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MANY-BODY THEORY

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FOREWORD

This report consists of the notes from a series of fifteen lectures on many-body theory given by Professor J. Robert Schrieffer at the Argonne National Laboratory in the Spring of 1961. The material contained herein is primarily addressed to solid state physicists who wish background in field theoretic techniques as applied to many-body problems. The concise style of the lectures has not been changed, nor has any effort been made to cover the subject completely. Save for minor additions of details and the inclusion of a few relevant references at the ends of sections the material is here given as presented in the lectures.

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MANY-BODY THEORY

by

J. R. Schrieffer

I. INTRODUCTION

Some of the many-body systems in which recent theoretical progress has been made are:

1. high and low-density electron gases;
2. superconductors;
3. imperfect Bose gas and its relation to superfluidity (He^4);
4. high-density Fermi gas with strong, short-range forces (He^3), infinite nuclear matter, finite nuclei.

Much of this progress was made through the use of the technique of quantum field theory, rather than conventional space representation. This is not essential, but it is useful in view of the fact that one can take over many results of quantum field theory into the many-body problem. In these lectures we shall first outline a field theoretical formalism appropriate to many-body problems and then discuss its application to the high-density electron gas and to superconductivity.

II. FORMALISM OF QUANTUM FIELD THEORY

A. Occupation Number Representation

Let us consider a system of n identical particles described in the Schrödinger representation by the Hamiltonian:

$$H(x_1 \dots x_n) = \sum_i \frac{p_i^2}{2m} + \sum_i V_1(x_i) + \frac{1}{2} \sum_{i \neq j} V_2(x_i, x_j) \quad . \quad (2.1)$$

The coordinate x_i labels the position and spin of particle i . Three-body potentials and higher interactions can be included in a straightforward manner, but for the moment we shall confine ourselves to two-body interactions.

The many-body Schrödinger equation is

$$H(x_1 \dots x_n) \Psi(x_1 \dots x_n, t) = i\hbar \frac{\partial \Psi(x_1 \dots x_n, t)}{\partial t} \quad . \quad (2.2)$$

We introduce a complete set of n -particle wave functions Φ . These are constructed as a properly symmetrized product of one-particle wave functions $u_k(x)$, which form a complete orthonormal set:

$$\int u_{k'}^*(x) u_k(x) dx = \delta_{kk'} \quad (\text{orthonormality}) \quad (2.3)$$

$$\sum_k u_k^*(x') u_k(x) = \delta(x-x') \quad (\text{completeness}) \quad . \quad (2.4)$$

The function Φ is then given by

$$\Phi = \mathcal{S} u_{k_1}(x_1) u_{k_2}(x_2) \dots u_{k_n}(x_n) \quad (2.5)$$

where $\mathcal{S} = (1/n!) \sum P$ in Bose statistics and $\mathcal{S} = (1/n!) \sum (-1)^P P$ in Fermi statistics and the summation is over all $n!$ possible permutations of the coordinates $x_1 \dots x_n$ and p is the order of the permutation. Rather than labeling Φ by the quantum numbers $k_1, k_2 \dots k_n$, we may specify the state by stating how many times each single particle state enters the product. Let this occupation number be n_k for state k . Then the set of numbers $n_1, n_2 \dots n_k$ uniquely specifies the symmetrized state $\Phi_{n_1, n_2 \dots n_k \dots}$. If we describe a system of n particles, we have clearly $\sum_k n_k = n$. For Fermi statistics the occupation numbers n_k are restricted to the values 0 and 1, whereas for Bose statistics they can have all possible positive integer values as well as 0. The functions $\Phi_{n_1 \dots n_k \dots}(x_1 \dots x_n)$ form a complete orthonormal set of n -particle functions for fermions when they are multiplied by the

factor $\sqrt{n!}$, whereas a multiplication factor $\sqrt{\frac{n!}{n_1!n_2!}}$ must be included to obtain a complete orthonormal set of Bose functions (Note: $0!$ is defined as unity). The orthonormality condition is

$$\int \Phi_{n_1, n_2, \dots}^* (x_1 \dots x_n) \Phi_{n_1, n_2, \dots} (x_1 \dots x_n) dx_1 \dots dx_n = \delta_{n_1, n_1} \delta_{n_2, n_2} \dots \quad (2.6)$$

In general, the total Schrödinger wave function may be expanded in the complete set of the $\Phi_{n_1 \dots n_k \dots}$:

$$\Psi(x_1 \dots x_n, t) = \sum A(n_1 \dots n_k \dots, t) \Phi_{n_1 \dots n_k \dots} (x_1 \dots x_n) \quad (2.7)$$

The coefficients $A(n_1 \dots n_k \dots, t)$ are now to be interpreted as the wave functions in the occupation number representation. Their norm gives the probability of finding n_k particles in state k .

B. Second Quantization for Bosons

For Bose statistics we introduce a set of operators a_k and $a_k^\dagger$ defined by

$$\begin{aligned} a_k^\dagger \Phi_{n_1 \dots n_k \dots} (x_1 \dots x_n) &= \sqrt{n_k + 1} \Phi_{n_1 \dots n_k + 1 \dots} (x_1 \dots x_{n+1}) \\ a_k \Phi_{n_1 \dots n_k \dots} (x_1 \dots x_n) &= \sqrt{n_k} \Phi_{n_1 \dots n_k - 1 \dots} (x_1 \dots x_{n-1}) \end{aligned} \quad (2.8)$$

The operator $a_k^\dagger$ (creation operator) creates an additional particle in state k , and a_k (annihilation operator) destroys a particle in state k . If $n_k = 0$ in Φ , the operator a_k gives 0.

We can see that $a_k^\dagger$ is the Hermitian conjugate of a_k by noting that the only nonvanishing matrix element of a_k is $(a_k)_{n_1 \dots n_k - 1 \dots}^{n_1 \dots n_k}$, which is equal to $\sqrt{n_k}$, and its Hermitian conjugate operator will have as its only nonvanishing matrix element $\left[(a_k)_{n_1 \dots n_k - 1 \dots}^{n_1 \dots n_k} \right]^* = (\sqrt{n_k})$; the operator which has only this nonvanishing matrix element is indeed $a_k^\dagger$ by definition. If we define a new operator $N_k = a_k^\dagger a_k$, it follows from definition (8) that its eigenvalue equation is

$$N_k \Phi_{n_1 \dots n_k \dots} (x_1 \dots x_n) = n_k \Phi_{n_1 \dots n_k \dots} (x_1 \dots x_n) \quad (2.9)$$

Therefore, N_k may be interpreted as the operator which measures the number of particles in state k (the number operator). We may now construct the operator N which measures the total number of particles in the system:

$$N = \sum_k N_k = \sum_k a_k^\dagger a_k \quad (2.10)$$

The commutation relations between the creation and destruction operators are easily established to be:

$$[a_k, a_{k'}^\dagger] = \delta_{kk'} \quad ; \quad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0 \quad . \quad (2.11)$$

For instance:

$$(a_k a_k^\dagger - a_k^\dagger a_k) \Phi_{n_1 \dots n_k \dots} = [(n_k + 1) - n_k] \Phi_{n_1 \dots n_k \dots} = 1 \Phi_{n_1 \dots n_k \dots} \quad .$$

The Hamiltonian can be expressed in the occupation number representation, and it can be seen that it becomes

$$H = \sum_{kk'} \langle k' | H_1 | k \rangle a_{k'}^\dagger a_k + \frac{1}{2} \sum_{k_1 k_2 k_1' k_2'} \langle k_1' k_2' | V_2 | k_1 k_2 \rangle a_{k_1'}^\dagger a_{k_2'}^\dagger a_{k_1} a_{k_2} \quad , \quad (2.12)$$

where

$$\langle k' | H_1 | k \rangle = \int u_{k'}^*(x) \left\{ \frac{p^2}{2m} + V_1(x) \right\} u_k(x) dx$$

and

$$\langle k_1 k_2 | V_2 | k_1' k_2' \rangle = \int u_{k_1'}^*(x_1) u_{k_2'}^*(x_2) V_2(x_1, x_2) u_{k_1}(x_1) u_{k_2}(x_2) dx_1 dx_2 \quad .$$

This can be proved by noticing that all matrix elements of Hamiltonian (12) with the complete set $\Phi_{n_1 \dots}$ are equal to the matrix elements as evaluated from the original Hamiltonian (1) in configuration space. We will not give the complete proof but will outline the way in which it can be obtained.

First, we evaluate all matrix elements of the Hamiltonian (12). The basic rule is to use the orthonormality of the set Φ and the definition (8) for creation and destruction operators. The wave function obtained by operating with (12) on the wave function to the right of the matrix element must be equal to the wave function on the left of the matrix element.

a) Diagonal elements

Only terms with $k = k'$ and $k_1 = k_1'$, $k_2 = k_2'$ or $k_1 = k_2'$, $k_2 = k_1'$ or $k_1 = k_2 = k_1' = k_2'$ give non-zero contribution because only these terms leave the wave function to the right unchanged. We have, then,

$$\begin{aligned} \langle \Phi_{n, n_2 \dots} | H | \Phi_{n, n_2 \dots} \rangle &= \sum_k \langle k | H_1 | k \rangle n_k \\ &+ \sum_{k_1 \neq k_2} n_{k_2} n_{k_1} \left\{ \langle k_1 k_2 | V_2 | k_1 k_2 \rangle + \langle k_2 k_1 | V_2 | k_1 k_2 \rangle \right\} \\ &+ \frac{1}{2} \sum_{k_1} n_{k_1} (n_{k_1} - 1) \langle k_1 k_1 | V_2 | k_1 k_1 \rangle \quad . \quad (2.13) \end{aligned}$$

b) Off-diagonal elements between wave functions which differ in the occupation numbers of two states i and j . Let the wave functions be:

$$\Phi \dots n_i n_j \dots \text{ and } \Phi \dots m_i m_j \dots$$

with

$$n_i + n_j = m_i + m_j$$

because the number of particles is fixed. The only matrix elements different from zero are those for which

$$\begin{aligned} \text{either } 1) \quad n_j &= m_j \mp 1 \quad n_i = m_i \pm 1 \\ \text{or } 2) \quad n_j &= m_j \mp 2 \quad n_i = m_i \pm 2 \end{aligned}$$

On choosing the upper signs, the matrix elements for the first case are

$$\begin{aligned} \langle k_i | H_1 | k_j \rangle \sqrt{(m_i+1)m_j} + \sum_{\ell} m_{\ell} \sqrt{(m_i+1)m_j} \\ (\langle k_{\ell} k_i | V | k_{\ell} k_j \rangle + \langle k_{\ell} k_i | V | k_j k_{\ell} \rangle) \end{aligned} \quad (2.14)$$

And for the second case

$$\frac{1}{2} \sqrt{m_i(m_i-1)(m_j+1)(m_j+2)} \langle k_j k_j | V_2 | k_i k_i \rangle$$

On choosing the lower signs, we have the same expressions with i and j interchanged

c) Off-diagonal elements between wave functions which differ in the occupation numbers of only 3 states: i , j , and ℓ . Those different from zero obey conditions of the type

$$n_i = m_i \pm 1 \quad ; \quad n_j = m_j \pm 1 \quad ; \quad n_{\ell} = m_{\ell} \mp 2$$

The matrix element with the upper choice of signs is

$$\frac{1}{2} \sqrt{(m_{\ell}+2)(m_{\ell}+1)m_j m_i} \left\{ \langle k_{\ell} k_{\ell} | V_2 | k_j k_i \rangle + \langle k_{\ell} k_{\ell} | V_2 | k_i k_j \rangle \right\} ;$$

with the lower choice of signs, we have

$$\frac{1}{2} \sqrt{(m_j+1)(m_i+1)(m_{\ell}-1)m_{\ell}} \left\{ \langle k_i k_j | V_2 | k_{\ell} k_{\ell} \rangle + \langle k_j k_i | V_2 | k_{\ell} k_{\ell} \rangle \right\} \quad (2.15)$$

d) Off-diagonal elements which differ in the occupational numbers of 4 states: k_i, k_j, k_ℓ , and k_s ; those different from zero obey the condition

$$n_i = m_i \mp 1 \quad ; \quad n_j = m_j \mp 1 \quad , \quad n_\ell = m_\ell \pm 1 \quad ; \quad n_s = m_s \pm 1 \quad .$$

The matrix element is

$$\sqrt{m_i m_j (m_\ell + 1) (m_s + 1)} \left\{ \langle k_\ell k_s | V_2 | k_i k_j \rangle + \langle k_\ell k_s | V_2 | k_j k_i \rangle \right\} \quad (2.16)$$

with the upper choice of signs. A matrix element of the same type, but with ℓ, s and i, j interchanged is obtained with the lower choice of signs.

The same matrix elements as in a), b), c), and d) are obtained from Hamiltonian (1). Let us consider as an example the last case; the same procedure will apply to the other cases. We want to evaluate

$$\left\langle \Phi \dots m_i - 1, m_j - 1, m_\ell + 1, m_s + 1 \left| \frac{1}{2} \sum_{pq} V_2(pq) \right| \Phi \dots m_i, m_j, m_\ell, m_s \right\rangle .$$

First of all, we can simplify the normalization constants by integrating over all variables other than p and q whatever p and q may be. We have

$$\begin{aligned} & \left[(m_i - 1)! (m_j - 1)! (m_\ell + 1)! (m_s + 1)! m_i! m_j! m_\ell! m_s! \right]^{-1/2} \\ & \left\langle u_i(1) \dots u_i(m_i - 1) u_\ell(m_i) \dots u_\ell(m_i + m_\ell) u_j(m_i + m_\ell + 1) \dots \right. \\ & \quad \dots u_j(m_i + m_j + m_\ell - 1) u_s(m_i + m_j + m_\ell) \dots u_s(m_i + m_j + m_\ell + m_s) \\ & \quad \left| \frac{1}{2} \sum_{pq} V_2(p, q) \right| P u_i(1) \dots u_i(m_i) u_\ell(m_i + 1) \dots u_\ell(m_i + m_\ell) \\ & \quad u_j(m_i + m_\ell + 1) \dots u_j(m_i + m_j + m_\ell) u_s(m_i + m_j + m_\ell + 1) \dots u_s(m_i + m_j + m_\ell + m_s) \rangle , \end{aligned}$$

where P indicates all possible permutations of particles. When $p = m_i$ and $q = m_i + m_j + m_\ell$, or vice versa, we obtain from the integral the quantity

$$\left\{ \langle k_\ell k_s | V_2 | k_i k_j \rangle + \langle k_\ell k_s | V_2 | k_j k_i \rangle \right\}$$

multiplied by a factor $m_i! m_j! m_\ell! m_s!$, because of the permutations which interchange particles on the same state on the wave function to the right. Because of the summation over p and q in the operator, we must consider the sum of all terms with

$$m_i \leq p \leq (m_i + m_\ell)$$

and

$$(m_i + m_j + m_\ell) \leq q \leq (m_i + m_j + m_\ell + m_s) \quad ;$$

this introduces another multiplicative factor $(m_{\ell}+1)(m_s+1)$. By multiplication of all factors with the normalization constants, we obtain

$$\sqrt{m_i m_j (m_{\ell}+1)(m_s+1)} \left\{ \langle k_{\ell} k_s | V_2 | k_i k_j \rangle + \langle k_{\ell} k_s | V_2 | k_j k_i \rangle \right\} ,$$

which is the same as equation (16).

