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Many-Body Perturbation Theory for Quantum Crystals. II. Ladder Approximation*

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Using the perturbation expansion for quantum crystals proposed in an earlier paper, we investigate here the ladder approximation. A summation of ladder diagrams to all orders is necessary since the interaction, e.g., a Lennard-Jones potential, is singular at short distances. The Bethe-Goldstone equation, describing the motion of two particles in a mean field due to the remaining lattice particles, is derived, and further approximations are discussed, leading to a simplified equation tractable by numerical methods. In this approximation, we calculate the ground-state energy, pressure, and compressibility of the isotopes of helium at various densities in the solid phase. The results are presented and agree quite well with experiments.

I. INTRODUCTION

In a previous paper,[1] hereafter referred to as I, we investigated a form of many-body perturbation theory designed specifically for quantum crystals. The proposed expansion is, at least at low temperatures, formally identical to the standard perturbation theory for spinless fermions. In the case of lattice particles having spin $\frac{1}{2}$, the "spinless fermions" are interacting with spins of $\frac{1}{2}$ attached to lattice sites. The expansion is found to be independent of the statistics of the lattice particles, except for the sign in the exchange term of the interaction.

The results given in I make it possible to use standard many-body methods in the treatment of quantum crystals. As a first step in this direction, we investigate in this paper the ladder approximation.

It has been shown, e.g., in the theory of nuclear matter,[2,3] that a summation of ladder diagrams to all orders produces sufficient short-range correlations to make a treatment of hard-core interactions possible. Since the interaction in quantum crystals is strongly repulsive at short distances, the ladder approximation is necessary, at least as a first step in a more complete perturbation treatment of quantum crystals.

A proper treatment of short-range correlations has been the subject of many previous papers.[4–14] Most of them used a variational treatment and a Jastrow-type trial wave function.[4–12] Several methods have been used to evaluate the energy expectation value: cluster expansion,[4–10] Monte-Carlo integration,[11] or integral equations known from the theory of classical dense gases.[12] Recently, Guyer[13,14] proposed a different method, based again on a cluster expansion of the ground-state energy and using a hierarchy of model Hamiltonians. He derived a two-particle equation describing the motion of a pair of particles in a mean field produced by the remaining lattice. This equation is very similar to the Bethe-Goldstone equation derived in this paper. We use similar approximations to reduce this equation to a form tractable by numerical methods.

The present paper is organized as follows. In Sec. II, we review the Brueckner theory and introduce some notations. Section III contains a derivation of the Bethe-Goldstone equation, the central equation in this paper, which describes the motion of a pair of particles interacting with the true interaction between themselves and moving in a mean field created from the remaining particles. This equation is considerably simplified if a pole approximation is used for the single-particle propagators. This is discussed in Sec. IV. In Sec. V we discuss a number of further approximations of the Bethe-Goldstone equation, reducing it to a form which can be treated with numerical methods. In Sec. VI, numerical results for the isotopes of helium are presented and discussed. Finally, the Appendix presents some numerical methods used in the solution of the Bethe-Goldstone equation.

II. REVIEW OF THE BRUECKNER THEORY

In this paragraph, we give a short review of the ladder approximation.[2,3] This also gives us the opportunity to introduce the notations used later. In the applications to ^{3}He we will not be interested in the nuclear spin system, assuming that we deal with temperatures high compared to the ordering temperature ($\approx 10^{-3}$ K). Following I, we have to solve the problem of a system of interacting spinless fermions having a Hamiltonian [Eqs. (I2.14) and (I2.15)]

$$H=\sum_{i}\sum_{m,n} c^{\dagger}_{im} T_{imin} c_{in} + \sum_{i>j}\sum_{\substack{mm' \\ nn'}} c^{\dagger}_{im} c^{\dagger}_{jn} \tilde{V}_{ij;mnm'n'} c_{jn'} c_{im'} \quad , \tag{2.1}$$

where T_{imin} are the matrix elements of the kinetic energy in a basis of Wannier states. $\tilde{V}$ is given by (I3.2), and the operators $c^{\dagger}$ and c are, within the approximations discussed in I, field operators for spinless fermions. In the case of ^{3}He, we would also have a term in H describing the coupling between "particles" and "spins" [(I6.2)] but in a high-temperature approximation for the spin system (2.1) is recovered.

