \tag{22}$$

This is the eigenvalue of the corresponding total momentum operator, which commutes with the Hamiltonian H . It is clear that p is an invariant to the ‘‘motion’’ of an eigenvalue as c varies continuously from ∞ to $-\infty$. For each solution set $\{k_j\}$, there is another set $\{k'_j\}$ that also solves Eq. (17), and is related to the former by

$$k'_j = k_j + 2\pi n_0. \tag{23}$$

The transformation $\{k_j\} \rightarrow \{k'_j\}$ amounts to shifting the total momentum by $6\pi n_0$. This means that any state can be mapped to another state in the central momentum strip $-3\pi < p \leq 3\pi$, and vice versa, by such a transformation. Thus we shall limit ourselves to study only those states having total momentum in this strip, namely, $n_p = -1, 0, 1$.

A convenient set of variables, especially when the three k 's are real, that uniquely define the state is p , δ_1 , and δ_2 , where δ_1 and δ_2 are, respectively, the relative momenta between particles 12 and 23, namely,

$$\delta_1 \equiv k_2 - k_1, \tag{24}$$

$$\delta_2 \equiv k_3 - k_2. \tag{25}$$

Note that, when real, the order assumed for k_j [Eq. (20)] implies that $\delta_j \geq 0$. The k 's are given in terms of these variables by

$$k_1 = \frac{1}{3}(p - 2\delta_1 - \delta_2), \tag{26}$$

$$k_2 = \frac{1}{3}(p + \delta_1 - \delta_2), \tag{27}$$

$$k_3 = \frac{1}{3}(p + \delta_1 + 2\delta_2), \tag{28}$$

and the energy takes the form

$$E = \frac{1}{3}[p^2 + 2(\delta_1^2 + \delta_2^2 + \delta_1\delta_2)]. \tag{29}$$

Combinations of Eqs. (18) and (19) give the two coupled equations for δ_1 and δ_2 ,

$$\delta_1 = i \ln \left[\left(\frac{c + i\delta_1}{c - i\delta_1} \right)^2 \frac{c - i\delta_2}{c + i\delta_2} \frac{c + i(\delta_1 + \delta_2)}{c - i(\delta_1 + \delta_2)} \right] + 2\pi n_1, \tag{30}$$

$$\delta_2 = i \ln \left[\left(\frac{c + i\delta_2}{c - i\delta_2} \right)^2 \frac{c - i\delta_1}{c + i\delta_1} \frac{c + i(\delta_1 + \delta_2)}{c - i(\delta_1 + \delta_2)} \right] + 2\pi n_2, \tag{31}$$

where, on the basis that the principal part of the logarithm is taken, n_1 is not necessarily equal to $m_2 - m_1$, nor is n_2 necessarily equal to $m_3 - m_2$. In fact, unlike m_j , n_j does not have to remain constant as a given ‘‘root’’ of the coupled equations $\{\delta_1(c), \delta_2(c)\}$ changes continuously with a variation of c . That is why we shall not classify the roots according to ‘‘local’’ values $\{n_1(c), n_2(c)\}$, but according to their values $\{n_1^0, n_2^0\}$ for no interaction, namely, for $c=0$. These are unambiguously related to the set of quantum numbers m_j ; see Eqs. (35) and (36) below. If, as c changes, the argument of one of the logarithms, say z_j , crosses the negative real axis (which is the branch cut for the principal part of the logarithm), its phase changes abruptly by $\pm 2\pi$, and the corresponding n_j has to jump up or down by one unit in order to

follow the root continuously. Of course, these discontinuities have no physical consequence, and merely reflect the choice made for the branch of the logarithm. For several formal manipulations and in particular for the object of obtaining asymptotic expressions, it is useful to avoid the discontinuities by continuing analytically the logarithm across the branch cut, i.e., by passing to the contiguous Riemann sheet when the argument z_j crosses the real, negative axis. This will be discussed further in Sec. IV to clarify the trajectories of the k_j 's as c changes smoothly.

There are certain symmetries of the parametrizations δ_1 , δ_2 , and p which can lead to energy degeneracies. The interchange $\delta_1 \rightleftharpoons \delta_2$, together with the change in sign of p , are equivalent to the changes $k_1 \rightleftharpoons -k_3$ and $k_2 \rightleftharpoons -k_2$ which, for real k 's, invert the order of Eq. (20) to $-k_1 > -k_2 > -k_3$. This is also equivalent to taking the complex conjugate of the wave function. Thus, if $k_1 \neq -k_3$ and/or $k_2 \neq 0$, these are two different states with the same energy, a twofold degeneracy. On the other hand, if $k_1 = -k_3$ and $k_2 = 0$, which is the special case that $\delta_1 = \delta_2$ and $p = 0$, then this symmetry reproduces the same state, the wave function is real, and the state is nondegenerate. In terms of the classification of the states of the central momentum strip by n_j^0 , it follows that interchanging n_1^0 and n_2^0 ($n_1^0 \neq n_2^0$) amounts to an interchange of δ_1 and δ_2 , and [see Eq. (37) below], to a change of the sign of p , so that all signs of the k 's are changed and the complex conjugate state is obtained. But, for the "diagonal" case $n_1^0 = n_2^0$, there is no degeneracy. These states are real and even under the parity transformation $x_j \rightarrow -x_j$.

A second symmetry of the parametrizations δ_1 , δ_2 , and p is the interchange $\delta_1 \rightleftharpoons -\delta_2$, while p remains unchanged. This is equivalent to the changes $k_1 \rightleftharpoons k_3$ and $k_2 \rightleftharpoons k_2$, which invert the order of Eq. (20) to $k_1 > k_2 > k_3$ but do not change the momenta themselves. But since the order of the k 's is immaterial, this is just another way of labeling the same state. In terms of n_j^0 , this means that (n_1^0, n_2^0) and $(-n_2^0, -n_1^0)$ are actually the same state.

Because of the stated symmetry relations and the fact that any eigenstate can be translated by the total momentum shift (23) to the central momentum strip, an exhaustive analysis of all possible states is achieved by examining the cases $n_2^0 \geq n_1^0 \geq 0$, since any other case is either equivalent to one of them or obtained by a simple transformation. An understanding of the behavior of the roots and their limiting properties for different ranges of c requires a detailed analysis of how to carry out the analytical continuation of the logarithms in Eqs. (30) and (31) as c varies. This is provided in the following sections. To keep track of the global picture, a handy summary of the results is provided in Sec. IX, and a set of figures illustrate the essential aspects.

III. REFERENCE CASE OF "NO INTERACTION"

For $c = 0$ there is no interaction, and the particles move freely. In this case,

$$e^{i\theta_j} = -1, \quad (32)$$

and with the present choice for the range of the θ_j 's,

$$\theta_{21} = \theta_{32} = \theta_{31} = -\pi. \quad (33)$$

It follows that

$$a(ijk) = 1, \quad (34)$$

$$\delta_1 = 2\pi n_1^0 = 2\pi(m_2 - m_1 - 1), \quad (35)$$

$$\delta_2 = 2\pi n_2^0 = 2\pi(m_3 - m_2 - 1). \quad (36)$$

Equivalently, the k_j 's are all real multiples of 2π . Due to the conventional order (20), only the case where $n_j^0 \geq 0$ needs to be considered in order to account for all the states of the system.

The total momentum in the central momentum strip for a state (n_1^0, n_2^0) is determined by noticing, from Eq. (27), that if k_2 is to be a multiple of 2π , then $p + \delta_1 - \delta_2$ has to be a multiple of 6π . For any pair n_1^0 and n_2^0 , and $p = 2\pi n_p$ ($n_p = 0, \pm 1$), there is only one possible solution for n_p , namely,

$$n_p = \begin{cases} 0 & \text{if } n_1^0 - n_2^0 = 3n \\ -1 & \text{if } n_1^0 - n_2^0 = 3n + 1 \\ 1 & \text{if } n_1^0 - n_2^0 = 3n + 2, \quad n = 0, \pm 1, \pm 2, \dots \end{cases} \quad (37)$$

For the states where one of the n_j^0 's is zero, two k 's are equal. The equality of two k 's can occur only at $c = 0$, and at certain critical c values discussed in Sec. V. (In general, for $c \neq 0$, the wave function vanishes if two k_j 's are equal.) For the ground state, $n_1^0 = n_2^0 = 0$, the three k_j 's are equal, and the wave function is a constant.

