MANY-BODY PERTURBATION THEORY FOR
QUANTUM CRYSTALS II: LADDER APPROXIMATION

by

Heinz Horner

**Solid State and Low Temperature
Physics Group**

SCHOOL OF PHYSICS AND ASTRONOMY

July, 1969

**UNIVERSITY OF MINNESOTA
MINNEAPOLIS, MINNESOTA**

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Many-Body Perturbation Theory for Quantum Crystals II:
Ladder Approximation

by

LEGAL NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Heinz Horner

Solid State and Low Temperature
Physics Group
School of Physics and Astronomy

University of Minnesota
Minneapolis, Minnesota

July 1969

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Work supported in part by the U. S. Atomic Energy Commission
under Contract No. AT(11-1) 1569.

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

Heinz Horner [†]

School of Physics and Astronomy, University of Minnesota
Minneapolis, Minnesota

Abstract

Using the perturbation expansion for quantum crystals proposed in an earlier paper¹⁾ we have investigated 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 calculated 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.

1. Introduction

In a previous paper¹⁾, hereafter referred to as I, we have investigated a form of many-body perturbation theory especially designed to treat quantum crystals. The proposed expansion is, at least at low temperatures, formally identical to the standard perturbation theory for spinless Fermions. In case of lattice particles having a spin $1/2$, the "spinless Fermions" are interacting with spins $1/2$ attached to each lattice site. 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 result of I makes it possible to use standard many-body methods in a 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, e.g. cluster expansion,⁴⁻¹⁰⁾ Monte Carlo integration¹¹⁾ or integral equations known from the theory of classical dense gas¹²⁾. Recently, Guyer^{13,14)} has proposed a different method based again on a cluster expansion of the ground state energy and using a hierarchy of model Hamiltonians. He derives 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 and we use similar approximations to reduce this equation to a form tractable by numerical methods.

The present paper is organized as follows. In Section 2, we review Brueckner theory and introduce some notation. Section 3 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 among 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, which is discussed in Section 4. In Section 5 we discuss a number of further approximations of the Bethe-Goldstone equation reducing it to a form which can be treated using numerical methods. In

Section 6, numerical results for the isotopes of helium are presented and discussed. Finally, in the Appendix, some numerical methods used in the solution of the Bethe-Goldstone equation are given.

2. A Review of Brueckner Theory

In this paragraph we give a short review of the Ladder approximation^{2,3} and this gives us also the opportunity to introduce the notations used later. In the applications to ³He we will not be interested in the nuclear spin system, assuming 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 (I, 2.14, 15)

$$H = \sum_i \sum_{m,n} c_{im}^\dagger T_{imin} c_{in} + \sum_{ij} \sum_{\substack{m m' \\ n n'}} c_{im}^\dagger c_{jn}^\dagger \tilde{V}_{ij; m n m' n'} c_{jn'} c_{im'} \quad (2.1)$$

where T_{imin} are the matrix elements of the kinetic energy in a basis of Wannier states. $\tilde{V}$ is given by (I, 3.2) and the operators $c^\dagger$ and c are, within the approximations discussed in

I field operators for spinless Fermions. In the case of ^3He we also would have a term in H describing the coupling between "particles" and "spins" (I, 6.2) but in a high temperature approximation for the spin system (2.1) is recovered.

We had split H into $H_0 + H'$ where (I, 2.14)

$$H_0 = \sum_i \sum_m c_{im}^\dagger \epsilon_m c_{im} \quad (2.2)$$

and we had added and subtracted a single particle potential u such that

$$T_{imin} + u_{imin} = \epsilon_n \delta_{mn} \quad (2.3)$$

We introduced unperturbed propagators

$$g_0(tt') = \frac{i}{\hbar} \delta_{ii'} \delta_{nn'} \exp\{-i\epsilon_n(t-t')\} \times \begin{cases} 1 - f(\epsilon_n) & i(t-t') > 0 \\ -f(\epsilon_n) & i(t-t') \leq 0 \end{cases} \quad (2.4)$$