Let us define some new operators which do not depend on state k but depend on the variable x as

$$\psi(x) = \sum_k u_k(x) a_k \text{ and } \psi^\dagger(x) = \sum_k u_k(x)^* a_k^\dagger . \quad (2.17)$$

They are called "wave field" operators and satisfy the commutation relations:

$$\begin{aligned} [\psi(x), \psi(x')^\dagger] &= \sum_{kk'} u_k(x) u_{k'}^*(x') [a_k, a_{k'}^\dagger] = \delta(x-x') \\ [\psi(x), \psi(x')] &= [\psi(x), \psi(x')]^\dagger = 0 . \end{aligned} \quad (2.18)$$

To clarify the usefulness of the wave field operators, we may notice that $\rho(x) = \psi^\dagger(x) \psi(x)$ represents the density of particles in the x space and the number operator is

$$N = \int \rho(x) dx = \sum_{kk'} a_{k'}^\dagger a_k \int u_{k'}^\dagger(x) u_k(x) dx = \sum_k a_k^\dagger a_k . \quad (2.19)$$

In many instances it is useful to have the Fourier transform of ρ , given by

$$\rho_q = \int e^{-iqx} \rho(x) dx = \sum_{kk'} a_{k'}^\dagger a_k \int e^{-iqx} u_{k'}^*(x) u_k(x) dx . \quad (2.20)$$

When the $u_k(x)$ are given simply by plane waves $e^{ik \cdot x}$ and we normalize in a box of unit volume, we have $k' = k - q$ and, consequently,

$$\rho = \sum_k a_{k'}^\dagger a_{k'+q} . \quad (2.21)$$

We may express the Hamiltonian operator in terms of the field variable $\psi(x)$; from formula (12) and the definition of the ψ we obtain

$$H = \int \psi^\dagger(x) H_1(x) \psi(x) dx + \frac{1}{2} \int \psi(x)^\dagger \psi(x')^\dagger V_2(x, x') \psi(x') \psi(x) dx dx' . \quad (2.22)$$

The order of the operators ensures that the term $i = j$ has been omitted in the two-body potential. If $V_2(x, x') = V_2(x - x')$, that is to say, if our two-body

operator is translationally invariant, the Hamiltonian can be written as

$$H = \int \psi^\dagger(\mathbf{x}) H_1(\mathbf{x}) \psi(\mathbf{x}) d\mathbf{x} + \frac{1}{2} \sum_{\mathbf{q}} V_2(\mathbf{q}) \eta(\rho_{\mathbf{q}}^\dagger \rho_{\mathbf{q}}) \quad , \quad (2.23)$$

where η is the normally ordered product such that all the $\psi^\dagger$ are placed to the left and all ψ to the right in the product. The proof is obtained by expanding $V_2(\mathbf{x}-\mathbf{x}')$ as its Fourier transform and using the definition of $\rho_{\mathbf{q}}^\dagger$.

The prescription for expressing an n-body interaction in the occupation number representation is now clear:

$$V_\nu = \frac{1}{\nu!} \int \psi^\dagger(\mathbf{x}_1) \dots \psi(\mathbf{x}_\nu) V_\nu(\mathbf{x}_1 \dots \mathbf{x}_\nu) \psi(\mathbf{x}_\nu) \dots \psi(\mathbf{x}_1) d\mathbf{x}_1 \dots d\mathbf{x}_\nu \quad . \quad (2.24)$$

From this point on we will suppress the variables $\mathbf{x}_1 \dots \mathbf{x}_n$ in Φ and represent Φ by

$$\Phi_{n_1 \dots n_i}(\mathbf{x}_1 \dots \mathbf{x}_n) = |n_1 \dots n_i \dots\rangle \quad . \quad (2.25)$$

In taking matrix elements the integral on space variables is understood. The n-body Schrödinger equation may now be expressed in the a_k language as

$$H\Psi(t) = i\hbar \frac{\partial \Psi(t)}{\partial t} \quad ,$$

where

$$\Psi(t) = \sum_{n_1, n_2 \dots} A(n_1, n_2, \dots, t) |n_1, n_2 \dots\rangle \quad (2.26)$$

and

$$H = H_1 + V_2 + \dots + V_\nu + \dots$$

as given in second quantization formalism.

C. Second Quantization for Fermions

For Fermi statistics we introduce creation and destruction operators $c_k^\dagger$ and c_k , formally given by equation (8), referred to the antisymmetric wave function. These operators satisfy an anticommutation relation:

$$\{c_k^\dagger, c_{k'}\} = \delta_{kk'}$$

and

$$\{c_k, c_{k'}\} = 0 = \{c_k^\dagger, c_{k'}^\dagger\} \quad , \quad (2.27)$$

where

$$\{A, B\} = AB + BA \quad .$$

It can be seen that this choice of commutation relations restricts the occupation number of the states k to 0 or 1 as required by Fermi statistics. In fact, $c_k c_k \Phi_{n_k} = 0 = \sqrt{n_k - 1} \sqrt{n_k} \Phi_{n_k - 2}$. With this restriction in mind, the definition of the operator c_k is

$$\begin{aligned} c_k \Phi_{\dots n_k} &= \Phi_{\dots n_k - 1} \quad \left\{ n_k = 1 \right. \\ &= 0 \quad \left\{ n_k = 0 \right. \\ c_k^\dagger \Phi_{\dots n_k} &= \Phi_{\dots n_k + 1 \dots} \quad \left\{ n_k = 0 \right. \\ &= 0 \quad \left\{ n_k = 1 \right. \quad . \end{aligned} \quad (2.28)$$

The Hamiltonian operator in the second-quantization formalism is given by

$$H = \sum_{k'ks} \langle k's | H_1 | ks \rangle c_{k's}^\dagger c_{ks} + \frac{1}{2} \sum_{ijklss'} \langle ij | V | lk \rangle c_{is}^\dagger c_{js}^\dagger c_{ks} c_{ls} \quad , \quad (2.29)$$

where s and s' label the spin of the particle.

The wave fields are defined as

$$\psi(x) = \sum_k u_k(x) c_k \quad ,$$

and they satisfy the anticommutation equations

$$\begin{aligned} \left\{ \psi(x), \psi(x')^\dagger \right\} &= \delta(x - x') \\ \left\{ \psi(x), \psi(x') \right\} &= 0 = \left\{ \psi^\dagger(x), \psi^\dagger(x') \right\} \quad . \end{aligned}$$

Note that in (2.29) the order of the destruction operators with regard to the matrix element indices is the inverse of that of the creation operators. The ν -body operator of equation (2.24) is

$$\begin{aligned} V_\nu &= \frac{1}{\nu!} \sum_{k'_\nu s'_\nu \dots k'_1 s'_1 k_\nu s_\nu \dots k_1 s_1} \langle k'_\nu \dots k'_1 | V_\nu | k_\nu \dots k_1 \rangle \\ &\quad c_{k'_\nu s'_\nu}^\dagger \dots c_{k'_1 s'_1}^\dagger c_{k_1 s_1} \dots c_{k_\nu s_\nu} \quad . \end{aligned} \quad (2.24')$$

The ordering is not entirely arbitrary because of sign changes arising from anticommutation of fermion operators; that of (2.29), (2.24'), (2.24), and (2.22) gives the correct sign for either fermion or boson operators.

References to Chapters II and III

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III. HEISENBERG AND INTERACTION REPRESENTATIONS

Until now we have been working in the "Schrödinger" picture, in which the wave function Ψ_S has all the time dependence and satisfies the equation

$$H \Psi_S(t) = i\hbar \frac{\partial \Psi_S(t)}{\partial t} . \quad (3.1)$$

An exact solution of equation (3.1) for the time dependence of the wave function Ψ_S is

$$\Psi_S(t) = e^{-i(t-t_0)H/\hbar} \Psi_S(t_0) . \quad (3.2)$$

It is convenient to make a unitary transformation into a new representation, in which the wave function is time independent and the time dependence of the problem is transferred to the operators. This representation is called the Heisenberg representation and is simply obtained by the transformation

$$\Psi_H = e^{i(t-t_0)H/\hbar} \Psi_S(t) . \quad (3.3)$$

In order to leave the observable quantities unaltered by the transformation, we must have for all operators in the new representation

$$\theta_H(t) = e^{iH(t-t_0)/\hbar} \theta_S e^{-iH(t-t_0)/\hbar} . \quad (3.4)$$

The Hamiltonian is unchanged in the new representation and only the operators which commute with the Hamiltonian remain time independent. All operators in the Heisenberg representation have a time dependence which is established by differentiating equation (3.4). It is given by the general operator equation

$$i\hbar \frac{\partial \theta_H}{\partial t} = [\theta_H, H] . \quad (3.5)$$

The field operator in the Heisenberg representation satisfies this last equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = [\psi(x,t), H] . \quad (3.6)$$

Because of the commutation properties of $\psi(x,t)$, this equation becomes, for both bosons and fermions,

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_1(x) + \int \rho(x') V_2(x,x') dx' \right) \psi(x,t) . \quad (3.7)$$

Thus it appears that the wave field $\psi(x,t)$ satisfies an effective Schrödinger equation in which the averaged potential enters in place of V_2 .

For purposes of perturbation expansions it is convenient to introduce a third picture in which the time dependence of the problem is divided between the operators and the wave functions. This is called the "interaction representation" and is defined by

$$|\Psi_I(t)\rangle = e^{itH_0/\hbar} |\Psi_S(t)\rangle \quad (3.8)$$

$$\theta_I(t) = e^{itH_0/\hbar} \theta_S e^{-itH_0/\hbar} \quad (3.9)$$

In this expression the Hamiltonian operator H has been divided into the sum of two terms, H_0 and H' . If H' vanishes, the interaction and the Heisenberg pictures become identical. In the presence of H' the time dependence of the field operators is governed by the zero-order Hamiltonian H_0 . The wave function Ψ_I is time dependent solely as a result of the interaction H' being present.

By inserting expression (3.8) for $|\Psi_S\rangle$ in terms of $|\Psi_I\rangle$ into Schrödinger's equation, we obtain

$$i\hbar \frac{\partial}{\partial t} |\Psi_I(t)\rangle = H'_I(t) |\Psi_I(t)\rangle \quad (3.10)$$

where $H'_I(t)$ is the perturbing Hamiltonian expressed in the interaction representation

$$H'_I(t) = e^{iH_0t/\hbar} H' e^{-iH_0t/\hbar} \quad (3.11)$$

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IV. GREEN'S FUNCTIONS IN THE MANY-BODY PROBLEM

A. Definition of One-particle Green's Function

In the many-body problem we are ultimately interested in predicting such quantities as the ground state energy of the system, thermodynamic properties, and nonequilibrium properties, such as electrical conductivity, absorption of quanta of external fields, etc. Thus we need certain excitation energies of the system, matrix elements of the coupling of the system to external fields, etc. Often conventional Raleigh-Schrödinger perturbation theory does not converge or does not give a convenient formalism for calculational purposes. Another approach is through Green's function methods, well known in quantum field theory. The excitation energies are found by searching for the poles of the Fourier transforms of the Green functions. To illustrate the method, let us consider the case of fermions of spin $\frac{1}{2}$ interacting with a two-body spin-independent potential. We define the one particle Green's function, G , by

$$G(x_1, t_1; x_2, t_2) = i \quad 0 | T[\psi(x_1, t_1) \psi^\dagger(x_2, t_2)] | 0 \rangle \quad , \quad (4.1)$$

where $|0\rangle$ represents the ground state wave function of H in the Heisenberg picture and the field operators are expressed in the Heisenberg picture as well. The symbol T indicates that the operators in the bracket are to be ordered chronologically so that earlier times are to the right. Minus signs arising from the anticommutation of the operators are to be included; however, all anticommutators arising from the ordering of the operators are to be neglected, that is,

$$G(x_1, t_1; x_2, t_2) = \begin{cases} i \quad 0 | \psi(x_1, t_1) \psi^\dagger(x_2, t_2) | 0 \rangle & t_1 < t_2 \\ -i \quad 0 | \psi^\dagger(x_2, t_2) \psi(x_1, t_1) | 0 \rangle & t_1 > t_2 \end{cases} \quad (4.2)$$

(We consider only spin up operators for the moment.)

If the system has translational invariance, we can put $x = x_1 - x_2$ and $\tau = t_1 - t_2$, and the Green function depends only on x and τ :

$$G(x_1, t_1; x_2, t_2) = G(x, \tau) \quad . \quad (4.3)$$

The Fourier transform of G with respect to x and τ is defined by

$$G(p, p_0) = \int e^{-i(px - p_0\tau)} G(x, \tau) d^3x d\tau \quad (4.4)$$

and

$$G(x, \tau) = \int e^{i(px - p_0\tau)} G(p, p_0) \frac{d^4p}{(2\pi)^4} \quad ,$$

where the four-momentum variable p , p_0 has been introduced. We may notice that

$$\sum_{\underline{p}} = \frac{1}{(2\pi)^3} \int d^3 \underline{p} \quad .$$

We shall use p for either the three-momentum or the four-momentum including p_0 , but the context will dispel any confusion.

