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Many-Body Perturbation Theory for Quantum Crystals. I[*]

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The possibility of a perturbation treatment for quantum crystals is investigated. It is found that the usual form of the unperturbed Hamiltonian, being a single-particle operator, is not suitable for this situation, since it does not produce correlations necessary in a theory of quantum crystals. These correlations prevent the unperturbed ground state or low excited states from containing multiply occupied lattice sites. An unperturbed Hamiltonian is proposed which generates these correlations but is no longer a single-particle operator. The rules for a diagrammatic representation of a perturbation expansion starting from this unperturbed Hamiltonian are given. They differ from the usual rules for Goldstone diagrams. In particular, the linked-cluster theorem is not valid. Adding and subtracting pairs of mutually cancelling diagrams, in a manner similar to that in which Pauli-principle–violating diagrams are treated in the standard perturbation theory for fermions, we find new rules which, at least at low temperatures, are identical to those for spinless fermions. This result is essentially independent of the statistics of the actual lattice particles. In the case where the lattice particles are actually fermions with spin $\frac{1}{2}$, e.g., ^{3}He, we find an expansion formally identical to the problem of spinless fermions interacting among themselves and with a set of spins $\frac{1}{2}$ localized at lattice sites.

I. INTRODUCTION

The outstanding feature of quantum crystals is the existence of large zero-point motion. This is caused by the light mass of the lattice particles, the isotopes of helium or molecular hydrogen, and by the fact that the van der Waals interaction is quite weak at distances of the order of the lattice constant. On the other hand, the strong repulsion at smaller distances produces short-range correlations which have to be contained in any first-principle calculation on quantum crystals. Numerous papers have dealt with this problem[1–11]; most of them are based on a Jastrow-type wave function and use variational methods.[1–9]

Another consequence of the large zero-point motion is the strong anharmonicity of the lattice vibrations even at zero temperature which prevents the use of ordinary lattice dynamics. This problem has been studied with the random-phase approximation (RPA)[12–17] and with summations to all orders of anharmonic phonon theory.[18–20] None of these papers, however, has given a consistent treatment of phonons and short-range correlations simultaneously. Some discussion has arisen as to which quantities should be identified with the actual phonon frequencies.[18, 20–22]

A third group of papers has been concerned with exchange in ^{3}He, and conceptually quite different approaches have been used.[4, 23–25]

In searching for a method to treat the three aspects – short-range correlations, phonons, and exchange – on a common basis, we have investigated the many-body perturbation theory. This approach is suggested by the fact that short-range correlations can be treated using Brueckner theory,[26, 27] as demonstrated, e.g., in the theory of nuclear matter. Phonons on the other hand can be obtained approximately from RPA. It therefore seems natural to try to combine both methods.

A careful examination of perturbation theory, however, reveals the fact that standard many-body methods[26, 28] cannot be applied directly to quantum crystals. The reason is that the usual form of the unperturbed Hamiltonian, being a single-particle operator, does not produce sufficient correlations in the unperturbed ground state or low excited states. The resulting perturbation series would converge extremely slowly if at all. This situation is similar to the theory of superconductivity where a canonical transformation has to be used first, and after doing this a perturbation theory in terms of quasiparticles is possible.

Naively, one would assume that a perturbation calculation in a crystal should start from a state having at each lattice site a particle sitting in a localized state, e.g., ground-state wave function of a harmonic oscillator. The unperturbed Hamiltonian would contain, besides the kinetic energy, an effective single-particle potential having a deep enough minimum at each lattice site. The problem arises from the fact that the unperturbed ground state mentioned above, having at each lattice site one particle in the lowest single-particle state, is highly degenerate. In the case of fermions, this state is degenerate with states having one or more doubly occupied lattice sites (sites occupied by two particles of opposite spin in the lowest single-particle state), and a corresponding number of vacancies. In the case of bosons, there are degenerate unperturbed states with even higher occupation numbers and corresponding numbers of vacancies. However, when the interaction is turned on, states with more than one particle on the same lattice site would develop into highly excited states. Such a situation would require the use of degenerate perturbation theory, which seems to be most difficult in this context.

In Sec. II, we propose an unperturbed Hamiltonian which actually lifts this degeneracy, but it is no longer a single-particle operator. The perturbation expansion for the partition function is discussed in Sec. III introducing diagrams similar to Goldstone graphs. The great disadvantage of this expansion is that the linked-cluster theorem is not valid. The rest of this paper is concerned with restoring the linked-cluster theorem.

There is an analog to this difficulty in the conventional perturbation expansion for a Fermi gas. Such an expansion obeys the linked-cluster theorem, but contains Pauli-principle-violating diagrams.[29] An expansion not containing those would not obey the linked-cluster theorem. The usual expansion could be recovered by adding pairs of mutually cancelling Pauli-principle-violating diagrams.

A similar method is used in Secs. IV, V, and VI to find an expansion in which the linked cluster theorem holds. Sections IV and V deal with spinless particles at zero and finite temperatures, respectively. In Sec. VI, the situation for fermions with spin $\frac{1}{2}$ is investigated. Section VII contains a summary and the Appendix contains a proof necessary for Secs. IV and V. The result is that the expansion, at least at low temperatures, can be brought into a form identical to the usual expansion for a system of spinless Fermions. This fact is independent of the statistics of the actual lattice particles (except for the exchange term in the interaction) as one would expect in a theory of quantum solids, since the overlap between neighboring particles is quite small. In the case of ^{3}He, we find that the “spinless Fermions” are coupled to a system of spins $\frac{1}{2}$ attached to the lattice sites.

The result of this paper enables one to use the standard methods developed in many-body theory, e.g., Brueckner theory or RPA. This opens the field for investigations which one may hope will lead to further developments in the theory of quantum crystals.