We had split H into H_0+H', where [(I2.14)]

$$H_0=\sum_i \sum_m c^{\dagger}_{im}\epsilon_m c_{im} \quad , \tag{2.2}$$

and we had added and subtracted a single-particle potential U such that

$$T_{imin}+U_{imin}=\epsilon_n \delta_{mn} \quad . \tag{2.3}$$

We introduced unperturbed propagators:

$$g_0(11')=(1/i)\delta_{ii'}\delta_{nn'}\exp[-i\epsilon_n(t-t')] \times\begin{pmatrix}1-f(\epsilon_n)\\ -f(\epsilon_n)\end{pmatrix}; \quad \begin{matrix} i(t-t')>0 \\ i(t-t')\leqslant 0\end{matrix} \quad . \tag{2.4}$$

The statistical weight functions $f(\epsilon)$ are given by (I5.2), but (as discussed in I) they can be replaced at low temperatures by Fermi functions:

$$f(\epsilon)=1/[e^{\beta(\epsilon-\mu)}+1] \quad , \tag{2.5}$$

where the "chemical potential" has to be between ϵ_0 and ϵ_1. Equation (2.4) now obeys the "quasi-periodicity condition"[15]

$$g_0(t-i\beta)=-g_0(t) \quad . \tag{2.6}$$

Introducing the Schrödinger operator

$$S(11')=\left[\left(i\frac{\partial}{\partial t}+\mu\right)\delta_{nn'}-T_{inin'}\right]\delta_{ii'}\delta(t-t'), \tag{2.7}$$

and $U(11')=U_{inin'}\delta_{ii'}\delta(t-t) \quad , \tag{2.8}$

we find $[S(13)-U(13)]g_0(32)=\delta(12) \quad , \tag{2.9}$

where we use the convention that repeated indices are summed, and repeated times are integrated over the interval $(0, -i\beta)$. We introduce in the usual way the renormalized propagator $g(12)$, which obeys the Dyson equation

$$[S(13)-M(13)]g(32)=\delta(12) \quad , \tag{2.10}$$

where $U(13)$ has canceled out. The mass operator is given by

$$M(12)=-iV(1324)g(43)-V(1354) \times g(56)g(47)g(83)\,T(6728) \quad , \tag{2.11}$$

and here we have used the vertex part of the two-particle propagator defined by

$$g(1234)=g(13)g(24)-g(14)g(23) +ig(15)g(26)\,T(5678)g(73)g(84) \quad . \tag{2.12}$$

In terms of diagrams, T is given by the sum of all connected skeleton diagrams having four terminals. T can be generated from irreducible kernels, e.g., by use of the Bethe-Salpeter equation:

$$T(1234)=K(1234)-iK(1536) \times g(68)g(75)\,T(8274) \quad . \tag{2.13}$$

Replacing the particle-hole irreducible kernel K by the potential leads to the RPA. Another possibility is to generate T from a particle-particle irreducible kernel R, containing all skeleton diagrams having four terminals, which cannot be cut into two parts by cutting two-particle lines. T is then given by

$$T(1234)=R(1234) + iR(1256)g(57)g(68)\,T(7834) \quad . \tag{2.14}$$

This equation is still exact, the ladder approximation is obtained by replacing R with the bare interaction

$$R(121'2')=V(121'2')=\delta_{ii'}\delta_{jj'}\delta(t_1-t_2) \times\delta(t_1-t'_1)\delta(t_2-t'_2)\,\tilde{V}_{ij;nmn'm'} \quad . \tag{2.15}$$

In this approximation the mass operator becomes

$$M(12)=-i\,T(1324)g(43) \quad . \tag{2.16}$$

The goal is now to find a self-consistent solution to Eqs. (2.10), (2.16), (2.14) and (2.15).

III. BETHE-GOLDSTONE EQUATION

To find self-consistent solutions to the set of equations (2.10), (2.14), and (2.16) without further approximations is at present impossible. We therefore have to discuss several steps to bring the problem into a tractable form. Since the direct term in (I3.2) is by far dominant and since we are not interested in exchange for the moment, we can neglect the exchange term in (I3.2). We introduce a $T(r_1\cdots r_4t)$ with

$$\begin{aligned}T(121'2')={}&\delta_{ii'}\delta_{jj'}\delta(t_1-t_2)\,\delta(t'_1-t'_2)\\&\times\int dr_1dr_2dr_3dr_4\,\varphi^*_m(r_1-R_i)\varphi^*_n(r_2-R_j)\\&\times T_{ij}(r_1r_2r_3r_4;t_1-t'_1)\,\varphi_{m'}(r_3-R_i)\\&\times\varphi_{n'}(r_4-R_j)\ .\end{aligned} \tag{3.1}$$

The δ functions are a consequence of the fact that the potential is instantaneous and diagonal in the lattice site indexes. Further, we have used the facts that $g(12)$ depends on t_1-t_2 only and is diagonal in the lattice site indexes. $\varphi_n(r)$ are wave functions of Wannier states at the origin, and R_i is the lattice vector to lattice site i. Although Eq. (3.1) does not determine T uniquely, we can choose it to be the solution to

$$\begin{aligned}T_{ij}(r_1r_2r_3r_4;t)={}&V(r_1-r_2)\,\delta(r_1-r_3)\\&\times\delta(r_2-r_4)\delta(t)+\int_0^{-i\beta}d\tau\int d\rho d\rho'\,V(r_1-r_2)\\&\times q_{ij}(r_1r_2\rho\rho';t-\tau)\,T_{ij}(\rho\rho' r_3r_4;\tau)\ ,\end{aligned} \tag{3.2}$$

where

$$\begin{aligned}q_{ij}(r_1r_2r_3r_4;t)={}&\sum_{mm'nn'}\varphi^*_m(r_1-R_i)\varphi^*_n(r_2-R_i)\\&\times g_{imim'}(t)\,g_{jnjn'}(t)\varphi_{m'}(r_3-R_i)\varphi_{n'}(r_4-R_j)\ .\end{aligned} \tag{3.3}$$