B. Noninteracting Free Electron Gas

To illustrate the use of the quantity $G(p, p_0)$, let us consider the particular case of free fermions without any interaction. Then,

$$H = H_0 = \sum_{\underline{p}} \epsilon_{\underline{p}}^0 c_{\underline{p}}^{\dagger} c_{\underline{p}} \quad , \quad (4.5)$$

where $\epsilon_{\underline{p}}^0 = \frac{p^2}{2m}$. The Fourier transform of $G_0(x, \tau)$ (the Green's function associated with H_0) with respect to x is

$$G_0(p, \tau) = i \langle 0 | T[c_{\underline{p}}(\tau) c_{\underline{p}}^{\dagger}(0)] | 0 \rangle \quad . \quad (4.6)$$

Using the anticommutation rules of the $c_{\underline{p}}$, we can show that

$$c_{\underline{p}}(\tau) = e^{-i\epsilon_{\underline{p}}^0 \tau} c_{\underline{p}}(0) \quad .$$

We then have for $G_0(p, \tau)$,

$$G_0(p, \tau) = \begin{cases} i \langle 0 | c_{\underline{p}} c_{\underline{p}}^{\dagger} | 0 \rangle e^{-i\epsilon_{\underline{p}}^0 \tau} & \tau > 0 \\ -i \langle 0 | c_{\underline{p}}^{\dagger} c_{\underline{p}} | 0 \rangle e^{-i\epsilon_{\underline{p}}^0 \tau} & \tau < 0 \end{cases} \quad , \quad (4.7)$$

which can be written, since $c_{\underline{p}}^{\dagger} c_{\underline{p}}$ is the number operator for state p , as

$$G_0(p, \tau) = \begin{cases} i e^{-i\epsilon_{\underline{p}}^0 \tau} (1 - n_{\underline{p}}) & \tau > 0 \\ -i e^{-i\epsilon_{\underline{p}}^0 \tau} n_{\underline{p}} & \tau < 0 \end{cases} \quad . \quad (4.8)$$

The occupation number $n_{\underline{p}}$ is equal to 1 for $p < p_F$ and equal to 0 for $p > p_F$, since in the ground state all single-particle states from $p = 0$ to $p = p_F$ are occupied and the rest are empty. We want now to prove that the complete Fourier transform of $G_0(x, \tau)$ is given by

$$G_0(p, p_0) = \frac{(-1)}{p_0 - \epsilon_p^0 + i\eta_p}, \quad (4.9)$$

where η_p is an infinitesimal quantity positive for $p > p_F$ and negative for $p < p_F$. This we establish by showing that (4.8) is given by the inverse time Fourier transform of (4.9), that is, by

$$\int_{-\infty}^{\infty} \frac{dp_0}{2\pi} e^{-ip_0\tau} \frac{(-1)}{p_0 - \epsilon_p^0 + i\eta_p}.$$

The integral is evaluated by using Cauchy's theorem and a contour of integration in the complex p_0 -plane which includes the entire real axis. For $\tau > 0$ the contour can be completed by an infinite semicircle Γ_+ in the lower half-plane along which $e^{-ip_0\tau}$ vanishes exponentially. For $\tau < 0$ the contour is completed by an infinite semicircle Γ_- in the upper half-plane. Because of η_p , the pole of the integrand is above the real axis for $p < p_F$ and below for $p > p_F$. The situation is presented in Figure 1, and for the integral in question we obtain (with $\eta_p \rightarrow 0$)

	$p > p_F$	$p < p_F$
$\tau > 0$	$i \exp(-i\epsilon_p^0 \tau)$	0
$\tau < 0$	0	$-i \exp(-i\epsilon_p^0 \tau)$

in agreement with (4.8).

Figure 1

We note that the pole of $G_0(p, p_0)$ is at $p_0 = \epsilon_p^0$ (η_p being infinitesimal), that is to say, at the single-particle energy. As we will see in detail later, under suitable conditions $G(p, p_0)$ has a pole corresponding to a single-particle-like excitation of the interacting system, in general at a complex $p_0 = E_p + i\Gamma_p$. The real part E_p gives the energy and the imaginary part Γ_p the decay rate of the excitation.

C. Spectral Representation of G for the Interacting Electron Gas

Consider now the general expression for $G(p, \tau)$ for a system of N interacting fermions, all with spin up:

$$G(p, \tau) = i \langle 0 | T \{ c_p(\tau) c_p^\dagger(0) \} | 0 \rangle$$

$$= \begin{cases} i \langle 0 | c_p e^{-iH\tau} c_p^\dagger | 0 \rangle e^{+iE_0^N \tau} & \text{for } \tau > 0 \\ -i \langle 0 | c_p^\dagger e^{iH\tau} c_p | 0 \rangle e^{-iE_0^N \tau} & \text{for } \tau < 0 \end{cases} \quad (4.10)$$

The latter equations result on introducing the explicit form of the Heisenberg operators; E_0^N is the ground state energy of the interacting system. By inserting between $c_p^\dagger$ and c_p the unit operator whose expression in terms of the complete set of eigenstates $|\Psi_n^{(N \pm 1)}\rangle$ of H for $N \pm 1$ particles is

$$1 = \sum_n |\Psi_n^{(N \pm 1)}\rangle \langle \Psi_n^{(N \pm 1)}|$$

we find

$$G(p, \tau) = \begin{cases} i \sum_n | \langle c_p^\dagger \rangle_{n,0} |^2 e^{-i(E_n^{N+1} - E_0^N) \tau} & \text{for } \tau > 0 \\ -i \sum_n | \langle c_p \rangle_{n,0} |^2 e^{i(E_n^{N-1} - E_0^N) \tau} & \text{for } \tau < 0 \end{cases} \quad (4.11)$$

The matrix elements are defined by

$$(c_p^\dagger)_{n,0} = \langle \Psi_n^{N+1} | c_p^\dagger | \Psi_0^N \rangle$$

$$(c_p)_{n,0} = \langle \Psi_n^{N-1} | c_p | \Psi_0^N \rangle \quad (4.12)$$

Since $c_p^\dagger$ increases the momentum of the system by p and the number of particles by one, the summation in equation (4.11) for $\tau > 0$ extends over eigenstates of $(N+1)$ particles with momentum p if the ground state has N particles and zero momentum. For $\tau < 0$ the sum on n runs over all eigenstates for $(N-1)$ particles and momentum $(-p)$.

We write

$$E_n^{N+1} - E_0^N = \epsilon_n^{N+1} + E_0^{N+1} - E_0^N = \epsilon_n^{N+1} + \mu(N) \quad ,$$

defining $\epsilon_n^{N+1} \equiv E_n^{N+1} - E_0^{N+1}$ as the excitation energy of the $(N+1)$ -particle system and $\mu(N)$ as the chemical potential. We shall assume that $\mu(N-1) = \mu(N)$, since we are concerned only with systems for which $N \gg 1$. With this assumption, we have

$$E_n^{N-1} - E_0^N = \epsilon_n^{N-1} - \mu(N) \quad .$$

The excitation energies ϵ_n^N are always non-negative. Inserting these definitions in (4.11), we obtain

$$G(p, \tau) = \begin{cases} i \sum_n |(c_p^\dagger)_{n,0}|^2 e^{-i[\epsilon_n^{N+1} + \mu(N)]\tau} & \text{for } \tau > 0 \\ -i \sum_n |(c_p)_{n,0}|^2 e^{+i[\epsilon_n^{N-1} - \mu(N)]\tau} & \text{for } \tau < 0 \end{cases} \quad (4.13)$$

We shall prove that the Fourier time transform $G(p, p_0)$ of (4.13) is given by

$$G(p, p_0) = - \int_0^\infty d\epsilon \left\{ \frac{\rho^+(p, \epsilon)}{p_0 - \mu - \epsilon + i\eta} + \frac{\rho^-(p, \epsilon)}{p_0 - \mu + \epsilon - i\eta} \right\} \quad , \quad (4.14)$$

where we have introduced the spectral densities

$$\left. \begin{aligned} \rho^+(p, \epsilon) &= \sum_n |(c_p^\dagger)_{n,0}|^2 \quad , \quad \epsilon < \epsilon_n^{N+1} < \epsilon + d\epsilon \\ \rho^-(p, \epsilon) &= \sum_n |(c_p)_{n,0}|^2 \quad , \quad \epsilon < \epsilon_n^{N-1} < \epsilon + d\epsilon \end{aligned} \right\} \quad (4.15)$$

The proof is analogous to that given for the free-field Green's function $G_0(p, p_0)$. Consider

$$\begin{aligned} G(p, \tau) &= \int_{-\infty}^\infty \frac{dp_0}{2\pi} e^{-ip_0\tau} G(p, p_0) \\ &= - \int_{-\infty}^\infty \frac{dp_0}{2\pi} e^{-ip_0\tau} \int_0^\infty d\epsilon \left\{ \frac{\rho^+(p, \epsilon)}{p_0 - \mu - \epsilon + i\eta} + \frac{\rho^-(p, \epsilon)}{p_0 - \mu + \epsilon - i\eta} \right\} \quad . \end{aligned} \quad (4.16)$$

We assume that the order of the p_0 and ϵ integrations may be reversed. For $\tau > 0$, the p_0 integration is effected by completing a contour with an arc in the lower half-plane. Since only the term with $\rho^+(p, \epsilon)$ has a pole in the lower half-plane, we obtain

$$G(p, \tau) = i \int_0^\infty d\epsilon \cdot e^{-i(\epsilon + \mu)\tau} \rho^+(p, \epsilon) \quad (\tau > 0) \quad . \quad (4.17)$$

For $\tau < 0$, we close a contour in the upper half-plane and obtain

$$G(p, \tau) = -i \int_0^\infty d\epsilon \cdot e^{i(\epsilon - \mu)\tau} \rho^-(p, \epsilon) \quad (\tau < 0) \quad . \quad (4.18)$$

With the definition (4.15) of $\rho^\pm(p, \epsilon)$, equations (4.17) and (4.18) are fully equivalent to (4.13), which thereby establishes the spectral representation stated in (4.14). The spectral representation (or Lehman representation) of G expresses G as an integral over free-field-like Green's functions

$$\frac{1}{p_0 - \mu \mp \epsilon \pm i\eta} \quad ,$$

with the spectral densities ρ^+ and ρ^- giving the strength of the contribution to G of states in an energy interval $d\epsilon$. Again, these states are the exact eigenstates of the full Hamiltonian. For the free Fermi gas, G_0 is given correctly by taking

$$\rho^+(p, \epsilon) = \delta(\epsilon - \epsilon_p + \mu)(1 - n_p) \quad (4.19)$$

$$\rho^-(p, \epsilon) = \delta(\epsilon + \epsilon_p - \mu)n_p \quad .$$

This follows directly from (4.20) and the representation of $\delta_\pm$ functions given immediately below.

The imaginary part of G is closely related to the ρ -functions. Using in equation (4.14) the well-known operational relation (see, e.g., Bethe and Salpeter, p. 41) for factors of an integrand

$$\frac{1}{p_0 - \mu - \epsilon \pm i\eta} = P\left(\frac{1}{p_0 - \mu - \epsilon}\right) \mp i\pi\delta(p_0 - \mu - \epsilon) \equiv \mp 2\pi i\delta_\pm(p_0 - \mu - \epsilon) \quad ,$$

where P indicates that a principal part is to be taken in integration, we can see that

$$\text{Im } G(p, p_0) = \begin{cases} \pi \int_0^\infty d\epsilon \rho^+(p, \epsilon) \delta(p_0 - \mu - \epsilon) = \pi \rho^+(p, p_0 - \mu) & p_0 > \mu \\ -\pi \int_0^\infty d\epsilon \rho^-(p, \epsilon) \delta(p_0 - \mu + \epsilon) = -\pi \rho^-(p, \mu - p_0) & p_0 < \mu. \end{cases} \quad (4.20)$$

Since ρ^+ and ρ^- are non-negative, the imaginary part of G changes sign at $p_0 = \mu$. We obtain a dispersion relation relating the real and imaginary parts $G(p, p_0)$ by substituting into the real part of (4.14) the expressions for ρ^+ and ρ^- from (4.20). The result is

$$\text{Re } G(p, p_0) = \frac{1}{\pi} P \int_\mu^\infty dp'_0 \frac{\text{Im } G(p, p'_0)}{p'_0 - p_0} - \frac{1}{\pi} P \int_{-\infty}^\mu dp'_0 \frac{\text{Im } G(p, p'_0)}{p'_0 - p_0} \quad (4.21)$$

D. Analytic Properties of $G(p, p_0)$ in the Complex p_0 -plane

If in equation (4.14) we replace ϵ by $(\epsilon + i\eta)$ in the first term and by $(-\epsilon + i\eta)$ in the second term, we have

$$\begin{aligned} G(p, p_0) &= \int_{-i\eta}^{-i\eta+\infty} d\epsilon \frac{\rho^+(p, \epsilon + i\eta)}{\epsilon - (p_0 - \mu)} + \int_{i\eta-\infty}^{i\eta} d\epsilon \frac{\rho^-(p, -\epsilon + i\eta)}{\epsilon - (p_0 - \mu)} \\ &\rightarrow \int_c d\epsilon \frac{F(p, \epsilon)}{\epsilon - (p_0 - \mu)}, \end{aligned} \quad (4.22)$$

where

$$F(p, \epsilon) = \begin{cases} \rho^+(p, \epsilon) & \epsilon > 0 \\ \rho^-(p, -\epsilon) & \epsilon < 0 \end{cases},$$

and the contour of integration c is shown in Figure 2.

Figure 2

Thus far, $G(p, p_0)$ has been defined only for real values of $p_0 - \mu$. We now extend the definition by writing

$$G(p, p_0) = \int_c d\epsilon \frac{F(p, \epsilon)}{\epsilon - (p_0 - \mu)} \quad (4.23)$$

as a function of the complex variable p_0 . Integrals of this type are known to define functions of p_0 which are analytic except possibly for values of $(p_0 - \mu)$ lying on the contour of integration c . In our case the contour c divides the complex plane into regions so that two different functions are defined:

$f_I(p_0 - \mu)$, which is analytic for $(p_0 - \mu)$ in region I

and

$f_{II}(p_0 - \mu)$, which is analytic for $(p_0 - \mu)$ in region II.

For real $(p_0 - \mu)$, $G(p, p_0)$ coincides with f_{II} for $p_0 - \mu < 0$ with f_I for $p_0 - \mu > 0$, as is evident from Figure 2. In general, f_I is not analytic for $(p_0 - \mu)$ in region II, and f_{II} is not analytic for $(p_0 - \mu)$ in region I. The function f_I is defined in region I by the integral (4.22) and in region II by its analytic continuation, and similarly for f_{II} . Since $F(p, \epsilon)$ is real, it is easily seen from (4.23) that at points lying infinitely close to the contour f_I in region I and f_{II} in region II are complex conjugates. From this it follows, for example, that the continuation of f_I^* into region II is f_{II} but that the continuation of f_I is not f_{II}^* .

