Complementary energy bounds for N-boson systems with linear pair potentials

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We study the ground-state energy of a system of N identical bosons, each having mass m, which interact in one dimension via the pair potential $V(x)=\gamma\,|\,x\,|$ and obey nonrelativistic quantum mechanics. It is shown that the energy is given by the formula $\varepsilon=C(N)(N-1)(\hbar^2/m)^{1/3}(\gamma N/2)^{2/3}$, where $1.01879<C(N)<1.02333$ for all $N\geq 2$. The lower bound is provided by the "equivalent two-body method" whereas the upper bound is derived by the use of collective field theory. The general relation between these complementary theories is investigated.

I. INTRODUCTION

We consider a system of N identical bosons which interact in one spatial dimension via central pair potentials and obey nonrelativistic quantum mechanics. The Hamiltonian for the N-particle system (with the kinetic energy of the center of mass removed) is given explicitly by

$$H=\frac{1}{2m}\sum_{i=1}^{N}p_i^2-\frac{1}{2Nm}\left[\sum_{i=1}^{N}p_i\right]^2+\sum_{\substack{i,j=1\\(i<j)}}^{N}\gamma f(x_{ij}/a)\;, \tag{1.1}$$

where m is the mass of a particle, $x_{ij}=x_i-x_j$ is a pair distance, $f(x)$ is the potential *shape*, a is a length parameter, and γ is the coupling constant. The main purpose of the present article is to study the linear potential whose shape is given simply by

$$f(x)=|\,x\,|\;. \tag{1.2}$$

This problem provides an opportunity to relate two well-established but complementary approaches to the many-body problem. These two methods start respectively from the rather different special cases, $N=2$ and $N\rightarrow\infty$, and they lead eventually to sharp energy bounds.

In Sec. II below we make use of the necessary permutation symmetry of the state vector to relate the energy of the N-particle system to the energy of a specially constructed two-particle system. This "reduction" to an "equivalent two-body problem" leads to an energy *lower* bound for the N-particle system. In Sec. III the collective field method is formulated in a way which permits the limit $N\rightarrow\infty$ to yield an energy *upper* bound valid for all *finite N*. It is interesting that a suitable formulation exists in which the complementary extreme cases $N=2$ and $N\rightarrow\infty$ become so "close" that we can determine the N-particle energy with error less than 0.23% for all $N\geq 2$.

II. THE EQUIVALENT TWO-PARTICLE PROBLEM

Soon after the neutron was discovered in 1932, Wigner and later Feenberg and others tried various ways[1] of relating the ground-state energy of a few-nucleon system to that of a specially constructed two-body system with a new mass and coupling constant. Sometimes the relationship was actually that of a variational upper bound but it was usually regarded simply as an *ad hoc* approximation. We shall give here a very brief outline of some rigorous results related to this idea and refer the reader to Ref. 2 for more technical details and literature.

One of the interesting points about the energy bounds is the fact that their quality depends on the system of relative coordinates used. We suppose that new coordinates are defined by $\xi=\underline{B}\mathbf{R}$, where $\xi=[\xi_i]$ and $\mathbf{R}=[x_i]$ are column vectors of the new and old coordinates, ξ_1 is the center-of-mass coordinate, and $\xi_2=(x_1-x_2)/\sqrt{2}$ is a pair distance. Our methods require these two coordinates and consequently the matrix $\underline{B}$ which must, of course, be invertible, has, without any further loss of generality, the form

$$\underline{B}=\begin{bmatrix}\frac{1}{\sqrt{N}} & \frac{1}{\sqrt{N}} & \frac{1}{\sqrt{N}} & \frac{1}{\sqrt{N}} & & \cdots & & \frac{1}{\sqrt{N}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & & \cdots & & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\end{bmatrix},$$

where rows 2 to N, which define the relative coordinates, are orthogonal to the first row. The column vectors $\mathbf{\Pi}$ and $\mathbf{P}$ of the new and old momenta are therefore related by $\mathbf{\Pi}=[\underline{B}^{-1}]^T\mathbf{P}$. The Hamiltonian (1.1) can also be rewritten in the form

$$H=\sum_{\substack{i,j=1\\(i<j)}}^{N}\left[\frac{1}{2Nm}(p_i-p_j)^2+\gamma f(x_{ij}/a)\right] . \tag{2.1}$$

