

Improving the Feshbach–Rubinow approximation

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The binding energy of three identical bosons is estimated by coupled differential equations that generalize the Feshbach–Rubinow approximation. This method turns out to be rather efficient, especially in the limit of vanishing binding.

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I. INTRODUCTION

There is no shortage of methods for solving the quantum-mechanical three-body problem: hyperspherical expansion, Faddeev equations, variational methods with a sophisticated search for the free parameters, Monte Carlo algorithms, etc. Each of them has merits and limitations. For instance, the hyperspherical expansion is a systematic scan of the Hilbert space and can come in several variants such as “potential harmonics” or “adiabatic.” However, it involves a rather delicate evaluation of the matrix elements of the potential within the basis of harmonics.

In the 1950s, a clever approximation, hereafter referred to as FR₁, was proposed by Feshbach and Rubinow [1]. It consists of seeking the bound-state wave function of three identical bosons of mass m as

$$\Psi(x, y, z) = \frac{u(r)}{r^{5/2}}, \quad r = \frac{x + y + z}{2}, \quad (1)$$

where $x = |\mathbf{r}_2 - \mathbf{r}_3|$, $y = |\mathbf{r}_3 - \mathbf{r}_1|$, and $z = |\mathbf{r}_1 - \mathbf{r}_2|$ measure the distances between particles. The S -wave ground state, indeed, depends on three scalar, translation-invariant, variables, which can be chosen as x , y , and z . The approximation consists of restricting to a function of their sum. Using astutely the stationary properties of the Schrödinger equation, Feshbach and Rubinow derived the radial function obeyed by the radial function $u(r)$ and energy E ,

$$-u''(r) + \frac{15}{4r^2}u(r) + 2mV_e(r)u(r) = \frac{14m}{15}u(r)E, \quad (2)$$

where the effective potential results from the projection of the interaction V ,

$$V_e(r) = \int V(x, y, z) d\tau, \quad (3)$$

$$\int d\tau = \frac{8}{r^5} \int_0^r y dy \int_{r-y}^r (2r - y - z)z dz.$$

This method has been applied to a variety of problems, in particular in nuclear physics [2], and is still used occasionally. However, in the case of baryon spectroscopy [3], the energy provided by FR₁ was found [4] not to be very accurate, as compared, e.g., with the hyperspherical expansion in

the approximation of a single partial wave, the so-called hyperscalar approximation (HA).

The most convincing success of FR₁ is perhaps in the domain of loosely bound systems as encountered, for instance, in studying Borromean binding [5]. The FR₁ approximation gives a good estimate of the coupling threshold¹ g_3 to be compared with the coupling threshold g_2 of two-body systems.

In Fig. 1, a comparison is made of the three-body binding energy of the simple pairwise exponential potential $V(x, y, z) = g \sum_x v(x)$, with $v(x) = -\exp(-x)$, computed from FR₁ and HA, as a function of the coupling g . The constituent mass is set to $m = 1$. The FR₁ method is clearly much better when the coupling threshold is approached, at $g \sim 1.2$.

The FR₁ method was improved by Bhaduri *et al.* and Lie *et al.* [2], and Rosenthal *et al.* [6] and in particular was adapted to deal with nonidentical particles. In spite of its simplicity, the Feshbach–Rubinow method was never extensively used probably because, unlike the HA and other standard methods, it was never presented as the starting point of a converging expansion. In the next section I suggest a possible remedy whereby the three-body wave function is written on a basis of orthogonal polynomials P_i with weight functions $u_n(r)$ that generalize the single $u(r)$ of FR₁ and obey coupled equations.

The ground-state energy obtained from these coupled equations is compared with the value given by standard variational methods. For estimating the quality of the wave function, the short-range correlation coefficient $\langle \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2) \rangle$ is also calculated. This quantity enters a number of decay or production rates and is notoriously hard to compute accurately. Its estimate is sometimes made easier by use of identities involving the derivative of the potential and centrifugal terms [4]. We restrict ourselves in this paper to a direct reading of the wave function at $\mathbf{r}_1 = \mathbf{r}_2$.