The statistical weight functions $f(\epsilon)$ are given by (I, 5.2), but as discussed in I we can replace them at low temperatures by Fermi functions

$$f(\epsilon) = 1 / [\exp\{\beta(\epsilon - \mu)\} + 1] \quad (2.5)$$

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

$$g_0(t - i\beta) = -g_0(t) \quad (2.6)$$

Introducing the Schrödinger operator

$$S(i i') = \left\{ \left(i \frac{\partial}{\partial t} + \mu \right) \delta_{nn'} - T_{in in'} \right\} \delta_{ii'} \delta(t - t') \quad (2.7)$$

and

$$U(i i') = U_{in in'} \delta_{ii'} \delta(t - t') \quad (2.8)$$

we find

$$\{ S(i i') - U(i i') \} g_0(i i') = \delta(i i') \quad (2.9)$$

where we use the convention to sum over indices appearing twice
 and to integrate over times appearing twice in the interval $0 \dots -i\beta$.
 We introduce in the usual way the renormalized propagator $g(i i')$
 which obeys the Dyson equation

$$\{ S(i i') - M(i i') \} g(i i') = \delta(i i') \quad (2.10)$$

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

$$\begin{aligned}
 M(12) = & -i V(1324) g(43) \\
 & - V(1354) g(56) g(47) g(83) \chi \\
 & \chi T(6728)
 \end{aligned}
 \tag{2.11}$$

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

$$\begin{aligned}
 g(1234) = & g(13) g(24) - g(14) g(23) \\
 & + i g(15) g(26) T(5678) g(73) g(84)
 \end{aligned}
 \tag{2.12}$$

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

$$\begin{aligned}
 T(1234) = & K(1234) - i K(1536) \chi \\
 & \chi g(68) g(75) T(8274)
 \end{aligned}
 \tag{2.13}$$

Replacing the particle hole irreducible kernel K by the potential would give the RPA.

Another possibility is to generate T from a particle-particle irreducible kernel R , containing all skeleton diagrams having four extremeities, which cannot be cut into two parts by cutting two particle lines. T is then given by

$$T(1234) = R(1234) + i R(1256) g(57) g(68) T(7834) \quad (2.14)$$

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

$$\begin{aligned} R(121'2') &= V(121'2') \\ &= \delta_{i_1 i_2} \delta_{j_1 j_2'} \delta(t_1 - t_2) \delta(t_1 - t_1') \delta(t_2 - t_2') \times \\ &\quad \times \tilde{V}_{ij; nm n'm'} \end{aligned} \quad (2.15)$$

In this approximation the mass operator becomes

$$M(12) = -i T(1324) g(43) \quad (2.16)$$

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

3. The 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 the present impossible. We therefore, have to discuss several steps to bring the problem into a tractable form. Since the direct term in (I, 3.2) is by far dominant and since we are not interested in exchange for the moment, we can neglect the exchange term in (I, 3.2). We introduce a $T(r_1 \dots r_4, t)$ by

$$\begin{aligned}
 T(i_1 i_2 i_3 i_4) &= \delta_{i_1 i_2} \delta_{i_3 i_4} \delta(t_1 - t_2) \delta(t_3 - t_4) \times \\
 &\times \int dr_1 dr_2 dr_3 dr_4 \varphi_m^*(r_1 - R_i) \varphi_n^*(r_2 - R_j) \times \\
 &\times T_{ij}(r_1, r_2, r_3, r_4; t_1 - t_4) \varphi_{m'}(r_3 - R_i) \varphi_{n'}(r_4 - R_j)
 \end{aligned}
 \tag{3.1}$$

The δ -functions are a consequence of the fact that the potential is instantaneous and diagonal in the lattice site indices. Further, we have used that $g(i_1 i_2)$ depends on $t_1 - t_2$ only and is diagonal in the lattice site indices. $\varphi_n(r)$ are wave functions of Wannier states at the origin and R_i is the lattice vector to

lattice site i . (3.1) does not determine T uniquely but we can choose it to be the solution to

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

where

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

Obviously (3.2) and (3.1) fulfills (2.14) with R replaced by V . Fourier transforming with respect to the time variable we find

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

where

$$T_{ij}(r_1, r_2, r_3, r_4; z_\nu) = \int_0^{-i\beta} dt e^{iz_\nu t} T_{ij}(r_1, r_2, r_3, r_4; t) \quad (3.5)$$

and

$$q_{ij}(r_1, r_2, r_3, r_4; z_\nu) = i \int_0^{-i\beta} dt e^{iz_\nu t} q_{ij}(r_1, r_2, r_3, r_4; t) \quad (3.6)$$

