

ARTICLES

Gravitating boson systems

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We study a system composed of N identical bosons interacting in three dimensions via attractive Yukawa pair potentials $V(r) = -e^{-\lambda r}/r$. Four approaches to the problem are related: the “equivalent two-body method,” translation-invariant Gaussian trial functions, collective field theory, and Hartree trial functions. Upper and lower energy bounds are given and are compared to some recent results which were obtained independently by an optimized Hartree method [M. Membrado, F. Pacheco, and J. Sañudo, Phys. Rev. A **39**, 4207 (1989)]. In the pure gravitational limit $\lambda \rightarrow 0$ the N -body energy is determined for all N and all values of the coupling with an error of less than 7.2%.

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I. INTRODUCTION

There is at least one good reason why the many-body problem in quantum mechanics may be easier to solve than the corresponding problem in classical mechanics: identical particles in quantum mechanics have no individuality. The states of a many-identical-particle system are either symmetric or antisymmetric under the permutation of the particle indices. This fact is a very powerful constraint which induces a kind of dynamic crystallography in which every pair of particles copies the motion of every other pair.

A system of N identical bosons interacting by attractive forces collapses as N increases: the “size” of the system diminishes to zero, and the binding energy per particle $|\mathcal{E}|/N$ increases without bound. It seems that fermions are necessary for stability. In the case of Coulomb interactions we have at our disposal detailed theoretical results [1–3] which characterize the relation between particle statistics and stability, and also the nature of the collapse in the unstable cases. A concise review of the “stability-of-matter” problem may be found in a recent article by Thirring [4]. By diminishing the coupling parameter γ of a general boson system as N increases (so that the product γN remains constant) we can arrange for \mathcal{E}/N to remain finite in the large- N limit. Just as in the large- N approximation, where \mathcal{N} is the number of spatial dimensions, suitable large- N limits can provide useful energy estimates, even for *finite systems*.

The main purpose of the present paper is to put together in a single framework some recent approaches to the N -boson problem so that the methodology and results may easily be compared. In Sec. II we introduce our formalism and discuss some general questions to do with the N -boson problem. We review, very briefly, the main results from the “equivalent two-body method” and the use of Gaussian wave functions, which have been described

in more detail in earlier articles [5,6]. In Sec. III we study the collective-field method which, it has been shown [7], yields the same upper energy bound as does the Hartree variational method, provided that the center-of-mass kinetic energy is removed. In Sec. IV these methods are applied to the specific example of the attractive Yukawa pair potential. We compare the results by expressing the energies in terms of a dimensionless parameter R which always lies in the range $-1 \leq R < 0$.

For the Yukawa problem, Membrado, Pacheco, and Sañudo [8] have derived a differential equation for the best Hartree upper bound: we are happy to report that their results and ours are close and consistent. This agreement is very welcome. Even though one is dealing with well-defined, and perhaps rather pure, many-body problems, there have been a number of differing results for such problems published in recent years. For example, Membrado, Pacheco, and Sañudo [8] report earlier Hartree results for the gravitational problem differing from theirs by a factor of 3. Meanwhile, in a study of the linear potential in one dimension [5] we found large discrepancies between our results and some earlier work based on collective-field theory. In the end we should like to understand fully how the different approaches to the problem are related and we should like to see them produce consistent results when they are applied to specific problems.

II. THE EQUIVALENT TWO-BODY METHOD AND GAUSSIAN TRIAL FUNCTIONS

In this section of the paper we summarize general results obtained from the “equivalent two-body problem” and by the use of Gaussian trial functions. We consider a system of N identical bosons each of mass m which interact via an attractive pair potential $V(\mathbf{r}) = \gamma f(r/a)$.

The Hamiltonian H for such a system (with the center-of-mass kinetic energy removed) is given by

$$H = \frac{1}{2m} \sum_{i=1}^N \mathbf{p}_i^2 - \frac{1}{2Nm} \left[\sum_{i=1}^N \mathbf{p}_i \right]^2 - \sum_{\substack{i,j=1 \\ i < j}}^N \gamma f(r_{ij}/a) \tag{2.1}$$

$$= \sum_{\substack{i,j=1 \\ i < j}}^N \left[\frac{1}{2Nm} (\mathbf{p}_i - \mathbf{p}_j)^2 + \gamma f(r_{ij}/a) \right]. \tag{2.2}$$

$$B = \begin{pmatrix} 1/\sqrt{N} & 1/\sqrt{N} & 1/\sqrt{N} & \dots & \dots & \dots & 1/\sqrt{N} \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 & & & & \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} & 0 & & & \\ \dots & & & & & & \\ \dots & & & & & & \\ 1/\sqrt{N(N-1)} & 1/\sqrt{N(N-1)} & \dots & \dots & \dots & \dots & -(N-1)/\sqrt{N(N-1)} \end{pmatrix}. \tag{2.3}$$