II. FORMALISM

The FR₁ ansatz is generalized as FR _{n} :

$$\Psi(x, y, z) = \frac{u_1(r)}{r^{7/2}} P_1(x, y, z) + \frac{u_2(r)}{r^{9/2}} P_2(x, y, z) + \dots, \quad (4)$$

¹ $g \geq g_3$ ensures a three-body bound state in the potential $\sum_{i < j} v(|\mathbf{r}_i - \mathbf{r}_j|)$, where v is attractive or, at least contains attractive parts.

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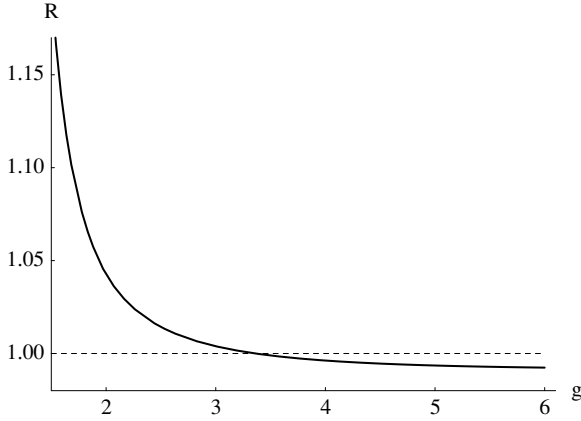


FIG. 1. Ratio of Feshbach–Rubinow to hyperscalar approximations of the three-body energy in a pairwise potential $-g \sum_{i<j} \exp(-r_{ij})$, as a function of the coupling g .

where P_n is a real and homogeneous polynomial of degree n , which is symmetrical. The first one is simply $P_1 = r$, and a truncation there corresponds to the original FR₁ method. Among the polynomials of degree $n = 1$ in x, y , and z , only $P_1 \propto x + y + z$, indeed, is symmetric. For $n > 1$, the polynomials $r^{n-1}P_1 \dots, rP_{n-1}$ are already included in the first terms of expansion (4); hence only a few genuinely new polynomials have to be introduced.² It is convenient to arrange P_n to be orthogonal. For $n = 2$, the new polynomial is

$$P_2(x, y, z) = \sqrt{\frac{3}{79}} [72r^2 - 49(x^2 + y^2 + z^2)], \quad (5)$$

where the coefficient is chosen such that $\int d\tau P_2^2 = r^2 \int d\tau P_1^2$.

If the expansion is truncated there, for testing purposes, the following set of coupled equations can be derived by straightforward calculus:

$$\begin{aligned} \alpha_{11}u_1'' + \frac{\beta_{11}}{r^2}u_1 + \alpha_{12}u_2'' + \frac{\beta_{12}}{r^2}u_2 + \gamma_{12}\frac{u_2'}{r} \\ + V_{11}u_1 + V_{12}u_2 &= \frac{7}{15}\epsilon u_1, \\ \alpha_{22}u_2'' + \frac{\beta_{22}}{r^2}u_2 + \alpha_{21}u_1'' + \frac{\beta_{21}}{r^2}u_1 + \gamma_{21}\frac{u_1'}{r} \\ + V_{21}u_1 + V_{22}u_2 &= \frac{7}{15}\epsilon u_2, \end{aligned} \quad (6)$$

with $\epsilon = 2mE$, $\alpha_{11} = -1$, $\alpha_{12} = \alpha_{21} = -2/(5\sqrt{237})$, $\alpha_{22} = -389/395$, $\beta_{11} = 15/4$, $\beta_{12} = -(93/10)\sqrt{3/79}$, $\beta_{21} = -95/(2\sqrt{237})$, $\gamma_{11} = \gamma_{22} = 0$, and $\gamma_{12} = -\gamma_{21} = -98/(5\sqrt{237})$. The 2×2 effective potential V_{ij} results from the projections

$$V_{ij} = 2m \int d\tau \hat{P}_i \hat{P}_j V(x, y, z), \quad (7)$$

with $\hat{P}_1 = 1$ and $\hat{P}_2 = P_2(x, y, z)/r^2$.

