General energy bounds for systems of bosons with soft cores

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We study a bound system of *N* identical bosons interacting by model pair potentials of the form *V*(*r*) $=$ λ sgn(*p*)*r*^{*p*}+ μ /*r*², λ > 0, μ ≥ 0. By using a variational trial function and the "equivalent two-body method," we find explicit upper and lower bound formulas for the *N*-particle ground-state energy in arbitrary spatial dimensions $d \ge 3$ for the two cases $p=2$ and $p=-1$. It is demonstrated that the upper bound can be systematically improved with the aid of a special large-*N* limit in collective field theory.

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I. INTRODUCTION

The principal subject of this paper is the ground-state energy of a system composed of *N* identical bosons bound together by pair potentials. Such systems usually collapse in the large-*N* limit; that is to say, the binding energy per particle rises with *N* to infinity $[1,2]$. In two earlier papers we studied gravitating boson systems $\lceil 3 \rceil$, and systems of bosons or fermions that interact by wide classes of purely attractive pair potential $[4]$. In the present paper we extend this work for the boson case to systems with pair potentials that bind the system but have a soft repulsive core of the form μ/r^2 . The methods we develop to analyze these systems may have application to models for Bose-Einstein condensates $[5,6]$ in which there is at present much renewed interest $[7-17]$. As in our earlier work, the goal of the present study is to provide simple general energy bounds as functions of the parameters m , λ , μ , and *N*. Since it is not difficult to do so, we also allow for an arbitrary number $d \geq 3$ of spatial dimensions.

Formulas for *N*-particle upper and lower energy bounds are derived for pair potentials $V_{ii} = V_0 f(r_{ii})$ whose shapes $f(r)$ are either harmonic oscillators with a soft core $f(r)$ $=$ $\lambda r^2 + \mu/r^2$, or Kratzer potentials $f(r) = -\lambda/r + \mu/r^2$. The shapes of these two potentials are shown in Fig. 1 for λ $=\mu=1$. The first of the models could perhaps be considered as a generalization of the soluble one-dimensional Calogero model $[18–20]$ to dimension $d \ge 3$. For such potentials, with minima $f(\hat{r})$ at $r = \hat{r} > 0$, provided there are enough spatial dimensions available $(d+1) \ge N$ for every pair distance to satisfy $r_{ij} = \hat{r}$, then, in classical mechanics the lowest energy would be equal to $\binom{N}{2}V_0 f(\hat{r})$. This expression provides a lower energy bound in both classical and quantum mechanics; our general energy bounds (valid for all $N \ge 2$) will show that this value is approached asymptotically for large V_0 in the limit $d \rightarrow \infty$; this is possible because the positive contribution from zero-point oscillations varies like $(N-1)(NV_0)^{1/2}$ and is eventually dominated by the static potential term.

The nonindividually of identical quantum-mechanical particles introduces a very powerful constraint that allows us to relate the *N*-body problem to a specially constructed (reduced) two-body problem having an overall factor of $N-1$ and a potential enhanced by *N*/2, corresponding respectively to the $N-1$ relative kinetic-energy operators and the $N(N)$ $-1/2$ pair potentials. This "equivalent two-body" notion, which is central to our approach to the study of these systems, will be formulated explicitly in Sec. II. The *N*-body energy $\mathcal E$ is described by function $E = F_N(v) = \mathcal E/(N-1)$, where $v = (N/2)V_0$, and V_0 is the coupling parameter (in units $\hbar = m = 1$). Since *v* includes the factor *N*, it follows that if we consider a *finite* value of *v* and let $N \rightarrow \infty$, this implies that $V_0 \rightarrow 0$. The well-known exactly soluble δ -potential problem in one dimension [21] provides a convenient illustration of the energy function $F(v)$. If $V(r)$ = $-V_0\delta(r)$, we have exactly

$$
\frac{\mathcal{E}}{N-1} = E = F_N(v) = -\frac{1}{6} \left[1 + \frac{1}{N} \right] v^2, \quad N \ge 2, \quad v = \frac{N}{2} V_0.
$$
\n(1.1)

FIG. 1. The shapes of the two potentials studied: the harmonic oscillator with soft core, $H = f(r) = \lambda r^2 + \mu r^{-2}$, and Kratzer's potential, $K=f(r)=-\lambda r^{-1}+\mu r^{-2}$, with $\lambda=\mu=1$ (units $\hbar=m=1$).