Obviously Eqs. (3.2) and (3.1) together satisfy Eq. (2.14), with R replaced by V. Fourier-transforming with respect to the time variable, we find

$$\begin{aligned}T_{ij}(r_1r_2r_3r_4;Z_\nu)={}&V(r_1-r_2)\delta(r_1-r_3)\delta(r_2-r_4)\\&+\int d\rho d\rho'\,V(r_1-r_2)\,q_{ij}(r_1r_2\rho\rho';z_\nu)\\&\times T_{ij}(\rho\rho' r_3r_4;z_\nu)\ ,\end{aligned} \tag{3.4}$$

where $T_{ij}(r_1r_2r_3r_4;z_\nu)$

$$=\int_0^{-i\beta}dt\,e^{iz_\nu t}\,T_{ij}(r_1r_2r_3r_4;t)\ , \tag{3.5}$$

and $q_{ij}(r_1r_2r_3r_4;z_\nu)$

$$=i\int_0^{-i\beta}dt\,e^{iz_\nu t}q_{ij}(r_1r_2r_3r_4;t)\ , \tag{3.6}$$

and $z_\nu=2i\pi\nu/\beta$ with ν an integer. To solve Eq. (3.4) it is convenient to introduce a correlated two-particle wave function $\psi(rr')$ such that

$$V(r-r')\psi_{imjn}(rr';z_\nu) =\int d\rho d\rho'\,T_{ij}(rr'\rho\rho';z_\nu)\varphi_m(\rho-R_i)\varphi_n(\rho'-R_j)\ . \tag{3.7}$$

Inserting this into Eq. (3.4), we find the integral equation

$$\psi_{imjn}(rr';z_\nu)=\varphi_m(r-R_i)\varphi_n(r'-R_j)+\int d\rho d\rho' \times q_{ij}(rr'\rho\rho';z_\nu)\,V(\rho-\rho')\psi_{imjn}(rr';z_\nu)\ . \tag{3.8}$$

The usual procedure to determine T is first to solve this (Bethe-Goldstone) equation to obtain

$$T_{imjnim'jn'}(z_\nu)=\int dr\,dr'\,\varphi^*_m(r-R_i)\varphi^*_n(r'-R_j) \times V(r-r')\psi_{im'jn'}(rr';z_\nu)\ . \tag{3.9}$$

IV. POLE APPROXIMATION FOR SINGLE-PARTICLE PROPAGATORS

Before proceeding with the discussion of the Bethe-Goldstone equation, we have to investigate the single-particle propagators and to introduce some approximations.

We Fourier-transform the Dyson equation (2.10) with respect to time:

$$(z_\nu+\mu)g_{imim'}(z_\nu)-\sum\nolimits_n[T_{imin}+M_{imin}(z_\nu)] \times g_{inim'}(z_\nu)=\delta_{mm'}\ , \tag{4.1}$$

where
$$g_{imim'}(z_\nu)=\int_0^{-i\beta}dt\,e^{iz_\nu t}g_{imim'}(t)\ , \tag{4.2}$$

$$M_{imim'}(z_\nu)=\int_0^{-i\beta}dt\,e^{iz_\nu t}M_{imim'}(t)\ , \tag{4.3}$$

and $z_\nu=2i\pi\nu/\beta$ with ν a half integer.

Neglecting the z_ν dependence of M we can find the basis of Wannier states, such that

$$T_{imin}+M_{imin}=\epsilon_n\delta_{mn}\ , \tag{4.4}$$

and then
$$g_{imin}(z_\nu)=(z_\nu-\epsilon_n+\mu)^{-1}\delta_{mn}\ , \tag{4.5}$$

and Fourier-transforming back,

$$g_{imin}(t)=\frac{1}{i}\delta_{mn}\exp[-i(\epsilon_n-\mu)t]\times[1-f(\epsilon_n-\mu)]$$
$$\times\, 0\,[-f(\epsilon_n-\mu)]\quad it\leqslant 0 \quad . \qquad (4.6)$$

Inserting this approximation into Eq. (3.3), we find

$$q_{ij}(r_1r_2r_3r_4;z_\nu)=\sum_{mn}\varphi^*_m(r_1-R_i)\,\varphi^*_n(r_2-R_j)$$
$$\times[1-f(\epsilon_m-\mu)-f(\epsilon_n-\mu)](z_\nu-\epsilon_m-\epsilon_n+2\mu)^{-1}$$
$$\times\varphi_m(r_3-R_i)\varphi_n(r_4-R_j)\,. \qquad (4.7)$$