II. UNPERTURBED HAMILTONIAN

A perturbation expansion for systems at finite temperatures[26, 28] usually starts from an expansion of the grand canonical partition function

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} \quad . \tag{2.1}$$

The Hamiltonian is split into an unperturbed part and a perturbation

$$H - \mu N = H_0 + H' \quad . \tag{2.2}$$

It is convenient to introduce “time-dependent” operators in the interaction picture ($\hbar = 1$)

$$A(t) = e^{iH_0 t} A e^{-iH_0 t} \quad , \tag{2.3}$$

and to allow for complex time arguments. The partition function can be expanded as

$$Z = Z_0 - i\int_0^{-i\beta} d\tau\, \mathrm{Tr}[H'(\tau)e^{-\beta H_0}] + (-i)^2 \int_0^{-i\beta} d\tau_1 \int_0^{\tau_1} d\tau_2\, \mathrm{Tr}[H'(\tau_1)H'(\tau_2)\, e^{-\beta H_0}] \tag{2.4}$$

$$+ (-i)^3 \int_0^{-i\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \int_0^{\tau_2} d\tau_3\, \mathrm{Tr}\,[H'(\tau_1)H'(\tau_2)H'(\tau_3)e^{-\beta H_0}] + \cdots \; ,$$

and $\quad Z_0 = \mathrm{Tr}\, e^{-\beta H_0}$ (2.5)

is the partition function for the unperturbed system. For this expansion to converge, it is crucial that the solution of the unperturbed system contains the essential features of the actual system. This is, for example, most evident in the theory of superconductivity, where an H_0 describing free particles is totally insufficient and a transformation to quasiparticles is necessary. More generally, for all systems having a symmetry lower than the actual Hamiltonian, it is essential to choose H_0 such that it has the lower symmetry of the system and not the full symmetry of H.

The usual choice of the unperturbed Hamiltonian is

$$H_0=\sum_s \int dr\,\Psi_s^\dagger(r)\left(-\frac{\nabla^2}{2m}+U(r)-\mu\right)\Psi_s(r)\,, \qquad (2.6)$$

where $U(r)$ could be the Hartree potential. In a crystal, $U(r)$ is expected to be periodic having the symmetry of the lattice, and in this case the eigenfunctions to H_0 are Bloch states. Introducing field operators for these states,

$$H_0=\sum_{kn} a^\dagger(kn)[\epsilon(kn)-\mu]a(kn)\quad , \qquad (2.7)$$

k is a wave vector inside the first Brillouin zone and n is a label for band and spin in the case of Fermions.

The density distribution of a particle around a lattice site even in the case of quantum solids is rather well concentrated compared to the electronic density distribution in metals. H_0 would describe lattice particles (e.g., He atoms or H_2 molecules) moving in bands, and as a consequence at least the lower bands are expected to be extremely narrow in comparison to the band gap. Neglecting the k dependence of ϵ, we might write Eq. (2.7) in terms of field operators for Wannier states:

$$H_0=\sum_{in} a^\dagger(in)[\epsilon(n)-\mu]a(in)\quad , \qquad (2.8)$$

where $a^\dagger$ and a create and annihilate particles in Wannier states near lattice site R_i and in a state with quantum number (band index) n.

For a crystal with N particles, we expect that the lattice constant is such that there are just N lattice sites. Turning on the interaction adiabatically we expect that the actual ground state will develop from an unperturbed state in which each lattice is occupied just by one particle in the lowest Wannier state. Unfortunately, this unperturbed state is highly degenerate with respect to H_0. For example, a state in which one lattice site is doubly occupied and another vacant has the same unperturbed energy as the one considered before. Such a state, however, will develop into a highly excited actual state when the interaction is turned on. In a calculation of the ground state, one would therefore have to apply degenerate perturbation theory, which is considerably more difficult in a many-body system. In an expansion of the partition function Eq. (2.4), these latter states would give rise to unreasonably large contributions, resulting in poor convergence of the expansion, if it converges at all.

From this discussion, we conclude that H_0 should be chosen such that the unperturbed ground state and low-lying excited states correspond to singly occupied lattice sites. States having multiply occupied lattice sites have much higher energy with respect to H_0. It seems reasonable to completely disregard the latter states for the present and to consider them, if necessary, separately. To do so, we introduce projection operators P_i such that

$$\begin{aligned} &P_i\,|\Psi\rangle = |\Psi\rangle, \quad \text{if } \textstyle\sum_n a^\dagger(in)a(in)\,|\,\Psi\rangle = |\Psi\rangle \\ &P_i\,|\,\Psi\rangle = 0\quad , \quad \text{otherwise}\,; \end{aligned} \qquad (2.9)$$

or using the Kronecker symbol (we use this notation instead of $\delta_{1,\,n}$ for typographical reasons)

$$P_i=\delta(1,n_i),\quad \text{where}\quad n_i=\textstyle\sum_n a^\dagger(in)a(in)\quad . \qquad (2.10)$$

Using these, we define

$$c(in)=a(in)P_i\ ,\quad c^\dagger(in)=P_i a^\dagger(in)\quad . \qquad (2.11)$$

These new operators commute (anticommute) if the lattice-site index is different:

$$[c^\dagger(in),\ c^\dagger(jm)]_\mp=[c^\dagger(in),c(jm)]_\mp=0,\quad i\neq j\ . \qquad (2.12)$$

Two operators having the same lattice-site index, however, do not obey simple commutation relations, but we will not need those.

