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Perturbation corrections to the variational ground-state energy of liquid ^{4}He

Felix J. Lee
Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, China

Deok Kyo Lee*
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

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The ground state of liquid ^{4}He is studied by means of a variation-perturbation procedure based on the method of correlated basis functions. The main purpose of the study is to evaluate leading corrections to the variational ground-state energy optimized in the Bijl-Dingle-Jastrow (BDJ) type of trial-wave-function space. The total energy correction consists of: (i) a two-ring type of second-order perturbation energy calculated by including the leading correction to the convolution approximation for the three-particle distribution function, (ii) eight three-ring types of third- and fourth-order perturbation energies computed with the use of convolution approximations for the three- and four-particle distribution functions, and (iii) contribution from the triple-dipole three-body interaction evaluated with the use of the Kirkwood superposition approximation. The formulation for the perturbation energies is given in terms of the liquid-structure function generated by the optimum BDJ-type wave function. The numerical values of the energy corrections are obtained by using the liquid-structure function determined by Pokrant. The resulting ground-state energy per particle is -7.16°K in close agreement with experimental value -7.20°K.

I. INTRODUCTION

Recently the ground state and low-lying excited states of liquid ^{4}He have been studied by many authors using the method of correlated basis functions.[1-11] In this approach, the ground state is usually described variationally by a Bijl-Dingle-Jastrow (BDJ) type of trial wave function

$$\Psi = A \prod_{i<j}^{N} \exp[\tfrac{1}{2}u(r_{ij})], \tag{1}$$

in which A is the normalization constant and N is the number of particles confined in a box of volume Ω. The correlation function $u(r)$ in Eq. (1) is determined by minimizing the expectation value of the Hamiltonian operator

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j}^{N} v(r_{ij}). \tag{2}$$

The two-body potential $v(r)$ does not appear explicitly in the formalism based on the method of correlated basis functions (except for the expression for the mean value of the potential energy) and nearly all of the important properties of low-lying states can be expressed in terms of the liquid structure function $S(k)$ and the number density $\rho = N/\Omega$. In the case of liquid ^{4}He, the procedure usually yields results in semiquantitative agreement with experimental observations. In the uniform limit and/or weak-coupling limit, however, results for the ground-state energy and excitation energy spectrum obtained in the correlated basis function approach agree exactly with those evaluated with substantially different methods[12-16] such as the occupation number formalisms developed by Bogoliubov[17] and by Bogoliubov and Zubarev.[18] Thus, the method of correlated basis functions based on the BDJ-type description of the ground state appears quite useful for model systems and also for the real physical system of liquid ^{4}He.

Although it is generally difficult to obtain the optimum form of the BDJ-type wave function in a direct way, any reasonably accurate variational description of the ground state by a nonoptimum form can be optimized in a systematic way by employing the paired-phonon analysis.[6,19] A very important relation in this optimization process (and also in the BDJ description of the ground state in general) is a formula for the correlation function $u(r)$ given as a functional in the liquid structure function $S(k)$ and/or the radial distribution function $g(r)$. It is often expressed

$$u(r) = \ln g(r) - \frac{1}{(2\pi)^3\rho}\int e^{i\vec{k}\cdot\vec{r}}\,\frac{[1-S(k)]^2}{S(k)}\,d\vec{k} + B(r), \tag{3}$$

where $B(r)$ is the sum of bridge diagrams. Equation (3) with the approximation

$$B(r) = 0 \tag{4}$$

is called the hypernetted chain (HNC) equation.[20,21] The Campbell-Feenberg results[6] for the optimum ground-state energy per particle indicate that the accuracy of the paired-phonon analysis is sensitive to the type of approximation used for $u(r)$, or, equivalently, $B(r)$.