If we now compute expectations with respect to translation-invariant boson functions, we find from Eq. (2.1) that $\langle H\rangle=\langle\mathcal{H}\rangle$, where the reduced two-body Hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H}=(N-1)\left[\frac{1}{2m\lambda}\Pi_2^2+\frac{N}{2}\gamma f(\sqrt{2}\xi_2/a)\right] \tag{2.2}$$

and the parameter λ is equal to the sum of the squares of the elements of the second row of the matrix $[\underline{B}^{-1}]^T$. For spatially antisymmetric states, the lower bound methods require more than one pair-distance coordinate so that $\underline{B}$ cannot be orthogonal and, in such cases, $\lambda>1$ (although the parameter λ is not quite a "coefficient of orthogonality"). If, for example, we use for our relative coordinates a set of $N-1$ pair distances, like ξ_2, then we find that $\lambda=2(N-1)/N$. For boson systems, the best results (that is to say, the highest *lower* energy bounds) are achieved with classical Jacobi coordinates for which $\underline{B}$ is *orthogonal* and therefore the parameter $\lambda=1$. We shall assume this value of λ for the remainder of our work in the present article.

If ψ represents a translation-invariant boson function then the lowest energy ε of the N-particle system is given by

$$\varepsilon=\inf_{\psi}\left\{\frac{(\psi,\mathcal{H}\psi)}{(\psi,\psi)}\right\} . \tag{2.3}$$

It is now convenient to define the dimensionless energy and coupling parameters E and v by

$$E=\frac{m\varepsilon a^2}{\hbar^2(N-1)},\quad v=\frac{m\gamma a^2N}{2\hbar^2} . \tag{2.4}$$

Equation (2.3) may then be further simplified and written in the form

$$E=F_N(v)=\inf_{\psi}\left\{\frac{(\psi,\mathbb{H}\psi)}{(\psi,\psi)}\right\} , \tag{2.5}$$

where the Hamiltonian $\mathbb{H}$ is defined in terms of the dimensionless variable $x=(x_1-x_2)/a=\sqrt{2}\xi_2/a$ and the derivative $D=d/dx$ by

$$\mathbb{H}=-D^2+vf(x) \tag{2.6}$$

and ψ is a translation-invariant N-boson function. We call the function $F_N(v)$ a *trajectory function* and the graph $(v,F_N(v))$, $v>0$, an *energy trajectory* for the N-boson problem. Since the permutation-symmetry constraint increases monotonically with N it is clear that, for each *fixed* v, the value of $F_N(v)$ increases monotonically with N. That is to say, $F_N(v)\geq F_M(v)$, $N>M$, and consequently we have

$$F_2(v)\leq F_N(v)\leq F_\infty(v) , \tag{2.7}$$

provided the limit $N\to\infty$ exists.

We now look at variational estimates of the energy. If we could find a translation-invariant boson function with the single-product form

$$\psi(\xi_2,\xi_3,\ldots,\xi_N)=\phi(\xi_2)g(\xi_3,\ldots,\xi_N) \tag{2.8}$$

then, by substituting this form in the right-hand side of Eq. (2.5), we see that an upper bound to $F_N(v)$ is given by the Rayleigh quotient

$$F_\phi(v)=\frac{(\phi,\mathbb{H}\phi)}{(\phi,\phi)} . \tag{2.9}$$

This last expression is exactly what we would use if we were to estimate variationally the bottom of the spectrum of $\mathbb{H}$, a one-particle (or *reduced* two-particle) Hamiltonian. The catch in all this is that (2.8) is a strong constraint for boson functions and it has in fact been proved[3] that the single-product form is achieved if and only if ψ is a Gaussian function. But in this case N disappears from the calculation and the result (which can still be minimized with respect to a scale parameter) provides an upper trajectory bound valid for all N: we call this $F_g(v)$. We can now summarize the results by writing

$$F_2(v)\leq F_N(v)\leq F_\infty(v)\leq F_g(v) , \tag{2.10}$$

where $F_g(v)$ is given by using $\phi(x)=e^{-\alpha x^2}$ in (2.9) and minimizing the resulting expression with respect to α. The corresponding energy bounds are recovered from the trajectory functions by using the following general expression:

$$\varepsilon=\left[\frac{\hbar^2}{ma^2}\right](N-1)F\left[\frac{m\gamma a^2N}{2\hbar^2}\right] . \tag{2.11}$$

The inequalities (2.10) are important because they reduce the N-body energy problem, approximately, to a study of the single-particle operator $\mathbb{H}$. The N dependence of the many-particle energy is captured by the general form (2.11) in which, very often, the trajectory function F_N does not *itself* vary strongly with N.