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

To solve (3.4) it is convenient to introduce a "correlated two-particle wave function" $\psi(r, r')$ such that

$$\begin{aligned} V(r-r') \psi_{imjn}(r, r'; z_\nu) = \\ = \int d\rho d\rho' T_{ij}(r, r', \rho, \rho'; z_\nu) \varphi_m(\rho - R_i) \varphi_n(\rho' - R_j) \end{aligned} \quad (3.7)$$

Inserting this into (3.4) we find the integral equation

$$\begin{aligned} \psi_{imjn}(r, r'; z_\nu) = \varphi_m(r - R_i) \varphi_n(r' - R_j) \\ + \int d\rho d\rho' q_{ij}(r, r', \rho, \rho'; z_\nu) V(\rho - \rho') \psi_{imjn}(\rho, \rho'; z_\nu) \end{aligned} \quad (3.8)$$

The usual procedure to determine T is to solve this equation, the Bethe-Goldstone equation first. Having the solutions we find

$$T_{imjn;im'jn'}(z_\nu) = \int d\mathbf{r} d\mathbf{r}' \varphi_m^*(\mathbf{r}-\mathbf{R}_i) \varphi_n^*(\mathbf{r}'-\mathbf{R}_i) \times \\ \times V(\mathbf{r}-\mathbf{r}') \psi_{im'jn'}(\mathbf{r}\mathbf{r}'; z_\nu) \quad (3.9)$$

4. Pole Approximation for the Single Particle Propagators

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

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

$$(z_\nu + i\mu) g_{imim'}(z_\nu) - \\ - \sum_n \{ T_{imin} + M_{imin}(z_\nu) \} g_{inim'}(z_\nu) = \delta_{mm'} \quad (4.1)$$

where

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

and

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

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

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

$$T_{imin} + M_{imin} = \epsilon_n \delta_{mn} \quad (4.4)$$

and then

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

and Fourier transforming back

$$g_{imin}(t) = \frac{1}{i} \delta_{mn} \exp[-i(\epsilon_n - \mu)t] \begin{cases} 1 - f(\epsilon_n - \mu) & \text{if } t > 0 \\ -f(\epsilon_n - \mu) & \text{if } t \leq 0 \end{cases} \quad (4.6)$$

Inserting this approximation into (3.3) we find

$$\begin{aligned}
q_{ij}(r_1, r_2, r_3, r_4; z_\nu) &= \sum_{mn} \varphi_m^*(r_1 - R_i) \varphi_n^*(r_2 - R_j) \times \\
&\times \left\{ 1 - f(\epsilon_m - \mu) - f(\epsilon_n - \mu) \right\} \left\{ z_\nu - \epsilon_m - \epsilon_n + 2\mu \right\}^{-1} \times \\
&\times \varphi_m(r_3 - R_i) \varphi_n(r_4 - R_j)
\end{aligned}
\tag{4.7}$$

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

$$h_i(r) \varphi_n(r - R_i) = \epsilon_n \varphi_n(r - R_i) \tag{4.8}$$

and a projection operator

$$P_i = \sum_n |\varphi_{in}\rangle \langle \varphi_{in}| \tag{4.9}$$

Using these we can write (4.7)

$$\begin{aligned}
q_{ij}(r_1, r_2, r_3, r_4; z_\nu) &= P_i P_j \left\{ z_\nu - h_i(r_1) - h_j(r_2) + 2\mu \right\}^{-1} \times \\
&\times \left\{ 1 - f(h_i(r_1) - \mu) - f(h_j(r_2) - \mu) \right\} \times \\
&\times \delta(r_1 - r_3) \delta(r_2 - r_4) P_i P_j
\end{aligned}
\tag{4.10}$$

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 (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 (4.10) we now can write the Bethe-Goldstone equation (3.8) in the form

$$\begin{aligned} & \{z_v + 2\mu - h_i(r) - h_j(r') - V(r-r') + \\ & + [f(h_i(r)-\mu) + f(h_j(r')-\mu)]V(r-r')\} \psi_{imjn}(rr'; z_v) = \\ & = \{z_v + 2\mu - \epsilon_m - \epsilon_n\} \varphi_{im}(r-R_i) \varphi_{jn}(r'-R_j) \end{aligned} \quad (4.11)$$