The problem of evaluating the leading correction to the ground-state energy minimized in the BDJ function space was considered by Davison and Feenberg,[5] who made an important observation

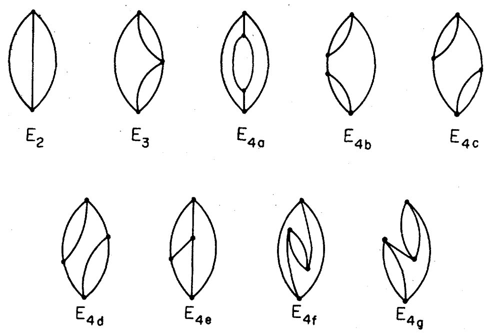

FIG. 1. Two- and three-ring diagrams considered in the calculation of the perturbation energy correction to the variational ground-state energy.

that the dominant contribution from non-BDJ components is the second-order perturbation energy generated by three-phonon vertices (E_2 in Fig. 1). They used the convolution approximation for the three-particle distribution function needed in the evaluation of the matrix element representing a collision process in which three phonons are created out of (or coalesce into) the ground-state substrate. The Davison-Feenberg formalism is expressed in terms of the liquid structure function that is generated by the optimum BDJ-type wave function.

Another important correction to the variational energy based on the many-body Hamiltonian of Eq. (2) is the contribution from the triple-dipole three-body interaction given by

$$v_3(\vec{r}_i, \vec{r}_j, \vec{r}_k) = \frac{V_0(1+3\cos\theta_1\cos\theta_2\cos\theta_3)}{r_{ij}^3 r_{jk}^3 r_{ki}^3}, \tag{5}$$

where θ_1, θ_2, and θ_3 are the interior angles of the triangle formed by particles at positions $\vec{r}_i$, $\vec{r}_j$, and $\vec{r}_k$, and $V_0 = 1.521 \times 10^3$ °K Å^9. Studies made on this contribution are reported in Refs. 5, 9, and 22–24.

In this paper, a more accurate calculation of the ground-state energy is presented by extending the Davison-Feenberg procedure. First, the interaction matrix elements appearing in the dominant (second order) perturbation energy correction is evaluated with higher accuracy by including the leading correction to the convolution approximation for the three-particle distribution function $p^{(3)}(1,2,3)$. Second, in addition to the dominant (second order) perturbation energy (represented by the two-ring diagram E_2 in Fig. 1), we evaluate eight three-ring energy corrections shown in Fig. 1, which are third- and fourth-order perturbation terms. Matrix elements needed for the three-ring diagrams are evaluated using the convolution approximations for the three- and four-particle distribution functions $p^{(3)}(1,2,3)$ and $p^{(4)}(1,2,3,4)$.

The Campbell-Feenberg results for the optimum BDJ-type ground-state description are based mainly on the use of the HNC and Percus-Yevick[25,26] approximations. A similar variational calculation was made later by Pokrant[10] by applying a compressibility consistent integral equation for the radial distribution function $g(r)$ to compute the sum of the bridge diagrams $B(r)$ in Eq. (3). Since the method employed by Pokrant is an attempt to obtain the best variational description by using an approximation superior to the HNC and Percus-Yevick approximations, our primary numerical results in the present study are based on the use of the optimum results for the ground-state energy and the liquid structure function $S(k)$ at the equilibrium density $\rho = 0.0218$ Å^{-3} given in Ref. 10.

The total correction to the variational ground-state energy is the sum of contributions from: (i) a two-ring energy diagram; (ii) eight three-ring energy diagrams; and (iii) the triple-dipole three-body interaction. The final result obtained here for the ground-state energy per particle is −7.16 °K, which compares favorably with experimental value −7.2 °K.[27] In many respects, the present analysis parallels the recent study of the energy spectrum of elementary excitations in liquid ^{4}He.[28]

II. FORMULATION OF ENERGY CORRECTIONS

The basic formalism necessary to evaluate the two- and three-ring perturbation energy corrections is developed in Ref. 28, where derivations of phonon functions and interaction matrix elements are given and many related subjects are discussed. To make the expressions for the perturbation energy corrections complete, we list here some of the useful results of Ref. 28.