E. Single-particle Excitation Energies and Lifetime

The physical significance of the function $G(p, \tau)$ is that of a probability amplitude for finding the system in the same state at $t = \tau > 0$ as it was at $t = 0$. This can be shown as follows. We choose phases so that the Heisenberg and Schrödinger pictures are identical at $t = 0$ for all states and operators. For the moment we will speak in the Schrödinger language. Let us create at $t = 0$ a particle in single-particle state p : the wave function for the system is then $c_p^\dagger |\Psi_0^S(0)\rangle$. At a later time τ the wave functions has evolved into $e^{-iH\tau} c_p^\dagger |\Psi_0^S(0)\rangle$. If the particle were created in state p at $t = \tau$ rather than at $t = 0$, the wave function would be $c_p^\dagger e^{-iH\tau} |\Psi_0^S(0)\rangle$. Thus the probability amplitude for finding the system at $t = \tau > 0$ in the same state as it was in at $t = 0$ is the scalar product of the two Schrödinger wave functions at time τ :

$$A(p, \tau) = \langle \Psi_0^S(0) | e^{iH\tau} c_p e^{-iH\tau} c_p^\dagger | \Psi_0^S(0) \rangle ,$$

which in the Heisenberg picture reads

$$A(p, \tau) = \langle 0 | c_p(\tau) c_p^\dagger(0) | 0 \rangle = -iG(p, \tau) . \quad (4.24)$$

From this physical significance of $G(p, \tau)$, it might be expected that its time dependence in a limited interval of time may be of the form

$$G(p, \tau) \sim e^{-i(E_p + \mu)\tau} e^{-\Gamma_p \tau}, \quad (4.25)$$

where E_p may be interpreted as the energy of a "quasi particle" excitation and $1/\Gamma_p$ as its lifetime for decay into other excitations. As is apparent from equation (4.8), this form is exact for the case of free particles with $\Gamma_p = 0$ and $E_p + \mu = \epsilon_p^0$.

Let us now examine analytically the behavior of $G(p, \tau)$ for large positive times. We carry out the ϵ integration in equation (4.17) by integrating along the contour indicated in Figure 3, where we have assumed that the analytic continuation of ρ^+ into the lower half-plane is analytic except for a simple pole at $\epsilon = E_p - i\Gamma_p$.

Figure 3

The integral consists, then, of the sum of two contributions, one arising from the residue at the pole and the other from the integration along the negative imaginary axis. For $\tau \gg 1/\Gamma_p$, the time dependence of $G(p, \tau)$ is determined by the first contribution only, and thus it reads

$$G(p, \tau) = r_p e^{-i(E_p + \mu)\tau} e^{-\Gamma_p \tau}, \quad (4.26)$$

where r_p is the residue of ρ^+ at its pole. From equation (4.20) we have

$$\begin{aligned} \rho^+(p, \epsilon) &= \frac{1}{\pi} \text{Im } G(p, \epsilon + \mu) = \frac{1}{\pi i} [G(p, \epsilon + \mu) - G^*(p, \epsilon + \mu)] \\ &= \frac{1}{\pi i} [f_I(\epsilon) - f_I^*(\epsilon)] \end{aligned} \quad (4.27)$$

However, the analytic continuation of f_I^* into the lower half-plane for $p_0 - \mu = \epsilon > 0$ is f_{II} , which is analytic in this region, and thus the poles of the analytic continuation of $\rho^+(p, \epsilon)$ into the lower half-plane for $\epsilon > 0$ coincide with the poles of the analytic continuation of $f_I(\epsilon) = G(p, \epsilon + \mu)$. Therefore we have the result that if there exists a simple pole of the analytic continuation of $G(p, p_0)$ in the lower half-plane for $p_0 > \mu$, this pole may be interpreted as giving the energy and lifetime of a quasi particle. If there are several singularities of the analytic continuation of G into the lower half-plane, the pole closest to the real axis will give the asymptotic behavior of G for large time. Equation (4.26) may also be interpreted as stating that if a particle is created in state p at $t = 0$, it has a probability amplitude r_p for being in the quasi-stationary state with energy E_p and damping rate Γ_p at $t = \tau$.

In a completely analogous way one can show that poles of the analytic continuation of $G(p, p_0)$ into the upper half-plane for $p_0 < \mu$ may be interpreted as giving the energy and damping rate of quasi holes.

F. Green's Function for a Bose Field

In terms of the Boson field coordinate $\phi_k = a_k + a_{-k}^\dagger$ ($\phi_k^\dagger = \phi_{-k}$), we define the boson Green's function for a translationally invariant system as

$$D(k, \tau) = i \langle 0 | T \{ \phi_k(\tau) \phi_k^\dagger(0) \} | 0 \rangle, \quad (4.28)$$

where $|0\rangle$ is the exact ground state of the system and all quantities are expressed in the Heisenberg picture. By inserting the complete set of eigenstates of H between ϕ and $\phi^\dagger$ we have (for the system with the given number N of particles, since ϕ and $\phi^\dagger$ do not change this number)

$$D(k, \tau) = \begin{cases} i \sum_n |(\phi_k^\dagger)_{n,0}|^2 e^{-i(E_n - E_0)\tau} & \text{for } \tau > 0 \\ i \sum_n |(\phi_k)_{n,0}|^2 e^{i(E_n - E_0)\tau} & \text{for } \tau < 0 \end{cases} \quad (4.29)$$

No minus sign arises from the chronological ordering since we are dealing with bosons. If we define

$$\Phi(k, \omega) d\omega = \sum_n |(\phi_k)_{n,0}|^2 = \sum_n |(\phi_{-k})_{n,0}|^2, \quad (4.30)$$

the sum extending over all states in the interval $\omega < E_n - E_0 < \omega + d\omega$, we find

$$D(k, \tau) = i \int_0^{\infty} \Phi(k, \omega) e^{-i\omega|\tau|} d\omega = \int_{-\infty}^{+\infty} D(k, k_0) e^{-ik_0\tau} \frac{dk_0}{2\pi} \quad (4.31)$$

It follows that the Fourier transform $D(k, k_0)$ is given by

$$D(k, k_0) = \int_0^{\infty} \Phi(k, \omega) \left\{ \frac{1}{\omega - k_0 - i\eta} + \frac{1}{\omega + k_0 - i\eta} \right\} d\omega, \quad (4.32)$$

where $\eta = 0^+$. From this integral one sees that the relation between the spectral density Φ and the imaginary part of D is

$$\text{Im } D(k, k_0) = \pi \Phi(k, |k_0|) > 0, \quad (4.33)$$

and the dispersion relation follows in the same manner as for G :

$$\text{Re } D(k, k_0) = \frac{1}{\pi} P \int_0^{\infty} \text{Im } D(k, k'_0) \left\{ \frac{1}{k'_0 - k_0} + \frac{1}{k'_0 + k_0} \right\} dk'_0. \quad (4.34)$$

By arguments similar to those used for G , one can show that the energy and lifetime of the quasi particles (bosons in this case) are given by the poles of the analytic continuation of $D(k, k_0)$ into the lower half of the complex k_0 plane.

References to Chapter IV

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V. PERTURBATION EXPANSION FOR THE GREEN'S FUNCTIONS

In order actually to evaluate the Green's functions, it is often convenient to express the true G 's or D 's as perturbation expansions involving the Green's functions for the system in the absence of interactions. More generally, if one makes a quite arbitrary dichotomy of the Hamiltonian and writes $H = H_0 + H_1$, then the expansion involves the Green's function appropriate to H_0 . The scheme is not necessarily limited to interactions H_1 which formally admit a perturbation type of expansion, since one can often perform partial summations of infinite series which eliminate divergencies otherwise present. The extent to which such rearrangements of terms lead to physically interesting results depends strongly on the nature of the system involved. By a judicious choice of terms in the partial summation, one can often obtain results which lead to qualitatively new features of the system, absent in the model system described by H_0 . We will discuss several examples of this later in this lecture series. Therefore in this scheme the physics is reduced to developing insight as to physical effects of various terms in the perturbation series and to developing techniques for summing the relevant terms.

A. Adiabatic Hypothesis

For the moment we restrict the discussion to that of a system of interacting spin- $\frac{1}{2}$ fermions. We write

$$H = H_0 + H_1$$

and choose the zero-order Hamiltonian to be sufficiently simple that the one-particle Green's function appropriate to H_0 can be found explicitly. For example, if H_0 is the kinetic energy, then

$$G_0(p, p_0) = \frac{(-1)}{p_0 - \epsilon_p + i\eta_p}$$

as we saw earlier, with $\epsilon_p = (p^2/2m)$.

We now introduce an interaction picture based on H_0 . In this picture, the ground state vector satisfies equations (3.10):

$$i \frac{\partial}{\partial t} |\Psi_0(t)\rangle = H_1(t) |\Psi_0(t)\rangle, \quad (\hbar = 1)$$

If we define the unitary matrix $U(t, t')$ by the equation

$$i \frac{\partial}{\partial t} U(t, t') = H_1(t) U(t, t') \quad (5.1)$$

subject to

$$U(t,t) = 1 \quad ,$$

it follows that

$$|\Psi_0(t)\rangle = U(t,t') |\Psi_0(t')\rangle \quad . \quad (5.2)$$

If $H_1(t')$ vanishes adiabatically as $t' \rightarrow \pm \infty$, then we assume that $|\Psi_0(-\infty)\rangle$ reduces to the ground state $|\Phi_0\rangle$ of H_0 . The formal solution of (5.1) is

$$\begin{aligned} U(t,t') &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{t'}^t dt_1 \dots \int_{t'}^t dt_n T \left\{ H_1(t_1) \dots H_1(t_n) \right\} \\ &= T \exp \left\{ -i \int_{t'}^t dt H_1(t) \right\} \quad . \end{aligned} \quad (5.3)$$

We verify that (5.3) satisfies (5.1) by differentiation:

$$\begin{aligned} i \frac{\partial}{\partial t} U(t,t') &= T \sum_{n \geq 0} i \cdot \frac{(-i)^n}{n!} \sum_{\nu=1}^n \int_{t'}^t dt_1 \dots \int_{t'}^t dt_{\nu-1} \int_{t'}^t dt_{\nu+1} \dots \int_{t'}^t dt_n \\ &\quad \cdot H(t_1) \dots H(t_{\nu-1}) H(t) H(t_{\nu+1}) \dots H(t_n) = H_1(t) U(t,t') \quad . \end{aligned}$$

The definition of the T product brings $H_1(t)$ to the left in each term of the expansion, and the symmetry of the integrands then gives the result. The inclusion of T in (5.3) is essential since $[H_1(t), H_1(t'')] \neq 0$ in general unless H_1 and H_0 commute. The unitary matrix $U(t,t')$ is also given, up to a unitary transformation independent of t and t' , by

$$U(t,t') = e^{iH_0 t} e^{-iH(t-t')} e^{-iH_0 t'} \quad , \quad (5.4)$$

as is easily seen from the differential equation plus boundary condition (5.1).

The U matrix has the properties:

$$\begin{aligned} \text{a)} \quad & UU^\dagger = 1 \\ \text{b)} \quad & U^\dagger(t,t') = U^{-1}(t,t') = U(t',t) \\ \text{c)} \quad & U(t,t') = U(t,t'') U(t'',t') \quad (\text{the group property}) \quad . \end{aligned} \quad (5.5)$$

By using the group property we have

$$|\Psi_0(0)\rangle = U(0, -\infty) |\Phi_0\rangle = U(0, \infty) U(\infty, -\infty) |\Phi_0\rangle = U(0, \infty) S |\Phi_0\rangle, \quad (5.6)$$

where $S \equiv U(\infty, -\infty)$ applied to $|\Phi_0\rangle$ can differ from $|\Phi_0\rangle$ by at most a phase factor, due to the adiabatic hypothesis made above.

We saw above that the operators in the interaction picture are given by

$$\theta_I(t) = e^{iH_0 t} \theta_S e^{-iH_0 t} = e^{iH_0 t} e^{-iHt} \theta_H(t) e^{iHt} e^{-iH_0 t},$$

where $\theta_H(t) = e^{iHt} \theta_S e^{-iHt}$ is the operator in the Heisenberg picture. Both the interaction picture and the Heisenberg picture are here chosen to be identical with the Schrödinger picture at $t = 0$, in consequence of which we have

$$U(t, 0) = e^{iH_0 t} e^{-iHt} \quad (5.7)$$

and can write

$$\begin{aligned} \theta_I(t) &= U(t, 0) \theta_H(t) U^\dagger(t, 0) \\ \theta_H(t) &= U^\dagger(t, 0) \theta_I(t) U(t, 0) \end{aligned} \quad (5.8)$$

With the aid of these relations we can express the Green's function in the interaction representation and shall obtain

$$G(p, \tau) \equiv i \langle \Psi_{0H} | T \{ c_{pH}(\tau) c_{pH}^\dagger(0) \} | \Psi_{0H} \rangle \quad (5.9)$$

$$= \frac{i \langle \Phi_0 | T \{ c_p(\tau) c_p^\dagger(0) S \} | \Phi_0 \rangle}{\langle \Phi_0 | S | \Phi_0 \rangle} \quad (5.10)$$

The quantities in (5.9) are all expressed in the Heisenberg representation, and those in (5.10) in the interaction representation.

We prove (5.10) first for $\tau > 0$. Carrying out the time-ordering while still in the Heisenberg picture,

$$G(p, \tau) = i \langle \Psi_{0H} | c_{pH}(\tau) c_{pH}^\dagger(0) | \Psi_{0H} \rangle.$$

Now we transform to the interaction picture. Using (5.6), (5.8), (5.5), and the adiabatic hypothesis incorporated in the forms

$$|\Psi_0(-\infty)\rangle = |\Phi_0\rangle, \quad S|\Phi_0\rangle = e^{i\phi}|\Phi_0\rangle,$$

we obtain

$$\begin{aligned} G(p, \tau) &= i \langle \Phi_0 | S^\dagger U^\dagger(0, \infty) \cdot U^\dagger(\tau, 0) c_p(\tau) U(\tau, 0) c_p(0) \cdot U(0, -\infty) | \Phi_0 \rangle \\ &= i e^{-i\phi} \langle \Phi_0 | U(\infty, \tau) c_p(\tau) U(\tau, 0) c_p(0) U(0, -\infty) | \Phi_0 \rangle \\ &= i e^{-i\phi} \langle \Phi_0 | T \left\{ U(\infty, \tau) c_p(\tau) U(\tau, 0) c_p(0) U(0, -\infty) \right\} | \Phi_0 \rangle. \end{aligned}$$

For any set of operators, $\alpha_1(t_1), \dots, \alpha_n(t_n)$, where any of the $\alpha_i(t_i)$ may be either fermion or boson and either creation or destruction operators,

and for any permutation $\begin{pmatrix} 1, 2, \dots, n \\ i_1, i_2, \dots, i_n \end{pmatrix}$, by definition

$$T \left\{ \alpha_1(t_1), \dots, \alpha_n(t_n) \right\} = \pm T \left\{ \alpha_{i_1}(t_{i_1}), \dots, \alpha_{i_n}(t_{i_n}) \right\}.$$

The upper (lower) sign holds if the permutation effects an even (odd) number of interchanges of order among the fermion factors alone. Now $H_1(t)$ and a fortiori $U(t, t')$ contains only products having an even number of fermion factors. Hence we can write

$$\begin{aligned} G(p, \tau) &= i e^{-i\phi} \langle \Phi_0(-\infty) | T \left\{ c_p(\tau) c_p^\dagger(0) U(\infty, \tau) U(\tau, 0) U(0, -\infty) \right\} | \Phi_0(-\infty) \rangle \\ &= i e^{-i\phi} \langle \Phi_0(-\infty) | T \left\{ c_p(\tau) c_p^\dagger(0) S \right\} | \Phi_0(-\infty) \rangle, \end{aligned}$$

which establishes (5.10) for $\tau > 0$. Clearly the same procedure will do for $\tau < 0$, and therefore (5.10) is proved generally.