The classification scheme used in the remainder of this paper, for the energy eigenvalues and states, is based on following δ_1 and δ_2 as continuous functions of c from the reference noninteracting system. A symbol such as (1,2) gives the values of the quantum numbers n_1^0 and n_2^0 , and identifies a given "root" $\{\delta_1(c), \delta_2(c)\}$ of the transcendental equations and the corresponding eigenstate (within the central strip of total momentum), irrespective of the value of c . Note that the three "quantum numbers" n_1^0 , n_2^0 , and n_p are equivalent to the set of quantum numbers $\{m_j\}$. The total momentum given in Eq. (37) is independent of the value of c , and the degeneracy of a root is also an invariant to the "motion" of the root with c .

IV. REAL k SOLUTIONS

On the assumption that the k_j 's all remain finite (and real), it follows that

$$\left. \begin{matrix} \theta_{21} \\ \theta_{32} \\ \theta_{31} \end{matrix} \right\} \rightarrow \begin{cases} 0 & \text{if } c \rightarrow \infty \\ -2\pi & \text{if } c \rightarrow -\infty, \end{cases} \quad (38)$$

with the consequence [see Eq. (18)] that

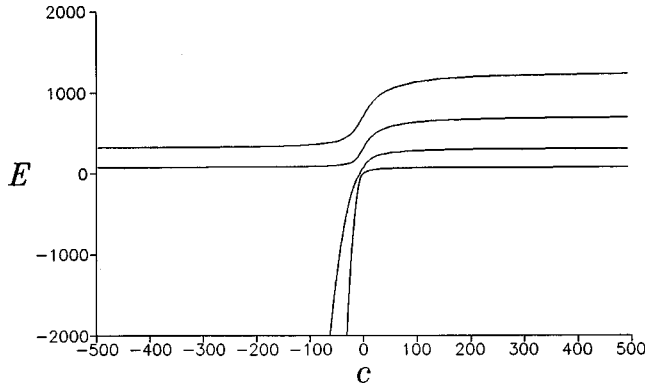


FIG. 1. $\langle E \rangle$ vs c for (n^0, n^0) . From bottom to top, $n^0=0, 1, 2$, and 3. The lines for $n^0=0$ and 1 extend to $-\infty$ as $c \rightarrow -\infty$.

$$\begin{aligned}
 -\infty \leftarrow c \rightarrow \infty, \\
 2\pi(m_1+2) \leftarrow k_1 \rightarrow 2\pi m_1, \\
 2\pi m_2 \leftarrow k_2 \rightarrow 2\pi m_2, \\
 2\pi(m_3-2) \leftarrow k_3 \rightarrow 2\pi m_3.
 \end{aligned} \tag{39}$$

Bounds on the k differences can be narrowed by examining separately the detailed properties of the θ 's for positive and negative c , by the following reasoning: On the basis of the chosen order for k_j [Eq. (20)], it follows that

$$k_3 - k_1 \geq k_2 - k_1, k_3 - k_2. \tag{40}$$

As a consequence, for $c > 0$ and $-\pi \leq \theta_{j'} \leq 0$ for $(j > \ell)$,

$$\tan\left(\frac{\theta_{31}}{2}\right) \leq \tan\left(\frac{\theta_{21}}{2}\right), \tan\left(\frac{\theta_{32}}{2}\right) \tag{41}$$

and

$$\theta_{31} \leq \theta_{21}, \theta_{32}, \tag{42}$$

so that

$$-\pi \leq \theta_{31} - \theta_{32} \leq 0 \tag{43}$$

and

$$\begin{aligned}
 2\pi n_1^0 - \pi &\leq 2\pi(m_2 - m_1) - \pi + 2\theta_{21} \\
 &\leq \delta_1 = k_2 - k_1 = 2\pi(m_2 - m_1) + 2\theta_{21} + \theta_{31} - \theta_{32} \\
 &\leq 2\pi(m_2 - m_1) + 2\theta_{21} \leq 2\pi(n_1^0 + 1).
 \end{aligned} \tag{44}$$

An analogous argument for $c < 0$ leads to

$$2\pi(n_1^0 - 1) < \delta_1 = k_2 - k_1 \leq 2\pi n_1^0 + \pi, \tag{45}$$

with the lower bound approached according to Eq. (39). Bounds for δ_2 involving n_2^0 have the same structure.

It is thus seen that if $n_1^0 \geq 2$ and $n_2^0 \geq 2$, then these k differences remain positive as c varies from ∞ to $-\infty$, with the consequence that the k_j 's are real for all c under these conditions. This also implies that the energy tends to a constant value for $|c| \rightarrow \infty$; see Fig. 1. For these states, the δ -function potential acts, for both very large positive and negative c ,

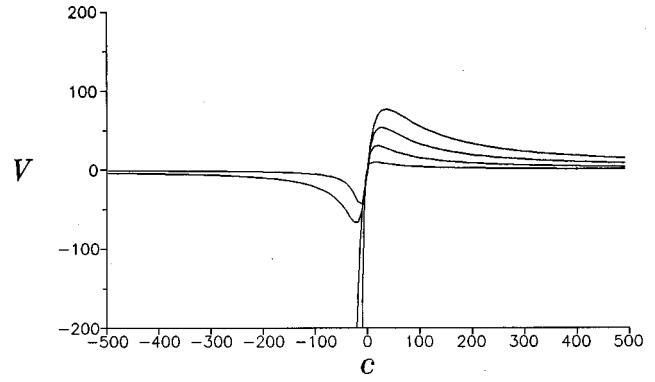


FIG. 2. $\langle V \rangle$ vs c for (n^0, n^0) . From bottom to top, $n^0=0, 1, 2$, and 3. The lines for $n^0=0$ and 1 extend to $-\infty$ as $c \rightarrow -\infty$.

effectively as an impenetrable barrier. That is, the wave function at the region boundaries, $x_i = x_j$, tends to zero. This can also be deduced from the jump conditions [Eq. (9)], since the derivatives produce only the finite k_j while c becomes infinite, so that consistency requires that ψ vanishes. The potential energy as a function of c decreases from zero to an intermediate minimum and then grows again toward zero as $c \rightarrow -\infty$, and vice versa for $c > 0$; see the Appendix and Fig. 2.

The above-deduced limitations on how δ 's change with c allow a more detailed discussion of these changes from the point of Eqs. (30) and (31). An appropriate starting point is to consider the limit of these equations when $c \rightarrow 0$, namely,

$$\delta_1 = i \ln \left[\left(\frac{\delta_1 - ic}{\delta_1 + ic} \right)^2 \frac{\delta_2 + ic}{\delta_2 - ic} \frac{(\delta_1 + \delta_2) - ic}{(\delta_1 + \delta_2) + ic} \right] + 2\pi n_1^0, \tag{46}$$

$$\delta_2 = i \ln \left[\left(\frac{\delta_2 - ic}{\delta_2 + ic} \right)^2 \frac{\delta_1 + ic}{\delta_1 - ic} \frac{(\delta_1 + \delta_2) - ic}{(\delta_1 + \delta_2) + ic} \right] + 2\pi n_2^0, \tag{47}$$

where the factors in the arguments have been rewritten to emphasize that the δ 's are in this limit the leading terms. The identification of n_j^0 is on the basis that, on expanding these equations as $c \rightarrow 0$, Eqs. (35) and (36) are obtained, namely,

$$\delta_1 = 2\pi n_1^0 + \frac{2n_1^0 n_2^0 + 2(n_2^0)^2 - (n_1^0)^2}{n_1^0 n_2^0 (n_1^0 + n_2^0) \pi} c + \dots, \tag{48}$$

with a symmetrical expression for δ_2 on interchanging n_1^0 and n_2^0 . These expansions are valid only if both $n_j^0 \neq 0$, while the exceptional cases are examined in Secs. VI and VII.