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The shape of the potential dictates the form v^2 of these energy curves, and there is a distinct curve for each value of $N \geq 2$. The curves of this particular example satisfy the general functional inequalities $[3]$

$$
F_2(v) \le E = F_N(v) \le F_\infty(v) \le F_\phi(v) \le F_G(v), \quad (1.2)
$$

where, as will be explained later, $F_{\phi}(v)$ is an upper bound obtained with the aid of collective-field theory in the large-*N* limit, and $F_G(v)$ is the upper-bound curve obtained by employing an *N*-body translation-invariant Gaussian trial wave function. The ordering of the $F_N(v)$ curves with *N* is a consequence of the monotonic increase in the severity of the boson-symmetrization constraint with increasing *N*. For the soluble δ -potential model we have [3] explicitly: $F_\infty(1)$ = $-1/6$, $F_{\phi}(1) = -0.164 868$, and $F_G(1) = -1/2\pi$. The family of densities used for the variational collective-field upper bound is given by

$$
\phi(r) = e^{-(r/b)^q}, \quad b, q > 0. \tag{1.3}
$$

The energy is minimized with respect to the positive scale and power parameters *b* and *q*. The effectiveness of this useful two-parameter family of trial densities is also demonstrated by the applications discussed in Secs. IV and V below. We conjecture that $F_{\phi}(v)$ is close to $F_{\infty}(v)$ for the more general problems considered in this paper but we know no way of proving such a claim at this time. For another well-known soluble problem, the *d*-dimensional harmonic oscillator $V(r) = V_0 r^2$, with $d \ge 1$, the inequalities (1.2) all collapse together to the common exact value $E = dv^{1/2}$.

II. *N***-BODY PROBLEM IN THE CENTRE-OF-MASS FRAME**

The Hamiltonian, with center of mass removed, for a system of *N* identical particles each of mass *m* interacting via central pair potentials may be written

$$
\mathcal{H} = \frac{1}{2m} \sum_{i=1}^{N} \mathbf{p}_i^2 - \frac{1}{2mN} \left(\sum_{i=1}^{N} \mathbf{p}_i \right)^2 + \sum_{j>i=1}^{N} V_0 f \left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a} \right),
$$
\n(2.1)

where V_0 and a are respectively the depth and range parameters of the potential with shape *f*. By algebraic rearrangement Eq. (2.1) may be rewritten in the more symmetrical form

$$
\mathcal{H} = \sum_{j>i=1}^{N} \left\{ \frac{1}{2mN} (\mathbf{p}_i - \mathbf{p}_j)^2 + V_0 f\left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}\right) \right\}.
$$
 (2.2)

We now define new coordinates by $\rho = BR$, where $\rho = [\rho_i]$ and $R = [\mathbf{r}_i]$ are column vectors of the new and old coordinates, respectively, and *B* is a real constant $N \times N$ matrix. For convenience we require all the rows of *B* to be unit vectors, we let the elements of the first row all be equal to $1/\sqrt{N}$, so that ρ_1 is proportional to the center-of-mass coordinate; we also require that the remaining $N-1$ rows of *B* be orthogonal to the first row, so that they define a set of $N-1$ relative coordinates. One more row is also fixed so that we have at least one pair distance at our disposal, namely,

$$
\rho_2 = \frac{\mathbf{r}_1 - \mathbf{r}_2}{\sqrt{2}}.\tag{2.3}
$$

For boson systems, we have found that Jacobi relative coordinates, for which *B* is orthogonal, are the most useful. Thus, corresponding to the transformation $\rho = BR$ of the coordinates, it follows that the column vector *P* of the associated momenta transforms to the new momenta $\Pi = [\pi_i]$ by the relation $\Pi = (B^T)^{-1}P = P$. If Ψ is any translation-invariant wave function for the *N*-body system composed of identical bosons, then we can write $[22,23]$ the following mean energy relation between the *N*-body and two-body systems:

$$
(\Psi, \mathcal{H}\Psi) = (\Psi, \mathbb{H}\Psi), \tag{2.4}
$$

where the "reduced" two-particle Hamiltonian H is given by

$$
H = (N - 1) \left[\frac{1}{2m} \pi_2^2 + \frac{N}{2} V_0 f \left(\frac{\sqrt{2} |\rho_2|}{a} \right) \right].
$$
 (2.5)