Notice that in (5.10) S is within the time-ordered product braces and is there to be represented by

$$S = \exp \left\{ -i \int_{-\infty}^{\infty} dt'' H_1(t'') \right\}.$$

Thus the time ordering applies both to τ and to the dummy variable t'' . The presence of $\langle \Phi_0 | S | \Phi_0 \rangle$ in the denominator of (5.10) cancels many phase factors from the numerator and greatly simplifies the perturbation

expansion for G . By expanding S in powers of H in the numerator, we have

$$G(p, \tau) = \frac{i}{\langle 0|S|0 \rangle} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} d\tau_1 \dots d\tau_n$$

$$\langle \Phi_0 | T \left\{ c_p(\tau) c_p^\dagger(0) H_1(\tau_1) H_1(\tau_2) \dots H_1(\tau_n) \right\} | \Phi_0 \rangle \quad (5.11)$$

In formula (5.11) the time variables $\tau_1, \dots, \tau_n$ are to be ordered chronologically with increasing time to the left and minus signs arising from anticommutation of the fermion operators are included in T as stated above. The denominator could also be put in a similar form by expanding S . If $H_1(t_i)$ is local in both space and time, we have

$$H_1(t_i) = \frac{1}{2} \int \psi^\dagger(x_i, t_i) \psi^\dagger(y_i, t_i) V(x_i - y_i) \psi(x_i, t_i) \psi(y_i, t_i) \delta(t_i - t_i') dx_i dy_i dt_i' \quad , \quad (5.12)$$

where we have inserted the delta function to emphasize that the interaction is local in time. More generally, one could replace the delta function by a kernel giving a nonlocal interaction in time, for example a potential due to virtual exchange of phonons which, as we will see, is important in the theory of superconductivity. In momentum space variables, H_1 has the form

$$H_1(t_i) = \frac{1}{2} \sum_q V_q \int \eta \left\{ \rho_q(t_i) \rho_q^\dagger(t_i') \right\} \delta(t_i - t_i') dt_i' \quad ,$$

where η indicates the normal ordered product as defined in equation 23 of

Section II is to be taken, and $\rho_q(t_i) = \sum_k c_k^\dagger(t_i) c_{k+q}(t_i)$ is the Fourier

transform of the particle density operator. More generally, for a potential which is local in time but nonlocal in space, we have

$$H_1(t_i) = \frac{1}{2} \sum_{k, k', q} (k+q, k'-q | V | k, k') \int c_{k+q}^\dagger(t_i) c_{k'-q}^\dagger(t_i') c_{k'}(t_i')$$

$$c_k(t_i) \delta(t_i - t_i') \cdot dt_i' \quad . \quad (5.13)$$

B. Perturbation Expansion Using Wick's Theorem

To evaluate the n^{th} -order term in the perturbation expansion of G , we require matrix elements of the form

$$\langle \Phi_0 | T \{ ABCD \dots \} | \Phi_0 \rangle ,$$

where A, B, C , etc., are either creation or annihilation operators, each with its own time variable. A systematic reduction of such expectation values to products of expectation values involving one c and one $c^\dagger$ is given by Wick's theorem.

Recall that a normally ordered product of operators, $N \{ ABC \dots \}$, is given by moving all creation operators to the left and all destruction operators to the right, including minus signs arising from anticommutation. In the fermion case, destruction operators are the c_k (destruction of electrons) for $k > k_F$ and $c_k^\dagger$ (destruction of holes) for $k < k_F$. In this way the ground state expectation value of a normal product is always zero, whereas the η used before gave zero only with respect to the bare vacuum with no particles. The contraction $\underline{AB}$ of a pair of operators AB is then defined by

$$T(AB) = N(AB) + \underline{AB} ,$$

that is, the contraction is the difference between the T and N products. In general, the contraction will be a c -number and a factor out of any matrix element.

Wick's theorem then states that a T product can be uniquely decomposed into a sum of N products as follows:

$$\begin{aligned} T(ABC \dots XYZ) = & N(ABC \dots XYZ) + N(\underline{AB} \dots XYZ) + \\ & N(\underline{AB} \dots XYZ) + \dots + N(\underline{ABC} \dots XYZ) + \\ & \dots, \text{etc.} , \end{aligned}$$

where $N(\underline{AB} \dots XYZ) = \underline{AB} N(\dots XYZ)$. All possible contractions are to be made and minus signs arising from anticommutation are to be included.

Note that the ground state expectation value of an N product vanishes unless $ABC \dots$ are all c -numbers, since there will be at least one annihilation operator on the right which gives zero when acting on $|\Phi_0\rangle$. If $ABC \dots$ are all creation operators, the expectation value obviously vanishes.

Therefore, the ground state expectation value of a T product is given by the sum of all possible N products involving only c-numbers, that is, the N products in which every annihilation operator is contracted with a creation operator.

To gain insight into the nature of the expansion, we consider a few low-order terms. For the moment we neglect $\langle \Phi_0 | S | \Phi_0 \rangle$ in the denominator of G.

The leading term (n=0) is

$$G^{(0)}(p, \tau) = i \langle \Phi_0 | T c_p(\tau) c_p^\dagger(0) | \Phi_0 \rangle = G_0(p, \tau) \quad (5.14)$$

Thus, the lowest approximation to G is G_0 . From the definition of a contraction, we can immediately obtain

$$\begin{aligned} \underline{c_p(\tau) c_p^\dagger(0)} &= \langle \Phi_0 | T \{ c_p(\tau) c_p^\dagger(0) \} | \Phi_0 \rangle \\ &- \langle \Phi_0 | N \{ c_p(\tau) c_p^\dagger(0) \} | \Phi_0 \rangle = -i G_0(p, \tau) \end{aligned} \quad (5.15)$$

Therefore the expansion of G in powers of H_1 will involve the zero-order Green's function G_0 .

The first-order term is

$$G^{(1)}(p, \tau) = i(-i) \langle \Phi_0 | T \left\{ c_p(\tau) c_p^\dagger(0) \int_{-\infty}^{+\infty} H_1(t) dt \right\} | \Phi_0 \rangle$$

This expression can be simplified by using for H_1 the second term of equation (23) of Section II for a two-body interaction on the free electron gas. We have, then,

$$\begin{aligned} G^{(1)}(p, \tau) &= \langle \Phi_0 | T \left\{ c_p(\tau) c_p^\dagger(0) \frac{1}{2} \sum_{q, k, k'} V_q \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' \delta(t-t') \right. \\ &\quad \left. c_{k+q}^\dagger(t) c_{k'-q}^\dagger(t') c_{k'}(t') c_k(t) \right\} | \Phi_0 \rangle \end{aligned} \quad (5.16)$$

With the aid of Wick's theorem we see there are two types of terms arising in $G^{(1)}$: a) Terms in which $c_p(\tau)$ and $c_p^\dagger(0)$ are contracted with each other while the operators in H_1 are not contracted with these operators. As we will see, these terms are cancelled by terms arising from $\langle \Phi_0 | S | \Phi_0 \rangle$ in the denominator of G and have no physical significance. b) Terms in which $c_p(\tau)$ and $c_p^\dagger(0)$ are each contracted with terms in H_1 . These terms are not cancelled by $\langle \Phi_0 | S | \Phi_0 \rangle$ and represent physical effects.

We will call terms of type a) and b) unlinked and linked terms, respectively. For the moment we neglect all unlinked terms.

There are two distinct types of linked terms in $G^{(1)}$, one which enters for $q \equiv 0$ and one for general q . For $q = 0$, we may contract $c_p^\dagger$ with either $c_{k'}$ or c_k . Since by momentum conservation

$$\underline{c_p(t_1)} \underline{c_{p'}^\dagger(t_2)} = \delta_{p,p'} \underline{c_p(t_1)} \underline{c_p^\dagger(t_2)} \quad , \quad (5.17)$$

it follows that if $c_p^\dagger$ and c_k are contracted, so must c_p and $c_{k'}^\dagger$. This leaves $c_{k'}^\dagger$ and c_k to be contracted in the T product. An identical term arises upon interchanging k and k' . We include both terms by neglecting the factor of $\frac{1}{2}$ in front of the interaction. The $q = 0$ contribution to $G^{(1)}$ is then

$$\sum_{k'} \int_{-\infty}^{+\infty} \int (-1) i(-i) V_0 [-i G_0(p, \tau-t)] [-i G_0(k', 0^-)] [-i G_0(p, t)] \delta(t-t') dt' dt \quad . \quad (5.18)$$

The factor (-1) arises from the anticommutation of the operators to bring them to the correct order for the contractions. The time 0^- in the middle G_0 is included to ensure the ordering $c_{k'}^\dagger c_k$ which occurs in H_1 .

It is helpful to introduce Feynman diagrams to interpret this expression. By reading the integrand from right to left we see that a particle created in state p at time zero propagates to time t , by $G_0(p, t)$, at which point it interacts with a particle in state k' , undergoing a forward scattering ($q \equiv 0$) and propagates on in state p until it is annihilated at time τ . A picture of this process is shown below.

The particle motions are represented by solid lines with arrows indicating that the particle moves in time in the direction of the arrow. The interaction is represented by a dashed line; the time $t = t'$ since the interaction was assumed to be instantaneous. The function $G_0(k', 0^-)$ is represented by a closed loop.

The second class of terms arising for general q is given by

$$i(-i) \sum_{k'} V_{k'-p} \int_{-\infty}^{+\infty} \int [-i G_0(p, \tau-t')] [-i G_0(k', 0^-)] [-i G_0(p, t)] \delta(t-t') dt' dt \quad (5.19)$$

This term, which is the exchange counterpart of the $q = 0$ term, is represented in the figure below.

The calculation is simplified by introducing the Fourier transform of all time-dependent quantities entering $G^{(1)}$. Thus, using

$$G_0(p, \tau) = \int_{-\infty}^{\infty} G_0(p, p_0) e^{-ip_0\tau} \frac{dp_0}{2\pi} \quad (5.20)$$

we have for the $q = 0$ term,

$$\begin{aligned} & -V_0 \sum_{k'} \int \left[-i G_0(p, p_0) e^{-ip_0(\tau-t)} \frac{dp_0}{2\pi} \right] \left[-i G_0(k', k'_0) e^{-ik'_0(0^-)} \frac{dk'_0}{2\pi} \right] \\ & \quad \cdot \left[-i G_0(p, p'_0) e^{-ip'_0(t)} \frac{dp'_0}{2\pi} \right] dt \\ & = -V_0 \sum_{k'} (-i)^3 \int \frac{dp_0}{2\pi} \frac{dp'_0}{2\pi} \frac{dk'_0}{2\pi} \cdot 2\pi \delta(p_0 - p'_0) e^{-ip_0\tau} e^{-ik'_0(0^-)} G_0(p, p_0) \\ & \quad \cdot G_0(p, p'_0) G_0(k', k'_0) \\ & = -V_0 \sum_{k'} \int \frac{dp_0}{2\pi} e^{-ip_0\tau} \int [-i G_0(p, p_0)]^2 [-i G_0(k', k'_0)] e^{-ik'_0(0^-)} \frac{dk'_0}{2\pi} \quad (5.21) \end{aligned}$$

Taking the Fourier transform with respect to τ we have the $q = 0$ contribution to $G^{(1)}$ given by

$$\begin{aligned} & [-i G_0(p, p_0)] \left\{ -V_0 \int \sum_{k'} [-i G_0(k', k'_0)] e^{-ik'_0(0^-)} \frac{dk'_0}{2\pi} \right\} [-i G_0(p, p_0)] \\ &= [-i G_0(p, p_0)] \left\{ -V_0 \sum_{k'} [-i G_0(k', \tau=0^-)] \right\} [-i G_0(p, p_0)] \quad , \end{aligned} \quad (5.22)$$

while the exchange term gives

$$-i G_0(p, p_0) \left\{ \sum_{k'} V_{k'-p} [-i G_0(k', \tau=0^-)] \right\} [-i G_0(p, p_0)] \quad . \quad (5.23)$$

We may draw new diagrams in the 4-momentum variables (p, p_0) rather than 3-momentum and time. The diagrams look identical with those above except there are no time labels and with each line is associated a 4-momentum, e.g., $p \equiv (p, p_0)$.

It is straightforward to show that there is a 1:1 correspondence between the terms in the perturbation expansion of $G(p, p_0)$ and the set of diagrams in which a particle enters from the right, leaves from the left, and undergoes all topologically distinct interactions in the intermediate state.

The general rules for obtaining the n^{th} -order term in $G(p, p_0)$ from Feynman diagrams are to include in the integrand as factors:

- 1) $i(-i)^n$ (arising partly from $(-i)^n/n!$; the $\frac{1}{n!}$ goes out if we count only topologically distinct diagrams since there are $n!$ equivalent terms corresponding to a given term arising in the Wick expansion in general);
- 2) a matrix element V_q at each vertex, where q is the 4-momentum transfer [note: if V is non-retarded, $V(q) = V|q|$];
- 3) a factor $\delta^4(\pm p_1 \pm p_2 \pm p_3 \pm p_4)$ conserving total 4-momentum at each vertex, where lines pointing away (toward) enter with a $+$ ($-$) sign in the delta function;
- 4) a factor $-i G_0(p)$ for each fermion line of 4-momentum p regardless of the direction of the line, where p is measured with respect to the arrow on the line;
- 5) (-1) for each closed loop in the diagram
- 6) and finally to integrate over the 4-momenta of all internal lines:

$$\int \frac{d^4 p_1}{(2\pi)^4} \dots \frac{d^4 p_i}{(2\pi)^4} \dots$$

As an illustration of these rules we calculate a typical second-order correction to G shown below:

which gives the contribution

$$(-1) i(-i)^7 G_0(p) \int \frac{d^4 q}{(2\pi)^4} V_q^2 G_0(p-q) \left[\int \frac{d^4 p'}{(2\pi)^4} G_0(p'+q) G_0(p') \right] G_0(p) .$$

C. Unlinked Diagrams and the Exclusion Principle

In addition to diagrams in which all parts of the graph are linked together, there are graphs of the form

The contribution of the total graph is the product of that of the linked portion and the contribution from the vacuum fluctuation

More generally, a given linked graph

will be multiplied by an arbitrary set of vacuum fluctuation graphs, which, when summed, are just cancelled by $\langle \Phi_0 | S | \Phi_0 \rangle$ occurring in the denominator of our expression for G . The cancellation is exact, however, only if we neglect the exclusion principle, since if a line in the linked portion accidentally corresponds to the same state as in the vacuum fluctuation this violates the exclusion principle. This difficulty can be overcome by consistently neglecting the exclusion principle in all graphs, since for every Pauli-principle-violating unlinked graphs there is a corresponding Pauli-principle-violating linked graphs which exactly cancels the unwanted term. For example,

is identically cancelled by

Therefore, the problem of calculating correction to G reduces to calculating the contribution of all linked graphs by consistently neglecting the Pauli principle.