Since $B^{-1} = B^T$, the column vectors $\mathbf{\Pi}$ and \mathbf{P} of the new and old momenta are related simply by $\mathbf{\Pi} = B\mathbf{P}$. We have exhibited this well-known matrix because it is important to note that the scheme we use is extensible. More specifically, as we increase N , each new relative coordinate is symmetric under the permutation of the previous $N-1$ particle indices. The significance of this can be understood by consideration of the following argument. If we have only two bosons, then the wave function $\Psi_2(\rho_2)$ must be a symmetric function of ρ_2 . If we now consider three bosons, then the new wave function $\Psi_3(\rho_2, \rho_3)$ must still be a symmetric function of ρ_2 and it must also satisfy one more condition so that it is invariant under *all* the permutations of the particle indices 1, 2, and 3 [the permutation group P_3 is generated by the exchange (12) and the 3-cycle (123)]. We see therefore that the necessary permutation-symmetry constraint of boson functions becomes more stringent as N increases.

If we now compute expectations with respect to translation-invariant boson functions, we find from Eq. (2.2) that $\langle H \rangle = \langle \mathcal{H} \rangle$, where the reduced two-body Hamiltonian \mathcal{H} is given by

$$\mathcal{H} = (N-1) \left[\frac{1}{2m} \mathbf{\Pi}_2^2 + \frac{N}{2} \gamma f(\sqrt{2}|\rho_2|/a) \right]. \tag{2.4}$$

Further simplification of our discussion of the general N -boson problem is possible if we introduce some dimensionless quantities by the following:

$$E = \frac{m \mathcal{E} a^2}{\hbar^2 (N-1)}, \quad v = \frac{m a^2 \gamma N}{2 \hbar^2}, \quad \mathbf{r} = \sqrt{2} \rho_2 / a = \mathbf{r}_{12} / a. \tag{2.5}$$

Let us suppose that Ψ_N is a translation-invariant boson function, that is to say, a square-integrable function of

In a careful discussion of the problem we must retain two symmetries: translation invariance and boson statistics. Therefore, even if it is uncomfortable, we must now deal with the question of relative coordinates.

We suppose that the new coordinates are the classical relative coordinates of Jacobi defined by $\rho = B\mathbf{R}$, where $\rho = [\rho_i]$ and $\mathbf{R} = [\mathbf{r}_i]$ are column vectors of the new and old coordinates, ρ_1 is the center-of-mass coordinate divided by $N^{1/2}$, $\rho_2 = (\mathbf{r}_1 - \mathbf{r}_2) / \sqrt{2}$, and B is the orthogonal matrix given explicitly by

the $N-1$ relative coordinates $\{\rho_i\}_{i=2}^N$ which is symmetric under the permutation of the N individual-particle indices. It follows that the ground-state energy of the N -boson problem may be written in the form

$$E = F_N(v) = \min_{\Psi_N} \frac{(\Psi_N, \mathfrak{H} \Psi_N)}{(\Psi_N, \Psi_N)}, \tag{2.6}$$

where \mathfrak{H} is the dimensionless one-particle Hamiltonian defined by

$$\mathfrak{H} = -\Delta + v f(r), \tag{2.7}$$

and Δ is the Laplacian with respect to \mathbf{r} .

For a given physical problem, the coupling parameter v varies with N . However, we *define* the "trajectory functions" F_N by (2.6) with the value of v fixed. Consequently, \mathfrak{H} does not depend on N , which enters the problem only as the number (plus 1) of Jacobi relative coordinates to be included in the wave function Ψ_N . As we observed above, the Jacobi coordinate ρ_{i+1} is symmetric under the permutation of the individual particles 1 through i . This means that the permutation-symmetry constraint on the minimization process (2.6) increases in severity monotonically with N ; this in turn implies that the N -boson trajectory functions satisfy the ordering relation:

$$F_N(v) \leq F_K(v), \quad 2 \leq N < K. \tag{2.8}$$

This relation says much more than that the energy increases with N . $F_N(v)$ is proportional to the N -boson energy \mathcal{E} divided by $N-1$, and meanwhile the product γN is held constant. The most interesting cases are the extremes $N=2$ and ∞ . Thus we have

$$E_L = F_2(v) \leq F_N(v) \leq F_\infty(v) = F_G(v) = E_U, \tag{2.9}$$

where the upper bound $F_G(v)$ is obtained by the use of a

Gaussian trial function, as will shortly be explained. The lower bound E_L is simply the exact lowest energy of the one-particle ("reduced" two-particle) Hamiltonian ξ . We refer [5-7] to this energy bound as an "equivalent two-body energy" because of the historical roots [9-12] of this notion from the early days of nuclear physics.