We construct an operator $h_i(r)$ having the Wannier states at lattice site i as eigenfunctions:

$$h_i(r)\varphi_n(r-R_i)=\epsilon_n\varphi_n(r-R_i)\quad , \qquad (4.8)$$

and a projection operator

$$P_i=\sum_n|\varphi_{in}\rangle\langle\varphi_{in}|\quad . \qquad (4.9)$$

Using these we can write Eq. (4.7) as

$$q_{ij}(r_1r_2r_3r_4;z_\nu)=P_iP_j[z_\nu-h_i(r_1)-h_j(r_2)+2\mu]^{-1}$$
$$\times[1-f(h_i(r_1)-\mu)-f(h_j(r_2)-\mu)]$$
$$\times\delta(r_1-r_3)\delta(r_2-r_4)P_iP_j\quad . \qquad (4.10)$$

We assumed that the overlap between Wannier states at different lattice sites is negligible. In this case P_i is essentially a projection operator into the Wigner-Seitz cell around R_i. Under this condition ψ [Eq. (3.8)] also will be essentially zero if one of its arguments is outside the corresponding Wigner-Seitz cell and we can replace the projection operators by unity.

Using Eq. (4.10) we now can write the Bethe-Goldstone equation [(3.8)] in the form

$$\{z_\nu+2\mu-h_i(r)-h_j(r')-V(r-r')+[f(h_i(r)-\mu)$$
$$+f(h_j(r')-\mu)]\,V(r-r')\}\psi_{imjn}(rr';z_\nu)$$
$$=(z_\nu+2\mu-\epsilon_m-\epsilon_n)\varphi_{im}(r-R_i)\,\varphi_{jn}(r'-R_j)\quad . \qquad (4.11)$$

To find the solutions of Eq. (4.11) we solve first the two-particle Schrödinger equation:

$$\{h_i(r)+h_j(r')+V(r+r')$$
$$+[f(h_i(r)-\mu)+f(h_j(r')-\mu)]V(r-r')\}\chi_{ij;\lambda}(rr')$$
$$=\eta_{ij;\lambda}\chi_{ij;\lambda}(rr')\quad . \qquad (4.12)$$

Then ψ can be expanded in terms of those eigenfunctions:

$$\psi_{imjn}(rr';z_\nu)=\sum_\lambda\frac{z_\nu+2\mu-\epsilon_m-\epsilon_n}{z_\nu+2\mu-\eta_{ij;\lambda}}$$
$$\times\langle\chi_{ij;\lambda}|\varphi_{im}\varphi_{jn}\rangle\,\chi_{ij;\lambda}(rr')\,. \qquad (4.13)$$

With Eq. (3.9), we find

$$T_{imjnim'jn'}(z_\nu)=\sum_\lambda\langle\varphi_{im}\varphi_{jn}|V|\chi_{ij;\lambda}\rangle$$
$$\times\frac{z_\nu+2\mu-\epsilon_m-\epsilon_n}{z_\nu+2\mu-\eta_{ij;\lambda}}\langle\chi_{ij;\lambda}|\varphi_{im'}\varphi_{jn'}\rangle. \qquad (4.14)$$

At low temperatures we are mainly interested in the matrix elements of T between low Wannier states. This means ϵ_m and ϵ_n in Eq. (4.14) are small; in this case the main contributions in Eq. (4.14) will come from the lowest eigenfunctions of Eq. (4.12). This argument is strengthened by the fact that the second matrix element in Eq. (4.14), as we will see, is essentially zero except for one particular state. Inverting the Fourier transformation [(3.5)] and using those arguments we find that the leading term is

$$T_{imjnim'jn'}(t)=\delta(t)\sum_\lambda{}'\langle\varphi_{im}\varphi_{jn}|V|\chi_{ij;\lambda}\langle\chi_{ij;\lambda}|\varphi_{im'}\varphi_{jn'}$$
$$\equiv\delta(t)\,T_{imjnim'jn'}\,. \qquad (4.15)$$

The sum over the eigenstates of Eq. (4.12) has to be restricted to the lowest states, since the z_ν-dependent term has been replaced by 1. The second matrix element in Eq. (4.15) actually will reduce the sum to essentially one term only.

Using Eq. (4.15) we find the mass operator [Eq. (2.16)]

$$M_{imim'}(z_\nu)=\sum_{jn}T_{imjnim'jn}f(\epsilon_n-\mu). \qquad (4.16)$$

V. FURTHER APPROXIMATIONS ON BETHE-GOLDSTONE EQUATIONS

To reduce the two-particle equation [(4.12)] to a form which can be attacked with numerical methods we have to discuss some further approximations. We also restrict further consideration to zero temperature, where

$$[h_i(r)+h_j(r')+V(r-r')-\eta_{ij;\lambda}]\chi_{ij;\lambda}(rr')$$
$$=\varphi_0(r-R_i)\int d\rho\,\varphi_0^*(\rho-R_i)V(\rho-r')\chi_{ij;\lambda}(\rho r')$$
$$+\varphi_0(r'-R_j)\int d\rho\,\varphi_0^*(\rho-R_j)V(r-\rho)\chi_{ij;\lambda}(r\rho). \qquad (5.1)$$

We assume that

$$h_i(r)=-\nabla^2/2m+U(r-R_i), \qquad (5.2)$$

where $U(r)$ is a local single-particle potential.

