

## Brillouin-Wigner perturbation procedure for elementary excitations in liquid $^4\text{He}$

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The energy spectrum of elementary excitations in liquid  $^4\text{He}$  is studied using the Brillouin-Wigner (BW) perturbation formalism in conjunction with the method of correlated basis functions. Phonon functions and interaction matrix elements associated with three- and four-phonon vertices are derived. Iteration of the BW energy series is carried out by including: (i) two one-ring types of second-order energy corrections evaluated with the inclusion of the leading correction to the convolution approximation for the three-particle distribution function, and (ii) six two-ring types of second-, third-, and fourth-order perturbation energies obtained with the use of the convolution approximations for the three- and four-particle distribution functions. The entire formulation is developed in terms of the liquid-structure function generated by the optimum Bijl-Dingle-Jastrow type of trial wave function. The resulting energy spectrum is found to agree with experimental results more closely than many earlier theoretical calculations.

### I. INTRODUCTION

Considerable progress has been made recently in the theoretical study of elementary excitations in liquid  $^4\text{He}$ . In particular, the excitation-energy spectrum has been derived by many authors using a wide variety of approximation methods including variational and perturbation approaches. One of the useful procedures which yield the spectrum in semiquantitative agreement with experimental measurements is the Brillouin-Wigner (BW) perturbation procedure employed by Jackson and Feenberg<sup>1</sup> (JF) in conjunction with the method of correlated basis functions.<sup>2</sup> Some novel points of this approach are (i) the unperturbed solution is not based on the approximation of the Hamiltonian operator, but rather on an appropriate variational choice of the wave function with the complete Hamiltonian, (ii) the two-body interaction potential, whose singular behavior near the origin often presents difficulties, does not appear explicitly, (iii) the entire formulation is given in terms of the liquid-structure function, which has no singularities yet contains nearly all of the correlation effects of the system, and (iv) addition of the two one-ring types of (second-order) perturbation corrections to the Bijl-Feynman (BF) excitation energy brings the computed spectrum considerably closer to the experimental results, indicating that the energy series probably converges rather rapidly.

The exact liquid-structure function (which is generated by the exact ground-state eigenfunction) is needed in the JF procedure, but such a liquid-structure function is quite difficult to obtain accurately. An attempt to overcome this difficulty has recently been made in Ref. 3, where the JF

formalism is slightly modified through the use of the optimum liquid-structure function, which is generated by the optimum Bijl-Dingle-Jastrow (BDJ) type of ground-state wave function. An actual numerical calculation of the optimum liquid-structure function was carried out by Campbell and Feenberg<sup>4</sup> using the paired-phonon analysis. Another advantage of using the optimum liquid-structure function is found in connection with the need for a formula expressing the three-particle distribution function as an explicit functional in the liquid-structure function or the radial distribution function. All available such formulas are derived with the assumption that the ground state is described by a BDJ-type wave function; very little study has been made for the case when the exact wave function is involved.<sup>5</sup> A useful formula for the three-particle distribution function employed in many recent studies of quantum fluids is the convolution approximation introduced by Jackson and Feenberg.<sup>1</sup> Improvement of this approximation has also been considered,<sup>6-8</sup> but its application to the calculation of the excitation spectrum has been made only in the limit of small wave vectors.<sup>9</sup>

In this paper the work of Ref. 3 is improved in two ways: (i) the leading correction to the convolution approximation for the three-particle distribution function is included in the evaluation of the two one-ring types of second-order perturbation energies considered in Ref. 3, and (ii) iteration of the BW energy series is carried out by including six important two-ring types of second-, third-, and fourth-order terms in addition to the two one-ring second-order terms (See Fig. 1). Our selection of the two-ring perturbation energy correc-

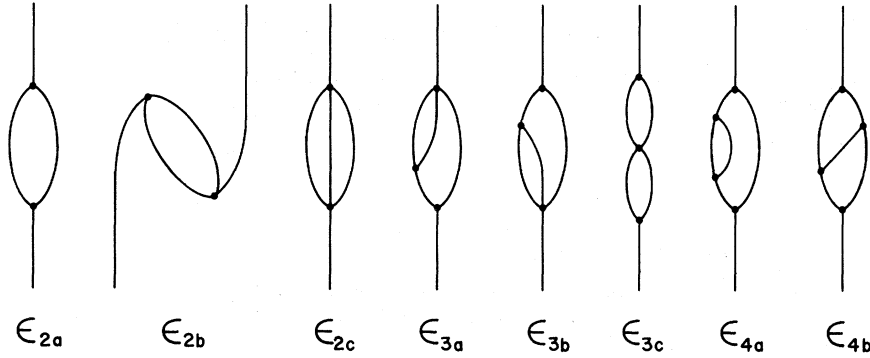


FIG. 1. Energy diagrams included in the calculation of  $\epsilon(k)$ .

tions are based on the observation that contributions from the matrix element representing a zero-to-three (or three-to-zero) phonon process are much smaller than those arising from other types of matrix elements. Consideration of the interaction matrix elements is limited to those representing three- and four-phonon vertices.

## II. BASIC RELATIONS

The system under consideration consists of  $N$  bosons interacting in a box of volume  $\Omega$  through a two-body potential  $v(r)$ , its Hamiltonian being

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

Unless stated otherwise, it will henceforth be assumed that the ground state is described by the optimum BDJ-type wave function of the form

$$\Psi_0 = |0\rangle = A \prod_{i<j}^N \exp\frac{1}{2}u(r_{ij}), \quad (2)$$

where

$$A = \left( \int \prod_{m<n}^N \exp u(r_{mn}) d\vec{r}_{1,2,\dots,N} \right)^{-1/2}. \quad (3)$$

The following basic quantities are useful in the study of low-lying states of the system: the collective coordinate

$$\rho_{\vec{k}} = \sum_{j=1}^N e^{i\vec{k}\cdot\vec{r}_j}, \quad (4)$$

the liquid-structure function

$$S(k) = N^{-1} \langle 0 | \rho_{\vec{k}} \rho_{-\vec{k}} | 0 \rangle, \quad k \neq 0, \\ S(0) = 0, \quad (5)$$

the radial distribution function

$$g(r) = 1 + \frac{1}{(2\pi)^3 \rho} \int [S(k) - 1] e^{i\vec{k}\cdot\vec{r}} d\vec{k} \\ \equiv 1 + h(r), \quad (6)$$

the  $n$ -particle distribution function

$$p^{(n)}(1, 2, \dots, n) \\ = N(N-1) \dots (N-n+1) \int \Psi_0^2 d\vec{r}_{n+1, n+2, \dots, N}, \quad (7)$$

and the BF formula for the excitation energy

$$\epsilon_0(k) = \hbar^2 k^2 / 2m S(k). \quad (8)$$

In Eq. (6)  $\rho = N/\Omega$  is the particle number density.

A useful form of the three-particle distribution function is the convolution approximation

$$p_c^{(3)}(1, 2, 3) = \rho^3 \left( 1 + h(r_{12}) + h(r_{23}) + h(r_{31}) \right. \\ \left. + h(r_{12})h(r_{23}) + h(r_{23})h(r_{31}) + h(r_{31})h(r_{12}) \right. \\ \left. + \rho \int h(r_{14})h(r_{24})h(r_{34}) d\vec{r}_4 \right), \quad (9)$$

which has extensively been used in a number of studies of quantum fluids. An improved approximation was considered in a recent investigation<sup>9</sup> of a long-wavelength-phonon spectrum in liquid <sup>4</sup>He; the formula is given by

$$p^{(3)}(1, 2, 3) = p_c^{(3)}(1, 2, 3) + \delta p_c^{(3)}(1, 2, 3), \quad (10)$$

where

$$\delta p_c^{(3)}(1, 2, 3) = \rho^3 \left( h(r_{12})h(r_{23})h(r_{31}) + \rho [h(r_{12}) + h(r_{23}) + h(r_{31})] \int h(r_{14})h(r_{24})h(r_{34}) d\vec{r}_4 \right. \\ \left. + \rho^2 \int \int d\vec{r}_4 d\vec{r}_5 h(r_{45}) [h(r_{14})h(r_{24})h(r_{25})h(r_{35}) + h(r_{34})h(r_{14})h(r_{15})h(r_{25}) + h(r_{24})h(r_{34})h(r_{35})h(r_{15})] \right. \\ \left. + \rho^3 \int \int \int d\vec{r}_4 d\vec{r}_5 d\vec{r}_6 h(r_{14})h(r_{25})h(r_{36})h(r_{45})h(r_{56})h(r_{64}) \right) \quad (11)$$

is the leading correction to the convolution approximation.<sup>10</sup>

The contributions from  $\delta p_c^{(3)}(1, 2, 3)$  usually enter into the formalism through the quantity<sup>8,9</sup>

$$\begin{aligned} \Delta(k, k', k'') & \\ & \equiv \frac{\rho^3}{N} \int d\vec{r}_{1,2,3} h(r_{12})h(r_{23})h(r_{31}) e^{i(\vec{k}\cdot\vec{r}_1+\vec{k}'\cdot\vec{r}_2+\vec{k}''\cdot\vec{r}_3)} \\ & = \frac{1}{(2\pi)^3\rho} \int d\vec{p} [S(p) - 1][S(\vec{p} + \vec{k}) - 1][S(\vec{p} - \vec{k}') - 1], \end{aligned} \quad (12)$$

in which

$$\vec{k} + \vec{k}' + \vec{k}'' = 0, \quad kk'k'' \neq 0. \quad (13)$$

### III. PHONON FUNCTIONS

The unperturbed normalized wave function

$$|\vec{k}\rangle = [NS(k)]^{-1/2} \rho_{\vec{k}} |0\rangle \quad (14)$$

describes the state with a single phonon whose energy is given by the BF formula (8). The leading perturbation corrections to the BF energy are one-ring diagrams, which involve only three-phonon vertices. To evaluate matrix elements of such three-phonon vertices, one needs two orthonormal phonon functions  $|\vec{k}, \vec{k}', \vec{k}''\rangle$  and  $|\vec{k}, \vec{k}', \vec{k}''\rangle$  as well as  $|\vec{k}\rangle$ . It will be noted that because of the constraints of Eq. (13)  $|\vec{k}, \vec{k}', \vec{k}''\rangle$  does not contain the (orthonormal) paired-phonon components, which is given by

$$|\vec{p}, -\vec{p}\rangle = [NS(p)]^{-1} [\rho_{\vec{p}}\rho_{-\vec{p}} - NS(p)] |0\rangle. \quad (15)$$