We split the actual Hamiltonian into three parts:

$$H=H_0+H'+\hat{H}\quad , \qquad (2.13)$$

where

$$\begin{aligned} H_0&=\sum_i\sum_{mn} c^\dagger(im)[T(im,in)+U(im,in)]c(in) \\ &=\sum_{in} c^\dagger(in)\epsilon(n)c(in)\quad , \end{aligned} \qquad (2.14)$$

$$\begin{aligned} H'=&\sum_{i>j}\ \sum_{m,m',n,n'} c^\dagger(im)c^\dagger(jn)[V(im,jn,in',jm') \\ &\pm V(im,jn,jn',im')]c(jn')c(im') \\ &-\sum_i\sum_{mn} c^\dagger(im)U(im,in)c(in)\quad . \end{aligned} \qquad (2.15)$$

Here T is the kinetic energy, V is the interaction, and U is some properly chosen single-particle potential.

The third part $\hat{H}$ contains the remaining terms and does not have matrix elements between two states, each having singly occupied lattice sites only.

Retaining states only having singly occupied lattice sites in evaluating the trace, and for the intermediate states, we end up with an expansion of the canonical partition function rather than the grand canonical, and a Hamiltonian $H = H_0 + H'$ only. This is the basic approximation of this paper. It corresponds to an expansion in a subspace of the N-particle Hilbert space, spanned by the states having each lattice site singly occupied.

This subspace actually depends on the particular choice of the single particle basis of Wannier states which was used to define the projection operators by Eq. (2.9). If, however, the overlap between states with different lattice site indices is sufficiently small, the Wannier states at a given lattice site form essentially a complete basis inside the corresponding Wigner-Seitz cell. Therefore, the actual choice of the Wannier function basis will not be critical as long as the overlap is sufficiently small. In actual calculations the basis will be determined self-consistently such that the single-particle propagators are diagonalized at low energies. In a Hartree calculation, this would amount to using the Hartree function as basis.

The restriction of the Hilbert space will not be crucial for most questions. For phenomena like formation of defects, diffusion, or especially exchange, however, states outside this subspace might play a role as intermediate states and at least some effects of these states should be included in a treatment of those phenomena. At present, we will not be concerned with these questions, leaving them for further investigation.

III. PERTURBATION EXPANSION OF THE PARTITION FUNCTION

The time dependence of the operators is given by Eq. (2.3). Using H_0 [Eq. (2.14)], we find

$$\begin{aligned} c^\dagger(in;t) &= \exp[i\epsilon(n)t]\, c^\dagger(in) \ , \\ c(in;t) &= \exp[-i\epsilon(n)t]\, c(in) \ . \end{aligned} \tag{3.1}$$

We introduce

$$\begin{aligned} \tilde{V}(ij;mnm'n') &= V(im, jn, im', jn') \\ &\quad \pm V(im, jn, jn', im') \ , \\ U(i, mn) &= U(im, in) \ . \end{aligned} \tag{3.2}$$

The expansion of the canonical partition function Eq. (2.4) becomes

$$\begin{aligned} \frac{Z}{Z_0} = 1 &- i \int_0^{-i\beta} d\tau \sum_{imm'} U(imm') \exp\{i[\epsilon(m) - \epsilon(m')]\tau\} \langle c^\dagger(im)\, c(im')\rangle_0 - i \int_0^{-i\beta} d\tau \sum_{i>j} \sum_{mm'nn'} \\ &\times \tilde{V}(ij;mnm'n') \exp\{i[\epsilon(m) + \epsilon(n) - \epsilon(m') - \epsilon(n')]\tau\} \langle c^\dagger(im)\, c(im')\, c^\dagger(jn)\, c\,(jn')\rangle_0 \\ &+ (-i)^2 \int_0^{-i\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \sum_{imm'} \sum_{jnn'} U(imm') U(jnn') \exp\{i[\epsilon(m) - \epsilon(m')]\tau_1\} \\ &\times \exp\{i[\epsilon(n) - \epsilon(n')]\tau_2\} \langle c^\dagger(im)\, c(im')\, c^\dagger(jn)\, c(jn')\rangle_0 + \cdots \ , \end{aligned} \tag{3.3}$$

where the unperturbed partition function

$$Z_0 = \mathrm{Tr}_N \exp(-\beta H_0) = [\textstyle\sum_n \exp(-\beta\epsilon_n)]^N \ , \tag{3.4}$$

and the unperturbed expectation value

$$\langle \mathrm{Op} \rangle_0 = Z_0^{-1}\, \mathrm{Tr}_N \mathrm{Op} \exp(-\beta H_0) \ . \tag{3.5}$$

Because of the commutation relations [Eq. (2.12)] the expectation values occurring in Eq. (3.3) factorize into expectation values, each containing c and $c^\dagger$ operators with the same lattice-site index only. A typical such factor would be

$$\langle c^\dagger(im_1)\, c(in_1)\, c^\dagger(im_2)\, c(im_2) \cdots c^\dagger(im_\nu)\, c(in_\nu)\rangle_0 = \delta(n_1 m_2)\, \delta(n_2 m_3) \cdots \delta(n_\nu m_1) \exp[-\beta\epsilon(m_1)] Z_0^{-1/N} \ . \tag{3.6}$$

In contrast to the usual perturbation expansion, where Eq. (3.6) would contribute $\nu!$ terms, this is the only contribution in our case.

We would like to express the perturbation expansion Eq. (3.3) in terms of diagrams similar to the Goldstone diagrams.[21] We use a vertical time axis and represent each matrix element of U or $\tilde{V}$ by a dashed line at the corresponding time level. The end points of these vertices are connected by lines with arrows forming closed loops.

Each such loop corresponds to an expectation value such as Eq. (3.6), each up-going line particle propagator contributes a factor $\delta(n,m)$, each down going line hole propagator, a factor $\delta(n,m)e^{-\beta\epsilon(n)}Z_0^{-1/N}$. Each loop carries a lattice-site index and can contain only one hole line. In a given diagram, all lattice site indices attached to different loops have to be different. To evaluate a given diagram we have the following rules: (a) Each vertex carries a time label, each propagator a band index, each loop of propagators a lattice-site index. Each loop can have only one hole line. (b) Each vertex contributes $-\frac{1}{2}i$ times the corresponding matrix element [Eq. (3.2]; each propagator, a factor $e^{-i\epsilon(n)(t-t')}$; and each hole propagator, in addition, a factor $e^{-\beta\epsilon(n)}Z_0^{-1/N}$. The quantity $\epsilon(n)$ is the energy corresponding to the band index n, t and t' are the starting and terminal time of the propagator. (c) Integrate over all times such that the given time order of the vertices is preserved, sum over all band indices and over all lattice-site indices such that no two of them are the same.