As c increases positively [always assuming the order of Eq. (20)], the phases of the factors in the arguments of the logarithms change; compare $\theta_{j'}$'s of Eq. (19), and the discussion of their behavior. On tracing this behavior as $c \rightarrow +\infty$, it is seen that the phase of the argument of each logarithm decreases by 2π , so this can be taken into account when changing Eqs. (46) and (47) into Eqs. (30) and (31) by setting $n_j(c \rightarrow \infty) = n_j^0 + 1$. For negative c , the phase changes are the opposite, and Eqs. (46) and (47) are appropriately changed into

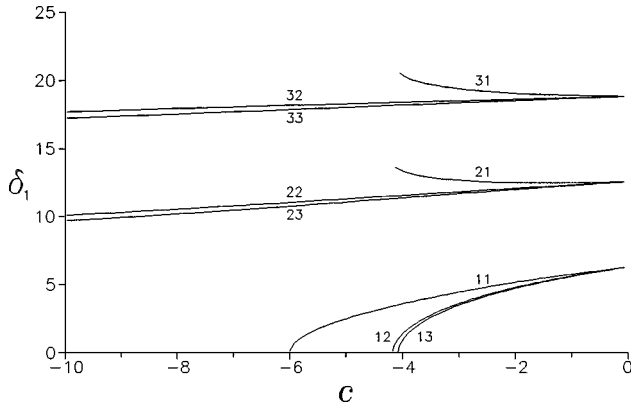


FIG. 3. δ_1 vs c . The numbers close to each line correspond to n_1^0 and n_2^0 . The figure for δ_2 is identical by interchanging n_1^0 and n_2^0 . The lines are only drawn up to the critical values of c where $\delta_1 = 0$ [for (1,1), (1,2); and (1,3)] or $\delta_2 = 0$ [for (2,1) and (3,1)]. For more negative values of c , the α - γ parametrization is used; see Figs. 5 and 6.

$$\delta_1 = i \ln \left[\left(\frac{-c - i\delta_1}{-c + i\delta_1} \right)^2 \frac{-c + i\delta_2}{-c - i\delta_2} \frac{-c - i(\delta_1 + \delta_2)}{-c + i(\delta_1 + \delta_2)} \right] + 2\pi(n_1^0 - 1), \quad (49)$$

$$\delta_2 = i \ln \left[\left(\frac{-c - i\delta_2}{-c + i\delta_2} \right)^2 \frac{-c + i\delta_1}{-c - i\delta_1} \frac{-c - i(\delta_1 + \delta_2)}{-c + i(\delta_1 + \delta_2)} \right] + 2\pi(n_2^0 - 1). \quad (50)$$

These are appropriate for expansions when $c \rightarrow -\infty$, but may of course be used for all values of c by analytic continuation. In the same vein, the related pair of equations with $n_j = n_j^0 + 1$ may be regarded as valid for all values of c by analytic continuation across the logarithm branch cut.

In summary, provided both $n_j^0 \geq 0$, then

$$\delta_j \underset{c \rightarrow \infty}{\sim} 2\pi(n_j^0 + 1) \left(1 - \frac{6}{c} \right) + O(c^{-2}), \quad (51)$$

while, provided both $n_j^0 > 1$, then

$$\delta_j \underset{c \rightarrow -\infty}{\sim} 2\pi(n_j^0 - 1) \left(1 + \frac{6}{-c} \right) + O(c^{-2}). \quad (52)$$

In contrast, if $n_1^0 = 1$, then δ_1 can approach 0 for finite negative c ; see Fig. 3. For more negative values of c , the k_j 's can become complex. The situation is similar for $n_2^0 = 1$. Section V discusses this situation. If any $n_j^0 = 0$, then δ_j vanishes at $c = 0$; see Sec. VI.

The case in which $n_1^0 = n_2^0$ is particularly simple to analyze. It follows from Eqs. (46) and (47), analytically continued for all values of c , that δ_1 and δ_2 satisfy the same equation and thus are equal, with the consequence that the three k 's for such an eigenstate remain equally spaced as c varies. After dropping the subscripts, and formally written for $c > 0$, the equation for the common δ is

$$\delta = i \ln \left[\frac{(c + i\delta)(c + 2i\delta)}{(c - i\delta)(c - 2i\delta)} \right] + 2\pi(n^0 + 1). \quad (53)$$

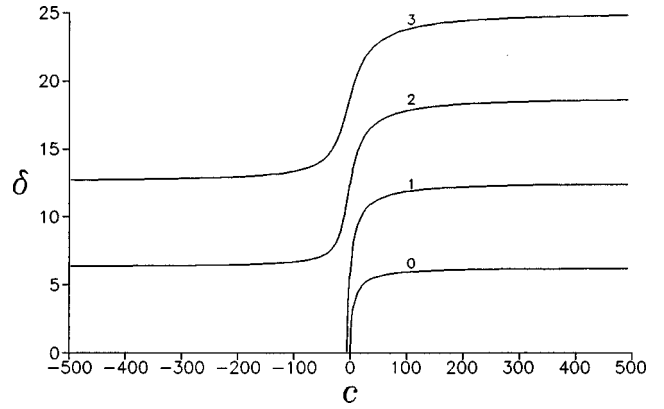


FIG. 4. δ vs c for (n^0, n^0) . From bottom to top, $n^0 = 0, 1, 2$, and 3.

Figure 4 illustrates how δ varies with c . By implicit differentiation,

$$\frac{d\delta}{dc} = \frac{6\delta(c^2 + 2\delta^2)}{c^2(c^2 + 5\delta^2) + 4\delta^4 + 6c(2\delta^2 + c^2)}. \quad (54)$$

If $n_1^0 = n_2^0 \neq 0$, Eq. (48) is consistent with the $c \rightarrow 0$ limit of this result.

V. STATES WITH AT LEAST ONE $n_j^0 = 1$: DIMER STATES

If one $n_j^0 = 1$, for definiteness $n_1^0 = 1$, then, from Eqs. (44) and (45), there is a possibility that δ_1 becomes 0 for some critical negative value $C(1, n_2^0)$ of c . Note that the equations for δ_1 and δ_2 are independent of p , so the critical value $C(1, n_2^0)$ has nothing to do with the value of p . [The discussion for the degenerate partner $(n_1^0, 1)$ follows similar lines, substituting n_1^0 with n_2^0 , δ_1 with δ_2 , and p with $-p$; see the discussion of the symmetries of this parametrization in Sec. II.] At a critical point $C(1, n_2^0)$, k_1 and k_2 become equal (if $n_2^0 = 1$ as well, all three k 's become equal), and the Bethe ansatz (12) form for the wave function is no longer valid because it vanishes. Of course, the normalization constant also vanishes, so that the normalized wave function does not vanish, but merely has a different functional form obtained by taking the limit as $c \rightarrow C(1, n_2^0)$ using the rule of l'Hospital. A similar case was found by Lieb and Liniger for one particular root in the case $N = 2$ [10].

Two different cases arise, according to whether $n_2^0 > 1$, or if $n_1^0 = n_2^0 = 1$. These cases are discussed in turn.