The two normalized functions

$$|\vec{k}, \vec{k}', \vec{k}''\rangle = [N^2 S(k')S(k'')]^{-1/2} \rho_{\vec{k}} \rho_{-\vec{k}'} \rho_{-\vec{k}''} |0\rangle \quad (16)$$

and

$$|\vec{k}, \vec{k}', \vec{k}''\rangle = [N^3 S(k)S(k')S(k'')]^{-1/2} \rho_{\vec{k}} \rho_{\vec{k}'} \rho_{\vec{k}''} |0\rangle \quad (17)$$

can be orthogonalized through the Gram-Schmidt method. An important quantity in this procedure is

$$S^{(3)}(k, k', k'') = \frac{1}{N} \int p^{(3)}(1, 2, 3) e^{i(\vec{k}\cdot\vec{r}_1+\vec{k}'\cdot\vec{r}_2+\vec{k}''\cdot\vec{r}_3)} d\vec{r}_{1,2,3} \quad (18)$$

$$\begin{aligned} |\vec{k}, \vec{k}', \vec{k}''\rangle & = |\vec{k}, \vec{k}', \vec{k}''\rangle - |\vec{k}, -\vec{k}\rangle \langle \vec{k}, -\vec{k} | \vec{k}, \vec{k}', \vec{k}''\rangle - |\vec{k}', -\vec{k}'\rangle \langle \vec{k}', -\vec{k}' | \vec{k}, \vec{k}', \vec{k}''\rangle \\ & \quad - |\vec{k}'', -\vec{k}''\rangle \langle \vec{k}'', -\vec{k}'' | \vec{k}, \vec{k}', \vec{k}''\rangle - |0\rangle \langle 0 | \vec{k}, \vec{k}', \vec{k}''\rangle \\ & = [N^3 S(k)S(k')S(k'')]^{-1/2} \{ \rho_{\vec{k}} \rho_{\vec{k}'} \rho_{\vec{k}''} - [1 + \Delta(k, k', k'')] [S(k)S(k')\rho_{\vec{k}}\rho_{-\vec{k}} + S(k)S(k'')\rho_{\vec{k}'}\rho_{-\vec{k}''} \\ & \quad + S(k)S(k')\rho_{\vec{k}''}\rho_{-\vec{k}}] - 2NS(k)S(k')S(k'')] \} |0\rangle. \end{aligned} \quad (25)$$

It can be shown that these orthogonalized functions are still normalized in the sense that

$$\langle -\vec{k}', -\vec{k}'' | -\vec{k}', -\vec{k}''\rangle = 1 + O(N^{-1}), \quad (26)$$

which can be evaluated in terms of  $S(k)$  if  $p^{(3)}(1, 2, 3)$  is given as an explicit functional in  $g(r)$ . In Appendix A we use the approximation of Eq. (10) for  $p^{(3)}(1, 2, 3)$  to derive

$$\begin{aligned} S^{(3)}(k, k', k'') & = [1 + \Delta(k, k', k'')] S(k)S(k')S(k'') \\ & \quad - S(k) - S(k') - S(k'') + 2. \end{aligned} \quad (19)$$

It is rather straightforward to obtain

$$\langle \vec{k} | -\vec{k}', -\vec{k}''\rangle = \langle 0 | \vec{k}, \vec{k}', \vec{k}''\rangle = \langle \vec{k}, -\vec{k} | \vec{k}, \vec{k}', \vec{k}''\rangle \quad (20)$$

$$= [N^{-1} S(k)S(k')S(k'')]^{1/2} [1 + \Delta(k, k', k'')], \quad (21)$$

in which use has been made of Eq. (19) and the relation

$$\begin{aligned} \rho_{\vec{k}} \rho_{\vec{k}'} \rho_{\vec{k}''} & \rightarrow N(N-1)(N-2) e^{i(\vec{k}\cdot\vec{r}_1+\vec{k}'\cdot\vec{r}_2+\vec{k}''\cdot\vec{r}_3)} \\ & \quad + N(N-1)(e^{i\vec{k}\cdot\vec{r}_{12}} + e^{i\vec{k}'\cdot\vec{r}_{12}} + e^{i\vec{k}''\cdot\vec{r}_{12}}) + N, \end{aligned} \quad (22)$$

where the arrow indicates equivalence in integrating over the variables  $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N$ . Although the equality relations of the three matrix elements expressed by Eq. (20) are expected as in the second-quantization formalism, we have actually shown this to be the case by evaluating each matrix element separately. The calculation of  $\langle \vec{k}, -\vec{k} | \vec{k}, \vec{k}', \vec{k}''\rangle$  is somewhat lengthy and involves  $p^{(5)}(1, 2, 3, 4, 5)$  in such a way that one can use the approximation

$$\begin{aligned} p^{(5)}(1, 2, 3, 4, 5) & = p^{(2)}(1, 2)p^{(3)}(3, 4, 5) \\ & \quad + (\text{distinct symmetric terms}), \end{aligned} \quad (23)$$

with the consequence that the resulting error is smaller at least by a factor of  $O(N^{-1})$ .

Equations (20) and (21) finally yield

$$\begin{aligned} |-\vec{k}', -\vec{k}''\rangle & \\ & = |-\vec{k}', -\vec{k}''\rangle - |\vec{k}\rangle \langle \vec{k} | -\vec{k}', -\vec{k}''\rangle \\ & = [N^2 S(k')S(k'')]^{-1/2} \{ \rho_{-\vec{k}'} \rho_{-\vec{k}''} - [1 + \Delta(k, k', k'')] \\ & \quad \times S(k')S(k'')\rho_{\vec{k}} \} |0\rangle, \end{aligned} \quad (24)$$

$$\langle \vec{k}, \vec{k}', \vec{k}'' | \vec{k}, \vec{k}', \vec{k}''\rangle = 1 + O(N^{-1}). \quad (27)$$

Other phonon functions necessary to evaluate two-ring types of perturbation energy corrections

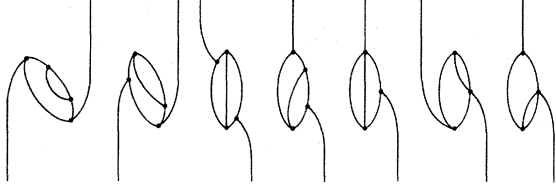


FIG. 2. Some of the third- and fourth-order energy diagrams neglected in the calculation of  $\epsilon(k)$ . Each diagram has at least one zero-to-three or three-to-zero phonon vertex, which is generally far smaller than one-to-two or two-to-one phonon vertex.

can be derived in a similar way. Nevertheless, the derivation is somewhat tedious, partly owing to the fact that  $p^{(4)}(1, 2, 3, 4)$  as well as  $p^{(3)}(1, 2, 3)$  is needed. The algebra can, however, be simplified by the use of the convolution approximations<sup>11</sup> for both  $p^{(3)}(1, 2, 3)$  and  $p^{(4)}(1, 2, 3, 4)$ . We surmise that these approximations for the two-ring diagrams considered in the present study introduce errors no greater than those arising from the use of the approximation (10) for the one-ring diagrams and/or the neglected terms [such as the neglected two-ring diagrams (some are shown in Fig. 2) and three-ring diagrams (all of which are neglected)].

Unless specified otherwise, the wave vectors  $\vec{k}_1$ ,

$\vec{k}_2$ ,  $\vec{k}_3$ , and  $\vec{k}_4$  are to be used in the rest of this paper under the assumption that they satisfy

$$\sum_{i=1}^4 \vec{k}_i = 0, \quad \vec{k}_i \neq 0 \neq \vec{k}_i + \vec{k}_j \quad (i, j = 1, 2, 3, 4). \quad (28)$$

Let us now introduce the normalized functions

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle = [N^3 S(k_1)S(k_2)S(k_3)]^{-1/2} \rho_{\vec{k}_1} \rho_{\vec{k}_2} \rho_{\vec{k}_3} |0\rangle, \quad (29)$$

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle = [N^4 S(k_1)S(k_2)S(k_3)S(k_4)]^{-1/2} \rho_{\vec{k}_1} \rho_{\vec{k}_2} \rho_{\vec{k}_3} \rho_{\vec{k}_4} |0\rangle. \quad (30)$$