These rules are quite similar to the usual rules for Goldstone diagrams,[26] with the additional restriction of one hole line per loop only, and the restriction of the lattice-site summations.

We would like to stress the fact that the only place where the statistics of the lattice particles enter is in the sign of the "exchange term" in the interaction (3.2). In situations where the overlap is small, the contribution of this term will be negligible and the calculation becomes independent of the statistics. This result is very natural in a theory of quantum crystals. It is confirmed by the close resemblance of solid ^{3}He and ^{4}He, in contrast to the liquids, at least at temperatures that are not so low that the nuclear spins in ^{3}He begin to play a role.

IV. GROUND-STATE ENERGY OF SPINLESS FERMIONS AND BOSONS

The calculation of the free energy $F=-kT\ln Z$ and of the ground-state energy $E=\lim F$ as $T\rightarrow 0$ is much simplified in the usual perturbation theory by the fact that disconnected diagrams simply contribute factors. Therefore F or E is given by the contribution of all connected diagrams. This fact, known as the linked-cluster theorem, is not valid in the present case because of the restrictions of the lattice-site summations in rule (c).

It is illuminating to examine for a moment a similar situation in the usual perturbation expansion for a Fermi gas. Such an expansion contains Pauli-principle-violating diagrams,[29] but to each such diagram exists another one cancelling its contribution exactly. In many cases, however, connected diagrams are cancelled by disconnected ones. Therefore, in an expansion which does not contain Pauli-principle-violating diagrams, the linked-cluster theorem would not be valid and one would find restrictions similar to those given in rule (c).

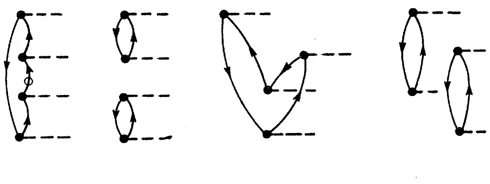
On the other hand, starting from such an expansion we could find the usual form adding mutually cancelling Pauli-principle-violating diagrams in an appropriate way. We will follow the same strategy in the present case.

We restrict our further consideration, for the time being, to bosons with spin 0 and to fermions, disregarding the spin degeneracy. The consideration of the spin degeneracy of Fermions with spin $\frac{1}{2}$ requires a slightly modified formulation which will be given in Sec. VI.

We first treat the case of zero temperature. There a hole line has to carry a band index of the band with lowest energy $n=0$, whereas, the band indices for particle lines are not restricted, including $n=0$. For each diagram with a particle line having band index $n=0$ we can find another one, not allowed according to the rules (a)–(c), giving exactly the same contribution. An example is given in Figs. 1(a) and 1(b), where the particle line carrying band index $n=0$ is marked by a 0. Similarly, we could find to each diagram having more than one hole line in a given loop, another one giving the same contribution, e.g., Figs. 1(c) and 1(d). In this case, both diagrams would be forbidden according to the rules (a)–(c).

We can restrict the summations of the band indices to $n\neq 0$ for particle lines and compensate this change in the rules by allowing diagrams of the type Fig. 1(b) having more than one loop for a given lattice-site index. We also can add diagrams containing parts given in Fig. 1(d) and subtract those of type Fig. 1(c) having more than one hole line per loop. In the Appendix, we investigate these cancellations more rigorously and find that this procedure of adding and subtracting mutually cancelling diagrams just gives all diagrams without the restrictions given in rules (a) and (c) concerning the lattice-site-index summations. More precisely, we find for spinless particles at zero temperature the following rules:

(i) The same as (a), except that the number of



(a) (b) (c) (d)

FIG. 1. Parts of mutually canceling diagrams.

hole lines is not restricted. (ii) The same as (b), except that each hole propagator contributes a factor $-\delta(n0)\exp[-i\epsilon(0)(t-t')]$ and each particle line $[1-\delta(n0)]\exp[-i\epsilon(n)(t-t')]$. A factor $(-1)^l$ has to be added, where l is the number of loops in the diagram. (iii) The same as (c), except that the lattice-site summation is not restricted.

The changed sign for hole lines and the factor $(-1)^l$ is introduced to give Figs. 1(c) and (d) opposite signs. Because of the form of the interaction [Eq. (2.15)], which is diagonal in the lattice-site index, all lines in a given loop still carry the same lattice-site index, but different loops with the same lattice-site index are allowed within one diagram. In this new diagrammatic expansion, disconnected diagrams simply contribute factors and the linked-cluster theorem is valid.

The new rules [(i)–(iii)] are exactly the rules for fermions in the usual Goldstone expansion[26]; they are, however, unchanged if we deal with bosons. As pointed out earlier, the only difference is the change in the sign of the exchange matrix element [Eq. (3.2)].

This result is not too surprising for a system of Fermions disregarding spin degeneracy. In this special case, the ground state of the usual unperturbed Hamiltonian [Eq. (2.8)] already is nondegenerate and has only singly occupied lattice sites. Since the interaction does not change the occupation numbers at each lattice site, the intermediate states also have singly occupied lattice sites and in this special case the correlations introduced by changing to the c and $c^\dagger$ operators are already present owing to the Pauli principle. As we will see in Sec. V, this is no longer true at finite temperatures.

Having rules (i)–(iii) the change to Feynman diagrams (without time axis) and the propagator renormalization follow standard procedures[28] and need not be discussed here.