D. Dyson's Equation

In general, $G(p)$ will be of the form

We shall derive an equation for $G(p)$ in terms of a quantity $\Sigma(p)$, called the irreducible self energy, which is defined to be the contribution of all distinct diagrams which cannot be divided into two sub-diagrams connected

only by a single solid line which carries the momentum p of the incoming line. Thus

$$-i\Sigma(p) = \text{[self-energy diagrams]} + \dots$$

For example, $\Sigma(p)$ does not include

In general, every contribution to $G(p)$ except for the zeroth-order contribution can be written as a product of three factors

$$\underbrace{\text{[diagram 1]}}_{\text{No. 1}} \underbrace{\text{[diagram 2]}}_{\text{No. 2}} \underbrace{\text{[diagram 3]}}_{\text{No. 3}} \quad (*)$$

where No. 2 is any one of the irreducible diagrams contribution to $\Sigma(p)$, and No. 3 is any possible reducible or irreducible diagram of $G(p)$. This provides a partition of all diagrams occurring in $G(p) - G_0(p)$, so that summing figure (*) over all choices of the specified types for No. 2 and No. 3 gives

$$[-i G(p)] = [-i G_0(p)] + [-i G_0(p)] [-i \Sigma(p)] [-i G(p)] \quad . \quad (5.24)$$

This is known as Dyson's equation. The problem of finding $G(p)$ is reduced to that of finding $\Sigma(p)$. We note that

$$G(p)^{-1} = G_0(p)^{-1} + \Sigma(p) \quad . \quad (5.25)$$

If we assume the major contribution to $G(p, \tau)$ comes from a single pole in $G(p, p_0)$, we see that, in accord with our discussion above, the quasi-particle energy E_p and the damping rate Γ_p are given by

$$E_p - i\Gamma_p = \epsilon_p + \tilde{\Sigma}(p, E_p - i\Gamma_p) \quad , \quad (5.26)$$

where $\tilde{\Sigma}$ is the analytic continuation of $\Sigma(p, p_0)$ into the lower half of the p_0 plane for $\epsilon_p > 0$. For $\Gamma \ll E_p$ we have, writing $\tilde{\Sigma} = \tilde{\Sigma}_0 + i\tilde{\Sigma}_1$,

$$\begin{aligned} E_p &= \epsilon_p + \tilde{\Sigma}_0(p, E_p) \\ \Gamma_p &= -\tilde{\Sigma}_1(p, E_p) \left\{ 1 - \left(\frac{\partial \tilde{\Sigma}_0}{\partial E_p} \right)_{p_0=E_p} \right\}^{-1} \end{aligned} \quad (5.27)$$

E Ground State Energy

We may express the ground state energy in terms of $G(p)$. Now G is of the form

$$G(p, \tau) = i \langle 0 | c_p(\tau) c_p^\dagger(0) | 0 \rangle \theta(\tau) - i \langle 0 | c_p^\dagger(0) c_p(\tau) | 0 \rangle \theta(-\tau) \quad , \quad (5.28)$$

where $\theta(\tau) = \begin{cases} 1 & \tau > 0 \\ 0 & \tau < 0 \end{cases}$ and all quantities are expressed in the Heisenberg representation. If we take the time derivative of G , we obtain

$$i \frac{\partial G(p, \tau)}{\partial \tau} = -\delta(\tau) \langle 0 | \{c_p(\tau), c_p^\dagger(0)\} | 0 \rangle - i \langle 0 | T \{ [H(\tau), c_p(\tau)] c_p^\dagger(0) \} | 0 \rangle \quad .$$

Writing $H = H_0 + H_1$, where $H_0 = \sum_p \epsilon_p \eta_p$, we obtain

$$\left(i \frac{\partial}{\partial \tau} - \epsilon_p \right) G(p, \tau) = -\delta(\tau) - i \langle 0 | T \{ [H_1(\tau), c_p(\tau)] c_p^\dagger(0) \} | 0 \rangle \quad .$$

By taking the Fourier transform of this equation with respect to τ , we have

$$G_0(p)^{-1} G(p) = 1 + i \int_{-\infty}^{\infty} e^{ip_0\tau} \langle 0 | T \{ [H_1(\tau), c_p(\tau)] c_p^\dagger(0) \} | 0 \rangle d\tau \quad . \quad (5.29)$$

Therefore, our definition of $\Sigma(p)$ from Dyson's equation is consistent with this relation if

$$\Sigma(p) G(p) = -i \int_{-\infty}^{\infty} e^{ip_0\tau} \langle 0 | T \{ [H_1(\tau), c_p(\tau)] c_p^\dagger(0) \} | 0 \rangle d\tau \quad . \quad (5.30)$$

If we multiply by a factor $e^{ip_0\eta}$, where $\eta \rightarrow 0^+$, and integrate with respect to p_0 over $-\infty < p_0 < \infty$, we obtain

$$\begin{aligned}
\int_C \frac{dp_0}{2\pi} \Sigma(p) G(p) &= -i \int d\tau \delta(\tau + \eta) \langle 0 | T \left\{ [H_1(\tau), c_p(\tau)] c_p^\dagger(0) \right\} | 0 \rangle \\
&= -i \langle 0 | T \left\{ [H_1(-\eta)] c_p^\dagger(0) \right\} | 0 \rangle \\
&= +i \langle 0 | c_p^\dagger(0) [H_1(0), c_p(0)] | 0 \rangle, \quad (5.31)
\end{aligned}$$

where on the left-hand side the integral is carried out over the contour shown below.

If H_1 includes only a two-body interaction, we see by inspection that

$$c_p^\dagger [H_1, c_p] = -2H_1.$$

Therefore, the ground state expectation value of H_1 is given by

$$\langle 0 | H_1 | 0 \rangle = \frac{i}{2} \int_C \frac{d^4 p}{(2\pi)^4} \Sigma(p) G(p). \quad (5.32)$$

To obtain the ground state expectation value of H_0 we note that

$$\begin{aligned}
\int_C e^{ip_0 \eta} G(p, p_0) \frac{dp_0}{2\pi} &= \int_C \frac{dp_0}{2\pi} \int_{-\infty}^{\infty} d\tau e^{ip_0(\tau + \eta)} G(p, \tau) \\
&= G(p, \tau=0^-) = -i \langle 0 | c_p^\dagger c_p | 0 \rangle = -i \langle 0 | \eta_p | 0 \rangle. \quad (5.33)
\end{aligned}$$

Thus, the expectation value of H_0 is

$$\langle 0 | H_0 | 0 \rangle = \sum_p \epsilon_p \langle 0 | \eta_p | 0 \rangle = i \sum_p \epsilon_p \int_C G(p) \frac{dp_0}{2\pi}, \quad (5.34)$$

so that the ground state energy may be expressed as

$$E_0 = i \int_C \frac{d^4 p}{(2\pi)^4} \left\{ \epsilon_p + \frac{1}{2} \Sigma(p) \right\} G(p) \quad (5.35)$$

Thus, if the system involves only two-body interactions, the one-particle Green's function suffices to determine the ground state energy.

F. Perturbation Series Including Bosons

If the Hamiltonian of the system involves a boson field ϕ which is coupled to the fermion field, it is straightforward to extend the above discussion to include virtual processes involving the bosons. Let

$$H = H_0 + H_1$$

where

$$H_0 = \left\{ \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}}^0 \left(a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + \frac{1}{2} \right) \right\}$$

and

$$H_1 = V_2 + \sum_{\mathbf{q}} g_{\mathbf{q}}^0 \phi_{\mathbf{q}} \rho_{-\mathbf{q}} \quad (5.36)$$

Here V_2 represents the two-body potential between fermions treated above, and the second term in H_1 represents the boson-fermion coupling. The rules for calculating $G(p)$ are extended to this problem by including three point vertices

representing emission or absorption of a boson (~~~~) as well as the four-point vertex

representing two particles scattering via V_2 . To the rules of Section B one adds the rules:

2') a matrix element $g_{\mathbf{q}}$ at each 3-point vertex, where $\mathbf{q}$ is the boson momentum ($g_{\mathbf{q}} = g_{\mathbf{q}}^*$).

3') a factor $(2\pi)^4 \delta(\pm p_1 \pm p_2 \pm q)$ at each 3-point vertex, where lines pointing away (toward) the vertex enter with a + (-) sign in the delta function. Here $q \equiv (q, q_0)$ is the 4-momentum of the boson.

4') a factor $-iD_0(q)$ for each boson line.

Thus, the lowest-order boson contribution to $G(p)$,

is given by

$$i(-i)^2 (-i)^4 G_0(p)^2 \int \frac{d^4 q}{(2\pi)^4} G_0(p-q) D_0(q) |g_q|^2.$$

One can use these generalized rules to calculate $D(q)$. For example,

$$\begin{aligned} -iD(q) = & \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \text{diagram 5} + \text{diagram 6} + \dots \\ & = -iD_0(q) + (-i)^2 (-i)^4 D_0(q)^2 \int \frac{d^4 p}{(2\pi)^4} G_0(p+q) G_0(p) |g_q|^2 + \dots \end{aligned}$$

As in the fermion case, it is useful to introduce a proper self-energy for bosons $\Pi(q)$ defined as the sum of all diagrams of the form

in which the diagrams in the circle cannot be divided into two parts connected only by a single boson line carrying momentum q . If we represent $D(q)$ by a heavy wavy line , it follows that

$$\text{wavy line} = \text{wavy line} + \text{wavy line} \circlearrowleft \pi(q) \text{wavy line}$$

$$-iD(q) = -iD_0(q) + [-iD_0(q)] [-i\pi(q)] (-iD(q)) \quad (5.37)$$

or

$$D(q)^{-1} = D_0(q)^{-1} + \pi(q) \quad (5.38)$$

Since

$$D_0(q) = \int_{-\infty}^{\infty} e^{iq_0\tau} D_0(q, \tau) d\tau = \frac{-2\omega_q^0}{q_0^2 - (\omega_q^0)^2 + i\eta} \quad (\eta = 0^+) ,$$

we have

$$D(q)^{-1} = \frac{q_0^2 - [\omega_q^0 + \pi(q)]^2 + \pi(q)^2}{-2\omega_q^0} \quad (5.39)$$

The energy and damping rate of the bosons are given by the poles of the analytic continuation of D into the lower half of the q_0 plane for $q_0 > 0$. Thus, the complex energy ω_q of the boson is given by

$$\omega_q^2 = \left\{ [\omega_q^0 + \tilde{\pi}(q)]^2 - \tilde{\pi}(q)^2 \right\}_{q_0 = \omega_q} \quad (5.40)$$

where $\tilde{\pi}(q)$ is the required analytic continuation of $\pi(q)$.

G. Polarization Propagator and Dielectric Constant

Returning to the fermion system with only two-body interactions, we note that the four-point vertex

is diagrammatically analogous to the exchange of a boson between two fermions. The analogy is even closer if we note that in higher order we have the related graphs

However, this series is just that for

$$\frac{\mathcal{V}(q) - V(q)}{[-iV(q)]^2} = \left[\frac{1}{\kappa(q)} - 1 \right] \frac{1}{[-iV(q)]} \quad (5.46)$$

Therefore, we have

$$\frac{1}{\kappa(q)} - 1 = -iV_q \int_{-\infty}^{\infty} e^{iq_0\tau} \langle 0 | T \{ \rho_{-q}(-\tau) \rho_q(0) \} | 0 \rangle d\tau \quad (5.47)$$

We now wish to clarify the connection between the dielectric constant as defined above from the time-ordered polarization propagator and the usual definition of a retarded dielectric constant. The retarded dielectric constant is defined by adding to the system an external charge density ρ_{ex} which produces an internal charge density ρ_{in} , and relating the 4-dimensional Fourier transforms of these charge densities by

$$\rho_{\text{total}}(q) = \rho_{\text{ex}}(q) + \rho_{\text{in}}(q) = \frac{1}{\kappa_r(q)} \rho_{\text{ex}}(q) \quad ,$$

or equivalently by

$$\rho_{\text{in}}(q) = \left(\frac{1}{\kappa_r(q)} - 1 \right) \rho_{\text{ex}}(q) \quad (5.48)$$

Since the external charge is turned on adiabatically from time $(-\infty)$ to time 0, the perturbation H' is

$$H'(t') = \int d^3 r \int d^3 r' \psi^\dagger(rt') \psi(rt') V_2(r-r') \rho_{\text{ex}}(r't') \quad (5.49)$$

To first order in H' , the state vector of the perturbed system is

$$|\Psi(t)\rangle = \left\{ 1 - i \int_{-\infty}^t dt' H'(t') \right\} |\Psi_0\rangle \quad (5.50)$$

(Here we work in the interaction representation, which coincides with the Heisenberg representation at time 0.) The expectation value of the induced charged density is

$$\rho_{\text{int}}(r,t) = \langle \Psi | \psi^\dagger(rt) \psi(rt) | \Psi \rangle - \langle \Psi_0 | \psi^\dagger(rt) \psi(rt) | \Psi_0 \rangle \quad (5.51)$$

Inserting (5.49) and (5.50) into (5.51) and neglecting second-order terms, we have

$$\rho_{in}(r_1, t) = i e^2 \int_{-\infty}^t dt' e^{\eta t'} \iint d^3 r d^3 r' \frac{\rho_{ex}(r', t')}{|r_1 - r'|} \langle \Psi_0 | [\rho(r_1, t'), \rho(r, t)] | \Psi_0 \rangle . \quad (5.52)$$

Taking $\tau = t - t'$ and the 3-momentum Fourier transform, we have

$$\begin{aligned} \rho_{in}(q, \tau) &= \rho_{ex}(q, \tau) i \frac{4\pi e^2}{q^2} e^{-\eta \tau} \langle \Psi_0 | [\rho(-q, \tau), \rho(q, 0)] | \Psi_0 \rangle , \text{ for } \tau > 0 \\ &= 0, \text{ for } \tau < 0 . \end{aligned} \quad (5.53)$$

The quantity in brackets on the right-hand side of (5.53) is similar to the propagator in (5.47), but we have here the commutator instead of the time-ordered product. To see the connection between the two expressions, we introduce a Lehman spectral representation of the time Fourier transforms of (5.53) and of (5.47). From (5.53) we obtain

$$\frac{1}{\kappa_r(q, q_0)} - 1 = \frac{4\pi e^2}{q^2} \sum_n |(\rho_q)_{no}|^2 \left\{ \frac{1}{q_0 + \omega_{no} + i\eta} - \frac{1}{q_0 - \omega_{no} + i\eta} \right\}, \quad (5.54)$$

where $(\rho_q)_{no}$ is the matrix element of ρ_q between the ground state of the system and the n^{th} excited state, and ω_{no} is the excitation energy for the n^{th} excited state. Introducing the spectral densities in the interval $\omega < \omega_{no} < \omega + d\omega$,

$$\begin{aligned} F(q, \omega) &= \frac{4\pi e^2}{q^2} \sum_{no} |(\rho_q)_{no}|^2 \quad \text{for } \omega > 0 \\ &= -F(q, \omega) \quad \text{for } \omega < 0 , \end{aligned}$$

we can write (5.54) as

$$\frac{1}{\kappa_r(q, q_0)} - 1 = \int_{-\infty}^{\infty} \frac{F(q, \omega)}{q_0 - \omega + i\eta} d\omega = \int_{C_r} \frac{F(q, \omega)}{q_0 - \omega} d\omega . \quad (5.55)$$

The contour C_r is a straight line just below the real axis in the complex ω -plane as shown in the following figure:

Expression (5.54), or its equivalent (5.55), is the Kramers-Heisenberg dispersion formula.

