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Method of correlated basis functions for the ground state of a one-dimensional many-particle boson system

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The method of correlated basis functions is used in the study of the ground-state properties of a one-dimensional system of bosons interacting through a repulsive δ-function potential. Ground-state energies are determined numerically for intermediate values of the coupling constant in three steps: (1) a trial form of the radial distribution function generated by the Bijl-Dingle-Jastrow (BDJ) type of wave function is introduced to obtain approximate ground-state energies, (2) the paired-phonon analysis is applied to improve the BDJ description of the ground state, and (3) leading corrections to the improved approximate energies are evaluted from the second-order perturbation energy generated by the three-phonon vertex. The obtained energy values are found to agree closely with the exact results calculated by Lieb and Liniger.

I. INTRODUCTION

Many recent theoretical studies on various many-particle boson systems are concerned with the method of correlated basis functions, which is often based on the variational description of the ground state with the use of a Bijl-Dingle-Jastrow[1] (BDJ) type of correlated wave function.[2] In the case of liquid ^{4}He, the procedure usually leads to semi-quantitative agreements with experimental observations. While it is generally rather difficult to find the optimum form of the BDJ-type wave function in a direct way, one can first start with a non-optimum wave function and then successively improve it to obtain the optimum or a near optimum form by using the paired-phonon analysis developed in Refs. 3 and 4. The application of the procedure to liquid ^{4}He generates a negative correction to the variational ground-state energy, considerably reducing the amount of the discrepancy with experimental results. In principle, the discrepancy may be attributed to non-BDJ components, but there are several other factors involved in the liquid-^{4}He problem, which make it difficult to estimate the non-BDJ contribution. They include (1) unavoidable experimental errors are not generally small enough to be neglected, (2) the ground-state energy cannot be measured at absolute zero, (3) the exact form of the two-body potential is not known in the theoretical calculation of the energy—it is often approximated by the Lennard-Jones potential, and (4) the three- (and more-) body potential terms are usually neglected in the theoretical determination. On the other hand, these types of difficulties do not exist if one considers a model system such as the charged-boson system,[5,6] but in most cases there are no results available for the *exact* ground-state energy (except for extreme limits of the coupling), with which the theoretical values obtained using an approximation method may be compared. However, the problem of the one-dimensional boson system with a δ-function potential is an exception, as exact results for many quantities including the ground-state energy were obtained not only in the limits of small and large couplings, but also at intermediate values of the coupling constant.[7]

In this paper, we present[8] evaluation of the ground-state energies of the one-dimensional boson system in three steps. First, a trial form of the radial distribution function is introduced to evaluate approximate ground-state energies in the BDJ-function space by using an improved hypernetted-chain (HNC) equation for the correlation function (Sec. II). Secondly, the BDJ description of the ground state is optimized by means of the paired-phonon analysis (Sec. III). Finally, leading energy corrections coming from a non-BDJ component are obtained by evaluating the second-order perturbation energy generated by three-phonon vertices[9] (Sec. IV). The obtained ground-state energies are found to agree quite closely with the exact values determined in Ref. 7. Very small improvements are made by the inclusion of the leading perturbation correction.

II. GROUND-STATE ENERGY IN A BDJ DESCRIPTION

The system under consideration[10] consists of N one-dimensional bosons interacting in a line of length L through a two-body potential

$$v(x) = 2c\delta(x)\ , \quad c > 0\ . \tag{1}$$

When the ground state is described by a BDJ-type wave function

$$\Psi = \prod_{i<j}^{N} e^{u(x_{ij})/2} \bigg/ \left(\prod_{m<n}^{N} \int e^{u(x_{mn})}\, dx_{12\cdots N} \right)^{1/2} , \tag{2}$$

the expectation value of the Hamiltonian of the system is given by (with $\rho = N/L$)

$$\frac{\langle H\rangle}{N} = \frac{\hbar^2\rho}{8m}\int \frac{du(x)}{dx}\frac{dg(x)}{dx}dx + \frac{\rho}{2}\int v(x)g(x)\,dx$$

$$= \frac{\hbar^2}{16\pi m\rho}\int k^2 W(k)[S(k)-1]\,dk$$

$$+\tfrac{1}{2}N\rho V(0) + \frac{1}{4\pi}\int V(k)[S(k)-1]\,dk \,, \qquad (3)$$

where

$$W(k) = \rho\int e^{ikx}u(x)\,dx \,, \qquad (4)$$

$$V(k) = \int e^{ikx}v(x)\,dx = 2c \,, \qquad (5)$$

and $g(x)$ and $S(k)$ are the radial distribution function and liquid-structure function defined, respectively, by