V. SPINLESS PARTICLES AT FINITE TEMPERATURES

We could try to generalize the results of Sec. IV to finite temperatures replacing the Kronecker symbols by statistical weight functions:

$$\begin{aligned} 1-\delta(n0) &\to 1-f(\epsilon(n)) \;, \\ -\delta(n0) &\to -f(\epsilon(n)) \;, \end{aligned} \tag{5.1}$$

where we choose

$$f(\epsilon(n)) = \exp[-\beta\epsilon(n)] \big/ \textstyle\sum_m \exp[-\beta\epsilon(m)] \;. \tag{5.2}$$

This choice contains the previous results as the $T\to 0$ limit. The cancellation of diagrams, e.g., Figs. 1(a) and 1(b) or Figs. 1(c) and 1(d), however, is no longer exact at finite temperatures. In the Appendix, we derive an expansion of expectation values of the form (3.6) in terms of semi-invariants. We introduce a single-particle function, analogous to the unperturbed single-particle Green's function in ordinary perturbation theory:

$$g_0(12) = -i\delta(i_1i_2)\delta(n_1n_2)\exp[-i\epsilon(n_1)(t_1-t_2)] \times \begin{pmatrix} 1-f(\epsilon(n_1)) \\ -f(\epsilon(n_1)) \end{pmatrix}; \quad \begin{matrix} i(t_1-t_2)>0 \\ i(t_1-t_2)\leqslant 0 \;, \end{matrix} \tag{5.3}$$

where $1\equiv(i_1n_1t_1)$ represents the lattice-site and band index and the purely imaginary time variable. In addition, we introduce

$$M_0(12) = i\delta(i_1i_2)\delta(n_1n_2) \times \exp[-i\epsilon(n_1)(t_1-t_2)]\, f(\epsilon(n_1)) \;, \tag{5.4}$$

and $M_0(12\cdots\nu;1'2'\cdots\nu')$

$$= \delta(i_1i_2)\delta(i_1i_3)\cdots\delta(i_1i_\nu)(-1)^{\nu-1}(\nu-1)! \times \begin{vmatrix} M_0(11') & M_0(12') & \cdots & M_0(1\nu') \\ M_0(21') & M_0(22') & \cdots & M_0(2\nu') \\ \cdots & \cdots & \cdots & \cdots \\ M_0(\nu1') & M_0(\nu2') & \cdots & M_0(\nu\nu') \end{vmatrix} . \tag{5.5}$$

In the Appendix, we show that expectation values of the form of Eq. (3.6) can be written[30]

$$-i\langle c^\dagger(1')c(1)\rangle_0 = -g_0(11') \;, \tag{5.6}$$

$$(-i)^2\langle c^\dagger(1')c(1)c^\dagger(2')c(2)\rangle_0 = g_0(11')g_0(22') - g_0(12')g_0(21') + M_0(12;1'2') \;, \tag{5.7}$$

$$\begin{aligned} &(-i)^3\langle c^\dagger(1')c(1)c^\dagger(2')c(2)c^\dagger(3')c(3)\rangle_0 \\ &= -g_0(11')g_0(22')g_0(33') + g_0(12')g_0(21')g_0(33') + \cdots \\ &\quad - g_0(12')g_0(23')g_0(31') - \cdots \\ &\quad - M_0(12;1'2')g_0(33') - \cdots + M_0(12;1'3') \\ &\quad \times g_0(32') + \cdots - M_0(123;1'2'3') \;. \end{aligned} \tag{5.8}$$

In general, we find for an unperturbed expectation value of $c^\dagger$ and c operators a sum of products, each formed from factors g_0, [Eq. (5.3)] and M_0, [Eq. (5.5)]. We have to sum over all possible ways to form such products, where products distinct only by the order of variables in a particular M_0 should be counted once only. Each product has a sign $(-1)^l$ where l is the number of loops, including those which would be formed if we connect the variables in M_0 in the order of appearance, i.e., in the last term of Eq. (5.8), 1 with $1'$, 2 with $2'$, and 3 with $3'$.

This expansion is valid for c operators at different lattice sites also, since the semi-invariants vanish if two lattice-site indices are not the same.

The time-dependent factors in Eq. (5.4) can easily be written as factors in front of the determinant, leaving a determinant which depends on the band indices only. If two of the band indices involved are the same, the determinant vanishes, since two rows or lines are the same. Thus, the maximal contribution arises if, e.g., $n_1=0$, $n_2=1$ and so on, and Eq. (5.5) will be proportional to

$$\exp[-\beta(\epsilon(0)+\epsilon(1)+\cdots\epsilon(\nu))]/\{\textstyle\sum_m \exp[-\beta\epsilon(m)]\}^{\nu} .$$

The expansion, therefore, is a low-temperature expansion, where the characteristic temperature is given by the energy difference between the lowest and the next band. In particular, at zero temperature all the M_0's vanish and we recover the result of Sec. IV.

A rather unpleasant feature is the fact that the statistical weight factor $f(\epsilon)$[Eq. (5.2)] is different from the usual Fermi function. As a consequence g_0 does not obey the usual quasiperiodicity condition[28]

$$g_0(t-i\beta)\neq -g_0(t) . \tag{5.9}$$

The lack of this symmetry makes the evaluation of diagrams sometimes more tedious. In actual calculations of quantum crystals, it is always possible to replace the function $f(\epsilon)$ [Eq. (5.2)] by a Fermi distribution function, since the temperature region of interest is always much lower than the gap between the lowest and the next-lowest band. The latter turns out to be of the order of the Debye temperature and the melting temperature is typically of the order of $\frac{1}{10}\Theta_D$. One has to have in mind the fact that low-temperature behavior is dominated by collective excitations, not by the single-particle properties.