It is convenient to define

$$F(k) = 1 - S(k), \tag{6}$$

$$\Delta(k, k', k'') = -\frac{1}{(2\pi)^3\rho}\int d\vec{p}\, F(p)F(\vec{p}+\vec{k})F(\vec{p}-\vec{k}'), \tag{7}$$

$$\Gamma(k, k', k'') = \frac{2}{(2\pi)^3\rho}\int d\vec{p}\,[p^2 + (\vec{p}+\vec{k})^2 + (\vec{p}-\vec{k}')^2] \times F(p)F(\vec{p}+\vec{k})F(\vec{p}-\vec{k}'), \tag{8}$$

where

$$\vec{k} + \vec{k}' + \vec{k}'' = 0, \quad kk'k'' \neq 0. \tag{9}$$

Then, the matrix elements of the perturbation operator

$$\delta H = H - \langle 0|H|0\rangle \tag{10}$$

are given by[28]

$$\begin{aligned}\langle\vec{k},\vec{k}',\vec{k}''\,|\,\delta H\,|\,0\rangle &= (\hbar^2/4m)[NS(k)S(k')S(k'')]^{-1/2}\\ &\quad\times\{[1+\Delta(k,k',k'')]\,[-\tfrac{1}{2}(k^2+k'^2+k''^2)S(k)S(k')S(k'')+k^2S(k')S(k'')+k'^2S(k'')S(k)+k''^2S(k)S(k')]\\ &\quad+(\vec{k}\cdot\vec{k}')S(k'')+(\vec{k}'\cdot\vec{k}'')S(k)+(\vec{k}''\cdot\vec{k})S(k')+\tfrac{1}{2}S(k)S(k')S(k'')\Gamma(k,k',k'')\}\,, \end{aligned}\tag{11}$$

$$\begin{aligned}\langle -k', -k''\,|\,\delta H\,|\vec{k}\rangle &= (\hbar^2/4m)[NS(k)S(k')S(k'')]^{-1/2}\\ &\quad\times[-\tfrac{1}{2}(k^2+k'^2+k''^2)S(k)S(k')S(k'')+k'^2S(k'')S(k)+k''^2S(k)S(k')\\ &\quad-k^2S(k')S(k'')+(\vec{k}'\cdot\vec{k}'')S(k)-(\vec{k}\cdot\vec{k}')S(k'')-(\vec{k}\cdot\vec{k}'')S(k')]\,, \end{aligned}\tag{12}$$

$$\begin{aligned}\langle\vec{k}_1,\vec{k}_2\,|\,\delta H\,|\,\vec{k}_3,\vec{k}_4\rangle = \frac{\hbar^2}{4mN}\left(\prod_{i=1}^{4} S(k_i)\right)^{1/2}\Bigg[&(\vec{k}_1+\vec{k}_3)^2F(\vec{k}_1+\vec{k}_3)+(\vec{k}_1+\vec{k}_4)^2F(\vec{k}_1+\vec{k}_4)+(\vec{k}_1+\vec{k}_2)^2\\ &-\tfrac{1}{2}[F(\vec{k}_1+\vec{k}_3)+F(\vec{k}_1+\vec{k}_4)]\sum_{i=1}^{4}\frac{k_i^{\,2}[1+F(k_i)]}{S(k_i)}\\ &-(\vec{k}_1+\vec{k}_2)\cdot\left(\frac{\vec{k}_1}{S(k_1)}+\frac{\vec{k}_2}{S(k_2)}-\frac{\vec{k}_3}{S(k_3)}-\frac{\vec{k}_4}{S(k_4)}\right)\\ &-\sum_{i=1}^{2}\sum_{j=3}^{4}S(\vec{k}_i+\vec{k}_j)\frac{\vec{k}_i\cdot\vec{k}_j}{S(k_i)S(k_j)}\Bigg]\,, \end{aligned}\tag{13}$$

$$\langle\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4\,|\,\delta H\,|\,0\rangle = 0\,,\tag{14}$$

where

$$\sum_{i=1}^{4}\vec{k}_i=0,\quad \vec{k}_i\neq 0\neq\vec{k}_i+\vec{k}_j\quad (i,j=1,2,3,4)\,,\tag{15}$$

and $|0\rangle$ is the optimum BDJ-type wave function and $S(k)$ is the optimum liquid structure function generated by $|0\rangle$. Equation (11) is evaluated with inclusion of the leading correction to the convolution approximation for $p^{(3)}(1,2,3)$ and Eqs. (12)–(14) are evaluated with convolution approximations for $p^{(3)}(1,2,3)$ and $p^{(4)}(1,2,3,4)$.[29-32]