It is now clear that the inequalities in (2.10) all collapse into equalities if and only if the potential has the harmonic-oscillator shape $f(x)=x^2$. The common value obtained in this special case is simply the bottom of the spectrum of $\mathbb{H}$ given in (2.6) with $f(x)=x^2$, that is to say

$$F_2(v)=F_N(v)=F_\infty(v)=F_g(v)=v^{1/2} . \tag{2.12}$$

In the more general case of power-law potentials with the form

$$f(x)=|x|^q,\quad q>0 . \tag{2.13}$$

Simple scaling arguments show that the corresponding energy trajectories are given by

$$E=F_N^{(q)}(v)=F_N^{(q)}(1)v^{2/(q+2)} . \tag{2.14}$$

In the special case of the linear potential $q=1$ we absorb the length parameter a into the coupling constant γ by setting $a=1$ and we then obtain from (2.11) and (2.14) the formula

$$\varepsilon = C(N)(N-1)\left[\frac{\hbar^2}{m}\right]^{1/3}\left[\frac{\gamma N}{2}\right]^{2/3}, \tag{2.15}$$

where, from (2.10) we have

$$F_2(1) \le C(N) \le F_\infty(1) \le F_g(1) . \tag{2.16}$$

$F_2(1)$ is the bottom of the spectrum of $\mathbb{H}$ and $F_g(1)$ is the best upper estimate of $\langle \mathbb{H} \rangle$ with respect to normalized Gaussian trial functions and, for the linear potential, the reduced Hamiltonian $\mathbb{H}$ is given by

$$\mathbb{H} = -D^2 + |x| . \tag{2.17}$$

It is well known that the bottom of the spectrum of $\mathbb{H}$ is given by the first zero of the derivative of Airy's function. Meanwhile, the estimate of $\langle \mathbb{H} \rangle$ by Gaussian functions (optimized with respect to scale) is obtained by an elementary computation. We therefore find

$$F_2(1) = 1.018\,793; \; F_g(1) = 3/2\pi^{1/3} = 1.024\,176\,1 , \tag{2.18}$$

where we have truncated the decimal approximations in the appropriate directions to preserve the energy bounds. Hence (2.17) and (2.18) determine the energy of the N-body problem with error less than 0.264% for all $N>2$. This results will be sharpened in the next section, with the aid of collective field theory.

III. THE COLLECTIVE FIELD METHOD

We first look for a formulation of the collective field method which will allow us to find the limiting trajectory function

$$F_\infty(v) = \lim_{N\to\infty} F_N(v)$$

for a given potential shape $f(x)$. We obtain Eq. (3.9), below, in which a variational upper bound $F_\phi(v)$ to $F_\infty(v)$ is provided in terms of the positive field density ϕ defined on $\mathbb{R}$ and normalized to one. We then show that a Gaussian "trial density" ϕ leads to the same upper estimate as we get when a Gaussian boson "trial function" ψ is used to estimate $F_\infty(v)$ via the original Hamiltonian H. This provides an interesting link between the two very different approaches to the many-body problem. From this result we then recover the well-known *exact* solution to the harmonic-oscillator problem for which the potential shape is $f(x)=x^2$.

The collective field method dates back to the early 1950s (Ref. 4) but recently it has been clarified and presented in a form suitable for our needs by Jevicki and Sakita.[5] There may still be some unresolved problems of a mathematical nature to do with this theory, particularly relating to the prelimit situation when N is finite. However, for the purposes of the present paper, our only interest is in the claims of the theory concerning the limiting energy per particle as N increases without bound, while the product γN is held constant: it is this limit that leads to $F_\infty(v)$. We have already resolved the question of the relation of this limiting energy trajectory to the corresponding trajectory for *finite* N because we know from (2.10) that $F_N(v) \le F_\infty(v)$.