For the same reasons, we can neglect in Eqs. (5.7), (5.8), and corresponding expressions, all terms containing M_0. With these two approximations, we recover an expansion identical to the usual perturbation expansion for Fermions. The statistics of the actual lattice particles again show up only in the sign of the "exchange term" in $\tilde{V}$ [Eq. (3.2)].

VI. FERMIONS WITH SPIN $\frac{1}{2}$

The method discussed in Sec. V cannot be used for Fermions with spin $\frac{1}{2}$. If we would simply allow for the spin degeneracy, e.g., enlarging the number of indices by a spin variable, M_0 [Eq. (5.5)] would no longer vanish at zero temperature or be small at low temperatures. The determinant in $M_0(12;1'2')$ would not always vanish at zero temperature since the band indices could be the same ($n=0$) if the spin indices are different. We would, therefore, have to retain all the M_0 of order 2, even at $T=0$.

The eigenfunctions to H_0 [Eq. (2.14)] have the property that they have at each lattice site just one particle. Since H_0 is also spin independent, or at least diagonal in the spin if an ordered state should be treated, the single-particle functions are products of a spatial part and a spin function. The Hilbert-space $\mathfrak{H}_N$ spanned by the states having each lattice site singly occupied is the product of a space spanned by spatial function, $\mathfrak{H}_R$ and a space spanned by spin functions $\mathfrak{H}_S$. If the unperturbed Hamiltonian and the interaction are spin independent H_0 and the contributions of H' due to U and the direct term act in $\mathfrak{H}_R$ only. The "exchange term" in (2.15) has for spin-independent interactions the form

$$V(in_1s_1, jn_2s_2, jn_4s_4, in_3s_3) = \delta(s_1s_4)\delta(s_2s_3)V(in_1, jn_2, jn_4, in_3) . \tag{6.1}$$

Its matrix elements with respect to the spin states have the same form as those of the usual Heisenberg Hamiltonian.

We would now like to characterize the states with each lattice site singly occupied in the following way.

We say each lattice site carries a spin $\frac{1}{2}$ and a "particle," meaning actually the spatial part of its total wave function. We introduce spin operators at each lattice site, represented by Pauli spin matrices, acting in the space spanned by two spin basis functions at each lattice site. We redefine the c and $c^\dagger$ operators [Eq. (2.11)] such that they act in the spatial part $\mathfrak{H}_R$ only, extending the Hilbert space by states having a spin, but no "particle," in the sense above, at a given lattice site. These states are unphysical, but we have to have in mind that they are introduced only as a trick and that the operators c and $c^\dagger$ always occur in pairs at the same time. Therefore, the energy of these states never occurs and the expansion actually is independent of these states as it should be.

Introducing spin operators and using the redefined c and $c^\dagger$ operators, the contribution of H' due to the exchange term can be written in a form similar to a Heisenberg Hamiltonian:

$$H' = \sum_{i>j}\sum_{mm'nn'} c^\dagger(im)c^\dagger(jn)V(imjnim'jn')c(jn')c(im') - \sum_{i>j}\sum_{mm'nn'} c^\dagger(im)c^\dagger(jn)V(imjnjn'im')$$
$$\times c(jn')c(im')[\tfrac{1}{2}+2\vec{s}(i)\cdot\vec{s}(j)] - \sum_i\sum_{mn} c^\dagger(im)U(imin)c(in) = \sum_{i>j}\sum_{mm'nn'} c^\dagger(im)c^\dagger(jn) \tag{6.2}$$

$$\times \tilde{V}(ij;mnm'n')c(jn')c(im') - \sum_i \sum_{mn} c^\dagger(im)U(imin)c(in) - 2\sum_{i>j} \vec{s}(i)\cdot\vec{s}(j)$$

$$\times \sum_{mm'nn'} c^\dagger(im)c^\dagger(jn)V(imjnjn'im')c(jn')c(im') \; ,$$

where now $\tilde{V}(ij;mnm'n') = V(imjnim'jn') - \frac{1}{2}V(imjnjn'im')$. (6.3)

In an expansion of the partition function, we can again add mutually cancelling diagrams and under the conditions discussed in the previous paragraph, i.e., at low temperatures, the c and $c^\dagger$ operators can be treated as field operators corresponding to spinless fermions. These "particles" interact via the last term in (6.2) with the "spins." This interaction has in spin space the usual form of a Heisenberg Hamiltonian. The exchange integral, however, is replaced by an operator in the "particle" space.[31]

In this form, the problem can be attacked by combining the standard perturbation-theoretical methods developed for fermions and for the Heisenberg model.

VII. SUMMARY

We have investigated the question as to what form of perturbation theory is applicable for quantum crystals. The usual choice of an unperturbed Hamiltonian as a single-particle operator cannot be used since it does not produce correlations essential in a theory of quantum crystals. These correlations prevent a lattice site from being occupied by more than one particle. An unperturbed Hamiltonian is proposed which provides these correlations but is no longer a single-particle operator.

Under the assumption that intermediate states having multiply occupied lattice sites can be disregarded completely, which is the basic approximation in this paper, we give a diagrammatic expansion starting from the proposed H_0. It is shown that this expansion is, at low temperatures, formally identical to the usual perturbation expansion for spinless Fermions.

This result is independent of the statistics of the actual lattice particles, except for the sign in the exchange term of the matrix elements of the interaction. In the case where the lattice particles are fermions with spin $\frac{1}{2}$ we find, within the framework of our basic approximation, an expansion formally identical to the usual expansion for spinless Fermions interacting among themselves and with a spin $\frac{1}{2}$ attached to each lattice site. This latter interaction has in spin space the form of the usual Heisenberg Hamiltonian. The exchange integral, however, is replaced by an operator in the space of the spinless fermions.

The validity of the basic approximation might be questionable to some degree if exchange is concerned. This problem has not been investigated and will be subject to further work.

