

One-Dimensional, Many-Body Calculation with a Correlated Gaussian Wave Function

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A two-parameter many-body correlated Gaussian wave function is used to calculate the expectation value of the Hamiltonian for N one-dimensional particles interacting through the one-dimensional analog of an atomic potential. Using a potential equal to four times the Slater-Kirkwood He-He potential, we calculate the optimum average interparticle separation, the ground-state energy, and the velocity of sound of the system as a function of particle mass. It is found that the correlated Gaussian always gives an improvement in energy compared with an uncorrelated Gaussian.

I. INTRODUCTION

UNCORRELATED Gaussian orbitals have been used by Bernardes and Primakoff¹ for the construction of a Heitler-London type trial wave function in a calculation of the ground-state properties of solid He³, and recently by Nosanow² and Mullin³ as factors in a Jastrow-type wave function for calculations on solid He³ and solid Ne, respectively. In this paper we wish to present a many-body calculation using a correlated Gaussian wave function. This calculation is intended to be a particularly straightforward application of a more general approach to the construction of trial wave functions appropriate to structured systems.

The general approach consists of using a wave function which is an appropriately symmetrized sum of all coordinate permutations of a function $\Psi(x_1, x_2, \dots, x_N)$ which has the property $P^{(i)}\Psi P^{(j)}\Psi < \Psi^2$, where $P^{(i)}$ and $P^{(j)}$ denote different permutations. The specific calculation will be that of the ground-state energy of a system of particles, confined to a ring, which interact with the one-dimensional analog of an atomic potential.

In the analysis, a two-parameter, N -particle wave function—the ground-state eigenfunction of the coupled-harmonic-oscillator Hamiltonian—will be used. One parameter b determines the average interparticle spacing; the other α essentially determines how strongly the particles resist overlapping each other. The circumference of the ring will be $L = Nb$ so that periodic boundary conditions can be applied and end effects eliminated.

The expectation value $E(b, \alpha)$ of a Hamiltonian

$$H = \sum (p_i^2/2m) + \sum_{i < j} V(x_i - x_j) \quad (1)$$

will be minimized with respect to b and α for various values of m . If the potential has a sufficiently strong attractive part, the minimum $E_0 = E(b_0, \alpha_0)$ will be negative and will occur at a finite value of b . This

¹ N. Bernardes and H. Primakoff, Phys. Rev. **119**, 968 (1960)

² L. H. Nosanow, Phys. Rev. Letters **13**, 270 (1964); the φ function used in this reference is not really a Gaussian, but can be analytically approximated by a Gaussian over a certain range of the variable.

³ W. J. Mullin, Phys. Rev. **134**, A1249 (1964).

corresponds, except for end effects, to the calculated equilibrium density of the solid into which the N particles would condense at absolute zero if placed on a ring whose circumference were greater than Nb_0 .

A comparison will be made between the results of this calculation of a calculation using uncorrelated Gaussian orbitals. It will be shown that the correlated function always yields a lower energy.

II. GENERAL CONSIDERATIONS

Consider the wave function

$$\Phi = \sum P\Psi(x_1, x_2, \dots, x_N), \quad (2)$$

where $\sum P$ means the appropriately symmetrized sum over all permutations of the variables. Suppose that Ψ has the property that $(P^{(i)}\Psi)(P^{(j)}\Psi)/\Psi^2 \approx 0$, where the superscripts denote different permutations, and that $\Psi(x_{n_1}, x_{n_2}, x_{n_3}, \dots)$ is only large when $x_{n_i+1} \approx x_{n_i} + b$. Then

$$\begin{aligned} \langle \Phi | \sum_{i < j} f(x_i - x_j) | \Phi \rangle / \langle \Phi | \Phi \rangle \\ \approx N \int |\Psi|^2 \sum_{i=2}^{N/2} f(x_i - x_1) dx / \int \Psi^2 dx, \quad (3) \end{aligned}$$

where the most convenient ordering of coordinates has been chosen, and where cross terms between different permutations have been dropped.⁴ It has also been tacitly assumed that periodic boundary conditions will be applied so that $x_{N+1} = x_1 + L$.