The orthogonalization procedure of these functions involves

$$S^{(4)}(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4) = \frac{1}{N} \int p^{(4)}(1, 2, 3, 4) \exp\left(i \sum_{j=1}^4 \vec{k}_j \cdot \vec{r}_j\right) d\vec{r}_{1,2,3,4} \quad (31)$$

as well as  $S^{(3)}(k, k', k'')$  defined by Eq. (18). Convolution approximations for  $p^{(3)}(1, 2, 3)$  and  $p^{(4)}(1, 2, 3, 4)$  lead to

$$S_c^{(3)}(k, k', k'') = S(k)S(k')S(k'') - S(k) - S(k') - S(k'') + 2, \quad (32)$$

$$S_c^{(4)}(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4) = \left( \prod_{i=1}^4 F(k_i) \right) \left( 1 - \sum_{i=1}^4 F^{-1}(k_i) - \frac{1}{2} \sum_{i < j}^4 F(\vec{k}_i + \vec{k}_j) \right) - \sum_{i, m, n}^3 [F(\vec{k}_m + \vec{k}_4) + F(\vec{k}_n + \vec{k}_4)] \times [F(k_i)F(k_4) + F(k_m)F(k_n)] + \sum_{i, j, m, n}^4 [F(k_i) + F(k_j)] F(\vec{k}_i + \vec{k}_j) F(k_m) F(k_n), \quad (33)$$

where

$$F(k) = 1 - S(k). \quad (34)$$

The primes on summation signs in Eq. (33) mean (i) no two or more indices are equal, (ii) the lower limit of each index is 1 unless specified otherwise, and (iii) summations are to be carried out such as to include *all distinct* terms. In the remainder, primes on summation signs are to be used with the same meanings. Equation (32) is simply the result of putting  $\Delta(k, k', k'') = 0$  in Eq. (19). The derivation of Eq. (33) is presented in Appendix B. It may be pointed out that the second term on the right-hand side of Eq. (33) is a symmetric function of  $\vec{k}_1, \vec{k}_2, \vec{k}_3$ , and  $\vec{k}_4$  because of the momentum conservation of Eq. (28).

Using Eqs. (32) and (33) and relations similar to Eq. (22), we find, after some algebra, the following results:

$$\langle -\vec{k}_4 | \vec{k}_1, \vec{k}_2, \vec{k}_3 \rangle = \langle 0 | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 \rangle = \langle \vec{k}_1, -\vec{k}_1 | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 \rangle \quad (35)$$

$$= \left( N^{-2} \prod_{i=1}^4 S(k_i) \right)^{1/2} [S(\vec{k}_1 + \vec{k}_2) + S(\vec{k}_1 + \vec{k}_3) + S(\vec{k}_1 + \vec{k}_4) - 2], \quad (36)$$

$$\langle \vec{k}_1 + \vec{k}_2, \vec{k}_3 | \vec{k}_1, \vec{k}_2, \vec{k}_3 \rangle = \langle \vec{k}_1 + \vec{k}_2, \vec{k}_3, \vec{k}_4 | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 \rangle \quad (37)$$

$$= [N^{-1} S(k_1)S(k_2)S(\vec{k}_1 + \vec{k}_2)]^{1/2}. \quad (38)$$

Again, Eqs. (35) and (37) are expected relations, which we have obtained through actual evaluation of each matrix element. It may be noted that, with  $\Delta(k, k', k'') = 0$  in Eq. (21), results for the matrix elements in Eqs. (21) and (37) are identical.

Finally the orthogonalized three- and four-phonon functions associated with four-phonon vertices become

$$\begin{aligned}
|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle &= |\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle - \sum'_{i,m,n} |\vec{k}_i + \vec{k}_m, \vec{k}_n\rangle \langle \vec{k}_i + \vec{k}_m, \vec{k}_n | \vec{k}_1, \vec{k}_2, \vec{k}_3\rangle - |-\vec{k}_4\rangle \langle -\vec{k}_4 | \vec{k}_1, \vec{k}_2, \vec{k}_3\rangle \\
&= [N^3 S(k_1)S(k_2)S(k_3)]^{-1/2} \left[ \rho_{\vec{k}_1}^- \rho_{\vec{k}_2}^- \rho_{\vec{k}_3}^- + 2S(k_1)S(k_2)S(k_3) \rho_{-\vec{k}_4}^- - \sum'_{i,m,n} S(k_m)S(k_n) \rho_{\vec{k}_i}^- \rho_{\vec{k}_m + \vec{k}_n}^- \right] |0\rangle, \quad (39)
\end{aligned}$$

$$\begin{aligned}
|\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle &= |\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle - \sum'_{i<j} |\vec{k}_i, \vec{k}_j, -\vec{k}_i - \vec{k}_j\rangle \langle \vec{k}_i, \vec{k}_j, -\vec{k}_i - \vec{k}_j | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle \\
&\quad - \sum'_{i=1}^4 |\vec{k}_i, -\vec{k}_i\rangle \langle \vec{k}_i, -\vec{k}_i | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle - |0\rangle \langle 0 | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle \\
&= \left( N^4 \prod_{i=1}^4 S(k_i) \right)^{-1/2} \left[ \rho_{\vec{k}_1}^- \rho_{\vec{k}_2}^- \rho_{\vec{k}_3}^- \rho_{\vec{k}_4}^- - \sum'_{i,j,m,n} S(k_i)S(k_j) X(\vec{k}_m, \vec{k}_n) \right. \\
&\quad \left. - \left( \prod_{i=1}^4 S(k_i) \right) \left( \frac{1}{2} \sum'_{i<j} S(\vec{k}_i + \vec{k}_j) - 2 \right) \left( \sum_{i=1}^4 \rho_{\vec{k}_i}^- \rho_{-\vec{k}_i}^- / S(k_i) - 3N \right) \right] |0\rangle, \quad (40)
\end{aligned}$$

where

$$X(\mathbf{k}, \mathbf{k}') = \rho_{\vec{k}}^- \rho_{\vec{k}'}^- \rho_{\vec{k}+\vec{k}'}^- - S(k)S(k') \rho_{\vec{k}}^- \rho_{-\vec{k}'}^- - S(k')S(k'') \rho_{\vec{k}}^- \rho_{-\vec{k}'}^- - S(k'')S(k) \rho_{\vec{k}}^- \rho_{-\vec{k}'}^- + 2NS(k)S(k')S(k''), \quad (41)$$

with  $\vec{k}'' \equiv -\vec{k} - \vec{k}'$ . As in the case of Eqs. (26) and (27), one can show that the orthogonalization procedure has altered the normalization relations only by  $O(N^{-1})$ :

$$\langle \vec{k}_1, \vec{k}_2, \vec{k}_3 | \vec{k}_1, \vec{k}_2, \vec{k}_3 \rangle = 1 + O(N^{-1}), \quad (42)$$

$$\langle \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 | \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 \rangle = 1 + O(N^{-1}). \quad (43)$$

#### IV. INTERACTION MATRIX ELEMENTS

We can now proceed to the evaluation of the matrix elements of the perturbation operator defined by

$$\delta H = H - \langle \vec{k} | H | \vec{k} \rangle. \quad (44)$$

The algebraic procedures are rather lengthy. Appendix C gives details of the derivation of the following expressions for the matrix elements needed for one- and two-ring diagrams:

$$\begin{aligned}
\langle \vec{k}, \vec{k}', \vec{k}'' | \delta H | 0 \rangle &= (\hbar^2/4m) [NS(k)S(k')S(k'')]^{-1/2} \{ [1 + \Delta(k, k', k'')] \\
&\quad \times [ -\frac{1}{2}(k^2 + k'^2 + k''^2)S(k)S(k')S(k'') + k^2S(k')S(k'') + k'^2S(k'')S(k) + k''^2S(k)S(k')] \\
&\quad + (\vec{k} \cdot \vec{k}')S(k'') + (\vec{k}' \cdot \vec{k}'')S(k) + (\vec{k}'' \cdot \vec{k})S(k') + \frac{1}{2}S(k)S(k')S(k'')\Gamma(k, k', k'') \}, \quad (45)
\end{aligned}$$

$$\begin{aligned}
\langle -\vec{k}', -\vec{k}'' | \delta H | \vec{k} \rangle &= (\hbar^2/4m) [NS(k)S(k')S(k'')]^{-1/2} \{ [1 + \Delta(k, k', k'')] \\
&\quad \times [ -\frac{1}{2}(k^2 + k'^2 + k''^2)S(k)S(k')S(k'') + k'^2S(k'')S(k) + k''^2S(k)S(k') - k^2S(k')S(k'') \\
&\quad + (\vec{k}' \cdot \vec{k}'')S(k) - (\vec{k} \cdot \vec{k}')S(k'') - (\vec{k} \cdot \vec{k}'')S(k') + \frac{1}{2}S(k)S(k')S(k'')\Gamma(k, k', k'') \}, \quad (46)
\end{aligned}$$

$$\Gamma(k, k', k'') = \frac{2}{(2\pi)^3 \rho} \int d\vec{p} [p^2 + (\vec{p} + \vec{k})^2 + (\vec{p} - \vec{k}')^2] F(p) F(\vec{p} + \vec{k}) F(\vec{p} - \vec{k}'), \quad (47)$$

$$\begin{aligned}
\langle \vec{k}_1, \vec{k}_2 | \delta H | -\vec{k}_3, -\vec{k}_4 \rangle &= \frac{\hbar^2}{4mN} \left( \prod_{i=1}^4 S(k_i) \right)^{1/2} \left[ (\vec{k}_1 + \vec{k}_3)^2 F(\vec{k}_1 + \vec{k}_3) + (\vec{k}_1 + \vec{k}_4)^2 F(\vec{k}_1 + \vec{k}_4) + (\vec{k}_1 + \vec{k}_2)^2 \right. \\
&\quad \left. - \frac{1}{2} [F(\vec{k}_1 + \vec{k}_3) + F(\vec{k}_1 + \vec{k}_4)] \sum_{i=1}^4 \frac{k_i^2 [1 + F(k_i)]}{S(k_i)} - (\vec{k}_1 + \vec{k}_2) \cdot \left( \frac{\vec{k}_1}{S(k_1)} + \frac{\vec{k}_2}{S(k_2)} - \frac{\vec{k}_3}{S(k_3)} - \frac{\vec{k}_4}{S(k_4)} \right) \right. \\
&\quad \left. - \sum_{i=1}^2 \sum_{j=3}^4 S(\vec{k}_i + \vec{k}_j) \frac{\vec{k}_i \cdot \vec{k}_j}{S(k_i)S(k_j)} \right], \quad (48)
\end{aligned}$$