The procedure described in this paper is not without ambiguity. To define occupation numbers at lattice sites we have introduced a complete set of Wannier states. Thus, the states omitted in our basic approximation depend on the particular choice of this basis. However, as long as the overlap between Wannier functions at different lattice sites is small, we expect negligible dependence on the further details of the basis chosen. In actual calculations, a self-consistency criterion will be used which reduces in a Hartree calculation to the choice of the Hartree states as basis.

In conclusion, we like to point out that we were able to bring the perturbation expansion, at least at low temperatures, into a form identical to the standard problem of spinless fermions and of a Heisenberg model. These problems have been widely studied and the methods developed there can be transferred to the case of quantum crystals. As a first step, the following paper[32] gives a discussion of the ladder approximation, which has to be used because the interaction in actual quantum crystals is singular.

VIII. ACKNOWLEDGMENT

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APPENDIX

We derive the expansion of expectation values of the form (3.6) in terms of semi-invariants [Eqs. (5.6)–(5.8)]. We introduce

$$F(12) = M_0(12) - i\lambda(1)\Theta(\,it_1 - it_2 - \eta) \times \delta(n_1 n_2)\exp[-i\epsilon(n_1)(t_1 - t_2)] \; , \quad \text{(A1)}$$

where M_0 is given by Eq. (5.4) and $\eta \to 0^+$. We have to have in mind that all the lattice-site indices in Eq. (3.6) are the same. Using Eq. (A1),

$$[1 + \Delta(1)]F(12) = g_0(12) \; , \quad \text{(A2)}$$

where g_0 is given by Eq. (5.3) and we have used the abbreviation

$$\Delta(1)F(12) = \frac{\delta}{\delta\lambda(1)} \, F(12) \Bigg\|_{\lambda \equiv 0} \; . \quad \textbf{(A3)}$$

We introduce

$$\mathfrak{F}(1\cdots n;\, 1'\cdots n') = (-1)^n \begin{vmatrix} F(11') & F(12')\cdots F(1n') \\ F(21') & F(22')\cdots F(2n') \\ \cdots & \cdots\cdots\cdots \\ F(n1') & F(n2')\ldots F(nn') \end{vmatrix} . \tag{A4}$$

Using these definitions, we can express Eq. (3.6):

$$(-i)^n \langle c^\dagger(1)c(1')c^\dagger(2)c(2')\cdots c^\dagger(n)c(n')\rangle_0$$

$$= \prod_{\nu=2}^{n} \Delta(\nu)\,\mathfrak{F}(1\cdots n;\, 1'\cdots n') \ . \tag{A5}$$

We must keep in mind that in Eq. (A5), $t_1 = t_1'$, $t_2 = t_2'$, and so on, and further $it_1 > it_2 \cdots > it_n$. Since

$$\Delta(1)F(12) = 0 \ , \quad \text{if } i(t_1 - t_2) < 0; \tag{A6}$$

$$\text{also} \quad \Delta(1)\mathfrak{F}(1\cdots n;\, 1'\cdots n') = 0 \ . \tag{A7}$$

We now write Eq. (A5) as

$$\prod_{\nu=1}^{n} [1 + \Delta(\nu)]\mathfrak{F}(1\cdots n,\, 1'\cdots n')$$

$$-\Bigg(\sum_{\nu_1 > \nu_2} \prod_{\nu_3 \neq \nu_1,\, \nu_2} \Delta(\nu_3) + \sum_{\nu_1 > \nu_2 > \nu_3}$$

$$\times \prod_{\nu_4 \neq \nu_1,\, \nu_2,\, \nu_3} \Delta(\nu_4) + \cdots + \sum_{\nu_1 > \nu_2} \Delta(\nu_1)\Delta(\nu_2)$$

$$+ \sum_{\nu} \Delta(\nu) + 1\Bigg)\, \mathfrak{F}(1\cdots n;\, 1'\cdots n') \ , \tag{A8}$$

where we have used the fact that as a consequence of Eq. (A7)

$$\prod_{\nu=1}^{n} \Delta(\nu)\mathfrak{F}(1\cdots n;\, 1'\cdots n')$$

$$= \prod_{\nu \neq \mu} \Delta(\nu)\mathfrak{F}(1\cdots n;\, 1'\cdots n') = 0 \ , \tag{A9}$$

if $\mu \neq 1$. The remaining terms arising from changing (A5)–(A8) are explicitly subtracted again.

$\mathfrak{F}(1\cdots n;\, 1'\cdots n')$ is just the antisymmetrized product of functions F [Eq. (A1)]. Since any permutation operator permuting indices in $\mathfrak{F}$ commutes with $\prod_\nu [1 + \Delta(\nu)]$, the first term in (A8) is just

$$\prod_\nu [1 + \Delta(\nu)]\mathfrak{F}(1\cdots n;\, 1'\cdots n')$$

$$= (-1)^n \begin{vmatrix} g_0(11') & g_0(12')\cdots g_0(1n') \\ g_0(21') & g_0(22')\cdots g_0(2n') \\ \cdots & \cdots\ \cdots\cdots \\ g_0(n1'), & g_0(n2')\ldots g_0(nn') \end{vmatrix}$$

$$= (-1)^n \textstyle\sum_P \delta_P P[g_0(11')g_0(22')\cdots g_0(nn')] \ , \tag{A10}$$

where P is a permutation operator acting on the indices $1\cdots n$. δ_P is 1 for an even permutation and -1 for an odd permutation. The sum runs over all permutations, i.e., over all elements of the symmetric group of order n.[33] Each element can be characterized by giving its cyclic structure, e.g., (123)(45)(67)(8), meaning that we have a cyclic permutation of the indices 1, 2, 3; that 4 and 5, and 6 and 7, are interchanged; and that 8 is not permuted. Usually cycles of length l, e.g., (8), are not explicitly written. A cyclic permutation acting on a product as the one in Eq. (A10) produces, in terms of diagrams, a "closed loop," e.g.,

$$(123)[g_0(11')g_0(22')\cdots g_0(nn')]$$

$$= g_0(12')g_0(23')g_0(31')g_0(44')\cdots g_0(nn') \ . \tag{A11}$$

It is easily seen that the factor δ_P together with $(-1)^n$ produces for a given permutation a factor $(-1)^l$, where l is the number of cycles, including cycles of length 1, or in terms of diagrams l is equal to the number of loops in the diagram generated by this permutation. Since we have to sum over all permutations, Eq. (A10) is just equal to the contribution of all diagrams which would be obtained if the c and $c^\dagger$ operators were field operators for fermions {except for a different definition of $f(\epsilon)$ [Eq. (5.2)]}.