Turning on the interaction in Eq. (5.1), we find a one-to-one correspondence between pairs of band indices mn and a corresponding λ. We write, using this correspondence,

$$\chi_{ij;mn}(rr')=f_{ij;mn}(rr')\varphi_m(r-R_i)\varphi_n(r'-R_j), \qquad (5.3)$$

and find with Eq. (5.2) an integrodifferential equation for f:

$$\left(-\frac{\nabla^2}{2m}-\frac{\nabla'^2}{2m}-\frac{\nabla\ln\varphi_m(r-R_i)}{m}\cdot\nabla-\frac{\nabla'\ln\varphi_n(r'-R_j)}{m}\cdot\nabla'\right.$$
$$\left.+V(r-r')-\eta_{ij;mn}+\epsilon_m+\epsilon_n\right)f_{ij;mn}(rr')$$
$$=\frac{\varphi_0(r-R_i)}{\varphi_m(r-R_i)}\int d\rho\;\varphi_0^*(\rho-R_i)V(\rho-r')f_{ij;mn}(\rho r')$$
$$\times\varphi_m(\rho-R_i)+\frac{\varphi_0(r'-R_j)}{\varphi_n(r'-R_j)}\int d\rho\;\varphi_0^*(\rho-R_j)$$
$$\times V(r-\rho)f_{ij;mn}(r\rho)\varphi_n(\rho-R_j). \tag{5.4}$$

This equation is considerably simplified if we assume that at least the lowest Wannier states can be approximated by oscillator eigenfunctions. Nosanow[8] has investigated this question and he found that this is a good approximation. To determine the ground-state energy we need only $f_{ij;00}(rr')$. We will concentrate on the treatment of this quantity. We use

$$\varphi_0(r-R_i)=(\alpha/\sqrt{\pi})^{3/2}\exp[-\tfrac{1}{2}\alpha^2(r-R_i)^2] \tag{5.5}$$

and introduce in Eq. (5.4) relative and center-of-mass coordinates $r\rightarrow R+\frac{1}{2}\rho$ and $r'\rightarrow R-\frac{1}{2}\rho$. We find

$$\left(-\frac{\nabla_R^2}{4m}-\frac{\nabla_\rho^2}{m}+\frac{\alpha^2}{m}(R-\tfrac{1}{2}R_i-\tfrac{1}{2}R_j)\cdot\nabla_R\right.$$
$$\left.+\frac{\alpha^2}{m}(\rho-R_i+R_j)\cdot\nabla_\rho+V(\rho)-\eta_{ij;00}+2\epsilon_0\right)f_{ij;00}(R\rho)$$
$$=\int d\rho'(\alpha/\sqrt{\pi})^3\exp(-\alpha^2\rho'^2)[V(\rho'+R_j-R-\tfrac{1}{2}\rho)$$
$$\times f_{ij;00}(\tfrac{1}{2}R+\tfrac{1}{4}\rho+\tfrac{1}{2}\rho'+\tfrac{1}{2}R_j;\;R+\tfrac{1}{2}\rho-\rho'-R_j)$$
$$+V(\rho'+R_i-R+\tfrac{1}{2}\rho)$$
$$\times f_{ij;00}(\tfrac{1}{2}\rho'+\tfrac{1}{2}R_i+\tfrac{1}{2}R-\tfrac{1}{4}\rho;\;\rho'+R_i-R+\tfrac{1}{2}\rho)]. \tag{5.6}$$

To simplify this equation further we assume that $f(R,\rho)$ depends on ρ only. The main contribution to T [Eq. (4.15)] will come from regions where $R\approx\frac{1}{2}R_i+\frac{1}{2}R_j$. We therefore neglect the R dependence of f and evaluate Eq. (5.6) at $R=\frac{1}{2}R_i+\frac{1}{2}R_j$, introducing $R_{ij}=R_i-R_j$:

$$\left\{-\frac{\nabla^2}{m}+\frac{\alpha^2}{m}(r-R_{ij})\cdot\nabla+V(r)-\eta_{ij;00}+2\epsilon_0\right\}f_{ij;00}(r)$$
$$=2(\alpha/\sqrt{\pi})^3\int d\rho\,\exp[-\alpha^2(\rho-\tfrac{1}{2}r-\tfrac{1}{2}R_{ij})^2]$$
$$\times V(\rho)f_{ij;00}(\rho). \tag{5.7}$$