The Lehman spectral representation of (5.47) differs from (5.55) only in the contour of integration, which is now just above the real axis for $\omega < 0$ and just below for $\omega > 0$, as shown below.

Since all excitation energies at zero temperature are positive, $\omega_{no} > 0$, $\kappa_r(q, q_0)$, and $\kappa_t(q, q_0)$ are identical for $q_0 > 0$. For $q_0 < 0$, the functions are complex conjugates. In passing, we note that the longitudinal sum

rule $\sum \omega_{no} |(\rho_q)_{no}|^2 = \frac{nq^2}{2m}$ holds.

H. Ground State Energy of the Fermi Gas

An expression for the ground state interaction energy may be obtained by integrating (5.47) over q_0 :

$$\begin{aligned}
\int_{-\infty}^{\infty} \left(\frac{1}{\kappa(q)} - 1 \right) \frac{dq_0}{2\pi} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iq_0\tau} \frac{dq_0}{(2\pi)} \langle 0 | T \left\{ \rho_{-q}(-\tau) \rho_q(0) \right\} | 0 \rangle d\tau \\
&= -iV_q \langle 0 | \rho_{-q}(0) \rho_q(0) | 0 \rangle .
\end{aligned} \tag{5.56}$$

Therefore we have

$$\begin{aligned}
\frac{1}{2} \sum_q V_q \langle 0 | \rho_{-q} \rho_q | 0 \rangle &= -\frac{1}{2} \sum_q \int_{-\infty}^{\infty} \text{Im} \left(\frac{1}{\kappa(q)} \right) \frac{dq_0}{2\pi} \\
&= -\frac{1}{2} \int \frac{d^4q}{(2\pi)^4} \text{Im} \frac{1}{\kappa(q)} ,
\end{aligned} \tag{5.57}$$

where we have used the fact that the left-hand side is manifestly real. However,

$$V_2 = \frac{1}{2} \sum_q' V_q \sum_{p,p'} c_{p+q}^\dagger c_{p'-q}^\dagger c_{p'} c_p = \frac{1}{2} \sum_q V_q \left\{ \rho_{-q} \rho_q^{-n} \right\} ,$$

where n is the number of fermions in the system. Thus,

$$\langle 0 | V_2 | 0 \rangle = -\frac{1}{2} \int \frac{d^4q}{(2\pi)^4} \text{Im} \frac{1}{\kappa(q)} - \frac{n}{2} \int \frac{d^3q}{(2\pi)^3} V_q . \tag{5.58}$$

A theorem of Pauli states that the ground state energy E of an interacting system is given in terms of a coupling constant integral by

$$E = E_0 + \int_0^1 \langle 0, \lambda | \lambda V_2 | 0, \lambda \rangle d\lambda , \tag{5.59}$$

where we write

$$H(\lambda) = H_0 + \lambda V_2$$

and $|0, \lambda\rangle$ is the ground state for coupling constant λ :

$$H(\lambda) |0, \lambda\rangle = E(\lambda) |0, \lambda\rangle .$$

The energy E_0 is the ground state energy of H_0 . Thus, we finally obtain the expression

$$E = E_0 - \frac{1}{2} \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d^3q}{(2\pi)^3} \left\{ \int_{-\infty}^{\infty} \frac{dq_0}{2\pi} \operatorname{Im} \frac{1}{\kappa(q, \lambda)} + \frac{n\lambda}{\lambda} V_q \right\} \quad (5.60)$$

Thus, a knowledge of the frequency- and wave-vector-dependent "dielectric constant" for all values of coupling constant suffices to determine the ground state energy. This is the result of Nozieres and Pines, and is often a convenient form for calculational purposes. Equation (5.60) can be written in a simpler form by using for the dielectric constant the expression (5.44) with $V_q = (4\pi e^2/q^2)\lambda$. The integral on λ can then be performed and the ground state energy is given by Hubbard's formula:

$$E = E_0 - \frac{1}{2} \left[+ \int \frac{d^3q}{(2\pi)^3} \frac{4\pi e^2}{q^2} - \int \frac{d^3q}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{dq_0}{2\pi} \operatorname{tg}^{-1} \frac{\kappa_2(q, q_0)}{\kappa_1(q, q_0)} \right] \quad (5.61)$$

In (5.61), κ_1 and κ_2 are the real and imaginary parts of the dielectric constant, respectively.

References to Chapter V

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VI. HIGH-DENSITY ELECTRON GAS

A. Discussion of the Hartree-Fock Approximation

We consider a free electron gas consisting of n electrons in a unit volume. Further, we assume there is a uniform background of total positive charge which makes the net charge of the system zero. The Hamiltonian is

$$H = \sum_{\mathbf{k}, s} \epsilon_{\mathbf{k}} n_{\mathbf{k}, s} + \frac{1}{2} \sum_{\mathbf{q} \neq 0} V_{\mathbf{q}} (\rho_{\mathbf{q}}^{\dagger} \rho_{\mathbf{q}} - n) \quad \left(V_{\mathbf{q}} = \frac{4\pi e^2}{q^2} \right) \quad (6.1)$$

We have introduced the spin variable $s = \pm \frac{1}{2}$ and the appropriate generalization of the field operators:

$$\begin{aligned} n_{\mathbf{k}s} &= c_{\mathbf{k}s}^{\dagger} c_{\mathbf{k}s} \\ \rho_{\mathbf{q}} &= \sum_{\mathbf{k}, s} c_{\mathbf{k}s}^{\dagger} c_{\mathbf{k}+\mathbf{q}, s} \end{aligned} \quad (6.2)$$

Due to translational invariance, the Hartree-Fock ground state is simply the Fermi sea Φ_0 :

$$\begin{aligned} c_{\mathbf{k}s}^{\dagger} |\Phi_0\rangle &= 0 & \mathbf{k} < \mathbf{k}_F \\ c_{\mathbf{k}s} |\Phi_0\rangle &= 0 & \mathbf{k} > \mathbf{k}_F \end{aligned} \quad (6.3)$$

The ground state energy is given in the Hartree-Fock approximation by

$$\begin{aligned} E_{H-F} &= \langle \Phi_0 | H | \Phi_0 \rangle = 2 \sum_{|\mathbf{k}| < k_F} \epsilon_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{q} \neq 0} V_{\mathbf{q}} [2f_{\mathbf{k}}(1-f_{\mathbf{k}+\mathbf{q}}) - n] \\ &= \frac{3}{5} n E_F - \sum_{\mathbf{q} \neq 0} V_{\mathbf{q}} f_{\mathbf{k}} f_{\mathbf{k}+\mathbf{q}} \end{aligned} \quad (6.4)$$

where $f_{\mathbf{k}} = \begin{cases} 1 & |\mathbf{k}| < k_F \\ 0 & |\mathbf{k}| > k_F \end{cases}$. The first term gives the kinetic energy in terms of the Fermi energy

$$E_F = \hbar^2 k_F^2 / 2m \quad ,$$

and $n = k_F^3 / 3\pi^2$. The second term, called the exchange energy, reduces the energy relative to the Hartree result $\frac{3}{5} n E_F$ due to electrons of parallel spin being kept apart by the exclusion principle. Physically, one can think

of each electron at a given point in space being surrounded by a local depletion of electrons of the same spin, this "hole" being called the "exchange hole."

It is convenient to introduce the parameter r_s by the equation

$$\frac{4\pi r_s^3 a_0^3}{3} = \frac{1}{n} \quad ,$$

where

$$a_0 = \hbar^2/me^2 \equiv \text{Bohr radius} \quad .$$

Then

$$k_F = \frac{1.92}{r_s a_0} \quad \left(1.92 = \pi \left(\frac{3}{2\pi}\right)^{2/3}\right)$$

$$E_F = \frac{3.70 \xi_0}{r_s^2} \quad ; \quad \xi_0 = \frac{e^2}{2a_0} \equiv \text{Rydberg} \quad .$$

The Hartree-Fock energy is given by

$$E_{H-F} = \frac{2.21 n \xi_0}{r_s^2} - \frac{0.916 n \xi_0}{r_s} \quad , \quad (6.5)$$

where the exchange term is obtained by replacing the sums over k and q in equation (6.4) by the corresponding integrals and performing the integrations.

This result suggests that in the high-density limit ($r_s \ll 1$) the Coulomb interactions should have a small relative effect on the ground state energy so that one might hope to use perturbation theory in this limit. This is more clearly seen by writing the Hamiltonian in reduced units. By setting $r = (r_s a_0) r'$ we have in configuration space

$$\frac{H}{\xi_0} = \frac{2}{r_s^2} \left(\sum_i \frac{P_i'^2}{2m} + r_s \sum_{i \neq j} \frac{1}{|r_{ij}'|} \right) \quad .$$

Thus, we expect the ground state energy to be expressed as

$$E_0 = n \xi_0 \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + B \log r_s + C r_s \log r_s + \dots \right) \quad , \quad (6.6)$$

with the dots indicating terms involving powers of r_s times powers of $\log r_s$. Why $\log r_s$ terms enter rather than a simple power series in r_s will be clear shortly.

A serious difficulty with the Hartree-Fock approximation in this problem is that the exchange energy leads to a vanishing density of single-particle states at the Fermi surface. This leads to a vanishing electronic specific heat rather than a specific heat proportional to T , as for the free electron gas. This result is easily traced to the long-range contribution of the Coulomb potential in the exchange energy. As we will see, an improved calculation leads to a screening of the Coulomb potential entering the exchange energy, and one obtains reasonable results for the density of states once again.

If we try to calculate corrections to Hartree-Fock by a perturbation technique based on Hartree-Fock states, we find a divergent result already in second order. The divergent term arises from particles in states k and $-p$ making a virtual transition to states $k+q$ and $-p-q$, respectively, and then returning to their initial states. This leads to the direct scattering contribution:

$$E_d^{(2)} = - \sum_q \sum_{\substack{|k+q| > k_F \\ |p+q| < k_F \\ |k| < k_F \\ |p| < k_F}} 2V_q^2 \frac{1}{\epsilon_{k+q} + \epsilon_{p+q} - \epsilon_k - \epsilon_p} , \quad (6.7)$$

which is divergent because $V_q = 4\pi e^2/q^2$ becomes infinite as $q \rightarrow 0$.

The second-order exchange contribution $E_{ex}^{(2)}$ is given by

$$E_{ex}^{(2)} = \sum_q \sum_{\substack{|k+q| > k_F \\ |p+q| > k_F \\ |k| < k_F \\ |p| < k_F}} V_q V_{q+k+p} \frac{1}{\epsilon_{k+q} + \epsilon_{p+q} - \epsilon_k - \epsilon_p} . \quad (6.8)$$

This term is finite because one of the singular matrix elements V_q in $E_d^{(2)}$ is replaced by V_{q+k+p} .

B. Random Phase Approximation in the Polarization Propagator

To get around this difficulty, Bohm and Pines introduced new variables in the problem, which are essentially the longitudinal electric field and vector potential for wave vectors q less than some cut-off k_C . By what is essentially a dynamical self-consistent field approximation, they were able to remove the singularities in the expression for the energy and obtain reasonable values for the electronic specific heat, etc.

A somewhat more complete treatment of this problem was given by Gell-Mann and Brueckner, who made a partial summation of infinite-order perturbation theory keeping the most divergent terms in each order. Their results for the ground state energy are nearly those of Bohm and Pines. Sawada derived the Gell-Mann-Brueckner results by a linearization of the field equations for operators of the form $c_{k+q}^\dagger c_{ks}$. As we will see, the linearization is essentially a time-dependent generalization of the Hartree scheme.

The general idea of this "random phase approximation," or time-dependent Hartree scheme, is to select those terms in n^{th} -order perturbation theory with the largest number of factors V_q , where q is a single momentum transfer handed from one electron-hole pair to another.

If we use the relation between the dielectric constant $\kappa(q)$ and the ground state energy, this approximation corresponds to keeping only the term

$$P_0(q) = \text{diagram}$$

in the irreducible polarization propagator. That this in fact corresponds to the approximation of piling up V_q as in the Gell-Mann-Brueckner summation is seen by noting that the ground state energy expression

$$E = \frac{3}{5} nE_F - \frac{1}{2} \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d^4q}{(2\pi)^4} \text{Im} \frac{1}{\kappa(q, \lambda)}$$

involves a summation over contributions each arising from a given wave q . Since

$$\frac{1}{\kappa(q, \lambda)} = \frac{1}{1 + i\lambda V_q P(q)} = 1 - i\lambda V_q P(q) + [i\lambda V_q P(q)] [i\lambda V_q P(q)] + \dots,$$

we see that E involves the imaginary part of the series

which describes a fixed momentum transfer q being passed from one particle-hole pair to the next, as required.