In this section we shall not use relative coordinates and therefore we shall work with the full Hamiltonian for the N-boson problem *including* the positive center-of-mass term $\mathcal{K}$, that is to say, with the Hamiltonian

$$H + \mathcal{K} = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 + \sum_{\substack{i,j=1\\(i<j)}}^{N} \gamma f(x_{ij}/a) . \tag{3.1}$$

By considering translation-invariant boson functions we see that the bottom of the spectrum of H is the same as the bottom of the spectrum of the operator $H+\mathcal{K}$. For Bose systems the principal idea is to treat the large N limit by a special device that builds in from the outset the necessary constraint of Bose symmetry. The most general operator which is symmetric in the $\{x_i\}$ is given formally by the expression

$$\hat{\rho}(x) = \sum_{i=1}^{N} \delta(x-x_i) . \tag{3.2}$$

We can use $\hat{\rho}(x)$ to construct boson functions as in the example

$$\sum_{i=1}^{N} \psi(x_i) = \int_{\mathbb{R}} \hat{\rho}(x)\psi(x)dx . \tag{3.3}$$

In general, boson functions can be constructed by means of a functional of the form

$$\psi(x_1, x_2, \ldots, x_N) = \Phi[\hat{\rho}] . \tag{3.4}$$

Consequently, the requirement that ψ satisfy Schrödinger's equation implies that the functional Φ satisfy a corresponding differential equation. This equation eventually leads to the following approximate expression for the total energy as a functional of a positive field density *function* ρ defined on $\mathbb{R}$,

$$\varepsilon[\rho] = \frac{\hbar^2}{8m}\int_{\mathbb{R}} \frac{[\rho'(t)]^2}{\rho(t)}dt + \frac{\gamma}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} \rho(s) f((s-t)/a)\rho(t)ds\,dt , \tag{3.5}$$

where

$$\int_{\mathbb{R}} \rho(t)dt = N . \tag{3.6}$$

As N is increased, the approximation becomes better and the functional $\mathcal{E}[\rho]$ approaches an upper estimate to the lowest energy of the system. Since we are interested *only* in the large-N limit we now transform the problem so that this limit can be approached. We define a new density $\phi(t)$ which is normalized to unity on $(-\infty,\infty)$ and we define $F_\phi(v)$ to be, essentially, the *limiting* energy per particle, where, from (2.4), $v = m\gamma a^2 N/2\hbar^2$ is kept *constant.* Thus we define the following:

$$\phi(t/a)=a\rho(t)/N$$

and therefore, (3.7)

$$\int_{\mathbb{R}}\phi(t')dt'=1, \quad t'=t/a$$

$$F_\phi(v)=\lim_{N\to\infty}\left[\frac{ma^2\varepsilon[\rho]}{\hbar^2 N}\right], \quad v=\frac{m\gamma a^2 N}{2\hbar^2}=\text{const} . \quad (3.8)$$

Since $(N-1)/N$ approaches 1 as N increases, we conclude from (3.5), (3.7), and (3.8) that the functional $F_\phi(v)$ provides an upper bound to the quantity $F_\infty(v)$ that we seek. Hence

$$F_\infty(v)\le F_\phi(v)=\frac{1}{8}\int_{\mathbb{R}}\frac{[\phi'(t)]^2}{\phi(t)}dt + v\int_{\mathbb{R}}\int_{\mathbb{R}}\phi(s)f(s-t)\phi(t)ds\,dt . \quad (3.9)$$

In the step from (3.5) to (3.9) we have first used dimensionless variables $s'=s/a$ and $t'=t/a$ and then dropped the primes on s and t in the final expression. All the results from collective field theory which we obtain are based on Eq. (3.9).

The next result is obtained by a simple calculation. We shall give enough of the details so that the calculation can easily be verified. We start with a normalized Gaussian density given by

$$\phi(t)=ce^{-4\alpha t^2}, \quad c=2\left[\frac{\alpha}{\pi}\right]^{1/2}, \quad \int_{\mathbb{R}}\phi(t)dt=1 . \quad (3.10)$$

This density is now substituted into the right-hand side of (3.9) leading to a function $E(\alpha)$ of the variational parameter α. More interestingly, we can rework the right-hand side of (3.9) so that, by using the change of variable $x=\sqrt{2}t$ and performing *one* of the potential-energy integrals, we obtain the result

$$E(\alpha)=\frac{(u,\mathbb{H}u)}{(u,u)} \quad \text{where } u^2(x)=\phi(t) . \quad (3.11)$$

Consequently, using a Gaussian *density* in (3.9) or a Gaussian *wave function* in (2.3) leads to precisely the same upper estimate for $F_\infty(v)$. When this common upper estimate is minimized with respect to the parameter α, we call the resulting approximate trajectory function $F_g(v)$.