$$g(x_{12}) = N(N-1)\rho^{-2}\int \Psi^2\,dx_{34\cdots N} \,, \qquad (6)$$

$$S(k) = 1 + \rho\int e^{ikx}[g(x)-1]\,dx \,. \qquad (7)$$

It is convenient to use $g(x)$, rather than $u(x)$, as the variational function.[11] To compute approximate ground-state energies, let us introduce a trial form[12]

$$g(x) = 1 - \alpha\left[1 - \beta\left(\frac{|x|}{a}\right)^p\right]\exp\left[-\left(\frac{|x|}{a}\right)^p\right], \qquad (8)$$

where

$$a = \frac{p}{2\alpha\rho(p-\beta)\Gamma(1+1/p)} \,, \quad p>0 \qquad (9)$$

and α, β, and p are variational parameters. The scale parameter a given by Eq. (9) is so chosen to satisfy the normalization condition

$$\rho\int [1-g(x)]\,dx = 1 \,. \qquad (10)$$

Besides Eq. (10), $g(x)$ or $S(k)$ must satisfy several other constraints. They include:

(a) At $x=0$, $g(x)\geq 0$ requires

$$\alpha \leq 1 \,. \qquad (11)$$

(b) At $\alpha=1$, for $s \ll a$,

$$g(x) = (1+\beta)(x/a)^p - (\tfrac{1}{2}+\beta)(x/a)^{2p} + \cdots \geq 0 \,, \qquad (12)$$

and consequently

$$\beta \geq -1 \ (\text{if } \alpha=1) \,. \qquad (13)$$

(c) For small k,

$$S(k) = \frac{2\alpha\rho a}{p}\left[\frac{(ka)^2}{2!}\Gamma\left(\frac{3}{p}\right)\left(1-\frac{3\beta}{p}\right) - \frac{(ka)^4}{4!}\Gamma\left(\frac{5}{p}\right)\left(1-\frac{5\beta}{p}\right)+\cdots\right], \qquad (14)$$

and hence $S(k)\geq 0$ requires

$$\beta \leq \tfrac{1}{3}p \ (\text{if } \alpha>0) \,. \qquad (15)$$

(d) Since a is a positive-valued scale parameter, Eq. (9) gives

$$p > \beta \ (\text{if } \alpha>0) \,. \qquad (16)$$

To evaluate $\langle H\rangle$ given by Eq. (3), we need a formula for $u(x)$ or $W(k)$ expressed in terms of $g(x)$ and/or $S(k)$. A useful one is the HNC approximation

$$u_{\mathrm{HNC}}(x) = \ln g(x) - \frac{1}{2\pi\rho}\int \frac{[1-S(k)]^2}{S(k)}e^{ikx}\,dk \,. \qquad (17)$$

An improved form is[13]

$$u(x) = u_{\mathrm{HNC}}(x) + \Delta u(x) \,, \qquad (18)$$

where

$$\Delta u(x) = \tfrac{1}{2}\rho^2\int\int dx_1\,dx_2\,h(x_1)h(x_2)h(x_{12})h(x_1-x)h(x_2-x) \,, \qquad (19)$$

$$h(x) = g(x) - 1 \,. \qquad (20)$$

Substitution of Eqs. (1) and (18) into Eq. (3) yields

$$\frac{\langle H\rangle}{N} = \frac{\hbar^2\rho^2}{2m}\gamma(1-\alpha) + \frac{\hbar^2\rho}{8m}\int\left(\frac{dg(x)}{dx}\right)^2\frac{1}{g(x)}dx + \frac{\hbar^2}{16\pi m\rho}\int\frac{[1-S(k)]^3}{S(k)}k^2\,dk$$
$$- \frac{\hbar^2}{16(2\pi)^3 m\rho^3}\int\int\int dk_1\,dk_2\,dk_3\,k_1^2[1-S(k_1)][1-S(k_2)][1-S(k_3)][1-S(k_{12})][1-S(k_{13})][1-S(k_{23})] \,, \qquad (21)$$

where

$$\gamma = 2mc/\hbar^2\rho \qquad (22)$$

is the dimensionless coupling constant.