$$\langle \vec{k}_1, \vec{k}_2, \vec{k}_3 | \delta H | -\vec{k}_4 \rangle = \frac{\hbar^2}{4mN} \left( \prod_{i=1}^4 S(k_i) \right)^{1/2} \left[ k_4^2 + \sum_{i<j} (\vec{k}_i \cdot \vec{k}_j) S(\vec{k}_i + \vec{k}_j) \left( \frac{1}{S(k_i)S(k_j)} - 1 \right) \right]$$

$$+ \sum_{i < j}^3 \left[ \frac{1}{2} - F(\vec{k}_i + \vec{k}_j) \right] \left( \frac{k_i^2 F(k_i)}{S(k_i)} + \frac{k_j^2 F(k_j)}{S(k_j)} \right) + \sum_{i=1}^3 \frac{\vec{k}_i \cdot \vec{k}_4}{S(k_i)} \Big], \quad (49)$$

$$\langle \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 | \delta H | 0 \rangle = 0. \quad (50)$$

### V. PERTURBATION PROCEDURE

In Ref. 3, the energy spectrum was evaluated by adding two one-ring diagrams ( $\epsilon_{2a}$  and  $\epsilon_{2b}$  in Fig. 1) to the BF energy formula (8). Both of these correction terms are second-order perturbation energies involving integrals of the form  $\int f(\vec{k}, \vec{k}') d\vec{k}'$ . Since there are no more nonvanishing one-ring diagrams, the next plausible step of improving the energy spectrum would be to include two-ring diagrams. However, there is an extremely large number of two-ring diagrams and the task of calculating all of them seems quite formidable, particularly because of the fact that they all contain integrals of the form  $\int \int g(\vec{k}, \vec{k}_1, \vec{k}_2) d\vec{k}_1 d\vec{k}_2$  that can be reduced (analytically) only to five-fold integrals.

In an attempt to simplify the evaluation of the contribution from the two-ring diagrams, we first observe in the second order that  $\epsilon_{2b}(k)$  is generally far smaller in magnitude than  $\epsilon_{2a}(k)$ . In Fig. 3 are plotted  $\epsilon_{2a}(k)$  (dashed line) and  $\epsilon_{2b}(k)$  (solid line), which were obtained from the iteration of the truncated BW energy series

$$\epsilon(k) = \epsilon_0(k) + \epsilon_{2a}(k) + \epsilon_{2b}(k) \quad (51)$$

by using the convolution approximation for  $p^{(3)}$  (1, 2, 3), as was done in Ref. 3. It is true that one can show the ratio  $\epsilon_{2b}(k)/\epsilon_{2a}(k)$  approaches unity in the limit of small wave vector (as indicated in Fig. 3), but in the small- $k$  region the BF spectrum is expected to be fairly accurate and thus the perturbation corrections are not significant anyway. On the other hand, in the roton region, which is a most important part,  $\epsilon_{2b}(k)$  is only about 1% of  $\epsilon_{2a}(k)$ . The overall smallness of the ratio  $\epsilon_{2b}(k)/\epsilon_{2a}(k)$  is mainly due to the fact that the matrix element representing the zero-to-three-phonon process is generally considerably smaller than that representing

the one-to-two-phonon process. To demonstrate this numerically, we have plotted  $\langle \vec{k}, \vec{k}', \vec{k}'' | \delta H | 0 \rangle$  and  $\langle -\vec{k}', -\vec{k}'' | \delta H | \vec{k} \rangle$  in Fig. 4 for the special configuration of equilateral triangle  $k = k' = k''$ . We obtained the results of Fig. 4 from Eqs. (45) and (46) with  $\Delta(k, k', k'') = 0 = \Gamma(k, k', k'')$ , which corresponds to the use of the convolution approximation of Eq. (9) in the evaluation of the matrix elements. Except for small  $k$  values, we find

$$|\langle \vec{k}, \vec{k}', \vec{k}'' | \delta H | 0 \rangle| \ll |\langle -\vec{k}', -\vec{k}'' | \delta H | \vec{k} \rangle|. \quad (52)$$

This observation may be used in finding a useful approximation to estimate the contribution from two-ring diagrams. In particular, we note that a great number of two-ring diagrams such as those shown in Fig. 2 contain zero-to-three and/or three-to-zero phonon processes, and only six two-ring diagrams shown in Fig. 1 do not contain such processes. In the present study, therefore, we extend the work of Ref. 3 by adding only these six perturbation corrections to the BW energy series (51). We believe that the other two-ring diagrams would make smaller contributions for the reason mentioned above.

Thus our entire perturbation consists of the eight energy terms shown in Fig. 1, and the energy series to be solved is<sup>12</sup>

$$\epsilon(k) = \epsilon_0(k) + \epsilon_{2a}(k) + \epsilon_{2b}(k) + \epsilon_{2c}(k) + \epsilon_{3a}(k) + \epsilon_{3b}(k) + \epsilon_{3c}(k) + \epsilon_{4a}(k) + \epsilon_{4b}(k). \quad (53)$$

As discussed in Ref. 3, use of the Rayleigh-Schrödinger perturbation formalism often presents difficulties associated with the vanishing of energy denominators, whereas no such singularities are encountered in the BW formalism. We therefore evaluate  $\epsilon(k)$  by iterating the BW energy series of Eq. (53). The explicit expressions of the perturbation energy corrections are

$$\epsilon_{2a}(k) = \frac{1}{2(2\pi)^3 \rho} \int d\vec{k}' \frac{|\langle \vec{k} | \delta H | \vec{k} - \vec{k}', \vec{k}' \rangle|^2}{\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}') - \epsilon_0(k')}, \quad (54)$$

$$\epsilon_{2b}(k) = \frac{1}{2(2\pi)^3 \rho} \int d\vec{k}' \frac{|\langle 0 | \delta H | \vec{k}, \vec{k}', -\vec{k} - \vec{k}' \rangle|^2}{\epsilon(k) - 2\epsilon_0(k) - \epsilon_0(k') - \epsilon_0(\vec{k} + \vec{k}')}, \quad (55)$$

$$\epsilon_{2c}(k) = \frac{1}{6(2\pi)^6 \rho^2} \int \int d\vec{k}_1 d\vec{k}_2 \frac{|\langle \vec{k} | \delta H | \vec{k} - \vec{k}_1, \vec{k}_{12}, \vec{k}_2 \rangle|^2}{\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_{12}) - \epsilon_0(k_2)}, \quad (56)$$

$$\epsilon_{3a}(k) = \epsilon_{3b}(k) = \frac{1}{2(2\pi)^6 \rho^2} \int \int d\vec{k}_1 d\vec{k}_2 \frac{\langle \vec{k} | \delta H | \vec{k} - \vec{k}_1, \vec{k}_1 \rangle \langle \vec{k}_1 | \delta H | \vec{k}_{12}, \vec{k}_2 \rangle \langle \vec{k} - \vec{k}_1, \vec{k}_{12}, \vec{k}_2 | \delta H | \vec{k} \rangle}{[\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_1)][\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_{12}) - \epsilon_0(k_2)]}, \quad (57)$$

$$\epsilon_{3c}(k) = \frac{1}{4(2\pi)^6 \rho^2} \iint d\vec{k}_1 d\vec{k}_2 \frac{\langle \vec{k} | \delta H | \vec{k} - \vec{k}_1, \vec{k}_1 \rangle \langle \vec{k} - \vec{k}_1, \vec{k}_1 | \delta H | \vec{k} - \vec{k}_2, \vec{k}_2 \rangle \langle \vec{k} - \vec{k}_2, \vec{k}_2 | \delta H | \vec{k} \rangle}{[\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_1)][\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_2) - \epsilon_0(k_2)]}, \quad (58)$$

$$\epsilon_{4a}(k) = \frac{1}{2(2\pi)^6 \rho^2} \iint d\vec{k}_1 d\vec{k}_2 \frac{|\langle \vec{k} | \delta H | \vec{k} - \vec{k}_1, \vec{k}_1 \rangle \langle \vec{k}_1 | \delta H | \vec{k}_{12}, \vec{k}_2 \rangle|^2}{[\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_1)]^2 [\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_{12}) - \epsilon_0(k_2)]}, \quad (59)$$

$$\epsilon_{4b}(k) = \frac{1}{(2\pi)^6 \rho^2} \iint d\vec{k}_1 d\vec{k}_2 \frac{\langle \vec{k} | \delta H | \vec{k} - \vec{k}_1, \vec{k}_1 \rangle \langle \vec{k}_1 | \delta H | \vec{k}_{12}, \vec{k}_2 \rangle \langle \vec{k} - \vec{k}_1, \vec{k}_1 | \delta H | \vec{k} - \vec{k}_2 \rangle \langle \vec{k} - \vec{k}_2, \vec{k}_2 | \delta H | \vec{k} \rangle}{[\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_1)][\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_1) - \epsilon_0(k_{12}) - \epsilon_0(k_2)][\epsilon(k) - \epsilon_0(\vec{k} - \vec{k}_2) - \epsilon_0(k_2)]}. \quad (60)$$