Now we turn to Gaussian trial functions. Suppose that the N -boson function could be factored in the form

$$\Psi(\rho_2, \rho_3, \dots, \rho_N) = \psi(\rho_2)g(\rho_3, \rho_4, \dots, \rho_N). \quad (2.10)$$

In this case, the expectation value on the right-hand side of (2.6) would reduce to $(\psi, \xi\psi)/(\psi, \psi)$, that is to say, the expectation of a one-body Hamiltonian ξ with respect to a one-body wave function $\psi(\rho_2)$. However, it has been proved [13] that the factored form (2.10) is possible for a boson function if and only if it is Gaussian. The upper bound $E_U = F_G(v)$ in (2.6) is therefore defined to be the result of using the trial function $\psi(\mathbf{r}) = e^{-\alpha r^2}$ and minimizing $\langle \xi \rangle$ with respect to the parameter α . Since v is held constant, and the N in Ψ cancels out with the factor g , we see that $F_G(v)$ is an upper bound for all $N \geq 2$. In the special case of the harmonic oscillator $f(r) = kr^2$, all the inequalities in (2.9) collapse to the well-known exact N -body solution $E = F_N(v) = 3v^{1/2}$. For this problem, the trajectory function F_N does not change at all with N for it always has the value $3v^{1/2}$. In many other cases, although the trajectory function F_N is not constant, it varies only very little with N so that the inequalities (2.9) may determine the N -boson energy surprisingly accurately. For example, in the case of the linear potential [7] the energy is determined by (2.9) with error less than 0.15%; by using the method described in the following section this error is reduced to 0.116%.

III. COLLECTIVE-FIELD THEORY AND HARTREE UPPER BOUNDS

The main difficulty with the N -boson problem is to satisfy the constraints of permutation symmetry and translation invariance simultaneously. One variational approach is to work with a translation invariant *Hamiltonian* but, instead of a boson function of the $N-1$ relative coordinates $\{\rho_{i>1}\}$, to employ a manifestly symmetric function $\theta_N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ of the N individual-particle coordinates. Provided θ_N is square integrable over $\prod_{i=1}^N d^3\mathbf{r}_i$ it follows that it is also square integrable over $\prod_{i=1}^N d^3\rho_i$ and, in a general Fourier analysis of θ_N in terms of functions of all the $\{\rho_i\}$, the dependence on ρ_1 could be expressed by a factor in each term, acting like a constant with respect to the Hamiltonian. It follows therefore that such a wave function, although it is not translation invariant, would generate an energy upper bound. That is to say, in our notation, we have

$$F_N(v) \leq \frac{(\theta_N, \xi\theta_N)}{(\theta_N, \theta_N)}. \quad (3.1)$$

The most convenient of such boson trial functions are of course Hartree products with the general form

$$\theta_N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \chi(\mathbf{r}_1)\chi(\mathbf{r}_2) \cdots \chi(\mathbf{r}_N). \quad (3.2)$$

We now introduce a "density function" ϕ defined by the relation

$$a^{-3}\phi(\mathbf{r}/a) = \chi^2(\mathbf{r}), \quad (3.3)$$

with the normalization

$$\int \chi^2(\mathbf{r})d^3\mathbf{r} = \int \phi(\mathbf{s})d^3\mathbf{s} = 1, \quad \mathbf{s} = \mathbf{r}/a. \quad (3.4)$$

In terms of the density ϕ we find [7] that the upper bound (3.1) can be expressed in the form

$$\begin{aligned} F_N(v) &\leq F_\phi(v) \\ &= \frac{1}{8} \int \frac{[\nabla\phi(\mathbf{s})]^2}{\phi(\mathbf{s})} d^3\mathbf{s} \\ &\quad + v \int \int \phi(\mathbf{s})f(|\mathbf{s}-\mathbf{s}'|)\phi(\mathbf{s}')d^3\mathbf{s}d^3\mathbf{s}'. \end{aligned} \quad (3.5)$$