Further simplifications can be achieved if we work with dimensionless quantities. We suppose that the translationinvariant *N*-body energy is $\mathcal E$ and we define the dimensionless energy and coupling parameters *E* and *v* by the expressions

$$
E = \frac{m\mathcal{E}a^2}{(N-1)\hbar^2}, \quad v = \frac{N_m V_0 a^2}{2\hbar^2}.
$$
 (2.6)

It is then natural to define a dimensionless versions of the reduced two-body Hamiltonian H and the relative coordinate ρ_2 by the relations

$$
H = \frac{m\mathbb{H}a^2}{(N-1)\hbar^2} = -\Delta + vf(r),
$$

$$
\mathbf{r} = \sqrt{2}\rho_2/a = (\mathbf{r}_1 - \mathbf{r}_2)/a, \quad r = ||\mathbf{r}||.
$$
 (2.7)

We note that the Hamiltonian *H* depends on *N only* through the dimensionless coupling parameter *v*. By the Rayleigh-Ritz (min-max) principle $[24–26]$, we have the following characterization of the *N*-body ground-state energy parameter *E* in terms of *H*:

$$
E = \min_{\Psi} \frac{(\Psi, H\Psi)}{(\Psi, \Psi)} = F_N(v),
$$
 (2.8)

where Ψ is a translation-invariant function of the $N-1$ relative coordinates (and spin variables, if any) that is symmetric under the permutation of the *N* individual-particle indices. The *N*-body energy $\mathcal E$ is recovered from E by inverting Eq. (2.6) . Thus we have explicitly

$$
\mathcal{E} = \frac{(N-1)\hbar^2}{ma^2} F_N \bigg(\frac{NmV_0 a^2}{2\hbar^2} \bigg). \tag{2.9}
$$

However, for the remainder of this paper we shall work with the dimensionless form $E = F_N(v)$: the problem is to find or approximate F_N . In each situation we shall have to specify the dimension *d* of physical space; usually $d=3$.

III. ENERGY BOUNDS

The energy bounds used in this paper are summarized in terms of the F functions by Eq. (1.2) . The history of the equivalent two-body method for boson systems has been described in the earlier papers $[3,4]$ and in the references therein. The main result is a general energy lower bound, which, for boson systems with orthogonal Jacobi relative coordinates, is given by

$$
F_2(v) \le E = F_N(v),\tag{3.1}
$$

where $F_2(v)$ is the lowest eigenvalue of the one-particle ("reduced" two-particle) Hamiltonian $H = -\Delta + vf(r)$. With equal simplicity, our weakest upper bound $F_G(N)$, provided by a Gaussian boson trial function Ψ , may also be expressed in terms of the one-body operator *H*. This is a consequence of the following argument. If and only if the symmetric translation-invariant function Ψ is Gaussian $[27,28]$, it may be factored in the form

$$
\Psi(\rho_2, \rho_3, ..., \rho_N) = \psi(\rho_2) \eta(\rho_3, \rho_4, ..., \rho_N). \tag{3.2}
$$

But the equivalence (2.4) then implies, in this case, that E $\leq (\psi, H\psi) \|\psi\|^{-2}$. This explains why the inequalities (1.2) collapse together in the case of the harmonic oscillator for which the exact one-body lowest eigenfunction of *H* is also Gaussian. In this argument we assume for the upper bound that $\langle H \rangle$ has been optimized with respect to the scale of the wave function. The boson symmetry of these Gaussian functions is demonstrated most clearly by the following algebraic identity:

$$
\sum_{j>i=1}^{N} (\mathbf{r}_{i} - \mathbf{r}_{j})^{2} = N \sum_{k=2}^{N} \rho_{k}^{2}.
$$
 (3.3)