The explicit expressions of the two- and three-ring perturbation energy diagrams shown in Fig. 1 are

$$E_2=-\frac{\Omega^2}{6(2\pi)^6}\int d\vec{k}\,d\vec{k}'\,\frac{|\langle\vec{k},\vec{k}',\vec{k}''\,|\,\delta H\,|\,0\rangle|^2}{\epsilon_0(k)+\epsilon_0(k')+\epsilon_0(k'')}\,,\tag{16}$$

$$E_3=\frac{\Omega^3}{4(2\pi)^9}\int d\vec{k}_{123}\,\frac{\langle 0\,|\,\delta H\,|\,\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle\vec{k}_2,-\vec{k}_1-\vec{k}_2\,|\delta H|\,\vec{k}_3,-\vec{k}_1-\vec{k}_3\rangle\langle\vec{k}_1,\vec{k}_3,-\vec{k}_1-\vec{k}_3\,|\,\delta H\,|\,0\rangle}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)][\epsilon_0(k_1)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_3)]}\,,\tag{17}$$

$$E_{4a}=-\frac{\Omega^3}{4(2\pi)^9}\int d\vec{k}_{123}\,\frac{|\langle 0\,|\delta H\,|\,\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle\vec{k}_1\,|\delta H\,|\vec{k}_1+\vec{k}_3,-\vec{k}_3\rangle|^2}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)]^2[\epsilon_0(k_2)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_2)+\epsilon_0(\vec{k}_1+\vec{k}_3)]}\,,\tag{18}$$

$$E_{4b}=E_{4c}=-\frac{\Omega^3}{4(2\pi)^9}\int d\vec{k}_{123}\,\frac{\langle 0\,|\delta H\,|\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle\vec{k}_2,-\vec{k}_1-\vec{k}_2\,|\delta H|-\vec{k}_1\rangle\langle-\vec{k}_1\,|\delta H\,|\vec{k}_3,-\vec{k}_1-\vec{k}_3\rangle\langle\vec{k}_1,\vec{k}_3,-\vec{k}_1-\vec{k}_3\,|\delta H\,|\,0\rangle}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)][2\epsilon_0(k_1)][\epsilon_0(k_1)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_3)]}\,,\tag{19}$$

$$\begin{aligned}E_{4d}&=-\frac{\Omega^3}{4(2\pi)^9}\\ &\quad\times\int d\vec{k}_{123}\,\frac{\langle 0\,|\delta H\,|\,\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle\vec{k}_1\,|\,\delta H\,|\vec{k}_1+\vec{k}_3,-\vec{k}_3\rangle\langle\vec{k}_2,-\vec{k}_1-\vec{k}_2\,|\delta H\,|-\vec{k}_1\rangle\langle-\vec{k}_1,-\vec{k}_3,\vec{k}_1+\vec{k}_3\,|\delta H\,|0\rangle}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)][\epsilon_0(k_2)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_2)+\epsilon_0(\vec{k}_1+\vec{k}_3)][\epsilon_0(k_1)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_3)]}\,,\end{aligned}\tag{20}$$

$$\begin{aligned}E_{4e}&=-\frac{\Omega^3}{(2\pi)^9}\\ &\quad\times\int d\vec{k}_{123}\,\frac{\langle 0\,|\delta H\,|\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle\vec{k}_1\,|\delta H|\,\vec{k}_1+\vec{k}_3,-\vec{k}_3\rangle\langle\vec{k}_2,-\vec{k}_3\,|\delta H|\,\vec{k}_2-\vec{k}_3\rangle\langle-\vec{k}_1-\vec{k}_2,\vec{k}_2-\vec{k}_3,\vec{k}_1+\vec{k}_3\,|\delta H\,|0\rangle}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)][\epsilon_0(k_2)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_2)+\epsilon_0(\vec{k}_1+\vec{k}_3)][\epsilon_0(\vec{k}_1+\vec{k}_2)+\epsilon_0(\vec{k}_1+\vec{k}_3)+\epsilon_0(\vec{k}_2-\vec{k}_3)]}\,,\end{aligned}\tag{21}$$