We have evaluated Eq. (21) numerically using the trial form of $g(x)$ given by Eq. (8). The approximate energies per particle E/N obtained by minimizing $\langle H\rangle/N$ with respect to α, β, and p are listed in Table I together with values of the optimum parameters. It can be seen that all of the values of these parameters satisfy the conditions given by Eqs. (11), (13), (15), and (16). It is interesting to note that the optimum value of β is zero for all values of γ. In Fig. 1, the solid line represents the liquid-structure function $S(k)$ evaluated with the optimum parameters at $\gamma=5$.

TABLE I. Ground-state energies and parameters. γ is the coupling constant defined by Eq. (22) and α, β, and p are variational parameters appearing in Eq. (8). $\hat{E}/N = E/N + \Delta E/N$ is the optimum energy per particle resulting from the paired-phonon analysis. $\mathcal{E}/N = \hat{E}/N + E_{2p}/N$ includes the second-order perturbation correction given by Eq. (35) but is nearly the same as E/N. Energies are given in units of $\hbar^2\rho^2/2m$.

γ	α	β	p	E/N	$\hat{E}/N$	E_{2p}/N	$\mathcal{E}/N$
1	0.49	0	0.92	0.653	0.638	-0.3×10^{-4}	0.638
2	0.63	0	0.95	1.085	1.050	-0.9×10^{-4}	1.050
3	0.71	0	0.97	1.407	1.352	-1.5×10^{-4}	1.352
4	0.77	0	0.98	1.659	1.586	-2.1×10^{-4}	1.586
5	0.80	0	1.02	1.888	1.796	-2.8×10^{-4}	1.796
6	0.83	0	1.04	2.065	1.956	-3.4×10^{-4}	1.956
7	0.86	0	1.06	2.216	2.091	-4.0×10^{-4}	2.091
8	0.88	0	1.08	2.346	2.205	-4.6×10^{-4}	2.205
9	0.89	0	1.09	2.459	2.307	-5.1×10^{-4}	2.307
10	0.90	0	1.10	2.560	2.397	-5.7×10^{-4}	2.396

III. OPTIMIZATION OF THE BDJ DESCRIPTION

The ground-state energies and liquid-structure functions obtained in Sec. II can be improved or optimized within the BDJ description by using the paired-phonon analysis first developed by Jackson and Feenberg[3] and later refined by Campbell and Feenberg.[4] In this procedure, $g(x)$ and $S(k)$ are generalized as

$$g(x_{12};\,\xi) = \frac{N(N-1)}{\rho^2 I(\xi)} \int \exp\left(\xi \sum_{i<j}^{N} v^*(x_{ij})\right) \Psi^2\, dx_{34\cdots N}\,, \tag{23}$$

$$S(k;\,\xi) = 1 + \rho \int [g(x;\,\xi) - g(\infty;\,\xi)]\, e^{ikx}\, dx\,, \tag{24}$$

where

$$v^*(x) = v(x) - \frac{\hbar^2}{4m}\frac{d^2u(x)}{dx^2}\,, \tag{25}$$

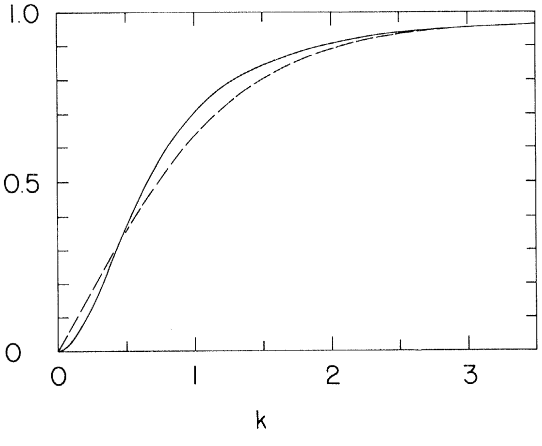

FIG. 1. Liquid-structure functions at $\gamma = 5$. The solid line represents the starting form of $S(k)$ generated by the trial radial distribution function of Eq. (8). The dashed line represents the optimum form $\hat{S}(k) = S(k) + \Delta S(k)$. ($k$ is given in unit of $mc/\hbar^2$.)

$$I(\xi) = \int \exp\left(\xi \sum_{m<n}^{N} v^*(x_{mn})\right) \Psi^2\, dx_{12\cdots N}\,. \tag{26}$$