The potentially better upper bound $F_{\phi}(N)$ is more complicated both to derive and to compute $[3]$. It is found by considering the collective field model in the large-*N* limit. The energy so obtained is an upper bound to $F_\infty(v)$ and this, in turn, may be closely approximated from above by optimizing the right-hand side of the following equation:

$$
F_N(v) \le F_\phi(v) = \frac{1}{8} \int \frac{[\nabla \phi(r)]^2}{\phi(r)} d^d r
$$

+
$$
+ v \int \int \phi(r) f(|r - r'|) \phi(r') d^d r d^d r', \qquad (3.4)
$$

where $\phi(r)$ is a trial probability density function (for interparticle distances) satisfying $\int \phi(r) d^d r = 1$. It has been shown [3] that if ϕ is Gaussian, and the energy is optimized with respect to a scale parameter, then the result $F_{\phi}(v)$ is identical to the upper bound $F_G(v)$ obtained with the aid of a scale-optimized translation-invariant Gaussian trial wave function. The wider possible choice of the form of the probability density ϕ allows us to transcend the Gaussian bound while still working essentially with a variational "function" of single variable for the *N*-body problem.

In order to facilitate the reproduction of our results and the application of the method to other problems, we make the following explicit technical remarks concerning the case *d* $=$ 3. It is very helpful to think of the probability density as a function $\phi(r) = w(r/b) = w(s)$, which depends on the remaining parameter *q*, to be discussed later. If we let *I* $=\int_0^\infty w(s) s^2 ds$, then the kinetic-energy integral becomes

$$
\langle E^{\text{kin}} \rangle = \frac{1}{8Ib^2} \int_0^\infty \frac{\left[w'(s)\right]^2}{w(s)} s^2 ds \tag{3.5}
$$

and potential-energy integrals for pure powers may be written

$$
\langle r^{p} \rangle = \frac{b^{p}}{I^{2}(p+2)} \int_{0}^{\infty} dt \, w(t) t
$$

$$
\times \int_{t}^{\infty} ds \, w(s) s \{ (s+t)^{p+2} - (s-t)^{p+2} \}, \quad p \neq -2.
$$
 (3.6)

For the case $p=-2$ we have instead

$$
\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{I^2 b^2} \int_0^\infty dt \, w(t) t \int_t^\infty ds \, w(s) s \ln \left(\frac{s+t}{s-t} \right). \tag{3.7}
$$

With the terms expressed in this form, the minimization over scale $b > 0$ can often be carried out explicitly yielding an algebraic expression that then needs to be minimized with respect to the remaining parameter *q*. We have explored various alternative forms for $w(s)$, such as $s^q \exp(-s²)$ and $\exp[-(s-q)^2]$, but have found it difficult to improve on the variable-power family $w(s) = \exp(-s^q)$ that we have used to obtain the results discussed in detail in Secs. IV and V below.

IV. HARMONIC OSCILLATOR WITH A SOFT CORE

We now choose the potential shape to be

$$
f(r) = \lambda r^2 + \frac{\mu}{r^2}, \quad \lambda > 0, \quad \mu \ge 0.
$$
 (4.1)

The lower bound $F_2(v)$ is given by the lowest eigenvalue of $H=-\Delta + v f(r)$ in *d* dimensions, a problem that is discussed, for example, in Ref. [29]. The Gaussian upper bound $F_G(v)$ is provided by minimizing the Rayleigh quotient $(\psi, H\psi) / (\psi, \psi)$ with respect to the scale variable α in $\psi(r)$ $= e^{-(1/2)\alpha r^2}$ in *d* dimensions. These calculations yield the following bounds on the N -boson energy parameter E [the energy itself is recovered essentially by multiplying *E* by *N* -1 , according to Eq. (2.10)]

$$
2(v\lambda)^{1/2} \left\{ 1 + \left[\mu v + \left(\frac{d}{2} - 1 \right)^2 \right]^{1/2} \right\} < E < (dv\lambda)^{1/2}
$$
\n
$$
\times \left[d + \frac{4v\mu}{d - 2} \right]^{1/2}, \quad d \ge 3. \tag{4.2}
$$