A. Case when $n_2^0 > 1$

The value of the critical point $C(1, n_2^0)$ and the behavior in its neighborhood, can be obtained by expanding Eqs. (49) and (50) for $\delta_1 \rightarrow 0$. For such a purpose it is useful to introduce the factors $u_j \equiv \delta_j/c$, $j = 1, 2$, and define $u_0 \equiv u_2(c = C)$ as the critical value of u_2 . After fairly extensive algebra, it follows that

$$c = C(1, n_2^0) + \frac{21 + 24u_0^2 + 8u_0^4}{6(1 + u_0^2)^2} u_1^2 + \dots, \quad (55)$$

with

$$C(1, n_2^0) = -4 - \frac{2}{1 + u_0^2}, \quad (56)$$

where u_0 is determined by the transcendental equation

$$3i \ln \frac{1 + iu_0}{1 - iu_0} + 2\pi(n_2^0 - 1) + 4u_0 + \frac{2u_0}{1 + u_0^2} = 0. \quad (57)$$

In the neighborhood of the critical point, u_2 changes according to

$$u_2 = u_0 - \frac{1}{2}u_1 + \frac{3 + 6u_0^2 + 2u_0^4}{6u_0(1 + u_0^2)}u_1^2 + \dots \quad (58)$$

It is seen that $\delta_1(c)$ has a square-root singularity at the critical point, being real for $c > C(1, n_2^0)$ and pure imaginary for $c < C(1, n_2^0)$. An analytic connection between real and imaginary branches of δ_1 can be made by attributing c with a small imaginary part. The association that is used in the following parametrization is consistent with c having a small negative imaginary part, essentially adding a small dissipative contribution to the Hamiltonian. It is also noticed from Eq. (56) that all the critical values of c lie between -6 and -4 . Actually, to three decimal places, the lowest critical value is $C(1, 2) = -4.163$, increasing toward -4 as u_0 and n_2^0 , increase. These aspects are illustrated in Fig. 3.

For $c < C(1, n_2^0)$, k_1 and k_2 become a complex conjugate pair, while k_3 remains real. The discussion of the root in this region is better examined by using a new set of real variables α and γ , defined by

$$\delta_1 = -2i\alpha, \quad (59)$$

$$\delta_2 = i\alpha - 3\gamma,$$

so that

$$k_1 = i\alpha + \gamma + p/3,$$

$$k_2 = -i\alpha + \gamma + p/3, \quad (60)$$

$$k_3 = -2\gamma + p/3.$$

This is consistent with Eq. (58) for $\alpha \rightarrow 0$, on the basis that both α and γ are real. This parametrization could of course be used for all c [with α possibly imaginary], since $\delta_1/2 = -i\alpha$ has the physical meaning of the relative momentum between particles 1 and 2, while 2γ is the relative momentum between the pair 12 and particle 3:

$$-i\alpha = \delta_1/2 = \frac{k_2 - k_1}{2}, \quad (61)$$

$$2\gamma = k_3 - \frac{p}{3} = \frac{2}{3} \left(k_3 - \frac{k_1 + k_2}{2} \right). \quad (62)$$

For real α , $1/\alpha$ gives a measure of the size of the ‘‘bound states’’ formed. Of course, in a finite box all states are, strictly speaking, bound, i.e., their energies are discrete and their spatial extension is limited by the box length. But when α is real, the state is localized even further so that the prob-

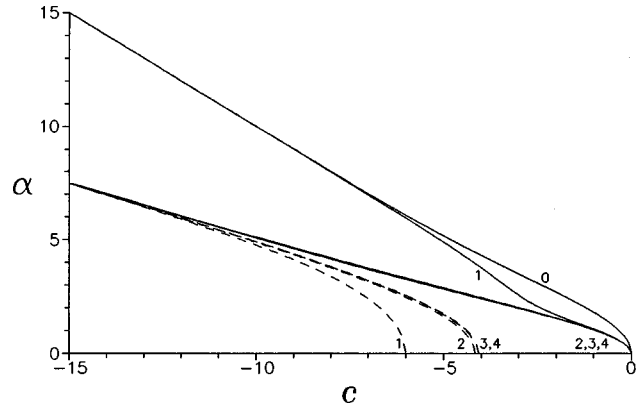


FIG. 5. α vs c . Solid lines: $n_1^0 = 0$. Dashed lines: $n_1^0 = 1$. The number close to the lines is n_2^0 .

ability of a pair of particles being close together has been significantly enhanced. In addition, the energy has a negative contribution [see Eq. (63) below], so that an energy gap arises in the spectrum between states with real or imaginary α ; see Fig. 1. Since these are all basic ingredients of proper bound states, this terminology seems justified.

With this parametrization, the total energy is decomposed into separate quadratic contributions from the three variables,

$$E = -2\alpha^2 + 6\gamma^2 + p^2/3, \quad (63)$$

and the system of transcendental equations takes the form

$$-2\alpha = \ln \left[\left(\frac{-c - 2\alpha}{-c + 2\alpha} \right)^2 \frac{-c - \alpha - 3i\gamma}{-c + \alpha + 3i\gamma} \frac{-c - \alpha + 3i\gamma}{-c + \alpha - 3i\gamma} \right], \quad (64)$$

$$i\alpha - 3\gamma = i \ln \left[\left(\frac{-c + \alpha + 3i\gamma}{-c - \alpha - 3i\gamma} \right)^2 \frac{-c + 2\alpha}{-c - 2\alpha} \frac{-c - \alpha + 3i\gamma}{-c + \alpha - 3i\gamma} \right] + 2\pi(n_2^0 - 1), \quad (65)$$

which corresponds to the correct phase form for $c < 0$, according to Eqs. (49) and (50). It is consistent to solve these equations maintaining α and γ real, which is also consistent with the local behavior Eq. (58), as $\alpha \rightarrow 0$. Before entering into the detailed analysis of the equations, it is worth examining Figs. 5 and 6 to quickly visualize the behavior of these

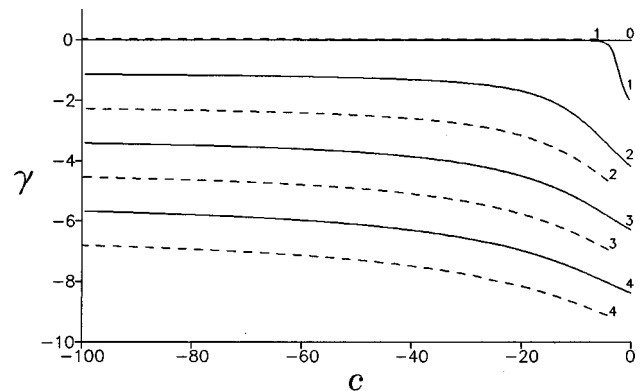


FIG. 6. γ vs c . Solid lines: $n_1^0 = 0$. Dashed lines: $n_1^0 = 1$. The number close to the lines is n_2^0 .

two parameters with c . Solid lines correspond to $n_1^0=0$ and dashed lines to $n_1^0=1$, whereas the numbers close to the different lines give n_2^0 . As c becomes more negative, α increases. This concentrates the wave function to where the particles are close together, and $\langle V \rangle$ and $\langle E \rangle$ become very large and negative; see, in Figs. 1 and 2, the lines for $n=0, 1$. A prominent feature in Fig. 5 is the grouping into two asymptotic behaviors for α , as $c \rightarrow -\infty$. These will be associated later with dimer and trimer configurations. Note also that all states with $n_1^0=0$ have a common critical point at $c=0$ (where $\alpha=0$), while for $n_1^0=1$ the critical points spread from $c=-6$ to -4 . Another interesting point is the quasi-invariance of α with respect to n_2^0 for $n_2^0 \geq 2$ at fixed c . These states have essentially the same binding strength and differ only by pair-single relative momentum, and possibly by total momentum. Figure 6 for γ has a simpler structure based on a rather regular pattern of lines with equally spaced asymptotic values. Except for the two cases (0,0) and (1,1) with $\gamma=0$ for all c 's, which corresponds to no relative motion between a particle pair and a single particle, when c becomes more negative, γ varies smoothly and tends to a constant value. When γ is essentially constant, c changes the strength of the attraction between the pair (i.e., the value of α), but not the motion of the third particle with respect to the pair.