²For three variables x, y , and z , the number p of symmetric polynomials of degree n does not exceed n until $n = 5$, and $(p - n)/n$ remains small for $n > 5$.

The coupled equations can be solved by several methods, for instance the discretization procedure described in [4]. In short, $r \in [0, +\infty[$ is mapped onto $x \in [0, 1[$, and if $u_i(r) = v_i(x)$, each v_i is expanded in Fourier series $v_i = \sum_n C_n \sin(n\pi x)$. The coefficients C_n are translated into the values $v_i(x_n)$ of the radial functions at equally spaced points $x_n = n/(N + 1)$, where N is the number of points. System (6) is reduced to a $2N \times 2N$ matrix equation for the quantities $v_i(x_n)$, and its eigenvalues give a good approximation to the energy levels of system (6).

The coefficient of short-range correlation,

$$\delta = \langle \Psi | \delta^{(3)}(\mathbf{x}) | \Psi \rangle / \langle \Psi | \Psi \rangle, \quad (8)$$

is given by

$$\delta_1 = \frac{\int_0^{+\infty} u^2 r^{-3} dr}{7\pi \int_0^{+\infty} u^2 dr}, \quad (9)$$

$$\delta_2 = \frac{15 \int_0^{+\infty} r^{-3} [u_1 - 26u_2 \sqrt{3/79}]^2 dr}{7\pi \int_0^{+\infty} [u_1^2 + u_2^2] dr},$$

for FR₁ and FR₂, respectively.

III. RESULTS

The method was first tested on the harmonic oscillator, $v(x) = x^2$, for which the exact solution is $E = 6\sqrt{3}/2 \simeq 7.3485$. FR₁ gives $E_1 = (36/7)\sqrt{15/7} \simeq 7.5284$, and FR₂ leads to a remarkable improvement, with $E_2 = 7.3537$. Meanwhile, the ratio of short-range correlation δ to the exact value $\delta_{\text{ex}} = (3/2)^{3/4} \pi^{-3/2}$ evolves from $\delta_1/\delta_{\text{ex}} = 1.57$ for FR₁ to $\delta_2/\delta_{\text{ex}} = 0.968$, again a dramatic improvement.

The linear potential $\sum_{i<j} r_{ij}/2 = r$ is diagonal in the basis of polynomials P_i , but is not exactly solvable because the kinetic energy is not diagonal. The results are $E_1 \simeq 3.906$ for FR₁ and $E_2 \simeq 3.8635$ for FR₂, to be compared with $E_{L=0} \simeq 3.8647$ and $E_{L \leq 4} \simeq 3.8633$ in the hyperspherical expansion with one and two partial waves, respectively [4]. The correlation coefficient is estimated to be $\delta_1 = 0.08488$ for FR₁ and $\delta_2 = 0.05592$ for FR₂. For comparison, $\delta \simeq 0.05689$ is obtained from four coupled hyperspherical waves [4], and $\delta \simeq 0.05702$ from 176 correlated Gaussians, a method that is presented shortly.

As for the short-range potentials, let us take again the example of the exponential potential, $v(x) = -g \exp(-x)$, already considered in the introduction. Figure 2 displays the ratio of FR₂ to FR₁ ground-state energy as a function of the coupling g : The improvement saturates at about 2% at large coupling and becomes more interesting in the domain of very weak binding.