In the special case that $f(x)=x^2$, we therefore find from (3.11), as we did in (2.12), that $F_g(v)=v^{1/2}$. Since we know from (2.12) that in this case $v^{1/2}$ is also a *lower* bound to $F_\infty(v)$, we again recover the result that $F_\infty(v)=F_g(v)=v^{1/2}$. Of course, from the point of view of collective field theory *alone,* the relationship between $F_\infty(v)$ and $F_N(v)$, for *finite N,* would still be unknown.

The advantage of the collective field equation (3.9), in general, is that it provides a way of systematically improving on $F_g(v)$. We can simply explore density functions variationally. This is what we do in Sec. IV in the case of the linear potential.

IV. THE LINEAR POTENTIAL

Even at a time when computation has become both cheap and comfortable, it is extremely useful to look at cases for which all the details of a theory can be worked out essentially by exact analytical methods. It turns out that the harmonic oscillator is "too good" because in this case the trajectory functions all coalesce into one, and also the equivalent two-body method and the collective field method yield the same results (for the large-N limit). The linear potential, however, does separate the distinct approaches.

As we found in Sec. III, the application of a Gaussian trial function or, in the collective field method, of a Gaussian density, leads to the same *upper* estimate to $F_\infty(v)$. If this upper bound is minimized with respect to a scale parameter we call the resulting trajectory function $F_g(v)$ and in the present problem we find for this trajectory function

$$F_\infty(v)\le F_g(v)=\frac{3v^{2/3}}{2\pi^{1/3}} . \quad (4.1)$$

Without help from the collective field method it would be very difficult, in general, to improve on the Gaussian upper bound (4.1) which is valid for *all* $N\ge 2$.

For the linear potential $f(x)=|x|$, the variational upper estimate (3.9) for $F_\infty(1)$ becomes

$$F_\infty(1)\le F_\phi(1)=\frac{1}{8}\int_{\mathbb{R}}\frac{[\phi'(t)]^2}{\phi(t)}dt + \int_{\mathbb{R}}\int_{\mathbb{R}}\phi(s)|s-t|\phi(t)ds\,dt , \quad (4.2)$$

where the positive density function $\phi(x)$ satisfies the normalization condition $\int_{\mathbb{R}}\phi(t)dt=1$. This optimization problem is certainly amenable to numerical methods. However, great care would have to be taken to preserve the bound in (4.2). We shall therefore proceed, as far as possible, with analytical methods.

We have tried a variety of one-parameter trial densities but they gave worse results than the Gaussian. However, the following two-parameter density, which includes the Gaussian as the special case $q=2$, gives satisfactory results:

$$\phi(t)=[bI(q)]^{-1}e^{-|t/b|^q} , \quad (4.3)$$

where b is a scale parameter and $I(q)$ is a normalization integral given by

$$I(q)=2\Gamma(1+1/q) . \quad (4.4)$$

We approach the minimum with respect to the two variational parameters b and q in two stages. First, we fix q and obtain the following expression for E:

$$E=\frac{K}{8Ib^2}+\frac{8Vb}{I^2} , \quad (4.5)$$

where K and V are the kinetic and potential energy integrals with the scale parameter $b=1$; that is to say,

$$K=\tfrac{1}{8}\int_{\mathbb{R}}\frac{[\phi'(t)]^2}{\phi(t)}dt=2q\Gamma(2-1/q) \quad (4.6)$$

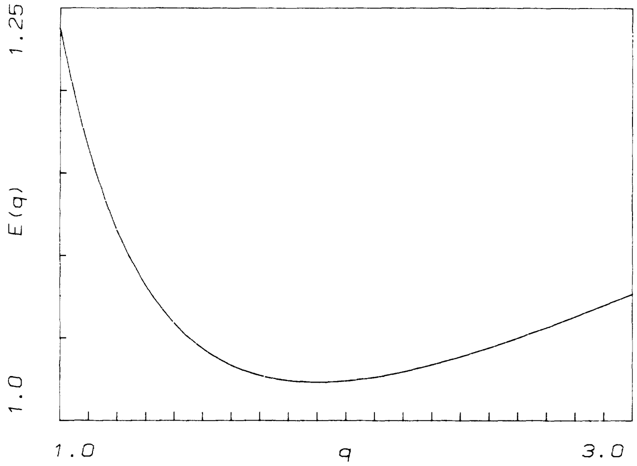

FIG. 1. The field theoretic expression (4.5) for the energy is first minimized with respect to scale parameter b and the figure shows the final minimization of $E(q)$ given by (4.9) with respect to the power parameter q.