In terms of

$$S'(k) = \left(\frac{dS(k;\,\xi)}{d\xi}\right)_{\xi=0}\,, \tag{27}$$

$$\omega(k) = \frac{S'(k)}{S(k)} - \frac{\hbar^2 k^2}{4m}\frac{1-S(k)}{S(k)}\,, \tag{28}$$

$$\epsilon(k) = \hbar^2 k^2/2mS(k)\,, \tag{29}$$

$$e(k) = [\epsilon^2(k) + 2\epsilon(k)\omega(k)]^{1/2}\,, \tag{30}$$

the corrections to $S(k)$ and E/N are given by

$$\Delta S(k) = -\frac{2\epsilon(k)\omega(k)S(k)}{e(k)[e(k)+\epsilon(k)]}\,, \tag{31}$$

$$\Delta E/N = -(4\pi\rho)^{-1} \int [\epsilon(k) + \omega(k) - e(k)]\, dk\,. \tag{32}$$

As can be seen from the above formulas, a most important quantity is $S'(k)$. Unfortunately, it is not easy to evaluate $S'(k)$ exactly. However, an approximate form can be obtained from the integral equation[2,4]

$$S'(k) = S^2(k)V^*(k) + \frac{S^2(k)}{2\pi\rho} \int \left(\frac{1}{S^2(k)} - 1\right) S'(k') \times [1 - S(k-k')]\, dk' \tag{33}$$

where

$$V^*(k) = \rho \int g(x) v^*(x) e^{ikx}\, dx\,, \tag{34}$$

whose derivation is based on the use of the HNC equation of Eq. (17). We have evaluated $S'(k)$ numerically by iterating Eq. (33) with the starting approximation $S'(k) = S^2(k)V^*(k)$; at $\gamma = 5$, this is represented by the dashed line in Fig. 2. The solid line in the figure is the solution for $S'(k)$. The HNC approximation was also used to evaluate $V^*(k)$.

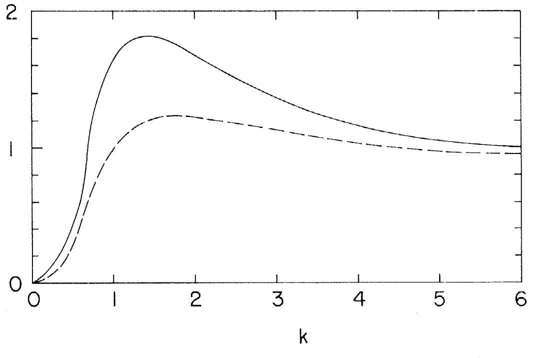

FIG. 2. Starting function and solution for $S'(k)$ (in units of $\hbar^2\rho^2/2m$). The dashed line represents the satrting function $S^2(k)V^*(k)$ and the solid line is the numerical solution obtained from Eq. (33) by an iteration process. (k is given in unit of $mc/\hbar^2$.)

The function $S(k)$ in Eq. (33) is, of course, generated by the trial form of $g(x)$ of Eq. (8).

The addition of $\Delta S(k)$ given by Eq. (31) to $S(k)$ yields the optimum liquid-structure function $\hat{S}(k) = S(k) + \Delta S(k)$. At $\gamma = 5$, this is represented by the dashed line in Fig. 1. Although $\hat{S}(k)$ does not seem to differ substantially from $S(k)$, there is an important difference. For small values of k, our numerical results for $\hat{S}(k)$ shows that $\hat{S}(k)$ is linear in k, whereas $S(k)$ is quadratic in k [see Eq. (14)]. It may be pointed out that all of the first three leading terms of the analytical formula for the optimum liquid-structure function obtained in an infinite series also exhibit linear behavior near $k = 0$.[14] Thus, there are strong indications that the correct form of $\hat{S}(k)$ is indeed linear in k near the origin. Our results for $\hat{E}/N = E/N + \Delta E/N$ obtained numerically from Eq. (32) are listed in Table I. We find that $\hat{E}$ is a considerable improvement over E.

We conclude this section by pointing out that our results for $\hat{S}(k)$ and $\hat{E}/N$ are not really the exact optimum quantities, since the HNC approximation was consistently involved in the determination of $S'(k)$. This means that we may have to repeat the entire procedure of optimization by using the obtained $\hat{S}(k)$ and $\hat{E}$ as the non-optimum starting liquid-structure function and energy. Our somewhat crude estimation for $\gamma = 5$ shows that very little changes are made for $\hat{S}(k)$ and $\hat{E}$ in this procedure and hence we have not carried out the second optimization.