The Gaussian trial wave function allows us to compute an approximate value for the mean-squared pair separation σ^2 a measure of the size of the system. We find

$$
\sigma^{2} = \langle (\mathbf{r}_{1} - \mathbf{r}_{2})^{2} \rangle = \frac{d}{2(v\lambda)^{1/2}} \left(1 + \frac{4v\mu}{d(d-2)} \right)^{1/2}.
$$
 (4.3)

We now look at some special cases. For the harmonic oscillator, $\mu=0$, the inequalities collapse to the exact value $E=d(v\lambda)^{1/2}$. The asymptotic forms of the bounds as $v\rightarrow\infty$ and μ > 0 are given by

$$
\sim 2v(\lambda \mu)^{1/2} \le E \le \sim 2v(\lambda \mu)^{1/2} \left(\frac{d}{d-2}\right)^{1/2}.
$$
 (4.4)

Thus for large *N* the energy per particle *E* increases like *N*, although the "size" of the system (as estimated by the Gaussian wave function) approaches the constant value σ $=[d/(d-2)]^{1/4}(\mu/\lambda)^{1/4}$. If *d* is now taken large, the asymptotic form of the energy approaches the classical expression $E = vf(\hat{r})$, where $\hat{r} = \sigma = (\mu/\lambda)^{1/4}$ is the position of the minimum of $f(r)$.

For the special case $d=3$ we obtain in general

$$
(v\lambda)^{1/2}[2+(1+4\,\mu v)^{1/2}]\leq E\leq (v\lambda)^{1/2}[9+12v\,\mu]^{1/2}.\tag{4.5}
$$

These results are shown in Fig. 2 along with the improved upper bound ("dashed" curve) obtained with the trial probability density function (1.3) . The extreme optimal $q(v)$ values in the range shown were $q(2)=2.8593, q(20)=4.460$. Hence the optimal probability density $\phi(r)$ is found to be quite far from Gaussian.

V. KRATZER POTENTIAL

The Kratzer potential has shape function given $[30-39]$ by

$$
f(r) = -\frac{\lambda}{r} + \frac{\mu}{r^2}, \quad \lambda > 0, \quad \mu \ge 0.
$$
 (5.1)

The *N*-particle lower bound $F_2(v)$ is provided by the lowest eigenvalue of $H=-\Delta + v f(r)$ in *d* dimensions, a problem that is discussed, for example, in Ref. $[40]$. Meanwhile an exactly similar calculation to that described in Sec. IV, with a Gaussian trial function, generates the corresponding upper bound. We find in this way that the energy parameter *E* satisfies the following inequalities:

$$
-\frac{(v\lambda)^2}{\left\{1+\left[(d-2)^2+4v\mu\right]^{1/2}\right\}^2} < E < -\frac{(v\lambda\gamma_d)^2}{\left[2d+\frac{8v\mu}{d-2}\right]}, \quad d \ge 3,
$$
\n(5.2)

FIG. 2. Bounds for the energy parameter $E(v) = \mathcal{E}/(N-1)$ of the *N*-boson system with pair potentials of the form $f(r) = V_0(r^2)$ $+r^{-2}$), as a function of $v = NV_0/2$. The graphs show: *U* the upper bound $F_G(v)$ found by a Gaussian trial function, *L* the lower bound $F_2(v)$ by the equivalent two-body method, and "dashed" the upper bound $F_{\phi}(v)$ by collective field theory.

where the *d*-dependent constant γ_d is given by

$$
\gamma_d = \frac{\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}, \quad \gamma_3 = \frac{2}{\sqrt{\pi}}.
$$
 (5.3)

The Gaussian trial wave function again allows us to compute an approximate value for the mean-squared pair separation. We find

$$
\sigma^2 = \langle (\mathbf{r}_1 - \mathbf{r}_2)^2 \rangle = \frac{d^3}{2(v\lambda \gamma_d)^2} \left(1 + \frac{4v\,\mu}{d(d-2)} \right)^2.
$$
 (5.4)