and

$$V=\frac{1}{8}\int_{\mathbb{R}}\int_{\mathbb{R}}\phi(s)\,|\,s-t\,|\,\phi(t)ds\,dt\ . \tag{4.7}$$

Even with the aid of Gaussian numerical integration it is uncomfortable to integrate over the absolute-value function. We therefore choose new variables obtained from (s,t) by a rotation by $\pi/4$ and obtain for the potential-energy integral

$$V=\int_0^{\infty}ds\,\phi(s)\int_s^{\infty}dt\,t\phi(t)\ . \tag{4.8}$$

By minimizing the expression in (4.3) with respect to b we find the following formulas for the minimum energy E and the critical value of b, as functions of q:

$$E=3\left[\frac{2KV^2}{I^5}\right]^{1/3}\ ;\quad b=\left[\frac{KI}{32V}\right]^{1/3}\ . \tag{4.9}$$

It is now safe to use computer technique and in Fig. 1 we exhibit the graph of $E=E(q)$. From the data for $E(q)$ we conclude that the minimum is at about $q=1.9$. Hence, our upper bound becomes

$$F_{\infty}(1)\le F_{\phi}(1)=E(1.9)<1.023\,323\ , \tag{4.10}$$

where we have truncated the result upwards to preserve the bound. The corresponding critical value of the scale parameter is $b=0.833\,624$. In Fig. 2 we exhibit the graph of the optimal density ϕ along with the optimal *Gaussian* density for which $q=2$.

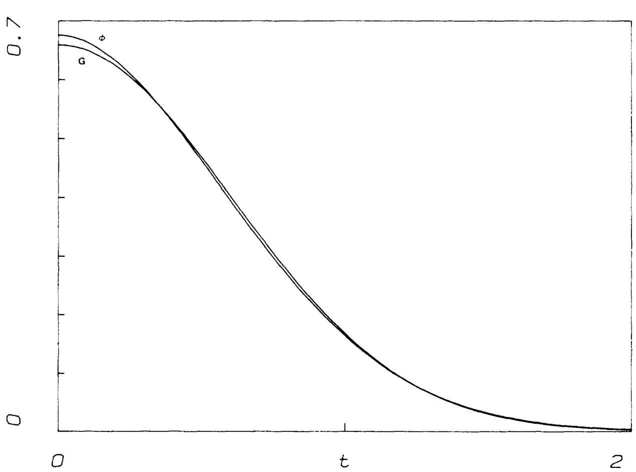

FIG. 2. The best Gaussian density G and the best density ϕ from the class (4.3) for the linear potential.

V. CONCLUSION

Our main specific result is that the energy of the N-boson problem (1.1) with the linear pair potential (1.2) and $a=1$ is given by the formula

$$\varepsilon=C(N)(N-1)\left[\frac{\hbar^2}{m}\right]^{1/3}\left[\frac{\gamma N}{2}\right]^{2/3}\ , \tag{5.1}$$

where the slowly varying function $C(N)$ is bounded by the inequalities

$$1.018\,797\,9<F_2(1)\le C(N)\le F_{\infty}(1)\le F_{\phi}(1)<1.023\,322\,7\ . \tag{5.2}$$

The formula (5.1) therefore determines the N-body energy with an errorless than 0.222% for all $N\ge 2$.

We have explained our methods in some detail partly because our specific results for the linear potential contradict the previously published data both of Muriel[6] and of Adric and Bardek.[7] The earlier work does not claim to provide energy bounds for finite systems. In the large-N limit, where comparison *is* possible, the earlier estimates for what we would call $C(\infty)$ are about 20% *lower* than our lower bound. One possible source for this difference may be the absence of explicit relative coordinates in the earlier work. As we noted in Sec. II, the use of $N-1$ pair distances for the relative coordinates in our theory would enhance the mass of the reduced problem by the factor of $\lambda=2(N-1)/N$; in the large-N limit this would decrease the lower bound by the factor $2^{-1/3}=0.794$.

More importantly, we have established a general relationship between the equivalent two-body method and collective field theory; this allows the field theoretic results to be used to estimate the energy of the many-body system even when N is *finite*. This is significant because it is far easier to perform variational calculations for the field density than it is to work with translation-invariant many-body wave functions. For the one exception to this general rule, the Gaussian wave function, we have proved that exactly the same results are obtained from the field theory if a Gaussian trial density is used. Thus, from a practical point of view, the field theoretical route to many-body ground-state energy upper bounds now appears to be in every way superior to direct Rayleigh-Ritz calculations.

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