The structure of the spectrum of energy levels can be described in terms of how the energy varies as the three quantum numbers n_1^0 , n_2^0 , and n_p change. This can be attributed to several types of "elementary excitations" which are associated with different physical effects. Within the central momentum strip, for states with complex k_j 's and for $-c$ large, these are as follows. (a) As n_2^0 varies, a change of relative pair-single motion by $\Delta_\gamma \approx \pi/3$, with α essentially constant and $|p|$ constant. In Fig. 6, this is not possible between all contiguous levels of γ , but only for those where $n_p=1$ and $n_{p'}=-1$; see Eq. (37). If one of the states has momentum zero, a jump to the nearest level necessarily implies, in addition to Δ_γ , an elementary total momentum jump $\Delta_p=2\pi$. (b) Transitions between a trimer and a dimer state or from a dimer to a pair-absent state, with $\delta_\alpha \approx -c/2$. (c) A minimum total momentum jump by 2π , with α and γ constant. This may only occur between the states (0,0) and (0,1) or (1,0). Any other transition changes γ . But α and γ may also stay constant if the system changes to a different momentum strip by a total momentum translation of $\Delta_p=6\pi$. Of course, multiples or combinations of these elementary excitations are possible, and complicate the spectrum considerably.

The detailed quantitative features of α and γ as functions of c are now examined. On the basis that α and γ are real, the real part of Eq. (65) is

$$\frac{3}{2}i \ln \left[\frac{(-c+\alpha-3i\gamma)(-c-\alpha-3i\gamma)}{(-c+\alpha+3i\gamma)(-c-\alpha+3i\gamma)} \right] = 3\gamma + 2\pi(n_2^0-1). \quad (66)$$

This provides upper and lower bounds for γ , namely,

$$-(4n_2^0-1)\pi/6 < \gamma < -(4n_2^0-7)\pi/6. \quad (67)$$

Equation (66) may also be written as

$$\arctan \left(\frac{6\gamma c}{c^2-9\gamma^2-\alpha^2} \right) = -\gamma - 2\pi(n_2^0-1)/3, \quad (68)$$

which is useful for the determination of the asymptotic behavior of α and γ .

It is also possible to solve for γ^2 in Eq. (64) in terms of α and c :

$$\gamma^2 = \frac{e^{-\alpha}(c-2\alpha)^2(c-\alpha)^2 - e^\alpha(c+2\alpha)^2(c+\alpha)^2}{9[e^\alpha(c+2\alpha)^2 - e^{-\alpha}(c-2\alpha)^2]}. \quad (69)$$

As $\alpha \rightarrow 0$, $\gamma^2(\alpha=0) = c^2(6+c)/[-9(4+c)]$. This is identical to Eq. (56) for the relation between δ_2 and c at a critical value of c .

The asymptotic behavior as $c \rightarrow -\infty$ is now investigated. According to Eq. (67), γ remains finite while α satisfies Eq. (64). Both positive and negative α are solutions to this equation, but since these just correspond to an interchange of k_1 and k_2 , only the positive root is examined. Equation (64) can be rewritten as an equation involving only real quantities, namely,

$$-2\alpha = \ln \left[\left(\frac{-c-2\alpha}{-c+2\alpha} \right)^2 \frac{(-c-\alpha)^2 + 9\gamma^2}{(-c+\alpha)^2 + 9\gamma^2} \right]. \quad (70)$$

The obvious (but invalid) approach to try when making an asymptotic expansion is to expand in powers of γ^2 , since the other factors involve c . This implies that α must also remain finite, and leads to the requirement that $c \rightarrow -6$, an inconsistency. It follows that either $(-c-2\alpha) \rightarrow 0$ or $(-c-\alpha) \rightarrow 0$ in the limit $c \rightarrow -\infty$. But it is noticed that as c changes from its critical value $C(1, n_2^0)$ to $-\infty$, α changes from 0 to its asymptotic behavior; however, the factors in the argument of the logarithm, $-c \pm 2\alpha$ and $(-c \pm \alpha)^2 + 9\gamma^2$, must remain positive, or an imaginary phase factor must be added to the right-hand side. Since such a case would imply that α becomes complex; this is not allowed. Another way to understand the preservation of sign of all factors is that if one of them becomes zero for a finite c (and α), the logarithm, and the left-hand side of the equation, would be infinite in absolute value, which is again inconsistent with the finite value of α on the right-hand side. The only form of α that maintains all factors positive is $\alpha = -\frac{1}{2}c + \beta$, with $\beta < 0$ and $\beta/c \rightarrow 0$ asymptotically. A straightforward expansion then gives

$$\beta = 3ce^{c/2} - 9c^2e^c + \dots, \quad (71)$$

$$\alpha = -\frac{1}{2}c + 3ce^{c/2} - 9c^2e^c + \dots,$$

and, from Eq. (68),

$$\gamma = -\frac{2\pi}{3}(n_2^0-1) \left[1 - \frac{8}{c} + \dots \right], \quad (72)$$

as the asymptotic expansions for both α and γ .

B. Case when $n_2^0 = n_1^0 = 1$

As previously mentioned, this implies that $\delta_1 = \delta_2$ for all c , and the common δ is determined by Eq. (53), which is appropriate for $c > 0$. Reexpressing this for $c < 0$, retaining a continuous relation for the phase, gives

$$\delta = i \ln \left[\frac{(-c - i\delta)(-c - 2i\delta)}{(-c + i\delta)(-c + 2i\delta)} \right], \quad (73)$$

and taking into account that $n^0 = 1$. Clearly $\delta = 0$ is a solution of this equation. But to find the corresponding critical value $C(1,1)$ of c , and the behavior in the neighborhood of this critical point, an expansion is needed. This is easily accomplished to yield

$$c = -6 + \frac{1}{6} \delta^2 + \dots \quad (74)$$

This immediately shows that the critical value is $C(1,1) = -6$, and that there is a square-root singularity of δ as a function of c . For $c < -6$, $\delta = -i\alpha$ is pure imaginary (negative imaginary if the same connection around the singularity is used as in Sec. V A). It follows that the k_j 's are given in terms of this parametrization by

$$\begin{aligned} k_3 &= -i\alpha + p/3, \\ k_2 &= p/3, \\ k_1 &= i\alpha + p/3, \end{aligned} \quad (75)$$

while α is determined by

$$\alpha = \ln \left(\frac{1 - 3\alpha' + 2\alpha'^2}{1 + 3\alpha' + 2\alpha'^2} \right), \quad (76)$$

where $\alpha' = \alpha/c$. [Contrast this with Eq. (60). The associations made for the k_j in Eq. (75) are more natural here, since $\delta_1 = \delta_2$ and the three k_j change continuously across the critical point, but in fact Eq. (60), with $\gamma = 0$, could be used as well because the state is defined by the three ‘‘momenta’’ regardless of the ordering convention.]

Clearly, if $\alpha' \rightarrow 0$ as $c \rightarrow -\infty$, then $\alpha \rightarrow 0$. But on expanding to look at the correction terms, this assumption implies that $c \rightarrow 6$, an inconsistent result. It follows that α grows to ∞ asymptotically. On the basis that only $\alpha > 0$ solutions are needed ($\alpha' < 0$), the vanishing of the denominator in the argument of the logarithm requires either $\alpha' \rightarrow -1$ or $\alpha' \rightarrow -\frac{1}{2}$ as $c \rightarrow -\infty$. Only the latter is consistent with no accumulation of phase, as c changes from -6 to $-\infty$, and the reality of α . [Note that, by a similar argument to the one below Eq. (70), the numerator and denominator in Eq. (76) must preserve their sign as c varies from -6 to $-\infty$, which implies the bound $2\alpha < -c$.] On setting $\alpha = -\frac{1}{2}c + \eta$, it follows on expansion that

$$\alpha = -\frac{1}{2}c + 3ce^{c/2} + \dots, \quad (77)$$

as the asymptotic behavior of α in this case.