$$E_{4f}=-\frac{\Omega^3}{4(2\pi)^9}\int d\vec{k}_{123}\,\frac{|\langle 0\,|\delta H\,|\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle 0\,|\delta H\,|\vec{k}_1,\vec{k}_3,-\vec{k}_1-\vec{k}_3\rangle\,|^2}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)]^2[2\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_2)+\epsilon_0(\vec{k}_1+\vec{k}_3)]}\,;\tag{22}$$

$$E_{4g}=-\frac{\Omega^3}{4(2\pi)^9}\times\int d\vec{k}_{123}\frac{|\langle 0|\delta H|\vec{k}_1,\vec{k}_2,-\vec{k}_1-\vec{k}_2\rangle\langle 0|\delta H|\vec{k}_1,\vec{k}_3,-\vec{k}_1-\vec{k}_3\rangle|^2}{[\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(\vec{k}_1+\vec{k}_2)][2\epsilon_0(k_1)+\epsilon_0(k_2)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_2)+\epsilon_0(\vec{k}_1+\vec{k}_3)][\epsilon_0(k_1)+\epsilon_0(k_3)+\epsilon_0(\vec{k}_1+\vec{k}_3)]}, \qquad (23)$$

where

$$\epsilon_0(k)=\hbar^2k^2/2mS(k) \qquad (24)$$

is the Bijl-Feynman formula for the excitation energy.

Since the system Hamiltonian [Eq. (2)] used in the variational calculation does not include the potential energy due to the triple-dipole three-body interaction of Eq. (5)

$$V_3=\sum_{1\leq i<j<k\leq N} v_3(\vec{r}_i,\vec{r}_j,\vec{r}_k), \qquad (25)$$

and its contribution is not very small,[5,9,22-24] another correction we need to consider along with the two- and three-ring energy terms is the mean value of V_3, which can be expressed

$$\langle V_3\rangle=\tfrac{1}{6}\Omega\int\int p^{(3)}(1,2,3)v_3(\vec{r}_1,\vec{r}_2,\vec{r}_3)\,d\vec{r}_1\,d\vec{r}_2\,. \qquad (26)$$

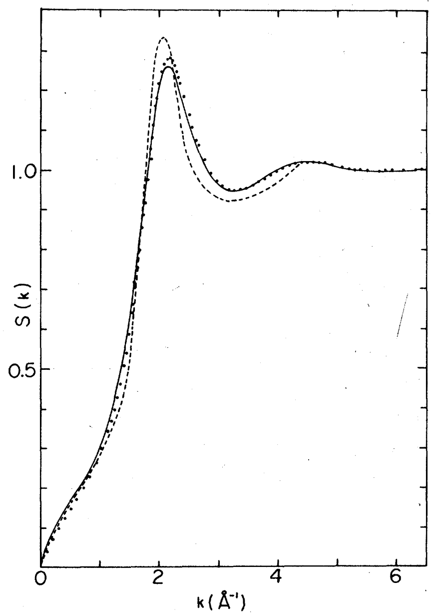

FIG. 2. Liquid structure functions of liquid ^{4}He. The solid line is the variational result evaluated by Pokrant (Ref. 10) and the dotted line is the Campbell-Feenberg result (Ref. 6) obtained using the paired-phonon analysis and the HNC approximation. The dashed line is the experimental result determined by x-ray scattering (Ref. 33).