## VI. NUMERICAL EVALUATION

The matrix elements in the expressions for the perturbation energy corrections (54)–(60) are given by Eqs. (45)–(49). These results are derived under the assumption that the ground state is described by the optimum BDJ-type wave function. It is quite obvious that if the exact wave function is involved, one would obtain different results for the matrix elements—for example,  $\langle \vec{k}, \vec{k}', \vec{k}'' | \delta H | 0 \rangle = 0$ . We must therefore use the liquid-structure function generated by the optimum BDJ-type wave function. The form of such a liquid-structure function to be used in the iteration of Eq. (53) is the Campbell-Feenberg result<sup>4</sup> obtained with the use of the hypernetted chain approximation, as it appears to be the best available.<sup>3</sup>

The two-ring diagrams in Fig. 1 involve, with the exception of  $\epsilon_{2c}(k)$ , one-to-two and/or two-to-one phonon processes given by Eq. (46), and thus their integrals are more difficult to evaluate than those of other diagrams. However, within our desired accuracy, the two-ring diagrams may be evaluated using

$$\begin{aligned} & \langle -\vec{k}', -\vec{k}'' | \delta H | \vec{k} \rangle_c \\ &= (\hbar^2/4m)[NS(k)S(k')S(k'')]^{-1/2} \\ & \times [-\frac{1}{2}(k^2 + k'^2 + k''^2)S(k)S(k')S(k'') + k'^2 S(k'')S(k) \\ & + k''^2 S(k)S(k') - k^2 S(k')S(k'')], \quad (61) \end{aligned}$$

which is obtained with the convolution approximation for  $p^{(3)}(1, 2, 3)$ . In fact, as mentioned earlier, the same convolution approximation is used in the derivation of Eqs. (48)–(50).

We thus carry out the numerical iteration of the BW energy series (53) by using Eqs. (45) and (46) for the one-ring diagrams and Eqs. (48), (49), and (61) for the two-ring diagrams. The iteration process for each value of  $k$  begins with the starting  $\epsilon(k)$  taken from the Cowley-Woods experimental measurements<sup>13</sup> and continues until two successive values differ by less than 0.8%. The number of iterations required for this accuracy does not exceed 4 for  $k \leq 2.56 \text{ \AA}^{-1}$ , the wave vector domain for which  $\epsilon(k)$  is computed in the present study. In most cases, three iterations were found to be sufficient. The obtained numerical results are pre-

sented in Table I and in Fig. 5. Our numerical calculations for several values of  $k$  show that the same results for  $\epsilon(k)$  can be obtained by starting with the BF spectrum  $\epsilon_0(k)$ , but in this case two or three more iterations are necessary. Nevertheless, iterations of the integral equation (53) generally converge rather rapidly in a stable fashion. In the numerical iteration processes, we have observed no singular behaviors that could indicate the possibility that the solution is not unique. Thus there is no particular reason to suspect that our numerical results for  $\epsilon(k)$  do not represent the true solution.

In Table I,  $\Delta\epsilon_{2ab}$  means the total energy shift of one-ring diagrams brought about by the addition of the leading correction  $\delta p_c^{(3)}(1, 2, 3)$  to the convolution approximation  $p_c^{(3)}(1, 2, 3)$ , and  $\epsilon_{2ab}^{(c)} \equiv \epsilon_{2a}^{(c)} + \epsilon_{2b}^{(c)} - \Delta\epsilon_{2ab}$  is the contribution from both of the two one-ring diagrams evaluated with the convolution approximation for  $p^{(3)}(1, 2, 3)$ . Examination of the results for  $\Delta\epsilon_{2ab}$  and  $\epsilon_{2ab}^{(c)}$  shows that addition of  $\delta p_c^{(3)}(1, 2, 3)$  to  $p_c^{(3)}(1, 2, 3)$  changes the total one-ring perturbation correction by less than 6% in the range  $k \leq 2.28 \text{ \AA}^{-1}$  and by about 8% near  $k = 2.56 \text{ \AA}^{-1}$ . This may mean that the convolution approximation  $p_c^{(3)}(1, 2, 3)$  is a reasonable form that can be used in the study of quantum fluids, or that  $\delta p_c^{(3)}(1, 2, 3)$  is

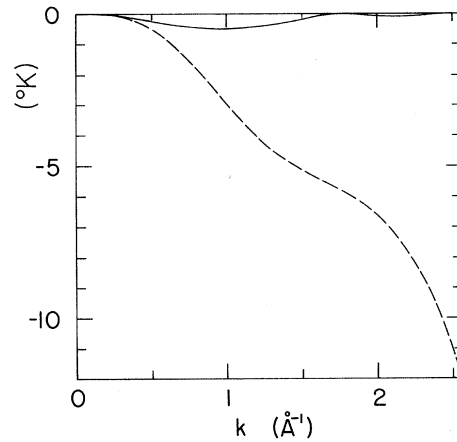


FIG. 3. Comparison of  $\epsilon_{2a}(k)$  (dashed line) and  $\epsilon_{2b}(k)$  (solid line) obtained from the iteration of the BW energy series (51).

only a small part of the total correction to  $p_c^{(3)}(1, 2, 3)$ . Use of the better-known Kirkwood superposition approximation  $p_K^{(3)}(1, 2, 3) = \rho^3 g(r_{12})g(r_{23})g(r_{31})$  would lead to much more complicated expressions for the phonon functions, matrix elements, and consequently the perturbation energy corrections. The importance of  $\delta p_c^{(3)}(1, 2, 3)$  may also be estimated by comparing  $\Delta(k, k', k'')$  with unity, since addition of  $\delta p_c^{(3)}(1, 2, 3)$  results in replacement of unity by  $1 + \Delta(k, k', k'')$  in many expressions. In Table II are listed the numerical values of  $\Delta(k, k', k'')$  for the equilateral configuration  $k = k' = k''$ .

In Fig. 5, curve A represents the BF excitation spectrum (8) and curve B (taken from Ref. 3) results from the BW energy series of Eq. (51). Curve C is the result of the present calculation obtained from the BW series (53). Curve D represents the experimental result obtained by Cowley and Woods<sup>13</sup> at 1.1 °K from inelastic neutron scattering. It may be pointed out that another experimental result by Henshaw and Woods<sup>14</sup> is nearly the same as curve D. The solid circles correspond to the theoretical values determined by Feynman and Cohen<sup>15</sup> in a variational calculation based on the backflow argument.

We find that our computed result for  $\epsilon(k)$  is in relatively good agreement with the experimental measurements. The minimum roton energy of this computed spectrum is 9.87 °K at  $k = 1.99 \text{ \AA}^{-1}$ , whereas the experimental value is about 8.7 °K at  $k = 1.9 \text{ \AA}^{-1}$ . Thus, it is seen that the addition of the six two-ring diagrams and the use of the better approximation for  $p^{(3)}(1, 2, 3)$  in one-ring diagrams bring a considerable improvement over the result

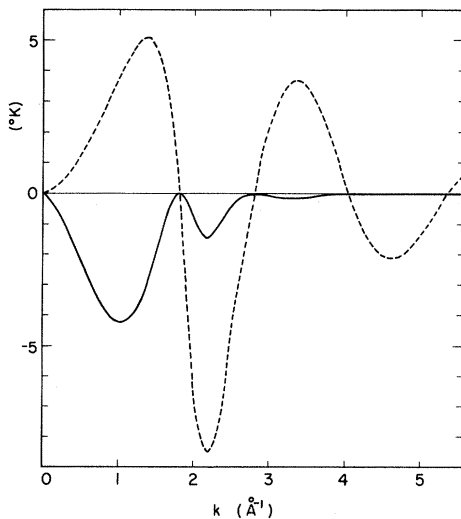


FIG. 4. Comparison of  $\langle \vec{k}, \vec{k}', \vec{k}'' | \delta H | 0 \rangle$  (solid line) and  $\langle -\vec{k}', -\vec{k}'' | \delta H | \vec{k} \rangle$  (dashed line) obtained, respectively, from Eqs. (27) and (28) for the configuration of equilateral triangle  $k = k' = k''$ .

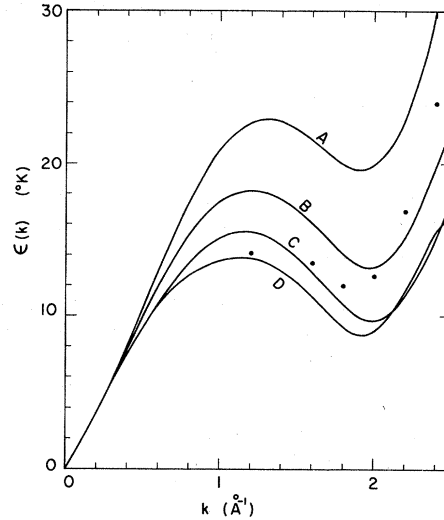


FIG. 5. Theoretical and experimental results for the energy spectrum of elementary excitations. Curve A represents the BF spectrum  $\epsilon_0(k)$ . Curve B (taken from Ref. 3) results from the BW energy series of Eq. (51), and Curve C is the result of the present calculation computed from the BW series of Eq. (53). Curve D represents the experimental values obtained by Cowley and Woods (Ref. 13). The solid circles are the variational results evaluated by Feynman and Cohen (Ref. 15).

obtained in Ref. 3. In particular, we note that all the corrections increase sharply beyond  $k = 2.28 \text{ \AA}^{-1}$ . Further improvements are expected to be made by including more perturbation energy corrections and by using still better approximations for  $p^{(n)}(1, 2, \dots, n)$  ( $n = 3, 4, \dots$ ), but the computational procedure would become extremely complicated as the degree of accuracy is increased. Also, use of an optimum liquid-structure function evaluated more accurately could yield an improved excitation spectrum.