VI. STATES WITH ONE $n_j^0 = 0$: DIMER AND TRIMER STATES

This group of states are of the form $(0, n_2^0)$, and of course their degenerate partners. Only the case $(0, n_2^0)$ is explicitly treated here, since its corresponding partner state is simply obtained by symmetry, specifically for the states when $c < 0$ by changing the sign of γ . For $c \rightarrow \infty$, these states fit into the formulation of Eq. (51), so no further discussion of this limit is needed.

As $c \rightarrow 0$, the starting point for the analysis is the pair of equations (46) and (47). Since $n_1^0 = 0$, δ_1 and c are to approach 0 simultaneously, and it is to be expected by analogy with the other cases that c will be proportional to δ_1^2 . This is confirmed by the following argument: Since $\delta_1 \rightarrow 0$, then the argument of the logarithm in Eq. (46) must approach 1. For the ratios of the terms involving δ_2 , these approach 1, since they are dominated by the common nonzero value of δ_2 . That leaves the square term. For this to approach 1, each factor must be dominated by the common δ_1 , which implies that it is the ratio c/δ_1 that is small and can be used as a variable for which the logarithm is expanded, as well as the ratios c/δ_2 and δ_1/δ_2 , all of which vanish as $c \rightarrow 0$. Explicitly, the expansions of Eqs. (46) and (47) are

$$\delta_1 = 4\frac{c}{\delta_1} - \frac{4c^3}{3\delta_1^3} - 2\frac{c\delta_1}{\delta_2^2} + O(\delta_1^4), \quad (78)$$

$$\delta_2 = 2\pi n_2^0 - 2\frac{c}{\delta_1} + \frac{2c^3}{3\delta_1^3} + 6\frac{c}{\delta_2} - 2\frac{c\delta_1}{\delta_2^2} + O(\delta_1^4).$$

It follows that c is proportional to δ_1^2 , as was to be deduced. Rearrangement of these series for $c \rightarrow 0$ gives the expansion in powers of δ_1 as

$$c = \frac{1}{4} \delta_1^2 + \left[\frac{1}{192} + \frac{1}{32(\pi n_2^0)^2} \right] \delta_1^4 + \dots, \quad (79)$$

$$\delta_2 = 2\pi n_2^0 - \frac{1}{2} \delta_1 + \frac{3\delta_1^2}{4\pi n_2^0} + \dots$$

For $c < 0$, the parametrization of Eq. (59) is appropriate. In the limit $c \rightarrow -0$, the ratio c/δ_1 transforms according to

$$\frac{c}{\delta_1} \rightarrow \frac{1}{4} \delta_1 \rightarrow -\frac{1}{2} i\alpha \leftarrow i\frac{c}{2\alpha}, \quad (80)$$

with the consequence that Eqs. (46) and (47) become

$$-2\alpha = \ln \left[\left(\frac{2\alpha + c}{2\alpha - c} \right)^2 \frac{(\alpha + c)^2 + 9\gamma^2}{(\alpha - c)^2 + 9\gamma^2} \right], \quad (81)$$

$$\begin{aligned} i\alpha - 3\gamma &= i \ln \left[\left(\frac{2\alpha - c}{2\alpha + c} \right) \left(\frac{i\alpha - ic - 3\gamma}{i\alpha + ic - 3\gamma} \right)^2 \left(\frac{-i\alpha - ic - 3\gamma}{-i\alpha + ic - 3\gamma} \right) \right] \\ &+ 2\pi n_2^0. \end{aligned} \quad (82)$$

It is also important to note that, as a consequence of the analytic continuation into the $c < 0$ region, $2\alpha + c > 0$ and $\gamma \rightarrow -\delta_2/3 < 0$. To avoid further singularities in the logarithmic expressions (which would lead to inconsistency between

right and left sides of the transcendental equations), these constraints must hold for all $c < 0$.

For exploring the behavior as $c \rightarrow -\infty$, Eq. (81) for α has an appropriate form for expansion about large $-c$ and α . But if one term in each of the factors is to dominate the expansion, then the result would imply that the logarithmic expression becomes finite, a result inconsistent with the left-hand side approaching $-\infty$. As a consequence, since $\alpha > -c/2$, either $\alpha \rightarrow -c/2$ or the combination $\alpha \rightarrow -c$ and $\gamma \rightarrow 0$ must occur. The first alternative is now shown to be valid only for $n_2^0 > 1$, while the second alternative is valid only if $n_2^0 = 1$.

The limiting case $\alpha = -\frac{1}{2}c + \beta$ leads to a straightforward expansion of Eq. (81),

$$-2\alpha = c - 2\beta = 2\ln\left(\frac{\beta}{-3c}\right) + \frac{22\beta}{3c} + \dots, \quad (83)$$

which can be rewritten as the equation

$$\beta = -3ce^{c/2} + 9c^2e^c + \dots \quad (84)$$

for β . As $c \rightarrow -\infty$, this vanishes exponentially. The behavior of γ is to be obtained from Eq. (82). But the dominant quantity c is multiplied by the phase factors $\pm i$, so that an asymptotic expansion carries along a phase change for the logarithm. On carefully analyzing how the various factors change as c changes from 0 to $-\infty$, a phase change of $e^{3\pi i}$ in the argument of the logarithm is found. The real part of Eq. (82) determines γ , which after expanding and rewriting gives

$$\gamma = -\left(\frac{2}{3}n_2^0 - 1\right)\pi\left(1 - \frac{8}{c}\dots\right). \quad (85)$$

Since it is required that $\gamma < 0$, it is seen that this expansion is only valid for $n_2^0 > 1$.

The limiting case $\alpha = -c + \eta$ also allows a straightforward expansion of Eq. (81), but in this case the resulting equation for η involves γ in the lowest-order term, namely,

$$\eta^2 + \gamma^2 = 36e^{-2}n_2^0c^2e^{2c}\left(1 - \frac{5\eta}{3c}\dots\right). \quad (86)$$

Since both η and γ are real, this implies that both these quantities must vanish asymptotically as $c \rightarrow -\infty$. In this case, Eq. (82) accumulates a phase $e^{3\pi i/2}$ in the argument of the logarithm when transforming the factors, so that they will be dominated by a positive real part in the limit. What is crucially different in this case from the previous one is the presence of finite complex factors $-3\gamma \mp i\eta$. As a result, the real part of Eq. (82) has the asymptotic expansion

$$-3\gamma = \frac{3}{2}\arctan\left(\frac{-\eta}{-3\gamma}\right) + \left(2n_2^0 - \frac{3}{2}\right)\pi - \frac{9\gamma}{2c} + \dots \quad (87)$$

As $c \rightarrow -\infty$, γ must vanish for this case, as was deduced from the expansion of the α equation. Thus, in the limit, the identity

$$\lim_{c \rightarrow -\infty} \arctan\left(\frac{\eta}{-3\gamma}\right) = \left(\frac{4}{3}n_2^0 - 1\right)\pi \quad (88)$$

must be satisfied. Since the magnitude of the arctangent is bounded by $\pi/2$, this identity can only be satisfied if $n_2^0 = 1$, in which case the limiting ratio of η and γ is determined by the condition $\eta = -3\gamma \tan(\pi/3)$. In summary, for $n_2^0 > 1$ the asymptotic behavior of α is $\alpha \rightarrow -c/2$, which gives states of the dimer type, while for $n_2^0 = 1$, $\alpha \rightarrow -c$, and all three particles are forced to be close to one another, a trimer state. These associations will be discussed in Sec. VIII.