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

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

Then ψ can be expanded in terms of those eigenfunctions

$$\psi_{imjn}(r, r'; z_v) = \sum_{\lambda} \frac{z_v + 2\mu - \epsilon_m - \epsilon_n}{z_v + 2\mu - \eta_{ij;\lambda}} \times \quad (4.13)$$

$$\times \langle \chi_{ij;\lambda} | \varphi_{im} \varphi_{jn} \rangle \chi_{ij;\lambda}(r, r')$$

With (3.9) we find

$$T_{imjn im'jn'}(z_v) = \sum_{\lambda} \langle \varphi_{im} \varphi_{jn} | V | \chi_{ij;\lambda} \rangle \times \quad (4.14)$$

$$\times \frac{z_v + 2\mu - \epsilon_m - \epsilon_n}{z_v + 2\mu - \eta_{ij;\lambda}} \langle \chi_{ij;\lambda} | \varphi_{im'} \varphi_{jn'} \rangle$$

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 (4.14) is small and in this case the main contributions in (4.14) will come from the lowest eigenfunctions of (4.12). This argument is strengthened by the fact that the second matrix element in (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

$$T_{imjn im'jn'}(t) = \delta(t) \sum_{\lambda} \langle \varphi_{im} \varphi_{jn} | V | \chi_{ij;\lambda} \rangle \times \quad (4.15)$$

$$\times \langle \chi_{ij;\lambda} | \varphi_{im'} \varphi_{jn'} \rangle$$

$$\equiv \delta(t) T_{imjn im'jn'}$$

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

Using (4.15) we find the mass operator (2.16)

$$M_{imim'}(z_v) = \sum_n T_{im;nim'n} f(\epsilon_n - \mu) \quad (4.16)$$

5. Further Approximations on the Bethe Goldstone Equation

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 the further considerations to zero temperature where

$$\begin{aligned} & \{ h_i(r) + h_j(r') + V(r-r') - \eta_{ij;\lambda} \} \chi_{ij;\lambda}(rr') = \\ & = \varphi_0(r-R_i) \int d\varrho \varphi_0^*(\varrho-R_i) V(\varrho-r') \chi_{ij;\lambda}(\varrho r') \\ & + \varphi_0(r'-R_j) \int d\varrho \varphi_0^*(\varrho-R_j) V(r-\varrho) \chi_{ij;\lambda}(r\varrho) \end{aligned} \quad (5.1)$$

We assume that

$$h_i(r) = -\frac{\nabla^2}{2m} + U(r-R_i) \quad (5.2)$$

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

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

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

and find with (5.2) an integro-differential equation for f

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

This equation is considerably simplified if we assume that at least the lowest Wannier states can be approximated by oscillator eigenfunctions. Nosanow⁸⁾ has investigated this question and he found that this is a good approximation. To determine the ground state energy we need only $f_{ij;00}(r,r')$ and we will concentrate on the treatment of this quantity. We use

$$\varphi_0(r-R_i) = (\alpha/\sqrt{\pi})^{3/2} \exp\{-\alpha^2(r-R_i)^2/2\} \quad (5.5)$$

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

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

To simplify this equation further we assume that $f(R, \rho)$ depends on ρ only. The main contribution to T (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 (5.6) at $R = \frac{1}{2} R_i + \frac{1}{2} R_j$ introducing $R_{ij} = R_i - R_j$

$$\begin{aligned} & \left\{ -\frac{\nabla^2}{m} + \frac{\alpha^2}{m} (r - R_{ij}) \cdot \nabla + V(r) - \eta_{ij;00} + 2\epsilon_0 \right\} f_{ij;00}(r) = \\ & = 2(\alpha/\sqrt{\pi})^3 \int d\rho \exp\{-\alpha^2(\rho - \frac{1}{2}r - \frac{1}{2}R_{ij})^2\} \times \\ & \times V(\rho) f_{ij;00}(\rho) \end{aligned} \quad (5.7)$$

As a last approximation we reduce this three-dimensional integro-differential equation to a one-dimensional equation assuming that $f(r)$ depends on $|r|$ only. In evaluating T (4.15) $f(r)$ is multiplied with a Gaussian having it's maximum at $r = R_{ij}$. We therefore should determine $f(r)$ as good as possible along the direction of R_{ij} solving (5.7) in this direction. We then obtain the one dimensional integro differential equation