As a last approximation we reduce this three-dimensional integrodifferential equation to a one-dimensional equation, assuming that $f(r)$ depends on $|r|$ only. In evaluating T[Eq. (4.15)], $f(r)$ is multiplied with a Gaussian having a maximum at $r=R_{ij}$. We therefore should determine $f(r)$ as accurately as possible along the direction of R_{ij}, solving Eq. (5.7) in this direction. We then obtain the one-dimensional integrodifferential equation

$$\left\{-\frac{1}{m}\left[\frac{\partial^2}{\partial r^2}+\left(\frac{2}{r}+\alpha^2R_{ij}-\alpha^2r\right)\frac{\partial}{\partial r}\right]+V(r)-\eta_{ij;00}+2\epsilon_0\right\}$$
$$\times f_{ij;00}(r)=4\alpha/\sqrt{\pi}\int_{-\infty}^{\infty}d\rho\,\frac{\rho+\frac{1}{2}r+\frac{1}{2}R_{ij}}{r+R_{ij}}\exp(-\alpha^2\rho^2)$$
$$\times V(\rho+\tfrac{1}{2}R_{ij}+\tfrac{1}{2}r)f_{ij;00}(\rho+\tfrac{1}{2}R_{ij}+\tfrac{1}{2}r). \tag{5.8}$$

Equations for the short-range correlation function $f_{ij;mn}(r)$ for excited states can be derived in the same way. To calculate the ground-state energy, however, we only need to know $T_{i0j0i0j0}$. In (4.15) then the following matrix element appears:

$$\langle\chi_{ij;mn}|\varphi_{i0}\varphi_{j0}\rangle=\int dr\,dr'\;\varphi_m^*(r-R_i)\varphi_n^*(r'-R_j)\chi$$
$$\times f_{ij;mn}(r-r')\varphi_0(r-R_i)\varphi_0(r'-R_j). \tag{5.9}$$

Since $f(r)$ is essentially constant at distances slightly greater than the hard-core radius and the main contribution to Eq. (5.9) comes from those regions, we find, with proper normalization of χ,

$$\langle\chi_{ij;mn}|\varphi_{i0}\varphi_{j0}\rangle\approx\delta_{m0}\delta_{n0}. \tag{5.10}$$

Using this we find the mass operator [Eq. (4.16)]

$$M(r-R_i)=\textstyle\sum_j\int d\rho\,|\varphi_0(\rho-R_{ij})|^2f_{ij;00}(r-\rho)V(r-\rho). \tag{5.11}$$

Equation (5.8) still depends on the parameter α which should be determined such that the Gaussian [Eq. (5.5)] gives the best fit to the lowest eigenfunction of the single-particle Hamiltonian [Eq. (5.2)], where U has to be replaced by Eq. (5.11). We determine α using a variational treatment such that the expectation value of (5.2) with the wave function (5.5) is minimal. In this variational procedure the α dependence of M [Eq. (5.11)] must of course be ignored.

The expression for the ground-state energy is similar to the Hartree approximation

$$E_0/N=\epsilon_0-\tfrac{1}{4}\textstyle\sum_i T_{i0j0i0j0}$$
$$=\tfrac{1}{2}\epsilon_0+3\alpha^2/8m. \tag{5.12}$$

The procedure to determine α mentioned above is equivalent to making E_0 stationary with respect to variations of α, again ignoring the α dependence of $f(r)$.

VI. PRESENTATION OF RESULTS

The integrodifferential equation [(5.8)] has been solved numerically for bcc ^{3}He, hcp ^{3}He, and hcp ^{4}He for various densities. Some aspects of this calculation are discussed in the Appendix. The standard form of a Lennard-Jones potential was used:

$$V(r)=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^6\right], \tag{6.1}$$

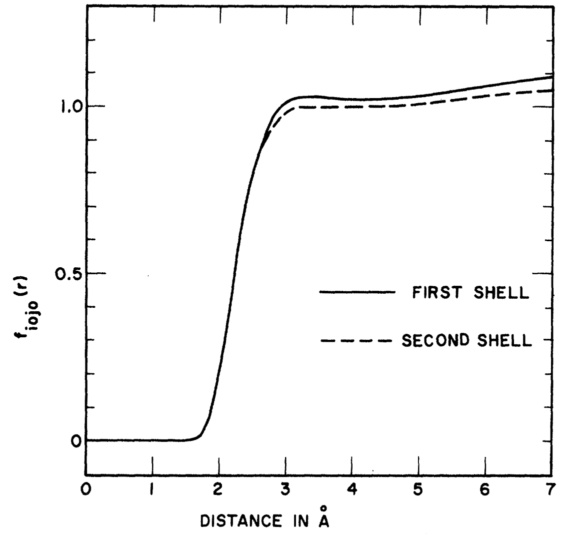

FIG. 1. $f_{i0j0}(r)$ for next and second-next neighbors in bcc ^{3}He.