As a final remark concerning our numerical results for the energy corrections listed in Table I, we point out that the ratio of the fourth-order  $\epsilon_4 = \epsilon_{4a} + \epsilon_{4b}$  to the third-order correction  $\epsilon_3 = \epsilon_{3a} + \epsilon_{3b} + \epsilon_{3c}$  is larger than unity (except for  $k \leq 0.37 \text{ \AA}^{-1}$ ). Although higher-order terms in a converging perturbation series are normally smaller in magnitude than lower order terms, our case here is somewhat different in that the magnitude of a perturbation-energy term generally depends on the degree of complexity of the term, or more specifically, on the number of rings contained in the energy diagram as in many formal perturbation series. This means that  $\epsilon_3$  and  $\epsilon_4$  are to be treated as corrections of the same order, since both involve two-ring diagrams. The same argument can be generalized to  $\epsilon_{2n-1}$  and  $\epsilon_{2n}$ , both of which contain  $n$ -ring diagrams. Two additional remarks must be made



TABLE I. Computed numerical values of the perturbation energy corrections. Wave vectors and energies are given in units of  $\text{\AA}^{-1}$  and  $^{\circ}\text{K}$ , respectively.

$k$	$\epsilon_0$	$\epsilon_{2ab}^{(2)}$	$\Delta\epsilon_{2ab}$	$\epsilon_{2c}$	$\epsilon_{3a} + \epsilon_{3b}$	$\epsilon_{3c}$	$\epsilon_{4a}$	$\epsilon_{4b}$	$\epsilon$
0.37	7.31	-0.50	-0.02	-0.46	-0.01	-0.07	-0.03	-0.00	6.21
0.65	14.22	-1.64	-0.05	-0.56	-0.03	-0.20	-0.23	-0.06	11.45
0.77	16.95	-2.36	-0.09	-0.60	-0.03	-0.22	-0.39	-0.11	13.15
0.85	18.55	-2.87	-0.12	-0.62	-0.04	-0.21	-0.51	-0.15	14.03
0.98	22.57	-3.63	-0.16	-0.65	-0.08	-0.16	-0.68	-0.22	14.99
1.10	22.00	-4.30	-0.21	-0.68	-0.14	-0.11	-0.80	-0.27	15.48
1.22	22.80	-4.84	-0.27	-0.73	-0.22	-0.05	-0.88	-0.31	15.50
1.34	22.96	-5.20	-0.31	-0.80	-0.30	0.02	-0.94	-0.36	15.08
1.46	22.53	-5.42	-0.33	-0.90	-0.34	0.07	-1.00	-0.41	14.21
1.59	21.68	-5.54	-0.31	-1.04	-0.35	0.09	-1.01	-0.45	13.08
1.71	20.64	-5.74	-0.24	-1.21	-0.35	0.06	-1.00	-0.46	11.69
1.83	19.77	-6.00	-0.16	-1.41	-0.32	-0.01	-0.94	-0.46	10.47
1.91	19.56	-6.33	-0.09	-1.55	-0.28	-0.07	-0.90	-0.47	9.86
1.95	19.62	-6.51	-0.06	-1.61	-0.26	-0.11	-0.89	-0.48	9.71
1.99	19.81	-6.69	-0.03	-1.66	-0.23	-0.15	-0.89	-0.49	9.67
2.03	20.14	-6.91	0.00	-1.70	-0.20	-0.20	-0.90	-0.50	9.72
2.07	20.61	-7.14	0.04	-1.74	-0.18	-0.25	-0.92	-0.53	9.89
2.11	21.24	-7.38	0.07	-1.77	-0.15	-0.30	-0.94	-0.56	10.21
2.16	22.02	-7.65	0.11	-1.78	-0.12	-0.36	-0.99	-0.60	10.64
2.28	25.26	-8.58	0.26	-1.79	-0.07	-0.59	-1.22	-0.76	12.51
2.56	36.36	-11.86	0.87	-1.75	-0.16	-1.44	-2.57	-1.44	18.02

here. First, because of the inequality of Eq. (52), there are many exceptions to the above general rule. For example, the one-ring diagram  $\epsilon_{2b}$  is almost always smaller in magnitude than most of the two-ring diagrams shown in Fig. 1 (see Fig. 3 and Table I). The second point has to do with the fact that energy dominators are negative definite (since they do not vanish for a convergent term) and hence whether or not the integrand of a perturbation-energy correction term changes the sign as integration variables vary depends on the form of the product of the interaction matrix elements. Therefore, among the energy corrections with the same number of rings, perturbation terms with the entire product of the matrix elements in the form of a square of an absolute value would be larger in magnitude than other types of perturbation terms. This is consistent with our numerical results given in Table I, since  $\epsilon_{2c}$  and  $\epsilon_{4a}$  are larger in magnitude than all the other two-ring diagrams in Fig. 1 (except for small values of  $k$ ). This second remark suggests that  $|\epsilon_{2n}/\epsilon_{2n-1}|$  is generally larger than unity, since the product of  $2n-1$  matrix elements in  $\epsilon_{2n-1}$  cannot be put as a square of an absolute value. Our numerical values of  $\epsilon_3$  and  $\epsilon_4$  are also consistent with this observation.

#### APPENDIX A: EVALUATION OF $S^{(3)}(k, k', k'')$

It is convenient to define a linear transform operator  $Y$  as

$$Y\{f(\vec{r}_1, \vec{r}_2, \vec{r}_3)\} = N^{-1}\rho^3 \int d\vec{r}_{1,2,3} f(\vec{r}_1, \vec{r}_2, \vec{r}_3) e^{i(\vec{k}\cdot\vec{r}_1 + \vec{k}'\cdot\vec{r}_2 + \vec{k}''\cdot\vec{r}_3)}, \quad (\text{A1})$$

so that

$$\Delta(k, k', k'') = Y\{h(r_{12})h(r_{23})h(r_{31})\}, \quad (\text{A2})$$

$$S^{(3)}(k, k', k'') = \rho^{-3}Y\{p^{(3)}(1, 2, 3)\}. \quad (\text{A3})$$

Evaluation of Eq. (A3) with the use of approximation formula (10) is rather straightforward, although it involves somewhat lengthy algebra.

The following results are obtained through repeated applications of the Fourier-integral theorem.

$$Y\{1\} = Y\{h(r_{12})\} = 0, \quad (\text{A4})$$

$$Y\{h(r_{13})h(r_{23})\} = F(k)F(k''), \quad (\text{A5})$$

TABLE II. Numerical values of  $\Delta(k, k', k'')$  for the equilateral configuration  $k = k' = k''$ . Wave vectors are given in units of  $\text{\AA}^{-1}$ .

$k$	$\Delta(k, k', k'')$	$k$	$\Delta(k, k', k'')$
0.08	-0.669	1.46	-0.155
0.16	-0.664	1.59	-0.110
0.24	-0.655	1.71	-0.0735
0.33	-0.641	1.83	-0.0449
0.37	-0.633	1.91	-0.0302
0.65	-0.544	1.95	-0.0242
0.67	-0.536	1.99	-0.0188
0.77	-0.491	2.03	-0.0143
0.79	-0.481	2.07	-0.0104
0.85	-0.452	2.11	-0.00717
0.98	-0.390	2.61	-0.00455
1.10	-0.327	2.28	+0.000129
1.22	-0.265	2.56	-0.00121
1.34	-0.207		

$$Y \left\{ \rho \int h(r_{14})h(r_{24})h(r_{34})d\vec{r}_4 \right\} = -F(k)F(k')F(k''), \quad (\text{A6})$$

$$Y \left\{ \rho h(r_{12}) \int h(r_{14})h(r_{24})h(r_{34})d\vec{r}_4 \right\} = -F(k'')\Delta(k, k', k''), \quad (\text{A7})$$

$$Y \left\{ \rho^2 \int h(r_{14})h(r_{34})h(r_{25})h(r_{35})h(r_{45})d\vec{r}_4d\vec{r}_5 \right\} = F(k)F(k')\Delta(k, k', k''), \quad (\text{A8})$$

$$Y \left\{ \rho^3 \int h(r_{14})h(r_{25})h(r_{36})h(r_{45})h(r_{56})h(r_{64})d\vec{r}_4d\vec{r}_5d\vec{r}_6 \right\} = -F(k)F(k')F(k'')\Delta(k, k', k''), \quad (\text{A9})$$

where  $F(k)$  is defined by Eq. (34). Substitution of the above relations into Eq. (A3) yields an expression, which can finally be simplified as given by Eq. (19).

Another useful quantity closely related to  $S^{(3)}(k,$

$k', k''$ ) is<sup>16</sup>

$$N^{-1} \langle 0 | \rho_{\vec{k}} \rho_{\vec{k}'} \rho_{\vec{k}''} | 0 \rangle = [1 + \Delta(k, k', k'')] S(k) S(k') S(k''), \quad (\text{A10})$$

which follows immediately from Eqs. (22) and (19).