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

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 need to know $T_{i_0j_0i_0j_0}$ only. In (4.15) occurs then the matrix element

$$\begin{aligned} \langle \chi_{ij;mn} | \varphi_{i_0} \varphi_{j_0} \rangle &= \int d\mathbf{r} d\mathbf{r}' \varphi_m^*(\mathbf{r}-\mathbf{R}_i) \varphi_n^*(\mathbf{r}'-\mathbf{R}_j) \chi \\ &\times f_{ij;mn}(\mathbf{r}-\mathbf{r}') \varphi_0(\mathbf{r}-\mathbf{R}_i) \varphi_0(\mathbf{r}'-\mathbf{R}_j) \end{aligned} \quad (5.9)$$

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

$$\langle \chi_{ij;mn} | \varphi_{i_0} \varphi_{j_0} \rangle \approx \delta_{m_0} \delta_{n_0} \quad (5.10)$$

Using this we find the mass operator (4.16)

$$M(\mathbf{r}-\mathbf{R}_i) = \sum_j \int d\mathbf{q} |\varphi_0(\mathbf{q}-\mathbf{R}_j)|^2 f_{ij;00}(\mathbf{r}-\mathbf{q}) V(\mathbf{r}-\mathbf{q}) \quad (5.11)$$

Eq. (5.8) still depends on the parameter α which should be determined such that the Gaussian (5.5) gives the best fit to the lowest eigenfunction of the "single particle Hamiltonian" (5.2), where $\mathcal{U}$ has to be replaced by (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 $M(5.11)$ has of course to be ignored.

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

$$\begin{aligned} E_0/N &= \epsilon_0 - \frac{1}{4} \sum_i T_{i \circ j \circ i \circ j \circ} \\ &= \frac{1}{2} \epsilon_0 + \frac{3 \alpha^2}{8 m} \end{aligned} \quad (5.12)$$

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

6. Presentation of Results

The integro differential equation (5.8) has been solved numerically for bcc ^3He , hcp ^3He and hcp ^4He for various densities. Some aspects of this calculation are discussed in the appendix. The standard form of a Lennard-Jones potential was used

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

with $\epsilon = 10.22 \text{ K}$ and $\sigma = 2.556 \text{ \AA}$. Fig. 1 shows the solution for next and second next pairs of neighbours for bcc ^3He at a density of 24 ccm/Mole. Fig. 2 shows the potential, the next neighbour two-particle correlation function without short range correlations

$$g_{ij}^0(r) = \exp \left\{ -\alpha^2 (r - R_{ij})^2 / 2 \right\} \quad (6.2)$$

and with short range correlations

$$g_{ij}(r) = f_{ij,\infty}(r) \exp \left\{ -\alpha^2 (r - R_{ij})^2 / 2 \right\} \quad (6.3)$$

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 ^4He at high densities). The experimental ground state energy for ^3He is of the order of $-.5 \text{ K}$ at 24 ccm/Mole. The main source of this discrepancy is the fact that phonons have not been included in this calculation. From other work it is known that this 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 ^3He and ^4He we find somewhat lower values compared to experiments, in the bcc phase of ^3He , 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. Fig. 5 also shows theoretical values deduced from a calculation by Morley and Kliwer²⁰⁾. Their treatment does not include short range correlations and the discrepancy with the experimental data is clear evidence of the importance of short range correlations even at higher densities.

7. 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 such a dense system as a quantum crystal. The unperturbed ground state, however, already contains correlations quite essential in a crystal. Therefore, the additional correlations which have to be produced by the summation of ladder diagrams are rather small. This can be seen e.g. from Fig. 2 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. Especially three-particle terms seem to be considerably less important in quantum solids than in translationally invariant systems.

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 curled bracket of (4.12) but instead the interaction $V(r-r')$ is in his calculation corrected by subtracting an effective force introduced earlier in his calculation. The effect of this correction is very similar to the effect of the additional term in (4.12) and the results from Guyers calculation are actually quite similar. The role of this effective force is somewhat related to the parameter α in the single particle wave function (5.5). In contrast to the present case no such self-consistency condition follows from his theory. Instead he proposes two alternative prescriptions to determine this effective force, where one turns out to be very similar to the present self-consistency condition.

Concluding we can say that the ladder-approach applied to quantum crystals represents an alternative method to treat short range correlations in quantum crystals. It is equivalent and in some respects superior to other means, especially 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.