IV. PERTURBATION CORRECTION

As mentioned in Sec. I, the ground-state energy $\hat{E}$ optimized in the BDJ-function space is not the exact energy eigenvalue. While there is no known simple procedure of evaluating the exact energy correction, Davison and Feenberg[9] derived the formula for the leading (second-order) perturbation energy correction generated by the three-phonon vertex. Their result is

$$\frac{E_{2p}}{N} = \frac{-1}{6(8\pi\rho)^2} \iint dk_1\, dk_2 \left(\prod_{i=1}^{3} \frac{[1-\hat{S}(k_i)]^2}{\hat{S}(k_i)} \right) \frac{1}{\langle \hat{\epsilon} \rangle} \times \left(2 \left\langle \frac{\hat{S}^2 \hat{\epsilon}}{1-\hat{S}} \right\rangle - \left\langle \frac{1}{1-\hat{S}} \right\rangle \langle \hat{S} \hat{\epsilon} \rangle \right)^2 , \tag{35}$$

where

$$k_1 + k_2 + k_3 = 0 , \tag{36}$$

$$\hat{\epsilon}(k) = \hbar^2 k^2 / 2m\hat{S}(k) , \tag{37}$$

$$\langle f \rangle = f(k_1) + f(k_2) + f(k_3) , \tag{38}$$

and $\hat{S}(k)$ is the liquid-structure generated by the optimum BDJ-type wave function.

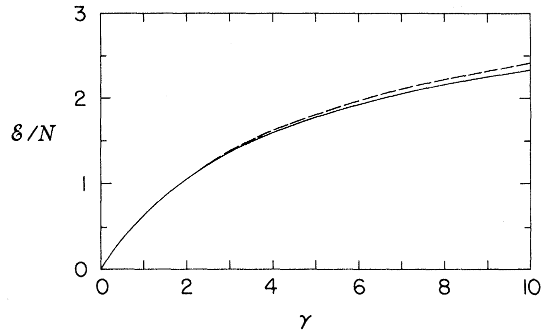

FIG. 3. Ground-state energies per particle in units of $\hbar^2\rho^2/2m$. The solid line is the exact result obtained in Ref. 7 and the dashed line represents $\mathcal{E}/N = \hat{E}/N + E_{2p}/N$. Note that the same dashed line can also represent $\hat{E}/N$, since E_{2p}/N is extremely small (see Table I).

Using the results for $\hat{S}(k)$ determined in Sec. III, we have evaluated the perturbation correction E_{2p}/N numerically. Results for E_{2p}/N and $\mathcal{E}/N = \hat{E}/N + E_{2p}/N$ are listed in Table I. It is seen that the leading non-BDJ contribution E_{2p}/N is so small that the numerical values of $\hat{E}/N$ and $\mathcal{E}/N$ are virtually the same for $\gamma \leq 10$. The magnitude of the ratio $E_{2p}/\mathcal{E}$ becomes larger as γ increases, but it is only about 0.02% at $\gamma = 10$. In the weak coupling expansion of the ground-state energy,[15] E_{2p} contributes about 0.16% to E_2—the total second-order energy term, which is of the same order of magnitude as E_{2p}. Similarly small contribution from non-BDJ components is found in the next-higher-order term E_3.[16] (Non-BDJ components make no contributions at all in zeroth and first orders in the energy series.)

In Fig. 3, the dashed curve represents our result for $\mathcal{E}/N$. In actuality, the same curve also represents $\hat{E}/N$ because of the extremely small difference between $\mathcal{E}/N$ and $\hat{E}/N$. The solid line in the figure, which represents exact ground-state-energy eigenvalues, is taken from Ref. 7. Comparison of the two curves in Fig. 3 reveals that the two results agree very closely although they were obtained with substantially different methods. The discrepancy generally becomes greater as γ increases, the maximum difference in the range $0 < \gamma \leq 10$ being about 3.7% at $\gamma = 10$. The close agreement here clearly demonstrates the accuracy and power of the method of correlated basis functions. It also indicates that the optimum or near-optimum form of the BDJ-type wave function can describe the ground state quite accurately.

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