This result has some interesting consequences, which are derived in more detail in Ref. [7]. First, in terms of our convention that the dimensionless coupling parameter v is fixed (so that the original coupling γ diminishes with increasing N so as to keep γN constant), it is evident that the upper bound F_ϕ is independent of N . Hence $F_\phi(v)$ is an upper bound to $F_\infty(v)$. Second, if we choose the Gaussian shape for the density ϕ , and we minimize $F_\phi(v)$ with respect to a scale parameter, then the result turns out to be identical to the Gaussian upper bound $F_G(v)$ which we found in Sec. II by the use of a *translation-invariant* Gaussian trial function. Hence, by using (3.5), we can find an upper energy bound (for all N) which is at least as good as the Gaussian upper bound $F_G(v)$. Lastly, (3.5) is exactly the expression obtained when collective-field theory [14-19] is applied to estimate the energy of the N -boson problem. However, it does not seem so clear from the rather complicated formulation of the latter theory that the expression $F_\phi(v)$ given in (3.5) is an upper bound to the quantity $F_\infty(v)$, as we now know it to be.

A very useful family of densities, which includes the Gaussian densities as a special case, is given by

$$\phi(\mathbf{s}) = (4\pi b^3 I)^{-1} w(s/b), \quad s = |\mathbf{s}|, \quad (3.6)$$

where the density function $w(t)$ is

$$w(t) = e^{-t^q}, \quad (3.7)$$

and the normalization integral I has the explicit form

$$I(q) = \int_0^\infty w^2(t)t^2 dt = \Gamma(3/q)/q. \quad (3.8)$$

If we use this family of densities and we minimize $F_\phi(v)$ with respect to both b and q , then we call the result $F_W(v)$. In summary we have

$$F_2(v) \leq F_N(v) \leq F_\infty(v) \leq F_W(v) \leq F_G(v). \quad (3.9)$$

From (2.5) we see that the N -body energy \mathcal{E} is recovered from the F functions by the general formula

$$\mathcal{E} = \frac{\hbar^2(N-1)}{ma^2} F \left[\frac{ma^2\gamma N}{2\hbar^2} \right]. \quad (3.10)$$

Since the exact trajectory functions $F_N(v)$, the Gaussian upper bound $F_G(v)$, and the Hartree upper bound $F_W(v)$

are all minimal with respect to scale changes, it follows [20] that *all* these results automatically satisfy the virial theorem.

IV. THE YUKAWA AND GRAVITATIONAL POTENTIALS

We now consider the Yukawa potential whose shape is given by

$$f(r) = -\frac{e^{-\lambda r}}{r}, \quad \lambda > 0. \quad (4.1)$$

Although it is clear from our general formulation that we need consider only *one* potential parameter, namely, the dimensionless coupling v , we have nevertheless introduced λ into the potential shape so that at any stage of the work we can easily recover the special case of the gravitational potential by the limit $\lambda \rightarrow 0$. Usually we shall set $\lambda = 1$ for the Yukawa potential.

All our results come from (3.9) and (3.10). The gravitational potential provides a useful guide to the energy range we need to consider. In that case we have

$$F_2(v) = -\frac{v^2}{4} \leq F_N(v) \leq F_\infty(v) \leq -\frac{2v^2}{3\pi} = F_G(v), \quad \lambda = 0. \quad (4.2)$$

The bounds F_2 and F_G for the pure gravitational problem were first found by Post [21]; later, some weaker bounds were obtained independently by Lévy-Leblond [22]. In contemplating such simple formulas, one must stop to remember that they bound the energy of the N -boson problem for all N and all values of the coupling γ . Meanwhile, since $-1/r < f(r)$, we know that $-v^2/4$ is a *lower* bound to $F_2(v)$ for $\lambda > 0$. Consequently, for the remainder of this section, we shall use, instead of F , the ratio R given generally by