In Fig. 3, my results are compared with those of one the fashionable methods on the market. It consists of expanding the wave function on the basis of correlated Gaussians,

$$\Psi(x, y, z) = \sum_i C_i \{ \exp[-(a_i \mathbf{v}^2 + 2b_i \mathbf{v} \cdot \mathbf{w} + c_i \mathbf{w}^2)/2] + \dots \}, \quad (10)$$

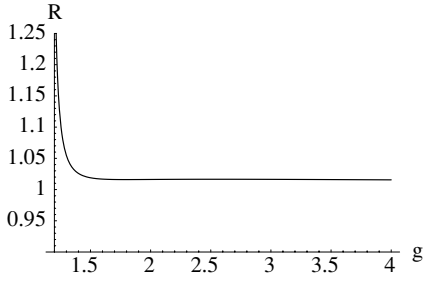


FIG. 2. Ratio of FR₂ to FR₁ approximations of the three-body energy in a pairwise potential $-g \sum_{i<j} \exp(-r_{ij})$ as a function of the coupling g .

written in terms of the Jacobi variables

$$\mathbf{v} = \mathbf{r}_2 - \mathbf{r}_1, \quad \mathbf{w} = \frac{2\mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_2}{\sqrt{3}}. \quad (11)$$

The dots in Eq. (10) are meant for Gaussians deduced by permutation of the particles. Suzuki and Varga [7] have pushed the method of a stochastic search of the parameters to a high degree of efficiency and have obtained very accurate estimates of binding energies in a variety of domains. Here we use the strategy of Hiyama *et al.* [8]: Gaussians with diagonal quadratic forms, i.e., $a_i \mathbf{v}^2 + c_i \mathbf{w}^2$, are first introduced, and if $a_i \neq c_i$, they are supplemented by the terms deduced by permutation, which includes an angular dependence through $\mathbf{v} \cdot \mathbf{w}$ and carry the same weight factor C_i to ensure Bose symmetry. The range parameters a_i and c_i are chosen to be any member of a geometric series $\{a, ar, ar^2, \dots, ar^{N-1}\}$. This means that, however large the number of terms, only two nonlinear parameters, a and r , are to be optimized. Note that $N = 2$ range parameters correspond to $N' = 8$ Gaussians, $N = 3$ to $N' = 21$, $N = 4$ to $N' = 40$, i.e., a fairly large number of terms.

The plots in Fig. 3 indicate that the FR₂ value is better than this variational estimate with $N = 2$, especially at vanishing binding, comparable with $N = 3$, and is defeated shortly by $N = 4$. This means that FR₂ is roughly equivalent to an expansion involving 40 correlated Gaussians, at least for this particular potential.

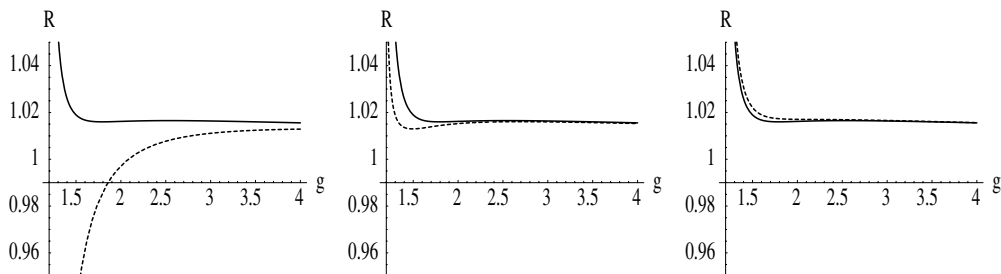


FIG. 3. Comparison of the energy in the exponential potential, as a function of the coupling g , for the FR₂ approximation (solid line), and the Gaussian expansion (dashed line) with $N = 2$ range parameters (left), $N = 3$ (centre) and $N = 4$ (right), corresponding to $N' = 8, 20, 40$ terms. For clarity, the energies are shown by their ratio to the FR₁ approximation.