VII. GROUND STATE: $n_1^0 = n_2^0 = 0$

Since n_1^0 and n_2^0 are equal, it follows that $\delta_1 = \delta_2 \equiv \delta$. Near $c = 0$ and for $c > 0$, the appropriate equation for determining δ is Eq. (46), which is modified for equal δ 's to be

$$\delta = i\ln\left[\frac{(\delta - ic)(2\delta - ic)}{(\delta + ic)(2\delta + ic)}\right]. \quad (89)$$

The behavior as $c \rightarrow \infty$ is covered by the expansion of Eq. (53), with an asymptotic form identical to Eq. (51). Since $\delta \rightarrow 0$ as $c \rightarrow 0$, it is necessary that the argument of the logarithm must approach 1, which requires that $c \rightarrow 0$ faster than does δ . Thus the expansion parameter is c/δ , so that, after expansion and rearrangement,

$$c = \frac{1}{3}\delta^2 + \frac{1}{108}\delta^4 + \dots \quad (90)$$

For $c < 0$, the parametrization of Eq. (75) is used, this being equivalent to $\delta = -i\alpha$ with $\alpha > 0$. The ratio $-ic/\delta$ for $c > 0$ thus becomes c/α for $c < 0$, and Eq. (89) becomes

$$\alpha = \ln\left[\frac{(\alpha - c)(2\alpha - c)}{(\alpha + c)(2\alpha + c)}\right]. \quad (91)$$

This is identical to Eq. (76), but now the constraint is that $\alpha > -c$. This constraint requires that as $c \rightarrow -\infty$, α must become infinite, and the expansion of the logarithm is about a singular point of the logarithm. The only possible form is $\alpha = -c + \eta$, with $\eta > 0$ approaching zero. After rearrangement, the resulting expansion gives

$$\eta = -6ce^c - 36c^2e^{2c} + \dots \quad (92)$$

which is consistent with η being positive.

VIII. TYPES OF STATES AND THEIR REPRESENTATION

The states are best represented as contour plots of the probability density (and of the phase if required) in a "ternary phase diagram" for the variables

$$\begin{aligned} r_{12} &= x_2 - x_1, \\ r_{23} &= x_3 - x_2, \\ r_{31} &= 1 + x_1 - x_3, \end{aligned} \quad (93)$$

constrained to the region R_{123} , $0 \leq r_{ij} \leq 1$. Note that these three coordinates always add up to 1. In this diagram the

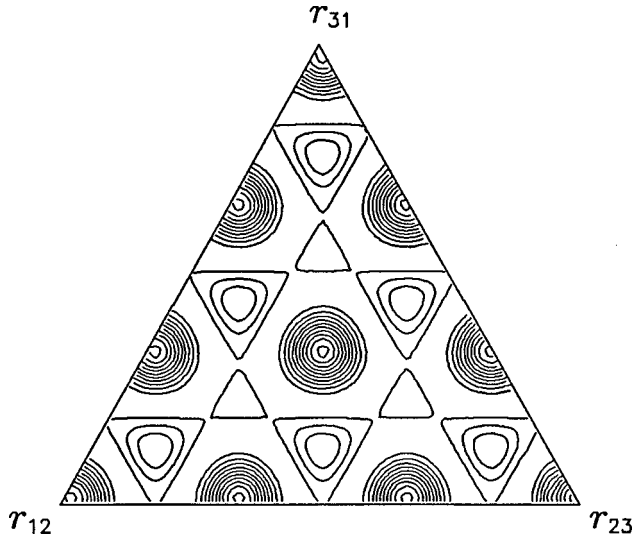


FIG. 7. Contour plot of the probability density of the state (3,3) at $c=1$. The interpretation of a “ternary phase” type of diagram is explained in the text.

coordinate points are represented in an equilateral triangle. Each of the base lines corresponds to one of the coordinates r_{ij} being zero, and each point in the base line corresponds to a particular location of the third particle at the right or left side of the pair ij (the closer to the vertex, the closer the third particle is to the pair). The lines parallel to the base are lines of constant r_{ij} . The value of r_{ij} increases from zero at the base to 1 at the opposite vertex (labeled as r_{ij} in the figures). The center of the triangle is the point where the three distances are equal to $\frac{1}{3}$. Near the vertex r_{ij} , the distance between particles j and i is also small (and tends to zero at the vertex itself); the difference from the basis region is that now the third particle is *between* the particles j and i .

In summary, bases are associated with two particles being together (dimer configurations), and vertices with the three particles being together (trimers). However, in a general state with three real k 's, there is no bias toward these configurations. Recall that the wave functions in R_{123} are linear combinations of six exponentials that can be obtained from the (123) form,

$$e^{i(k_1x_1+k_2x_2+k_3x_3)}, \quad (94)$$

by permuting the k 's in all possible manners. The probability density (square modulus) of any of these real k plane-wave terms is constant; in other words, in these plane waves none of the particle configurations is favored. The interference between the six different plane waves, however, destroys the spatial homogeneity (except for the ground state at $c=0$), and provides some structure with maxima and minima; see Fig. 7. The complex k case is different, see Figs. 8 and 9 for examples of trimer and dimer states. Equation (94) for the (123) exponential may now be written, using the parametrization in Eq. (60), as

$$e^{i(x_1+x_2+x_3)p/3} e^{i\gamma(x_1+x_2-2x_3)} e^{\alpha(x_2-x_1)}, \quad (95)$$

where the plane wave for the center-of-mass motion, a plane wave for relative motion of the pair 12 with respect to particle 3, and a real exponential can be recognized; for $\alpha > 0$,

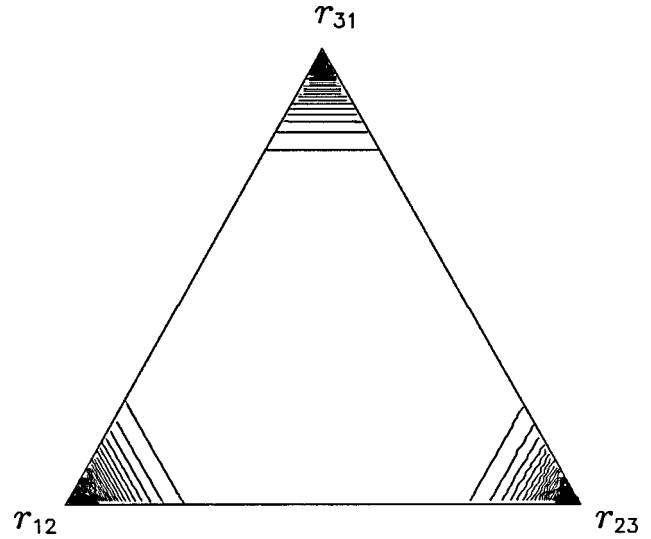


FIG. 8. Contour plot of the probability density of the state (0,0) at $c=-9$.

the exponent is positive, and it favors the trimer configuration of the vertex ($r_{12}=1$). By permuting k_1 and k_2 , one finds instead, in the term (213), a negative exponent that favors the dimer configurations $r_{12}=0$. Of course the other two pairs, 13 and 23, also have a corresponding set of dimer and trimer contributions, so that the six terms of the wave function can be separated into two groups: Three of them, (123), (231), and (312), represent trimer configurations, and the other three, (213), (132), and (321), represent dimer configurations. The relative weights among them are determined by the amplitudes a_{ijk} . For “trimer states,” the three trimer terms dominate the linear combination, and the energy becomes, as $c \rightarrow -\infty$, the energy of an actual trimer state (for three particles on an infinite line). For “dimer states,” there is also significant density along the edges of the triangle (not only at the vertices), and the energy tends to the energy of the actual dimer (on the infinite line), plus the contributions from relative motion of the dimer with the free particle and