Equation (3) is most easily justified when

$$N \langle \Psi | P^{(i, i+1)} \Psi \rangle / \langle \Psi | \Psi \rangle \ll 1,$$

with

$$\langle \Psi | P^{(i, i+n)} \Psi \rangle \sim \langle \Psi | P^{(i, i+1)} \Psi \rangle^n;$$

$$N^2 \langle \Psi | P^{(i, i+1, i+2)} \Psi \rangle / \langle \Psi | \Psi \rangle \ll 1; \dots,$$

where the superscript on P denotes the cycles into which

⁴ Notational conveniences which will be followed in the remainder of the paper have been introduced: $\Psi \equiv \Psi(x_1, x_2, x_3, \dots, x_N)$, i.e., all of the coordinates listed in order; $\Psi(x_{m_1}, x_{m_2}, \dots, x_{m_n})$ will mean that the n variables given explicitly are in that order while all the rest are in the same order as in Ψ ; and, $dx \equiv dx_1 dx_2 \dots dx_N$. Symmetrized wave functions will always be denoted by Φ and unsymmetrized wave functions by Ψ .

the permutation can be resolved.⁵ We shall discuss in Sec. V how well the wave function which will be given in Eq. (6) and used as a basis for numerical calculations in this paper meets the above criteria. Meanwhile we shall use Eq. (3).

We also note that, to the extent to which Eq. (3) is valid, expectation values of two-body operators are the same whether the particles considered are bosons or fermions. This is not surprising in view of Girardeau's⁶ result that the energy spectrum of one-dimensional Bose and Fermi systems are identical when the two-body potential has a rigid core.

III. GROUND-STATE ANALYSIS

A possible choice for Ψ is the well-known ground-state eigenfunction of the coupled-harmonic-oscillator Hamiltonian

$$H^{(1)} = \sum (\hat{p}_i^2/2m) + \frac{1}{2}\Omega^2 \sum (x_{i+1} - x_i - b)^2. \quad (4)$$

Under the substitutions $x_{n+1} - x_n - b = q_{n+1} - q_n$, and the canonical transformation $q_n = (1/\sqrt{N})\sum_s e^{ins}Q_s$, $\hat{p}_n = \sum_s e^{-ins}P_s$, $H^{(1)}$ assumes the form of the Hamiltonian for a sum of uncoupled harmonic oscillators. The corresponding unnormalized ground-state wave function⁷ is

$$\Psi_Q = \exp\left\{-\frac{m}{2\hbar}\sum \omega_s Q_s^* Q_s\right\}, \quad (5)$$

where $\omega_s^2 = \Omega^2(2 \sin s/2)^2/m$ and $s = 2\pi l/N$, $-N/2 < l \leq N/2$. Unnormalized wave functions will be used throughout this paper. The summation sign without explicit limits will be used to denote a sum over the entire range of the indicated index.

At this point, a departure from the conventional⁸ treatment will be made and the wave function will be re-expressed in terms of the q_n . The result is

$$\Psi_1 = \exp\left\{-\alpha^2 \sum_{nn'} g(n-n')q_n q_{n'}\right\}, \quad (6)$$

where $\alpha^2 = 2\Omega m^{1/2}/\pi\hbar$ and

$$g(m) = \frac{\pi}{2N} \frac{\sin \pi/N}{\cos(2\pi m/N) - \cos(\pi/N)}. \quad (7)$$

For N large and $(n-n')/N$ small, $g(m)$ may be approximated by the larger of

$$g'(m) = (1 - 4m^2)^{-1} \quad (8a)$$

or

$$g'(m) = [1 - 4(|m| - N)^2]^{-1}. \quad (8b)$$

⁵ See, e.g., E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), p. 124.

⁶ M. Girardeau, *J. Math. Phys.* **1**, 516 (1960).

⁷ See, e.g., E. M. Henley and W. Thirring, *Elementary Quantum Field Theory* (McGraw-Hill Book Company, Inc., New York, 1962), pp. 1-21.

⁸ The author has been unable to find a development in the literature exactly paralleling that occurring between Eqs. (6) and (9) here. However, R. M. Fowler and T. E. Sterne [*Rev. Mod. Phys.* **4**, 635 (1932)] have discussed the form of the wave function in coordinate space for three particles coupled by a harmonic potential.