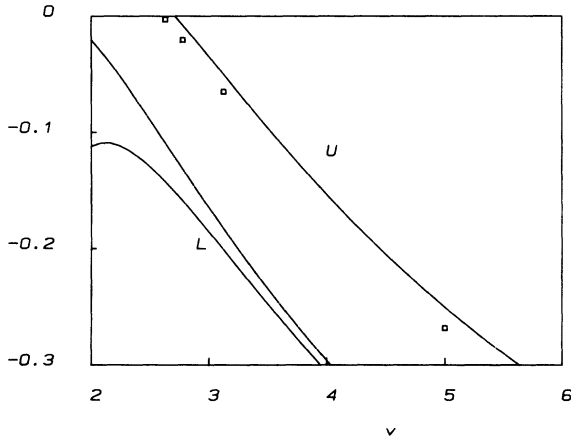


FIG. 1. The energy ratio $R = 4F(v)/v^2$ for the Yukawa potential $V(r) = -ve^{-r}/r$. U corresponds to the upper bound $F_G(v)$ found with the aid of a Gaussian trial function. The lower bound L corresponds, respectively, to $F_2(v)$, which is the lowest eigenvalue of the one-particle Hamiltonian $\mathfrak{H} = -\Delta + V(r)$, and the convenient formula $-(1-2/v)^2 - 0.224/v$, which is, in turn, a lower bound to $F_2(v)$. The discrete data (\square) are Hartree upper bounds from Ref. [8].

$$R(v) = \frac{4F(v)}{v^2} \geq -1 \quad (4.3)$$

to represent energies. For large v the ground-state wave function is concentrated near $r=0$ and the energy is essentially that of the gravitational potential. Hence, even with $\lambda > 0$, we can recover the gravitational results from the Yukawa ratios by taking the limit:

$$\lim_{v \rightarrow \infty} R(v) = R(\infty) = R(1)|_{\lambda=0}. \quad (4.4)$$

We now turn to the Yukawa potential $\lambda = 1$. The computation for the Gaussian upper bound $R_G(v)$ is very straightforward and needs no further comment here. We shall, however, give some details to do with the Hartree upper bound. We have to substitute the density (3.6) into the expression (3.5), integrate, and then minimize with respect to b and q . We obtain the following energy expression (before minimization):

$$E(v, b, q) = \frac{K}{8Ib^2} + vJ, \quad (4.5)$$

where I is given by (3.8), K is given by

$$K = \int_0^\infty \frac{[w'(s)]^2}{w(s)} s^2 ds = (1+q)\Gamma(1+1/q), \quad (4.6)$$

and the potential-energy integral J may be written

$$J(b, q) = \frac{2}{\lambda b^2 I^2} \int_0^\infty dt w(t) t \sinh(\lambda bt) \times \int_t^\infty w(s) s e^{-\lambda bs} ds. \quad (4.7)$$

Two advantages of writing J in this form are that integrations over the absolute-value function are avoided, and the gravitational limit $\lambda \rightarrow 0$ is easy to obtain analytically. In order to find $R_w(v)$ we must minimize $E(v, b, q)$ with respect to b and q , and then multiply by $4/v^2$.

In Figs. 1 and 2 we exhibit the lower bound $R_2(v)$, the

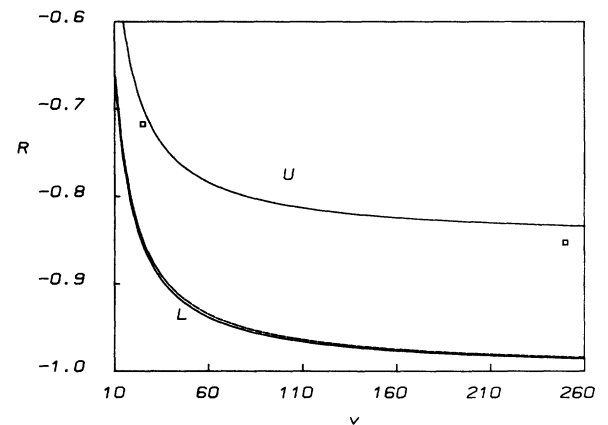


FIG. 2. The energy ratio $R = 4F(v)/v^2$ for the Yukawa potential $V(r) = -ve^{-r}/r$. This graph is a continuation of Fig. 1. In the gravitational (or Coulomb) limit $v \rightarrow \infty$ we have $R_2(\infty) = -1$, $R_G(\infty) = -8/3\pi$, $R_w(\infty) = -0.866$, and $R_M(\infty) = -0.868$. We suspect that the *exact* gravitational solution is close to -0.866 but a higher lower bound is required to confirm this conjecture.