#### APPENDIX B: EVALUATION OF $S^{(4)}(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4)$

The convenient definition of the linear-transform operator used in this appendix is given by

$$Z \{ f(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \} = N^{-1} \rho^4 \int d\vec{r}_{1,2,3,4} f(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \exp \left( i \sum_{j=1}^4 \vec{k}_j \cdot \vec{r}_j \right). \quad (\text{B1})$$

Thus Eq. (31) becomes

$$S^{(4)}(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4) = \rho^{-4} Z \{ p^{(4)}(1, 2, 3, 4) \}, \quad (\text{B2})$$

which is to be evaluated here with the use of the convolution approximation<sup>17,18</sup>

$$\begin{aligned} p_c^{(4)}(1, 2, 3, 4) = & \rho^4 \left( 1 + \sum_{i,j}^4 h(r_{ij}) + \sum_{i,j,m}^4 h(r_{im})h(r_{jm}) + \rho \sum_{i,j,m}^4 \int h(r_{i5})h(r_{j5})h(r_{m5})d\vec{r}_5 \right. \\ & + \sum_{i,j,m,n}^4 h(r_{ij})h(r_{mn}) + \sum_{i,j,m,n}^4 h(r_{ij})h(r_{jm})h(r_{mn}) + \sum_{i,j,m,n}^4 h(r_{in})h(r_{jn})h(r_{mn}) + \rho \int \prod_{i=1}^4 h(r_{i5})d\vec{r}_5 \\ & \left. + \rho \sum_{i,j,m,n}^4 \int h(r_{i5})h(r_{j5})h(r_{m5})h(r_{n5})d\vec{r}_5 + \rho^2 \sum_{i,j,m,n}^4 \int h(r_{i5})h(r_{j5})h(r_{m6})h(r_{n6})h(r_{56})d\vec{r}_5d\vec{r}_6 \right). \quad (\text{B3}) \end{aligned}$$

We need the following formulas of the  $Z$  transform, which can be derived without much difficulty:

$$\begin{aligned} Z\{1\} &= Z\{h(r_{12})\} = Z\{h(r_{13})h(r_{23})\} \\ &= Z\{h(r_{12})h(r_{34})\} = Z \left\{ \rho \int \prod_{i=1}^3 h(r_{i5})d\vec{r}_5 \right\} = 0, \quad (\text{B4}) \end{aligned}$$

$$Z\{h(r_{12})h(r_{23})h(r_{34})\} = -F(k_1)F(k_4)F(\vec{k}_1 + \vec{k}_2), \quad (\text{B5})$$

$$Z \left\{ \prod_{i=1}^3 h(r_{i4}) \right\} = - \prod_{j=1}^3 F(k_j), \quad (\text{B6})$$

$$Z \left\{ \rho h(r_{14}) \int \prod_{i=2}^4 h(r_{i5})d\vec{r}_5 \right\} = F(\vec{k}_1 + \vec{k}_4) \prod_{j=1}^3 F(k_j), \quad (\text{B7})$$

$$Z \left\{ \rho \int \prod_{i=1}^4 h(r_{i5})d\vec{r}_5 \right\} = \prod_{j=1}^4 F(k_j), \quad (\text{B8})$$

$$\begin{aligned} Z \left\{ \rho^2 \int h(r_{15})h(r_{26})h(r_{35})h(r_{46})h(r_{56})d\vec{r}_5d\vec{r}_6 \right\} \\ = -F(\vec{k}_1 + \vec{k}_2) \prod_{j=1}^4 F(k_j). \quad (\text{B9}) \end{aligned}$$

Using Eqs. (B3)–(B9), it is easy to show that Eq. (B2) reduces to the result given by Eq. (33).

#### APPENDIX C: EVALUATION OF INTERACTION MATRIX ELEMENTS

The results given by Eqs. (45)–(50) can be derived by extending the procedure first developed by Davison and Feenberg<sup>19</sup> in their study of the ground state of liquid <sup>4</sup>He. The following basic definitions and relations are useful:

$$W(\beta) \equiv \exp \left[ \beta \sum_{i < j}^N \left( v(r_{ij}) - \frac{\hbar^2}{8m} \sum_{n=1}^N \nabla_n^2 u(r_{ij}) \right) \right], \quad (\text{C1})$$

$$I(\beta) \equiv \langle 0 | W(\beta) | 0 \rangle, \quad (\text{C2})$$

$$S(k; \beta) \equiv [NI(\beta)]^{-1} \langle 0 | W(\beta) \rho_{\vec{k}} \rho_{-\vec{k}} | 0 \rangle, \quad (\text{C3})$$

$$\left(\frac{d}{d\beta} S(k; \beta)\right)_{\beta=0} = \frac{\hbar^2 k^2}{4m} [1 - S(k)], \quad (\text{C4})$$

$$\Delta(k, k', k''; \beta) \equiv \frac{1}{(2\pi)^3 \rho} \int d\vec{p} [S(p; \beta) - 1] [S(\vec{p} + \vec{k}; \beta) - 1] [S(\vec{p} - \vec{k}'; \beta) - 1], \quad (\text{C5})$$

$$\Gamma(k, k', k'') \equiv \frac{8m}{\hbar^2} \left(\frac{d}{d\beta} \Delta(k, k', k''; \beta)\right)_{\beta=0}, \quad (\text{C6})$$

$$\langle \mathcal{F} \Psi_0 | \delta H | \mathcal{G} \Psi_0 \rangle = \frac{N \hbar^2}{2m} \int \Psi_0^2 [(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) - \frac{1}{4} \nabla_1^2 (\mathcal{F}^* \mathcal{G})] d\vec{r}_{1,2,\dots,N} + \left(\frac{d}{d\beta} \frac{1}{I(\beta)} \langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle\right)_{\beta=0}. \quad (\text{C7})$$

It may be remarked that the result for  $\Gamma(k, k', k'')$  given by Eq. (47) follows directly from Eqs. (C6) and (C4). The interaction matrix elements are evaluated with suitable choices for functions  $\mathcal{F}$  and  $\mathcal{G}$  in the formula of Eq. (C7).

To simplify lengthy algebraic expressions in the remainder of this Appendix, we let

$$\begin{aligned} S &= S(k), \quad S' = S(k'), \quad S_n = S(k_n), \\ \Delta &= \Delta(k, k', k''), \quad \Gamma = \Gamma(k, k', k''), \\ S(\beta) &= S(k; \beta), \quad S'(\beta) = S(k'; \beta), \quad \Delta(\beta) = \Delta(k, k', k''; \beta). \end{aligned} \quad (\text{C8})$$

Evaluation of  $\langle \vec{k}, \vec{k}', \vec{k}'' | \delta H | 0 \rangle$  begins with our choice of the functions  $\mathcal{F}$  and  $\mathcal{G}$  as

$$\mathcal{F} = (N^3 S S' S'')^{-1/2} [\rho_{\vec{k}} \rho_{\vec{k}'} \rho_{\vec{k}''} - (1 + \Delta)(S' S'' \rho_{\vec{k}} \rho_{-\vec{k}} + S S'' \rho_{\vec{k}'} \rho_{-\vec{k}'} + S S' \rho_{\vec{k}''} \rho_{-\vec{k}''} - 2N S S' S'')], \quad (\text{C9})$$

$$\mathcal{G} = 1. \quad (\text{C10})$$

We thus have

$$(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) = 0, \quad (\text{C11})$$

$$\begin{aligned} \nabla_1^2 (\mathcal{F}^* \mathcal{G}) &= 2(N^5 S S' S'')^{-1/2} \left\{ -\frac{1}{2} (k^2 + k'^2 + k''^2) \rho_{\vec{k}} \rho_{-\vec{k}} \rho_{\vec{k}'} \rho_{-\vec{k}'} - (\vec{k}' \cdot \vec{k}'') \rho_{\vec{k}} \rho_{-\vec{k}} - (\vec{k} \cdot \vec{k}'') \rho_{\vec{k}'} \rho_{-\vec{k}'} - (\vec{k} \cdot \vec{k}') \rho_{\vec{k}''} \rho_{-\vec{k}''} \right. \\ &\quad \left. + (1 + \Delta) [k^2 S' S'' (\rho_{\vec{k}} \rho_{-\vec{k}} - N) + k'^2 S S'' (\rho_{\vec{k}'} \rho_{-\vec{k}'} - N) + k''^2 S S' (\rho_{\vec{k}''} \rho_{-\vec{k}''} - N)] \right\}, \end{aligned} \quad (\text{C12})$$

and consequently

$$\begin{aligned} \frac{N \hbar^2}{2m} \int \Psi_0^2 [(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) - \frac{1}{4} \nabla_1^2 (\mathcal{F}^* \mathcal{G})] d\vec{r}_{1,2,\dots,N} \\ = \frac{\hbar^2}{4m} (N S S' S'')^{-1/2} \left[ -\frac{1}{2} (1 + \Delta) (k^2 + k'^2 + k''^2) S S' S'' + (\vec{k} \cdot \vec{k}') S' S'' + (\vec{k}' \cdot \vec{k}'') S + (\vec{k}'' \cdot \vec{k}) S' \right. \\ \left. + (1 + \Delta) (k^2 S' S'' + k'^2 S' S + k''^2 S S') \right], \end{aligned} \quad (\text{C13})$$

in which Eq. (A10) is used. Using Eqs. (C1)–(C6), we also find

$$\langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle = (N S S' S'')^{-1/2} I(\beta) \left\{ [1 + \Delta(\beta)] S(\beta) S'(\beta) S''(\beta) - (1 + \Delta) [S' S'' S(\beta) + S'' S S'(\beta) + S S' S''(\beta) - 2S S' S''] \right\}, \quad (\text{C14})$$

$$\left(\frac{d}{d\beta} \frac{1}{I(\beta)} \langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle\right)_{\beta=0} = \frac{\hbar^2}{8m} \left(\frac{S S' S''}{N}\right)^{1/2} \Gamma. \quad (\text{C15})$$

Substitution of Eqs. (C13) and (C15) into Eq. (C7) leads to the result given by Eq. (45).