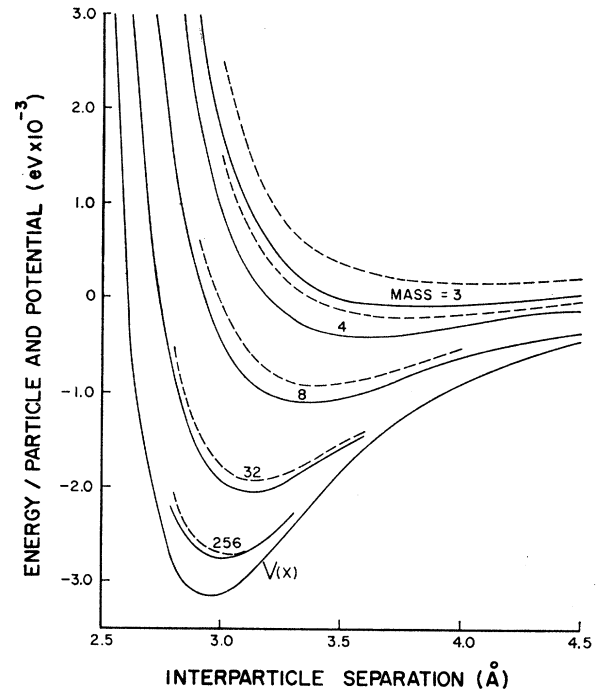


FIG. 1. Optimum energy per particle for various particle masses as a function of average interparticle separation and two-body interaction $V(x)$ as a function of particle separation x . Energies for correlated and uncorrelated Gaussian wave functions are given by the solid and dashed curves, respectively.

Since $\sum g(n-n')=0$, the function Ψ_1 is translationally invariant, and the permutation (x_1, x_2, \dots, x_N) leaves the value of Ψ_1 unchanged. Thus such permutations should be excluded from the sum over all permutations.

If all of the coordinates except for q_m are considered fixed, the dependence of the wave function upon q_m can be written

$$\Psi_1 = \exp\left\{-\alpha^2 \sum_{nn' \neq m} [g(n-m) - g(n-m)g(n'-m)]q_n q_{n'}\right\} \times \exp\left\{-\alpha^2 [q_m + \sum_{n \neq m} g(n-m)q_n]^2\right\}. \quad (9)$$

The second factor makes Ψ_1 a maximum for $q_m = -\sum_{n \neq m} g(n-m)q_n q_m$ and, since the $g(k)$ drop off rapidly as the argument increases, the m th particle will be constrained primarily to lie between q_{m+1} and q_{m-1} . Thus, the function Ψ_1 is equal to unity when all of the q_i are equal to zero or a constant, but, by adjusting α , it can be made to become very small as two particles approach each other.

The definition we have chosen for the q_n , namely $q_{n+1} - q_n = x_{n+1} - x_n - b$, applies only to $\Psi_1(x_1, x_2, \dots, x_N)$ and implies that $q_n = x_n - nb + \text{constant}$. In the customary definition, the constant is equal to zero and for convenience we shall also choose this value. Thus the argument of the exponential in Eq. (6) is $-\alpha^2 \sum_{nn'} g(n-n') \times (x_n - nb)(x_{n'} - n'b)$; however, it should be noted that

in constructing Φ out of Ψ_1 , the coordinate indices are permuted, but the numbers which are coefficients of b and arguments of g are not. Since Eq. (3) allows us to work with one particular permutation, we have merely chosen the most convenient one in the expression just given.

Further development is straightforward. Using H as defined in Eq. (1), and noting that

$$\sum \frac{p_i^2}{2m} \Psi_2 = \left(\frac{2\hbar\Omega}{\pi\sqrt{m}} - \frac{\Omega^2}{2} \sum (x_{i+1} - x_i - b)^2 \right) \Psi_2$$

we obtain

$$E(b, \alpha) = N \left\{ \frac{2\hbar\Omega}{\pi\sqrt{m}} + \int [V(y) - \frac{1}{2}\Omega^2(y-b)^2] \times \psi^2(y) dy / \int \psi^2(y) dy \right\}, \quad (10)$$

where $E(b, \alpha) \equiv \langle \Phi | H | \Phi \rangle / \langle \Phi | \Phi \rangle$, the transformation $\frac{1}{2}(x_2 + x_1) = X$, $x_2 - x_1 = y$ has been made,

$$\psi^2(y) = \int \Psi_1^2(y, X, x_3, \dots, x_N) dX dx_3, \dots, dx_N, \quad (11)$$

and it has been assumed that $V(2b) \ll V(b)$.⁹ From the form of Eq. (10) it is clear that if all the coordinates but two are integrated out, the argument of the exponent will be a quadratic form in the remaining two coordinates. Furthermore, the center-of-mass dependence on these two coordinates should vanish because the two particles are no longer constrained to be at any particular point on the ring. Thus we can take