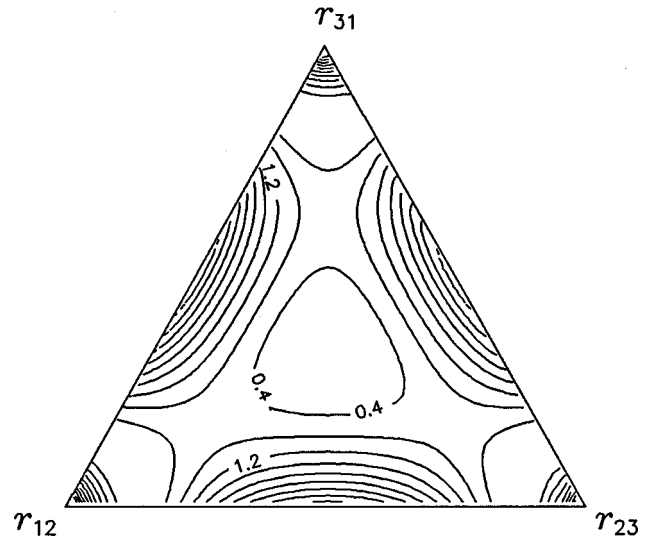


FIG. 9. Contour plot for the probability density of the state (0,2) at $c=-9$.

of the center-of-mass motion. This is consistent with our expectation of reproducing infinite line results in the limit of a large box. As a concrete example, the (unnormalized) states (0,0) and (1,1) for $c \leq -6$ are examined: In both cases $\gamma = p = 0$, and they can be written, using Eqs. (12), (15), (16), and (91), as

$$\psi = e^{\alpha r_{12}} + e^{\alpha r_{23}} + e^{\alpha r_{31}} + \frac{2\alpha - c}{2\alpha + c} (e^{-\alpha r_{12}} + e^{-\alpha r_{23}} + e^{-\alpha r_{31}}). \quad (96)$$

As $c \rightarrow -\infty$, the factor multiplying the dimer terms in parentheses tends to 3 for (0,0) (which makes this contribution negligible) but to ∞ for (1,1). Figure 8 shows the ground state (0,0) for negative c .

An important aspect of these associations is that the trimer or dimer character changes continuously along a given root as c varies, and only asymptotically ($c \rightarrow -\infty$) is the separation between trimer and dimer states unambiguous. For any finite negative c , the complex k roots have nonzero dimer and trimer components. Note, for example, how the state (0,1) goes from dimer-dominated to trimer-dominated behavior as c becomes more negative in Fig. 5. In the same vein, even though the threshold between real and complex k is well defined, and it occurs at a critical value of c , there are no dramatic (discontinuous) changes in the wave function, and the energy varies smoothly with c (see Fig. 1) in the neighborhood of the critical c values. However, a different qualitative behavior (of the energy and state probability density) becomes clear when comparing the states below and above the critical point as the distance from C increases. Thus the critical values indicate a transition of the root from one character, without pair formation, to another where dimers or trimers can be recognized.

IX. SUMMARY

A model of three bosons subject to δ -function interactions and periodic boundary conditions has been analyzed. In particular, a description of the eigenstates and their behavior has been given in terms of three momenta k_i , $i = 1, 2, 3$, or two sets of alternative parametrizations, δ_1 , δ_2 , and p and α , γ , and p , convenient, respectively, for the cases where the k 's are real or complex. The roots can be primarily classified according to whether the three momenta remain real, or not, for all c . In the second case the wave function tends to concentrate asymptotically around dimer or trimer configurations, and the energy decreases quadratically with c as $c \rightarrow -\infty$. The critical values of c required to form the bounds (go from real to complex k 's) have been provided.

The main features of the root behavior as c varies are now summarized. [Using the symmetry properties or total momentum translations, the behavior of any other state is obtained from the ones we consider explicitly, namely states (n_1^0, n_2^0) , $n_1^0 \leq n_2^0$, in the central momentum strip, $n_p = 0, \pm 1$.] Relations satisfied by all roots are as follows.

(i) The total momentum p (within the central strip) is given from n_1^0 and n_2^0 by Eq. (37). It is constant as c varies for a given root. The total energy varies according to (29) or (63).

$$(ii) \delta_j(c=0) = 2\pi n_j^0.$$

(iii) $\delta_j \rightarrow 2\pi(n_j^0 + 1)$ as $c \rightarrow \infty$.

The different particular cases are characterized by the following properties:

(i) (0,0): $C(0,0) = 0$, $p = 0$, $\gamma = 0$, and $\alpha \sim -c$ as $c \rightarrow -\infty$. The ground state is a nondegenerate state with trimer character.

(ii) (0,1): $C(0,1) = 0$, $\alpha \sim -c$, and $\gamma \rightarrow 0$ as $c \rightarrow -\infty$. Asymptotic trimer character. Similar to the ground state, but it has a degenerate partner and $p \neq 0$.

(iii) $(0, n_2^0 > 1)$: $C(0, n_2^0) = 0$, $\gamma \rightarrow (-2/3n_2^0 + 1)\pi$, and $\alpha \sim -c/2$ as $c \rightarrow -\infty$. Dimer character.

(iv) $(1, n_1^0 \geq 1)$: $-6 \leq C(1, n_2^0) < -4$, $\gamma \rightarrow -2\pi/3(n_2^0 - 1)$, and $\alpha \sim -c/2$ as $c \rightarrow -\infty$. Also dimer character, but it takes a stronger interaction to achieve in comparison to the previous group.

(v) $(n_1^0 > 1, n_2^0 \geq n_1^0)$: Real k_i for all c 's, $\delta_j(\pm\infty) = 2\pi n_j^0 \pm 1$. The energy tends to a constant value as $|c| \rightarrow \infty$.

It is hoped that the root structure found and the techniques developed for its study will be useful for an examination of variants of the model involving different interactions and/or an arbitrary number of particles. Since all eigenstates can be obtained for a given c , one of the possible applications of the present work is the simulation of time-dependent rearrangement processes using a discretized basis. In this context, it may serve as a reference exact model to compare with approximate wave-function propagation methods based on periodic boundary conditions [9]. The model may also permit an explicit comparison between the classical concepts of "bound pair" and "free" particles, and their collisional rearrangements with their quantum counterparts. The origin of the difficulties in the quantum case is that the Hamiltonian for the three (or N -) body system does not commute with the Hamiltonian of a pair, so that using the concept of the bound pair in a gas (or in a box) is a delicate matter [33].

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APPENDIX: NORMALIZATION AND POTENTIAL ENERGY

Expression (12) for the wave function is not normalized. For the analysis of the energy spectrum, this does not have any effect. However, the calculation of physical expectation values, and in particular of the potential energy, requires a normalized function. This requires the evaluation of the inner product $\langle \psi | \psi \rangle$, where $|\psi\rangle$ is the unnormalized total wave function given explicitly by Eq. (12) in the region R_{123} . The contribution of the six regions is identical, so

$$\langle \psi | \psi \rangle = 6 \int_0^1 dx_3 \int_0^{x_3} dx_2 \int_0^{x_2} dx_1 |\psi(k_1, k_2, k_3; x_1, x_2, x_3)|^2. \quad (A1)$$

This integral is decomposed into 36 terms with integrals of the general form

$$\int_0^1 dx_3 \int_0^{x_3} dx_2 \int_0^{x_2} dx_1 e^{i(\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3)}, \quad (\text{A2})$$

where the α 's are combinations of momenta of the form $-k_j^* + k_i$, ($i, j = 1, 2, 3$). These integrals can of course be solved explicitly, but the result is so lengthy that it is not reported here. In order to handle all terms efficiently, it is useful to classify the possible types of integrals. There are

three cases: ($\alpha_j = 0, j = 1, 2, 3$), ($\alpha_j = 0, \alpha_k + \alpha_i = 0$), and ($\alpha_j \neq 0, j = 1, 2, 3$). In all cases the sum of the α 's is zero, $\sum_j \alpha_j = p - p = 0$.

Once $\langle \psi | \psi \rangle$ is obtained, the (dimensionless) potential energy involves a simpler integration because of the δ functions, namely,

$$\langle V \rangle = \frac{6c}{\langle \psi | \psi \rangle} \int_0^1 dx_3 \int_0^{x_3} dx_1 |\psi(x_1, x_1, x_3)|^2. \quad (\text{A3})$$

Again, all integrals involved can be carried out.

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