TABLE I. Values of the ratio $R = 4E/v^2$ for the Yukawa potential $V(r) = -ve^{-\lambda r}/r$, with $\lambda = 1$. R_L is the lower bound obtained by the equivalent two-body method, R_M is an optimal Hartree upper bound from Ref. [8], R_W is our Hartree upper bound, and R_G is the upper bound obtained with the aid of a Gaussian trial function. The limit $v \rightarrow \infty$ corresponds to the gravitational (or Coulomb) special case $\lambda = 0$.

v	R_L	R_M [8]	R_W	R_G
2.631 58	-0.109	-0.002 88	-0.001 16	0.008 45
2.777 78	-0.132	-0.020 5	-0.018 7	-0.007 71
3.125	-0.183	-0.065 0	-0.062 9	-0.050 2
5.0	-0.397	-0.268	-0.266	-0.250
25.0	-0.849	-0.717	-0.714	-0.698
250.0	-0.983	-0.852	-0.849	-0.833
∞	-1.0	-0.868	-0.866	-0.849

Gaussian upper bound $R_G(v)$, and some Hartree upper bounds (\square) from Membrado, Pacheco, and Sañudo [8]. The lowest curve in these figures is a lower bound to $R_2(v)$ which we found useful in connection with a study of screened Coulomb potentials [23,24], namely, the left-hand side of the inequalities:

$$-(1-2/v)^2 - 0.224/v \leq R_2(v) \leq -(1-2/v)^2. \quad (4.8)$$

The point of (4.8), which we established with the aid of a soluble comparison Hulthén potential, is that it is very convenient to have a *formula* for the lower bound instead of a task involving the numerical solution of Schrödinger's equation. However, the analytical approximation of the *one*-body Yukawa problem is another story [25].

Our own Hartree results are very close to those of Membrado, Pacheco, and Sañudo, and slightly above them; this is completely consistent with their theory which finds the *best* Hartree upper bound. These various results are compared in the Table I.

V. CONCLUSION

A system of N bosons interacting via attractive pair potentials must collapse. This process can be defeated by weakening the coupling parameter γ in such a way that the product γN is held constant. This device leads to a well-defined theoretical problem for all N . The energy \mathcal{E} of the system may be written quite generally in the form

$$\mathcal{E} = \frac{\hbar^2(N-1)}{ma^2} F_N \left[\frac{ma^2\gamma N}{2\hbar^2} \right], \quad (5.1)$$

where the "trajectory function" $F_N(v)$ depends on the potential shape $f(r)$ and on N . We have proved that, for each v , $F_N(v)$ increases monotonically with $N \geq 2$. In many instances, however, F_N does not vary very much with N . For such problems, $F_2(v)$ and $F_\infty(v)$ are not far apart, and therefore the entire family of many-body trajectories is sandwiched between close outer bounds. Since a Gaussian trial function provides an upper bound to $F_\infty(v)$, a sufficient criterion for close bounds (for all N) is that a Gaussian trial function would provide a good estimate for the energy of the *one*-body problem with Hamiltonian \mathfrak{H} .

In the case of the Yukawa pair potential, we have explored a more general upper bound than $F_G(v)$, provided by a Hartree trial function with two-parameter single-particle factors of the form $\exp[-(r/b)^q]$. Our results for this problem are very close to those of Membrado, Pacheco, and Sañudo, who, for certain values of v , find the energy corresponding to the best Hartree wave function. In the gravitational limit ($v \rightarrow \infty$), we have to find just one number, the limiting "ratio" R_∞ , which, from Table I, is determined by the inequality

$$R_2 = -1 \leq R_\infty \leq -0.866 = R_W < R_G = -8/3\pi. \quad (5.2)$$

The mean value of the bounds $R = -0.933$ therefore determines R_∞ with error less than 7.2%. At this time we cannot with certainty say more.

However, we have studied [6] the counterpart of the Coulomb (or gravitational) problem in *one* dimension, namely, the delta-function potential $-\delta(x)$. These two problems scale in the same way: consequently the energies in both cases are proportional to v^2 . For the one-dimensional problem we have the advantage of an exact solution for all N . In the notation of the present article we have [6]

$$R_N = -\frac{2}{3} \left[1 + \frac{1}{N} \right] < R_W = -0.659472. \quad (5.3)$$

Thus, for the δ -function potential, the Hartree upper bound is about 1% above the exact value $R_\infty = -\frac{2}{3}$. We may also have attained this quality of upper bound for the gravitational problem: the only way to be sure about that would be to devise a better lower bound, for example, by using the method of Hill [26]. Even though such security is hard to come by, it is well worth pursuing because it helps us enormously in scientific endeavor if we can know with certainty exactly what our physical theories predict.

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