8. Appendix

To solve the integro differential equation (5.8) we used the following procedure. f has to be normalized according to (5.10), i.e.

$$\alpha/\sqrt{2\pi} \int_{-\infty}^{\infty} d\rho \frac{1}{r_{ij,00}}(\rho) \frac{\rho + R_{ij}}{R_{ij}} \exp(-\alpha^2 \rho^2/2) = 1 \quad (8.1)$$

The integro differential equation was solved iteratively. Starting from an initial function $f(r)$, normalized according to (8.1), 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 finding solutions to the inhomogeneous and to the homogeneous equation integrating from small r outwards and 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 their first derivative. The eigenvalue, considered as parameter in this "inhomogeneous differential

equation", was determined such that the new f -function again was normalized according to (8.1). The new f finally was used to calculate a new right hand side of (5.8). This procedure is sufficiently fast and rapidly converging.

ACKNOWLEDGEMENTS

It is a pleasure for the author to thank L. H. Nosanow for many critical and helpful discussions and for a reading of the manuscript. A discussion with R. A. Guyer also should be acknowledged.

REFERENCES

- * Work supported in part by the U. S Atomic Energy Commission under Contract No. AT(11-1) 1569.
- + Present Address: Institut Max von Laue-Paul Langevin.
8046 Garching b. München. Reaktorgelände.

- 1. H. Horner, (to be published).
- 2. See e.g. D. J Thouless: The Quantum Mechanics of Many-Body Systems. Academic Press, New York and London (1961).
- 3. B. D. Day, Rev. Mod. Phys. 39, 719 (1967) and references cited.
- 4. Nosanow, L. H., and G. L. Shaw: Phys. Rev. 119, 968 (1962).
- 5. Nosanow, L. H., Phys. Rev. Letters 13, 270 (1964).
- 6. Mullin, W. J., Phys. Rev. 134, A1249 (1964).
- 7. Nosanow, L. H., and W. J. Mullin, Phys. Rev. Letters 14, 133 (1965).
- 8. Nosanow, L. H., Phys. Rev. 146, 120 (1966).
- 9. Hetherington, J. H., W. J. Mullin and L. H. Nosanow, Phys. Rev. 154, 175 (1967).
- 10. K. A Brueckner and J. Frohberg, Prog. Theoret. Phys. (Kyoto), Suppl. (1965); J. H. Frohberg, Ph.D. dissertation, Univ. of Calif./San Diego, 1967, unpublished.
- 11. J-P. Hansen and D. Levesque, Phys. Rev. 165, 293 (1968).
- 12. W. E. Massey and C-W. Woo, Phys. Rev. 169, 241 (1968);
C-W. Woo and W. E. Massey, Phys. Rev. (to be published).

13. R. A. Guyer, Solid State Comm. 7 315 (1969) and Solid State Physics (to be published).
14. R. A. Guyer, B. Sarkissian (to be published).
15. L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics W. A. Benjamin, Inc. New York, 1962).
A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloskinski, Methods of Quantum Field Theory in Statistical Physics (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963).
16. D. O. Edwards, R. C. Pandorf, Phys. Rev. 140, A816 (1965).
17. J. S. Dugdale, J. P. Franck, Phil. Trans. R. Soc. 275, 1 (1964).
18. S. G. Sydoviak, R. L. Mills, E. R. Grilly, Phys. Rev. Lett. 4 495 (1960).
19. D. O. Edwards, J. L. Baum, D. F. Brewer, J. G. Daunt, A. S. McWilliams, Helium Three, Ohio State University Press, Columbus, (1960).
20. G. L. Morley, K. L. Kliever, Phys. Rev. 180 245 (1969).
21. E. D. Adams, G. C. Straty, E. L. Wall, Phys. Rev. Lett. 15 549 (1965).

FIGURE CAPTIONS

- Fig. 1: $f_{iojo}(r)$ for next and second next neighbours in bcc ^3He .
- Fig. 2: Lennard-Jones Potential, two-particle correlation function for next neighbours in bcc ^3He . Without short range correlations (dashed) and with short range correlations (solid).
- Fig. 3: Ground state energy for ^3He and ^4He vs. density. This work (H), ref. 13 (G) ref 9 (HMN) and ref. 8 (N).
- Fig. 4: Pressure vs. density. This work (solid), ref. 16 (E.P.), ref. 17 (D. F.), ref. 18 (circles), ref. 19 (squares).
- Fig. 5: Compressibility vs. density. This work (solid) ref. 20 (solid M.K.) ref. 17 (D. F.) ref. 16 (E.P.) ref. 21 (A.S.W.)