For the pure gravitational case $\mu=0$ the energy inequalities become

$$
-\frac{(v\lambda)^2}{(d-1)^2} \le E < -\frac{(v\lambda\gamma_d)^2}{2d}.\tag{5.5}
$$

The asymptotic forms of the bounds as $v \rightarrow \infty$ and $\mu > 0$ are given by

$$
\sim -\frac{v\lambda^2}{4\mu} \le E \le \sim -\frac{v\lambda^2}{4\mu} M(d),
$$

where $M(d) = \left[\frac{\gamma_d^2(d-2)}{2} \right]$. (5.6)

The function $M(d)$ increases monotonically with d to 1; $M(3) = 2/\pi \approx 0.636 62$; $M(8) > 0.9$. Thus, as for the previ-

FIG. 3. Bounds for the energy parameter $E(v) = \mathcal{E}/(N-1)$ of the *N*-boson system with pair potentials of the form $f(r) = V_0$ $(-r^{-1}+r^{-2})$, as a function of $v=NV_0/2$. The graphs show: *U* the upper bound $F_G(v)$ found by a Gaussian trial function, *L* the lower bound $F_2(v)$ by the equivalent two-body method, and "dashed" the upper bound $F_{\phi}(v)$ by collective field theory.

ous model, the energy per particle *E* increases like *N*. Meanwhile the size (as estimated by the Gaussian wave function) approaches the constant value $\sigma = [2\sqrt{2}d/\gamma_d(d-2)](\mu/\lambda)$. If *d* is now taken large, the asymptotic form of the energy (again) approaches the classical expression $E = v f(\hat{r})$, in which $\hat{r} = \sigma = 2 \mu/\lambda$ is the position of the minimum of $f(r)$.

For the special case $d=3$ we obtain in general

$$
-\frac{(v\lambda)^2}{[1+(1+4v\mu)^{1/2}]^2} < E < -\frac{(v\lambda)^2}{\pi\left[\frac{3}{2}+2v\mu\right]}.\tag{5.7}
$$

The bounds for three dimensions are shown in Fig. 3, along with the improved upper bound ("dashed" curve) obtained

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with the trial probability density function (1.3) . The extreme optimal $q(v)$ values in the range shown were for this problem: $q(2)=2.0017$, $q(20)=3.237$. The optimal probability density (in this family) is found to be almost Gaussian for small $v < 3$ but very different from Gaussian for larger values of *v*.

VI. CONCLUSION

The main purpose of this paper is to derive general bounds for the energy of *N*-boson systems that are bound together by pair potentials with soft cores. We have examined two such models and we have provided upper and lower bound formulas valid for all $N \ge 2$ and $d \ge 3$, and for all values of the potential parameters that bind the system. These bounds are expressed in terms of the energy parameter $E = \mathcal{E}/(N-1) = F_N(v)$, where (in units with $\hbar = m = 1$) *v* $=NV_0/2$. If the potential shape is such that $F_2(v)$ is close to $F_\infty(v)$, then we obtain close upper and lower bounds valid for all $N \ge 2$. The upper bound $F_G(v)$ provided by a Gaussian trial function may be improved to $F_{\phi}(v)$, which is derived by using a (possibly non-Gaussian) trial probability density ϕ in a limiting form of collective field theory. In order to do significantly better one might hand craft a trial wave function for a particular $f(r)$ and *N*. Of course, to be secure about this wave function one would still need to find a good lower bound, a goal usually not easy to achieve. The global results we have obtained show that these boson systems are asymptotically bounded by expressions of the form $\mathcal{E} \sim cN^2$; if *d* is also large, we have shown that the heuristic classical expression $\mathcal{E} = \binom{N}{2} V_0 f(\hat{r})$ is reached asymptotically. Since the many-body problem continues to offer a serious challenge for direct numerical solution, it is very helpful to have some explicit analytic upper and lower energy bounds and size estimates for model systems such those discussed in this paper.

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