with $\epsilon = 10.22$ °K and $\sigma = 2.556$ Å. Figure 1 shows the solution for next and second-next pairs of neighbors for bcc ^{3}He at a density of 24 cm^3/mole.[22,23] Figure 2 shows the potential, the next-neighbor two-particle correlation function without short-range correlations

$$g^0_{ij}(r) = \exp[-\tfrac{1}{2}\alpha^2(r-R_{ij})^2]\,, \tag{6.2}$$

and with short-range correlations

$$g_{ij}(r) f_{ij;00}(r)\ \exp[-\tfrac{1}{2}\alpha^2(r-R_{ij})^2]\,. \tag{6.3}$$

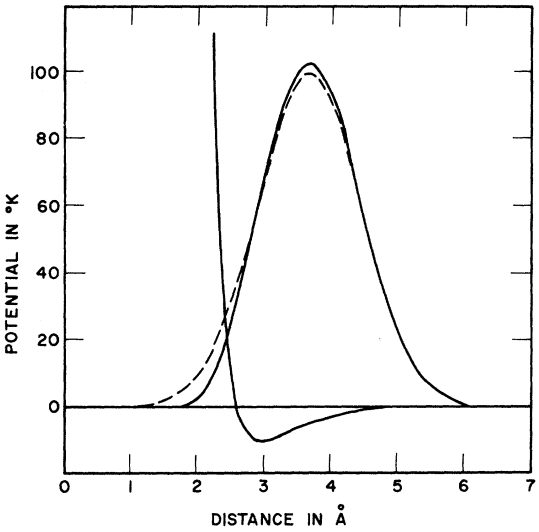

FIG. 2. Lennard-Jones Potential, two-particle correlation function for next neighbors in bcc ^{3}He. Without short-range correlations (dashed) and with short-range correlations (solid).

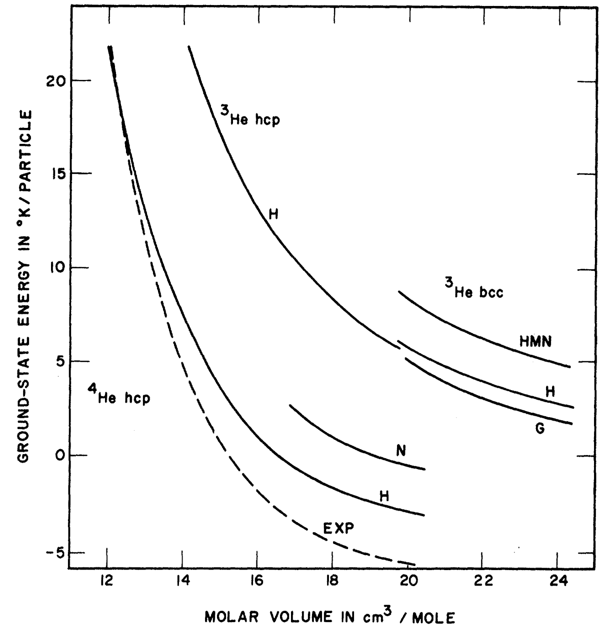

FIG. 3. Ground-state energy for ^{3}He and ^{4}He versus density. This work (H); Ref. 13 (G); Ref. 9 (HMN); and Ref. 8 (N).

The ground-state energy as a function of density is shown in Fig. 3, together with previous calculations. The results are consistently higher than the experimental values (except for ^{4}He at high densities). The experimental ground-state energy for ^{3}He is of the order of -0.5 K at 24 cm^3/mole. The main source of this discrepancy is the fact that phonons have not been included in this calculation. From other work,[24] it is known that this

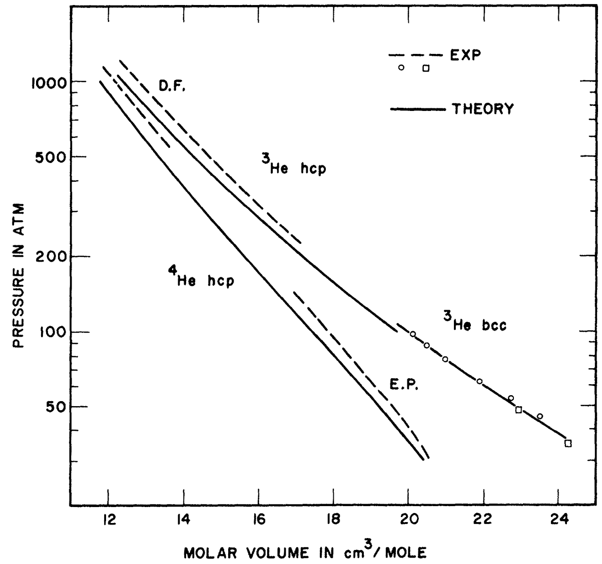

FIG. 4. Pressure versus density. This work (solid); Ref. 16 (E.P.); Ref. 17 (D.F.); Ref. 18 (circles); Ref. 19 (squares).

would bring a lowering of approximately 2 K per particle. The accuracy of this calculation is also insufficient to predict the bcc-hcp phase transition at the experimental density. Pressure data obtained from the volume dependence of the ground-state energy are presented in Fig. 4. In the hcp phase of ^{3}He and ^{4}He we find somewhat lower values than the experimental ones; in the bcc phase of ^{3}He, however, the agreement is very good.