III. NUMERICAL EVALUATION

As we have already pointed out, the expressions for the perturbation energy corrections given in Sec. II are based on the condition that the liquid structure function $S(k)$ and the unperturbed energy $\langle 0|H|0\rangle$ are obtained in the optimum BDJ-type description of the ground state. Although no *exact* results for such $S(k)$ and $\langle 0|H|0\rangle$ are available at the present time, many authors[1-11] carried out approximate optimization calculations obtaining semiquantitative agreements with experimental observations. In particular, the results obtained by Pokrant[10] appear to be suitable in the numerical evaluation of the perturbation energy corrections and the contribution from the three-body interaction given in Sec. II. We surmise that the error introduced from the use of the Pokrant's results for $S(k)$ (solid line in Fig. 2) and $\langle 0|H|0\rangle$ (Table I) is not significantly greater than those associated with (i) the approximations involved in the evaluation of interaction matrix elements; (ii) the truncation of the energy perturbation series after the three-ring diagrams; and/or (iii) the approximation [Eq. (27)] used in evaluating $\langle V_3\rangle$ of Eq. (26).

Our computed numerical results (obtained with Pokrant's data) for the energy corrections given by Eqs. (16)–(23) and (26) appear in Table I. The Kirkwood superposition approximation

$$p^{(3)}(1,2,3)=\rho^3g(r_{12})g(r_{23})g(r_{31}) \qquad (27)$$

TABLE I. Numerical values of the energy terms included in the evaluation of the ground-state energy per particle of liquid ^{4}He at the equilibrium density $\rho=0.0218$ Å^{-3}. Energies are given in units of °K/atom.

Energy terms	Numerical values
$\langle 0\|H\|0\rangle/N$	−6.60
E_2N	−0.465
E_3/N	−0.0393
E_{4a}/N	−0.0399
E_{4b}/N	−0.0591
E_{4c}/N	−0.0591
E_{4d}/N	−0.0267
E_{4e}/N	−0.0195
E_{4f}/N	−0.0026
E_{4g}/N	−0.0026
$\langle V_3\rangle/N$	+0.154
E/N	−7.16

was used in Eq. (26) to compute $\langle V_3\rangle$. The final result for the ground-state energy per particle is

$$E/N=(\langle 0|H|0\rangle+E_2+E_3+E_{4a}+E_{4b}+E_{4c}+E_{4d}+E_{4e}+E_{4f}+E_{4g}+\langle V_3\rangle)/N = -7.16\,{}^\circ\mathrm{K}, \tag{28}$$

which agrees closely with the experimental value $-7.2\,{}^\circ$K.

It may be instructive to make some remarks here in connection with the present calculation of the ground-state energy:

(a) Evaluation of E_2/N [Eq. (16)] with the use of the convolution approximation for $p^{(3)}(1,2,3)$, which is equivalent to the approximation $\Delta(k,k',k'')=0=\Gamma(k,k',k'')$ in Eq. (11), yields $E_2/N=-0.520\,{}^\circ$K. This means that inclusion of the leading correction to the convolution approximation for $p^{(3)}(1,2,3)$ results in the energy shift of $+0.055\,{}^\circ$K for E_2/N.

(b) The total contribution from the three-ring diagrams is $E_{3\,\mathrm{ring}}/N=-0.2488\,{}^\circ$K, which is about 54% of the second-order (two ring) correction. This may seem to suggest that the perturbation energy series does not converge fast at least in low orders. On the other hand, we can also regard $(E_{3\,\mathrm{ring}}+\langle V_3\rangle)/N=-0.0948\,{}^\circ$K (20% of E_2/N) as the second-lowest-order energy correction. It is, therefore, difficult to estimate the degree of importance for the higher-order corrections.