$$\psi^2(y) = \exp[-2c\alpha^2(y-b)^2]. \quad (12)$$

It can be found that $c = \pi^2/16$ by noting that $\langle \Psi_2 | \frac{1}{2}\Omega \sum (q_{i+1} - q_i)^2 | \Psi_2 \rangle$ is well known from the problem of the coupled harmonic oscillators so that the value of the second integral in Eq. (10), which depends on c , is known and c can be determined. Equation (10) then becomes

$$\frac{E(b, \alpha)}{N} = \frac{\hbar^2\alpha^2}{2m} + \frac{\alpha}{2} \left(\frac{\pi}{2} \right)^{1/2} \times \int V(y) \exp\left[\frac{-\pi^2\alpha^2(y-b)^2}{8} \right] dy. \quad (13)$$

⁹ The neglect of all but nearest-neighbor interactions is not really necessary and is primarily made to simplify the form of Eq. (10). The most distant interactions may be included by adding to Eq. (10) the terms

$$\sum_n \int \psi_n^2(y_n) V(y_n) dy_n / \int \psi_n^2(y_n) dy_n,$$

where

$$X_n = \frac{1}{2}(x_1 + x_{n+2}) \quad y_n = x_{n+2} - x_1$$

and

$$\psi_n^2 = \int \Psi^2 dX_n dx_2 \cdots dx_{n+1} dx_{n+3} \cdots dx_N.$$

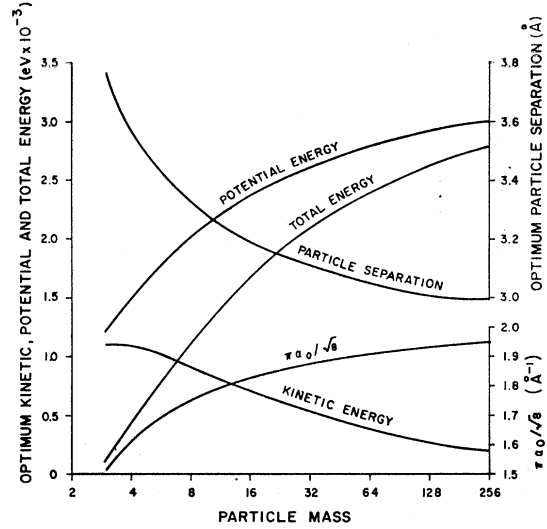


Fig. 2. Values of optimum kinetic energy, potential energy, total energy, particle separation and $\pi\alpha_0/\sqrt{8}$ as a function of particle mass.

Since the kinetic-energy term is proportional to α^2 and the width of the Gaussian to $(1/\alpha)$ it is clear that there must be an optimum value of α for which ψ^2 does not overlap the hard core very strongly and the kinetic energy is not too large.

IV. NUMERICAL RESULTS

A. Results with Correlated Wave Function

The numerical work involved in minimizing E with respect first to α and then to b has been accomplished by means of an IBM-7094 computer program. It was found that, for particles of atomic weight 4, a bound system would not result if a one-dimensional analog of the Slater-Kirkwood¹⁰ He-He potential were used; an interaction equal to four times this potential was arbitrarily chosen and this gave binding. The exact potential used was

$$V(y) = 1925 \exp(-4.6y) - 3.725/y^6, \quad (14)$$

where the units are eV and Å.

The singularity in the potential at $y=0$ was avoided by simply starting the numerical integration at 1 Å. The ratio of the value of $|V(y)\psi^2(y)|$ at this point to the value at the potential minimum was typically 10^{-4} . Thus the value of the integral would be unaffected by any assumed nonsingular behavior for $y < 1$ Å.

A graph of this potential and of the minimum value of E/N for various values of b are given by the solid-line curves of Fig. 1 for particles of various atomic weights. The graph has not been extended to values of b much greater than the optimum value b_0 ; in this region the wave function Φ forces an unstable configuration upon the system and becomes a poorer trial wave

¹⁰ J. C. Slater and J. G. Kirkwood, Phys. Rev. 37, 682 (1931).