For further checking, a basis of correlated exponential functions has also been used, namely,

$$\psi(x, y, z) = \sum_i C_i [\exp(-a_i x - b_i y - c_i z) + \dots], \quad (12)$$

where the ellipses indicate terms deduced by circular permutations of $\{a_i, b_i, c_i\}$. Wave functions of this type have been used in pioneering works on few-charge systems and in recent high-precision calculations of atomic systems [9]. The strategy of Ref. [8] can also be applied, to avoid numerical instabilities in the minimization process, by restricting all range parameters a_i, b_i, \dots , to belong to a single geometric series. Note that, with suitable constraints on these range parameters, this method can mimic the FR1 method ($a_i = b_i = c_i \forall_i$) or its generalization [6] by Rosenthal and Haracz (RH), ($\{a_i, b_i, c_i\} \propto \{a_1, b_1, c_1\} \forall_i > 1$), $r^{5/2} u(r)$ being described as a sum of exponentials. This provides a check of the numerical solution of the radial FR1 equation or its RH analog.

In Ref. [6], indeed, Rosenthal and Haracz proposed replacing the symmetric ansatz $F(r) = u(r)/r^{5/2}$, $2r = x + y + z$ of FR1 with

$$\Psi(x, y, z) = F(\eta_1 x + \eta_2 y + \eta_3 z) + \dots, \quad (13)$$

where the ellipses correspond to the permutation of x, y , and z to restore the symmetry of the wave function. This method results in an integrodifferential equation for F , whose solution is further optimized when η_2 and η_3 are varied empirically (a normalization $\eta_1 = 1/2$ can be adopted).

In Table I, a comparison is made of the values obtained for the ground-state energy and correlation coefficient in the exponential potential at coupling $g = 1.4$ and of the critical coupling g_3 at which three-body binding occurs. FR₁ and FR₂ are compared with RH, as well as with the Gaussian expansion GN with up to N different values of the range parameters, and its analog EN with exponentials.

At least with this potential, and for this domain of coupling close to the stability threshold, the generalization of the Feshbach–Rubinow approximation with two coupled differential equations, FR₂, appears to be more efficient than the single integrodifferential equation RH. The ground-state energy, short-range correlation, and coupling threshold approach the exact value to about 1% accuracy for the simple exponential potential.

TABLE I. Ground-state energy E_3 and correlation coefficient δ for an exponential potential with coupling $g = 1.4$, and critical coupling g_3 for three-body binding, with FR₁, FR₂, and RH methods and variational calculations with correlated Gaussian (G) or exponential (E) basis functions with a varying number of allowed range parameters.

	$G2$	$G4$	$G8$	$E2$	$E4$	$E5$	FR ₁	RH	FR ₂
$-E_3$	0.03055	0.03575	0.03586	0.03466	0.03583	0.03586	0.03468	0.03475	0.03542
δ	0.00840	0.00972	0.01000	0.01251	0.01005	0.01002	0.01212	0.01224	0.01091
g_3	1.2194	1.1613	1.1563	1.2158	1.1587	1.1560	1.1751	1.1649	1.1644

IV. OUTLOOK

In this paper, the Feshbach–Rubinow method is generalized by the expansion of the ground-state wave function of three identical bosons on orthogonal polynomials of the interparticle distances. The coefficients of these polynomials are functions of the sum of distances and obey coupled equations that can be derived by calculus and solved numerically. The results obtained with two equations provide a dramatic improvement in the case of confining potentials, for which the single-equation version of this method was known to be inaccurate. For the short-range potentials, the results are also significantly better and become really excellent in the limit of loose binding.

The method is compared with standard variational expansion schemes with correlated exponentials or Gaussians that imply solving an eigenvalue equation whose result is minimized by varying the range parameters. The generalized Feshbach–Rubinow method requires solving coupled differential equations, similar to those of the hyperspherical expansion, i.e., after suitable discretization, solving once an eigenvalue equation of higher dimension.

Further investigations would be necessary to check the convergence when the number of equations is increased, and for excited states. It is rather straightforward to include more components in expansion (4), write down and solve the coupled equations that generalize system (6). The accuracy of the method should also be probed for potentials with hard core, which often occur in applications. The case of particles with different masses or interaction properties also deserves further work. The binding energy and wave function of the positronium ion and other two-electron atoms, which were the subject of interesting developments of the Feshbach–Rubinow method, will be studied in a forthcoming paper within the formalism of coupled equations.

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