(c) We have also evaluated the energy corrections using the Campbell-Feenberg results for the optimum liquid structure function obtained with the use of the HNC approximation (dotted line in Fig. 2). The numerical results are

$$\begin{aligned}
&\langle 0|H|0\rangle/N=-4.04\,{}^\circ\mathrm{K},\\
&E_{2\,\mathrm{ring}}/N=E_2/N=-0.623\,{}^\circ\mathrm{K},\\
&E_{3\,\mathrm{ring}}/N=(E_3+E_{4a}+E_{4b}+E_{4c}+E_{4d}+E_{4e}+E_{4f}+E_{4g})/N\\
&\qquad=-0.3275\,{}^\circ\mathrm{K},\\
&\langle V_3\rangle/N=+0.156\,{}^\circ\mathrm{K},\\
&E/N=(\langle 0|H|0\rangle+E_{2\,\mathrm{ring}}+E_{3\,\mathrm{ring}}+\langle V_3\rangle)/N\\
&\qquad=-4.83\,{}^\circ\mathrm{K}.
\end{aligned} \tag{29}$$

We note that the result for E/N here is quite different from that obtained using Pokrant's $S(k)$. The most likely source of the discrepancy is the use of the HNC approximation. Since all of the bridge diagrams are entirely neglected in this approximation, the above result for the variational ground-state energy per particle ($-4.04\,{}^\circ$K), in particular, is believed to be less accurate than Pokrant's value ($-6.60\,{}^\circ$K) obtained by including the sum of the bridge diagrams.

(d) A form of improved HNC equation derived in a series-expansion method gives[34]

$$B(r)=-\tfrac{1}{2}\rho^2\int\int d\vec{r}_1\,d\vec{r}_2[g(r_1-1]\times[g(r_2)-1)][g(r_{12})-1]\times[g(\vec{r}_1-\vec{r})-1][g(\vec{r}_2-\vec{r})-1]. \tag{30}$$

We have evaluated the contribution from Eq. (30) to the variational ground-state energy per particle using the Campbell-Feenberg $S(k)$ based on the HNC approximation. The obtained numerical value is $-0.3343\,{}^\circ$K and hence

$$\langle 0|H|0\rangle/N=-4.37\,{}^\circ\mathrm{K},\quad E/N=-5.17\,{}^\circ\mathrm{K}. \tag{31}$$

Although the correction due to Eq. (30) is in the right direction, consideration of the leading bridge diagram alone seems to leave enough room for further improvement.

(e) The two-body potential function $v(r)$ used to obtain the numerical results for $\langle 0|H|0\rangle/N$ [Eqs. (29) and (31)] is the 6-12 Lennard-Jones potential

$$v(r)=4\epsilon[(\sigma/r)^{12}-(\sigma/r)^6], \tag{32}$$

with[35] $\epsilon=10.22\,{}^\circ$K and $\sigma=2.556$ Å.

(f) A three-ring diagram of second-order perturbation correction involving

$$|\langle 0|\delta H|\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4\rangle|^2\Big/\sum_{i=1}^{4}\epsilon_0(k_i),\quad \sum_{i=1}^{4}\vec{k}_i=0 \tag{33}$$

is not included in Fig. 1, since it vanishes because of the relation given by Eq. (14).

(g) Finally, it may be remarked that the explicit expressions for the three-ring perturbation energy diagrams given by Eqs. (17)-(23) are based on the use of the relations

$$\langle\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\vec{k}_1,\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle=\langle\vec{k}_1|\vec{k}_1\rangle\langle\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle, \tag{34}$$

$$\langle\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\delta H|\vec{k}_1,\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle=\langle\vec{k}_1|\vec{k}_1\rangle\langle\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\delta H|\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle, \tag{35}$$

so that

$$\frac{\langle\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\delta H|\vec{k}_1,\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle}{(\langle\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n\rangle\langle\vec{k}_1,\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'|\vec{k}_1,\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle)^{1/2}}=\frac{\langle\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\delta H|\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle}{(\langle\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n|\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_n\rangle\langle\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'|\vec{k}_2',\vec{k}_3',\ldots,\vec{k}_m'\rangle)^{1/2}}. \tag{36}$$

We proved Eqs. (34) and (35) for the matrix elements involved in the three-ring diagrams. Since the proof is quite lengthy, it is not presented here. Equation (36) justifies considering only the lines entering and leaving a solid (black) circle in writing the matrix elements corresponding to a diagram. The complete set of lines cut by a horizontal line drawn between two adjacent solid circles is involved in the energy denominator.

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