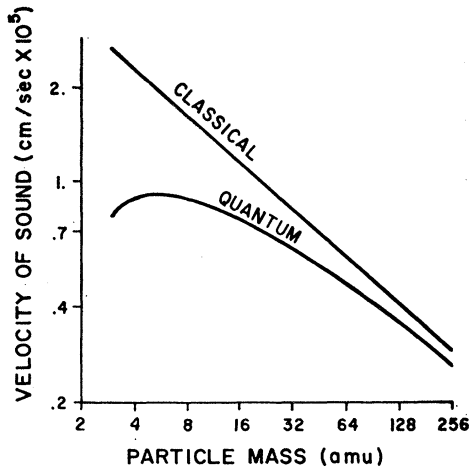


Fig. 3. Classical and calculated quantum-mechanical velocity of sound as a function of particle mass.

function since, as b increases, the average potential which a particle sees looks less and less like a harmonic potential. This latter point is illustrated by the fact that E became positive for sufficiently large values of b in all systems for which binding was obtained. It should be noted that for $b > 3.26 \text{ \AA}$ the second derivative of the potential is negative so that the particles will on the average reside on a local potential maximum.

In order to show the effect of particle mass, a plot of $\pi\alpha_0/\sqrt{8}$, b_0 , E_0 , and the kinetic- and potential-energy contributions to E_0 for various values of particle mass is given in Fig. 2. Thus the fact is demonstrated that a particle can be more sharply localized for the same expenditure of kinetic energy as its mass increases.

It is a straightforward matter to obtain the compressibility and from this the long-wavelength limit of the velocity of sound as a function of particle mass from the numerical results presented in Fig. 1. The results of such a calculation are shown in Fig. 3 together with the velocity of sound $c = y_0[V''(y_0)/m]^{1/2}$ of the corresponding classical system in which the equilibrium separation of the particles is y_0 and the potential minimum is $V(y_0)$.

B. Comparison with Uncorrelated Gaussian

It is a straightforward calculation to show that if, instead of Ψ_1 ,

$$\Psi_2 = \exp\left\{-\frac{(\pi\alpha/8)^2}{2} \sum q_n^2\right\}$$

had been chosen originally, Eq. (13) would have been

$$E'(b, \alpha)/N = (\pi^2/8)(E_K(b, \alpha)/N) + E_V(b, \alpha)/N,$$

where $E_K(b, \alpha) + E_V(b, \alpha) = E(b, \alpha)$ and E_K and E_V have their most obvious meaning. Thus, for any value of b , the optimum Ψ_1 will always give a lower energy than

the optimum Ψ_2 . This improvement will be greatest in loosely bound systems where the kinetic and potential energies are almost equal.

The minimum values of E'/N for various values of b are shown by the dashed curves of Fig. 1.

V. DISCUSSION

An inspection of Ψ_1 shows that

$$\Psi_1 P^{(i, i+1)} \Psi_1 \approx \exp[-(\pi\alpha b)^2/8] \Psi_1^2$$

so that Ψ_1 satisfies the first of the criteria given in Sec. II only when $N \ll \exp[(\pi\alpha b)^2/8]$. Using a typical value of α from Fig. 2, one obtains $N \ll 10^{13}$. For the purposes of this paper, it will simply be assumed that a large but finite system is being treated, i.e., $1 \ll N \ll 10^{13}$, and that, since it would be very odd if a calculation diverged at $N \approx 10^{13}$, the results are probably valid in the limit $N \rightarrow \infty$.

We intend to treat the permutation problem in greater detail in a subsequent publication and to give a systematic method by which contributions from permutation terms can be assessed. The resolution of this problem is necessary if one wishes to explore a more interesting system—one in which the particles are penetrable—using this one-dimensional model. As pointed out by Lieb and Liniger,¹¹ a system of one-dimensional penetrable particles is the closest one-dimensional analogy to a three-dimensional, intermediate density system. In addition, the effects of statistics will be apparent only when $\Psi P \Psi$ terms are retained.

The numerical results obtained in this paper are probably not very accurate—at least for the lower mass systems. The reason for this is that the Gaussian does not cutoff rapidly enough when the hard cores of the particles begin to overlap; the width of the optimum Gaussian is then too narrow and the kinetic energy is too high. The main purpose of this paper is to show that the right correlated Gaussian function can be easily handled in a many-body calculation, and that such a function leads to an improvement in the energy over a calculation using an uncorrelated function. Thus it is possible that an improved Jastrow-type trial wave function could be constructed using a three-dimensional correlated Gaussian as a factor. We intend to investigate this possibility in the future.

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¹¹ E. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963).