Next, to evaluate  $\langle -\vec{k}', -\vec{k}'' | \delta H | \vec{k} \rangle$ , we let

$$\mathcal{F} = (N^2 S' S'')^{-1/2} [\rho_{-\vec{k}'} \rho_{-\vec{k}''} - (1 + \Delta) S' S'' \rho_{\vec{k}}], \quad (\text{C16})$$

$$\mathcal{G} = (NS)^{-1/2} \rho_{\vec{k}}. \quad (\text{C17})$$

The relations

$$(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) = - (N^5 S S' S'')^{-1/2} [(\vec{k} \cdot \vec{k}') \rho_{\vec{k}'} \rho_{-\vec{k}'} + (\vec{k} \cdot \vec{k}'') \rho_{\vec{k}''} \rho_{-\vec{k}''} + N(1 + \Delta) k^2 S' S''], \quad (\text{C18})$$

$$\begin{aligned} \nabla_1^2 (\mathcal{F}^* \mathcal{G}) &= 2(N^5 S S' S'')^{-1/2} \left[ -\frac{1}{2} (k^2 + k'^2 + k''^2) \rho_{\vec{k}} \rho_{\vec{k}'} \rho_{\vec{k}''} - (\vec{k} \cdot \vec{k}') \rho_{\vec{k}''} \rho_{-\vec{k}''} - (\vec{k}' \cdot \vec{k}'') \rho_{\vec{k}} \rho_{-\vec{k}} \right. \\ &\quad \left. - (\vec{k}'' \cdot \vec{k}) \rho_{\vec{k}'} \rho_{-\vec{k}'} + (1 + \Delta) k^2 S' S'' (\rho_{\vec{k}} \rho_{-\vec{k}} - N) \right] \end{aligned} \quad (\text{C19})$$

can be used to obtain

$$\begin{aligned} & \frac{N\hbar^2}{2m} \int \Psi_0^2 [(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) - \frac{1}{4} \nabla_1^2 (\mathcal{F}^* \mathcal{G})] d\vec{\Gamma}_{1,2,\dots,N} \\ &= \frac{\hbar^2}{4m} (NSS'S'')^{-1/2} \left[ \frac{1}{2} (1+\Delta) (k'^2 + k''^2 - k^2) SS'S'' - (1+\Delta) k^2 S'S'' + (\vec{k}' \cdot \vec{k}'') S - (\vec{k} \cdot \vec{k}') S'' - (\vec{k} \cdot \vec{k}'') S' \right]. \end{aligned} \quad (C20)$$

It is rather straightforward to show

$$\langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle = (NSS'S'')^{-1/2} I(\beta) \{ - (1+\Delta) S(\beta) S' S'' + [1+\Delta(\beta)] S(\beta) S'(\beta) S''(\beta) \}, \quad (C21)$$

$$\left( \frac{d}{d\beta} \frac{1}{I(\beta)} \langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle \right)_{\beta=0} = \frac{\hbar^2}{4m} \frac{1}{(NSS'S'')^{1/2}} \left\{ \frac{1}{2} \Gamma SS'S'' + (1+\Delta) [k'^2 S'' S(1-S') + k''^2 SS'(1-S'')] \right\}. \quad (C22)$$

Combining Eqs. (C21) and (C23) we obtain Eq. (46).

The procedure of evaluating other matrix elements (which represents four-phonon vertices) involves somewhat lengthy algebra, but the method is basically the same. Therefore for each case we present only results for the two terms on the right-hand side of Eq. (C7). The convolution approximations are used for  $p^{(3)}(1, 2, 3)$  and  $p^{(4)}(1, 2, 3, 4)$ .

For matrix element  $\langle \vec{k}_1, \vec{k}_2 | \delta H | -\vec{k}_3, -\vec{k}_4 \rangle$ , we have

$$\mathcal{F} = (N^2 S_1 S_2)^{-1/2} (\rho_{\vec{k}_1} \rho_{\vec{k}_2} - S_1 S_2 \rho_{\vec{k}_1 + \vec{k}_2}), \quad (C23)$$

$$\mathcal{G} = (N^2 S_3 S_4)^{-1/2} (\rho_{-\vec{k}_3} \rho_{-\vec{k}_4} - S_3 S_4 \rho_{-\vec{k}_3 - \vec{k}_4}), \quad (C24)$$

$$\begin{aligned} \int \Psi_0^2 [(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) - \frac{1}{4} \nabla_1^2 (\mathcal{F}^* \mathcal{G})] d\vec{\Gamma}_{1,2,\dots,N} &= -\frac{1}{2} N^{-2} (S_1 S_2 S_3 S_4)^{1/2} \left[ \frac{1}{2} [F(\vec{k}_1 + \vec{k}_3) + F(\vec{k}_1 + \vec{k}_4)] \sum_{i=1}^4 k_i^2 \right. \\ &\quad \left. + (\vec{k}_1 + \vec{k}_2) \left( \frac{\vec{k}_1 + \vec{k}_2}{S_1} - \frac{\vec{k}_3}{S_3} - \frac{\vec{k}_4}{S_4} \right) - (\vec{k}_1 + \vec{k}_2)^2 + \sum_{i=1}^2 \sum_{j=3}^4 S(\vec{k}_i + \vec{k}_j) \frac{\vec{k}_i \cdot \vec{k}_j}{S_i S_j} \right], \end{aligned} \quad (C25)$$

$$\begin{aligned} \left( \frac{d}{d\beta} \frac{1}{I(\beta)} \langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle \right)_{\beta=0} &= \frac{\hbar^2}{4m} \left( \frac{S_1 S_2 S_3 S_4}{N^2} \right)^{1/2} \left( (\vec{k}_1 + \vec{k}_3)^2 F(\vec{k}_1 + \vec{k}_3) + (\vec{k}_1 + \vec{k}_4)^2 F(\vec{k}_1 + \vec{k}_4) \right. \\ &\quad \left. - [F(\vec{k}_1 + \vec{k}_3) + F(\vec{k}_1 + \vec{k}_4)] \sum_{i=1}^4 \frac{k_i^2 F_i}{S_i} \right). \end{aligned} \quad (C26)$$

Equations (C25) and (C26) readily lead to Eq. (48).

In the case of  $\langle \vec{k}_1, \vec{k}_2, \vec{k}_3 | \delta H | -\vec{k}_4 \rangle$ , the function  $\mathcal{F}$  is defined by Eq. (39) and

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3\rangle = \mathcal{F} |0\rangle. \quad (C27)$$

The other function  $\mathcal{G}$  is given by

$$\mathcal{G} = [NS_4]^{-1/2} \rho_{-\vec{k}_4}. \quad (C28)$$

After some algebra, one obtains

$$\begin{aligned} \int \Psi_0^2 [(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) - \frac{1}{4} \nabla_1^2 (\mathcal{F}^* \mathcal{G})] d\vec{\Gamma}_{1,2,\dots,N} &= \frac{1}{2N^2} (S_1 S_2 S_3 S_4)^{1/2} \left[ \sum_{i=1}^4 \left( \frac{k_i^2 F_i}{S_i} + \frac{\vec{k}_i \cdot \vec{k}_4}{S_i} \right) - 2 \frac{k_4^2 F_4}{S_4} \right. \\ &\quad \left. + \sum_{i < j}^3 (\vec{k}_i \cdot \vec{k}_j) S(\vec{k}_i + \vec{k}_j) \left( \frac{1}{S_i S_j} - 1 \right) \right], \end{aligned} \quad (C29)$$

$$\left( \frac{d}{d\beta} \frac{\langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle}{I(\beta)} \right)_{\beta=0} = -\frac{\hbar^2}{4mN} (S_1 S_2 S_3 S_4)^{1/2} \sum_{i < j}^3 F(\vec{k}_i + \vec{k}_j) \left( \frac{k_i^2 F_i}{S_i} + \frac{k_j^2 F_j}{S_j} \right), \quad (C30)$$

and consequently Eq. (49) is obtained.

Finally, for  $\langle \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 | \delta H | 0 \rangle$ , we determine the function  $\mathcal{F}$  from Eq. (40) such that

$$|\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4\rangle = \mathcal{F} |0\rangle. \quad (C31)$$

Also,

$$\mathcal{G} = 1. \quad (C32)$$

These functions lead to the results

$$\int \Psi_0^2 [(\nabla_1 \mathcal{F}^*) \cdot (\nabla_1 \mathcal{G}) - \frac{1}{4} \nabla_1^2 (\mathcal{F}^* \mathcal{G})] d\vec{r}_{1,2,\dots,N} = \frac{-1}{2N^2} (S_1 S_2 S_3 S_4)^{1/2} \left( \sum_{n=2}^4 [F(\vec{k}_1 + \vec{k}_n) + 1] (\vec{k}_1 + \vec{k}_n)^2 - \sum_{i=1}^4 k_i^2 \right), \quad (\text{C33})$$

$$\left( \frac{d}{d\beta} \frac{\langle \mathcal{F} \Psi_0 | W(\beta) | \mathcal{G} \Psi_0 \rangle}{I(\beta)} \right)_{\beta=0} = \frac{\hbar^2}{8mN} (S_1 S_2 S_3 S_4)^{1/2} \sum_{i < j}^4 F(\vec{k}_i + \vec{k}_j) (\vec{k}_i + \vec{k}_j)^2. \quad (\text{C34})$$

Equation (C7) then becomes

$$\langle \vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4 | \delta H | 0 \rangle = -\frac{\hbar^2}{2mN} \vec{k}_1 \cdot \sum_{i=1}^4 \vec{k}_i, \quad (\text{C35})$$

which reduces to Eq. (50) because of the momentum conservation expressed by Eq. (28).

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