We now have to investigate the remaining terms in Eq. (A8). We consider for simplicity

$$\Delta(m+1)\Delta(m+2)\cdots\Delta(n)\mathfrak{F}(1\cdots n;\, 1'\cdots n') \ , \tag{A12}$$

where $n \geq m \geq 2$. A generalization to an arbitrary term in Eq. (A8) is trivial. We introduce antisymmetrizers

$$A(1\cdots\nu) = \frac{1}{\nu!} \sum_{P \in S_\nu} \delta_P P \ , \tag{A13}$$

where S_ν contains all permutations of the indices $1\cdots\nu$. Since $\mathfrak{F}$ is already antisymmetric,

$$A(1\cdots\nu)\mathfrak{F}(1\cdots n;\, 1'\cdots n') = \mathfrak{F}(1\cdots n;\, 1'\cdots n') \ . \tag{A14}$$

We associate to each element of S_m an operator consisting of products of antisymmetrizers such that the indices in one cycle are just the indices in one antisymmetrizer. We also insert a factor δ_P. Thus, with $P = (123)(45)(6)\cdots(m)$, the operator

$$O_P(1\cdots m) = (-1)^2 A(123)(-1)A(45) \tag{A15}$$

is associated.

Because of Eq. (A14), and since the number of even permutations is equal to the number of odd permutations,

$$\sum_{P\in S_m} O_P(1\cdots m)\mathfrak{F}(1\cdots n;1'\cdots n')=0\ , \qquad \text{(A16)}$$

or

$$\sum_{P\in S_m;\ P\neq 1} O_P(1\cdots m)\mathfrak{F}(1\cdots n;1'\cdots n')$$
$$=-\mathfrak{F}(1\cdots n;1'\cdots n')\ . \qquad \text{(A17)}$$

Operators associated with permutations which are distinct only by the order in which the same variables occur in a given cycle are the same. For example, the operator associated with $P=(132)(45)$ is equal to Eq. (A15). For a permutation having cycles of length $n_1, n_2, \ldots$, there are just $(n_1-1)!(n_2-1)!\cdots$ identical operators since there are $(n-1)!$ different cyclic permutations in S_n.

We now have to investigate the diagrams created by acting with a given operator $O_Q(1\cdots m)$ on $\mathfrak{F}$. We write $\mathfrak{F}$ explicitly as

$$\mathfrak{F}(1\cdots n;\ 1'\cdots n')=(-1)^n\sum_{P\in S_n}\delta_P P$$
$$\times[F(11')F(22')\cdots F(nn')]\ . \qquad \text{(A18)}$$

We investigate one single term on the right-hand side, corresponding to a certain arrangement of closed loops, in terms of diagrams. Acting with $O_Q(1\cdots m)$ on this term produces, except for a numerical factor, functions similar to $M_0(1\cdots\nu;1'\cdots\nu')$ [Eq. (5.5)], each one corresponding to a cycle in Q. The difference with M_0 is that they are constructed from functions $F(12)$ instead of $M_0(12)$ [Eq. (5.4)] but for $\lambda\equiv 0$ they are equal.

Again we get for a given O_Q identical contributions from different P in Eq. (A18) if these are distinct only by permutations of numbers occurring in the same cycle of Q. There are just $n_1!n_2!\cdots$ such terms if Q has cycles of length $n_1 n_2\cdots$. Summation over all such terms and over all identical operators O_Q thus gives $n_1!(n_1-1)!n_2!\times(n_2-1)!\cdots$ terms. The factors $n_1!n_2!\cdots$ are cancelled by the factors $1/\nu!$ in Eq. (A13), whereas the factors $(n_1-1)!(n_2-1)!\cdots$ occur explicitly in $M_0(1\cdots n_1;1'\cdots n_1')$ [Eq. (5.5)].

We use Eq. (A17) in (A8) such that in each term the variables in O_Q are just those not occurring in the products of $\Delta(n)$ operators [Eq. (A3)]. After the execution of the Δ operators and setting $\lambda\equiv 0$ we get a sum of products, each containing at least one $M_0(1\cdots;1'\cdots)$ [Eq. (5.5)]. We now collect all terms having the same factors $M_0(\cdots;\cdots)$, e.g., $M_0(123;1'4'5')M_0(45;2'6')$, and find that they give, e.g.,

$$(-1)^n M_0(123;1'4'5')M_0(45;2'6')\prod_{\nu=6}^{n}[1+\Delta(\nu)]$$
$$\times{\sum_P}'\,\delta_P PF(63')F(77')\cdots$$
$$=(-1)^n M_0(123;1'4'5')M_0(45;2'6')$$
$$\times{\sum_P}'\,\delta_P Pg(63')g(77')\cdots\ , \qquad \text{(A19)}$$

where ${\sum}'_P$ runs over all permutations of the numbers not contained in the M_0 factors.

Since we have to sum over all different configurations of function $M_0(\cdots;\cdots)$ and each configuration occurs once, we obtain just the expansion given in Sec. V. The first terms of this expansion are given in Eqs. (5.6)–(5.8).

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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-