Finally, Fig. 5 shows the compressibility. Again the agreement between theory and experiment is better in the bcc phase; however, even in the hcp phase the agreement is quite good. Figure 5 also shows theoretical values deduced from a calculation by Morley and Kliewer.[20] Their treatment does not include short-range correlations; the discrepancy with the experimental data is clear evidence of the importance of short-range correlations even at higher densities.

VII. DISCUSSION

As a first application of the perturbation expansion developed in I we investigated in this paper the ladder approximation. In translationally invariant systems this approximation is a low-density expansion and it is not at all clear that it should work in a system as dense as a quantum crystal. The unperturbed ground state, however, already contains correlations quite essential in a crystal. Therefore, the additional correlations which must be produced by the summation of ladder diagrams are rather small. This can be seen, e.g., from Fig. 2, by comparing the two-particle correlation functions with and without short-range correlations. A comparison with experiments indeed shows that the ladder approximation is rather good for quantum solids. In particular, three-particle terms seem to be considerably less important in quantum solids than in translationally invariant systems.

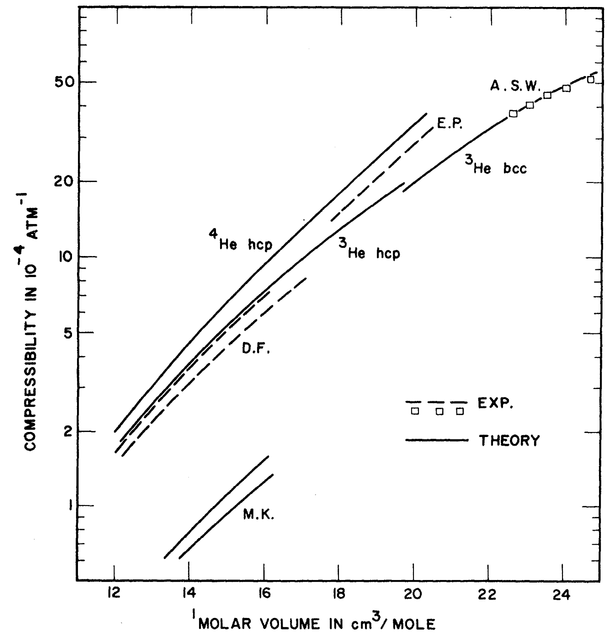

FIG. 5. Compressibility versus density. This work (solid); Ref. 20 (solid M.K.); Ref. 17 (D.F.); Ref. 16 (E.P.); Ref. 21 (A.S.W.).

The central equation in this paper is the Bethe-Goldstone equation [(3.8)] and the two-particle Schrödinger equation [(4.12)]. This second equation is similar to a corresponding equation derived by Guyer[13,14] using a cluster expansion of the ground-state energy. The main difference is that his equation does not contain the last term in the curly bracket of Eq. (4.12). Instead, the interaction $V(r-r')$ in his calculation is corrected by substracting an effective force introduced earlier in his calculation. The effect of this correction is very similar to the effect of the additional term in Eq. (4.12), and the results from Guyer's calculation are actually quite similar to those presented here. In contrast to the present case no self-consistency condition follows from his theory for the parameter α in the single-particle wave function [Eq. (5.5)]. Instead, he proposes two alternative prescriptions to determine his effective force; one turns out to be very similar to the present self-consistency condition.

In conclusion, we can say that the ladder approach applied to quantum crystals represents an alternative method of treating short-range correlations in quantum crystals. It is equivalent and in some respects superior to other means, in particular, to the use of Jastrow factors. Its main advantage is certainly that it has to be considered as the first step in a unified treatment of quantum crystals using many-body perturbation theory.

APPENDIX

To solve the integrodifferential equation [(5.8)] we used the following procedure. f has to be normalized according to Eq. (5.10), i.e.,

$$\alpha/(2\pi)^{1/2}\int_{-\infty}^{\infty} d\rho\, f_{ij;00}(\rho)[(\rho+R_{ij})/R_{ij}]\exp(-\tfrac{1}{2}\alpha^2\rho^2)=1 . \tag{A1}$$

The integrodifferential equation was solved iteratively. Starting from an initial function $f(r)$, normalized according to (A1), the right-hand side of (5.8) was calculated and treated as an inhomogeneity to the left-hand side. This "inhomogeneous differential equation " was solved by finding solutions to the inhomogeneous and to the homogeneous equation integrating from small r outwards, a second set, integrating from large r inwards. The inhomogeneous and homogeneous solutions were added and constant factors in front of the homogeneous solution were chosen such that at some intermediate distance the resulting two solutions matched in value and in first derivative. The eigenvalue, considered as a parameter in this "inhomogeneous differential equation," was determined so that the new f function again was normalized according to Eq. (A1). The new f finally was used to recalculate the right-hand side of (5.8). This procedure is sufficiently fast and rapidly converging.

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