By using the rules for diagrams in momentum space, we have

$$P_0(q) = (-1)2 \int \frac{d^4p}{(2\pi)^4} [-iG_0(p+q)] [-iG_0(p)] \quad , \quad (6.9)$$

where the factor two arises from the sum over 2 spin directions in the closed loop. Inserting the expressions for $G_0(p)$, we find

$$P_0(q) = 2 \int \frac{d^4p}{(2\pi)^4} \frac{1}{(p_0 + q_0 - \epsilon_{p+q} + i\eta_{p+q})} \frac{1}{(p_0 - \epsilon_p + i\eta_p)} \quad (6.10)$$

$$\text{with } \eta_p = \begin{cases} 0^+ & \text{for } p > p_F \\ 0^- & \text{for } p < p_F \end{cases} .$$

In performing the p_0 integral there are three possible cases:

a) If both $\vec{p}$ and $\vec{p} + \vec{q}$ are on the same side of the Fermi surface, then both poles are on the same side of the real axis. If the contour on the opposite side of the real axis is closed, we see that the integral vanishes.

b) If $\vec{p}$ is below and $\vec{p} + \vec{q}$ is above the Fermi surface, by closing the contour above we get a contribution

$$+ 2i \int \frac{d^3p}{(2\pi)^3} \frac{f_p(1-f_{p+q})}{q_0 + \epsilon_p - \epsilon_{p+q} + i\eta} \quad (\eta = 0^+) \quad (6.11)$$

$$\text{where } f_p = \begin{cases} 1 & p < p_F \\ 0 & p > p_F \end{cases} .$$

c) If $\vec{p}$ is above and $\vec{p} + \vec{q}$ is below the Fermi surface, we close below and obtain

$$-2i \int \frac{d^3p}{(2\pi)^3} \frac{f_{p+q}(1-f_p)}{q_0 + \epsilon_p - \epsilon_{p+q} - i\eta} \quad (\eta = 0^+) \quad (6.12)$$

Thus we have

$$P_0(q, q_0) = 2i \int \frac{d^3p}{(2\pi)^3} \left[\frac{f_p(1-f_{p+q})}{q_0 + \epsilon_p - \epsilon_{p+q} + i\eta} - \frac{f_{p+q}(1-f_p)}{q_0 + \epsilon_p - \epsilon_{p+q} - i\eta} \right] \quad (6.13)$$

which can also be written as

$$P_0(q, q_0) = +2i \int \frac{d^3p}{(2\pi)^3} f_p(1-f_{p+q}) \left\{ \frac{1}{q_0 - (\epsilon_{p+q} - \epsilon_p) + i\eta} - \frac{1}{q_0 + (\epsilon_{p+q} - \epsilon_p) - i\eta} \right\} \quad (6.14)$$

The real and imaginary parts of $\kappa(q, q_0)$ defined by

$$\kappa(q, q_0) = 1 + iV_q P(q, q_0) \equiv \kappa_1 + i\kappa_2$$

can be immediately obtained by separating the integration in (6.14) into a delta function and a principal part integral as done in Chapter IV. The result is

$$\kappa_1(q, q_0) = 1 - 2V_q P \int \frac{d^3p}{(2\pi)^3} f_p(1-f_{p+q}) \frac{2(\epsilon_{p+q} - \epsilon_p)}{q_0^2 - (\epsilon_{p+q} - \epsilon_p)^2} \quad (6.15)$$

where P indicates that a principal value integral is to be performed and

$$\kappa_2(q, q_0) = 2\pi V(q) \int \frac{d^3p}{(2\pi)^3} f_p(1-f_{p+q}) [\delta(q_0 - \epsilon_{p+q} + \epsilon_p) + \delta(q_0 + \epsilon_{p+q} - \epsilon_p)] \quad (6.16)$$

The integrations in (6.15) and (6.16) are elementary and straightforward, but a bit tedious. One obtains explicit expressions for the real and imaginary parts of the dielectric constant first given by Lindhart:

$$\kappa_1(q, q_0) = 1 + 2 \frac{e^2 m k_F}{\pi q^2} \left\{ 1 + \frac{1}{2} \frac{k_F}{q} \left[1 - \left(\frac{mq_0}{q k_F} + \frac{q}{2 k_F} \right)^2 \ln \left| \frac{1 + \left(\frac{mq_0}{q k_F} + \frac{q}{2 k_F} \right)}{1 - \left(\frac{mq_0}{q k_F} + \frac{q}{2 k_F} \right)} \right| \right] - \frac{1}{2} \frac{k_F}{q} \left[1 - \left(\frac{mq_0}{q k_F} - \frac{q}{2 k_F} \right)^2 \ln \left| \frac{1 + \left(\frac{mq_0}{q k_F} - \frac{q}{2 k_F} \right)}{1 - \left(\frac{mq_0}{q k_F} - \frac{q}{2 k_F} \right)} \right| \right] \right\} \quad (6.15a)$$

and

$$\kappa_2(q, q_0) = \begin{cases} 0 & \text{when } 2mq_0 > q^2 + 2qk_F \\ 0 & \text{when } q > 2k_F \text{ and } 2mq_0 < q^2 - 2qk_F \\ + 2e^2 m^2 \frac{q_0}{q^3} & \text{when } q < 2k_F \text{ and } 2mq_0 < |q^2 - 2qk_F| \\ + \frac{e^2 m k_F^2}{q^3} \left\{ 1 - \left(\frac{mq_0}{q k_F} - \frac{q}{2 k_F} \right)^2 \right\} & \text{when } |q^2 - 2qk_F| < 2mq_0 < |q^2 + 2qk_F| \end{cases} \quad (6.16a)$$

By expressing the quantities in equations (6.15a) and (6.16a) in terms of $x = q/k_F$ and $y = q_0/\epsilon_F$, where $\epsilon_F = k_F^2/2m$, one can show that $\kappa_1 - 1$ and κ_2 are proportional to the quantity $0.33 r_s$, where r_s is the radius in Bohr units of a sphere whose volume is equal to the volume per electron. Thus the random phase approximation includes only the terms for which $\kappa_1 - 1$ and κ_2 are linear in r_s , and at large electron densities this is an accurate approximation.

For $q_0 = 0$, formula (6.16) gives $\kappa_2(q, 0) = 0$ and the static dielectric constant $\kappa_1(q, 0)$ is given by

$$\kappa_1(q, 0) = 1 + 0.66 r_s \left(\frac{k_F}{q} \right)^2 u(q/2k_F) \quad , \quad (6.17)$$

where

$$u(x) = \frac{1}{2} \left[1 + (2x)^{-1} (1-x^2) \ln \left| \frac{1+x}{1-x} \right| \right] \quad . \quad (6.18)$$

The important characteristics of $u(x)$ are that:

- a) $u(\infty) = 0$, so that $\kappa_1 \simeq 1$.
 $q \rightarrow \infty$

b) $u(1) = \frac{1}{2}$, so that $\kappa \simeq 1 + 0.165 r_s$.
 $q \rightarrow 2k_F$

c) $u(0) = 1$, so that for $q \rightarrow 0$ one obtains the classical Thomas-Fermi result for the dielectric constant.

d) $\frac{du}{dq} \rightarrow \infty$ as $q \rightarrow 2k_F$.

The situation for $q_0 = 0$ is represented in the figure below, where the quantity $1/\kappa(q,0)$ as obtained from equations (6.17) and (6.18) is compared with the Thomas-Fermi result.

As pointed out by Kohn et al., $1/\kappa(q,0)$ has an infinite slope at $q = 2k_F$, which leads to the screened Coulomb potential being proportional to

$$\frac{\cos(2k_F r + \phi)}{r^3} \quad (6.19)$$

in the limit $k_F r \rightarrow \infty$, rather than to $e^{-\alpha r}/r$ as in the Thomas-Fermi approximation. There now appears to be good experimental support for these corrections to the Thomas-Fermi approximation which arise from the sharpening of the Fermi surface.

For $q_0 \neq 0$ we notice that the imaginary part of the dielectric constant is different from zero only when q_0 and q are so related that it is possible to satisfy the conditions imposed by the delta functions in (6.16), that is to say when

$$q^2 - 2qk_F < q_0^2 < q^2 + 2qk_F \quad .$$

The situation is illustrated in the following figure where a function $q_0(q)$ is also indicated for which $\kappa_1 = 0$.

For large frequency, that is, $q_0 \gg q^2 + 2qk_F/2m$, and small q , we have $\kappa_2 = 0$ and one obtains from (6.16a):

$$\kappa_1(q, q_0) = 1 - \frac{\omega_p^2}{q_0^2}, \quad (6.20)$$

where $\omega_p = \sqrt{4\pi n e^2/m}$ is the classical electron plasma frequency.

From the integral representation for $1/\kappa(q)$ we see that a pole of $1/\kappa(q)$ corresponds to the existence of a physical excitation of the system. Thus for $q_0 = \omega_p$ we find the plasmon collective excitation. As q increases, the plasmon frequency slightly increases, as indicated in the figure, and then for sufficiently large q the plasmons are damped by the electron-hole pairs which exist in the region where $\kappa_2 \neq 0$, so that they are no longer well-defined elementary excitations of the system.

One can now insert the RPA expression for $\kappa(q)$ into the ground state energy expression (5.61) and obtain E . One then finds the correlation energy is given by the Gell-Mann-Brueckner result:

$$E_c \equiv E_0 - E_{H-F} = 0.0622 \ln r_s - 0.096 + O(r_s) \quad .$$

The electronic specific heat, relative to that for a noninteracting Fermi gas of the same density, is

$$C/C_F = [1 + 0.0833 r_s(-\ln r_s - 0.203) + \dots]^{-1} .$$

C. Linearized Equation Method for the RPA.

As Sawada and Sawada, Brueckner, Fukuda and Brout have shown, the same results can be obtained from the equations of motion for the field operators. Consider the operator

$$\rho_{ks}^\dagger(q) = c_{k+qs}^\dagger c_{ks} ,$$

in the Heisenberg representation. The time rate of change of this operator is given by

$$[H, \rho_{ks}^\dagger(q)] = \nu_k(q) \rho_{ks}^\dagger(q) + [V, \rho_{ks}(q)] ,$$

where $\nu_k(q) = \epsilon_{k+q} - \epsilon_k$. The commutator of V with ρ will involve a product of four fermion operators. To find the operators $\mu_\alpha^\dagger(q)$ which create excited states of the system we require

$$[H, \mu_\alpha^\dagger(q)] = \Omega_\alpha(q) \mu_\alpha^\dagger(q) , \quad (6.24)$$

where $\Omega_\alpha(q)$ is the excitation energy of the α^{th} state. It is clear that neither $\rho_{ks}(q)$ nor any linear combination of these operators can form eigenoperators $\mu_\alpha^\dagger(q)$ of the full equations of motion. The random phase approximation corresponds to linearizing the equations of motion by replacing a product of two operators $c_{ks}^\dagger c_{ks}$ occurring in the $[V, \rho]$ commutator by its expectation value in the Fermi sea. We then obtain

$$[H, \rho_{ks}^\dagger(q)] = \nu_k(q) \rho_{ks}^\dagger(q) + V(q)(f_k - f_{k+q}) \sum_{k', s'} \rho_{k', s'}(q) , \quad (6.25)$$

where

$$\langle \Phi_0 | c_{ks}^\dagger c_{ks} | \Phi_0 \rangle \equiv f_k = \begin{cases} 1 & k < k_F \\ 0 & k > k_F \end{cases} .$$

Notice that, after linearization, only a single momentum transfer q enters. The full V - ρ commutator involves both q and an arbitrary wave vector q' . The random phase approximation corresponds to neglect of correlations introduced by couplings between different q 's.

The linearized equations are easily solved to give the dispersion relation

$$1 = 2V(q) \sum_k \frac{f_k - f_{k+q}}{\Omega_\alpha(q) - \nu_k(q)} = 4V(q) \sum_k \frac{f_k}{\Omega_\alpha^2(q) - \nu_k^2(q)} \quad (6.26)$$

for the frequencies $\Omega_\alpha(q)$. If we work in a finite box, one root $\Omega_\alpha(q)$ of the dispersion relation sits between each unperturbed level $\nu_k(q)$. These correspond to the scattering eigenstates of a particle-hole pair. There will be a "bound" state split off from the continuum which corresponds to the plasmon mode, as is seen below.

Knowing the eigenfrequencies, we can find the transformation relating the eigenoperators $\mu_\alpha^\dagger(q)$ and the operators $\rho_{ks}^\dagger(q)$, say

$$\rho_{ks}^\dagger(q) = \sum_\alpha \left\{ f_{k\alpha}(q) \mu_\alpha^\dagger(q) + g_{k\alpha}(q) \mu_\alpha(-q) \right\} \quad (6.27)$$

The ground state interaction energy is then given by use of the fact that

$$\mu_\alpha(q)|0\rangle \equiv 0$$

for all α and q . That is, $|0\rangle$ is the vacuum for the excitations created by $\mu_\alpha^\dagger(q)$. In this way, one can obtain the results of the RPA for E . This equation of motion approach is a most useful alternative to the Green's function scheme, as we shall see in the case of the superconductor.

References to Chapter VI

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VII. THEORY OF SUPERCONDUCTIVITY

To illustrate other systems in which non-perturbative results have been obtained through the use of field theoretic methods, we consider an idealized model of a superconducting metal.

For simplicity, consider a system of unit volume containing n electrons which interact via a two-body potential which, in practice, is considered to arise from the Coulomb interaction and an effective potential due to virtual exchange of phonons. The latter is known to be attractive for sufficiently small energy transfer and large momentum transfer in the 4-point vertex.

A. The Pairing Interaction

We now know the superconducting state differs from the so-called normal state in that there exist long-range correlations between particles of opposite spin and momentum. These long-range correlations lead to a gap in the single-particle excitation and to flow properties of the electron assembly which is characteristic of a superfluid. To see how these pairing correlations come about, we consider the transition amplitude for a pair of particles with zero center of mass momentum and opposite spin, defined by

$$(p', -p' | t_{q_0} | p, -p) = (p', -p' | V | p, -p) + i \int \frac{d^4 p''}{(2\pi)^4} (p', -p' | V | p'', -p'') G_0(p'' + q) G_0(-p'') (p'', -p'' | t_{q_0} | p, -p) \quad , \quad (7.1)$$

or, diagrammatically by

$$\left(\begin{array}{c} p' \leftarrow \\ -p' \leftarrow \end{array} \right| \boxed{t} \left| \begin{array}{c} p \leftarrow \\ -p \leftarrow \end{array} \right. = \begin{array}{c} p' \leftarrow \quad \quad \quad p \\ -p' \leftarrow \quad \quad \quad -p \end{array} \quad + \quad \begin{array}{c} p' \leftarrow \quad \quad \quad p'' \\ -p' \leftarrow \quad \quad \quad -p'' \end{array} \left| \boxed{t} \left| \begin{array}{c} p \leftarrow \\ -p \leftarrow \end{array} \right. \right) \quad .$$

If we approximate V by a factorizable potential,

$$(p', -p' | V | p, -p) = \lambda w_p^* w_p \quad . \quad (7.2)$$

It is straightforward to show that t is given by

$$(p', -p' | t_{q_0} | p, -p) = \frac{\lambda w_p^* w_p}{1 + \lambda \phi(q_0)} \quad , \quad (7.3)$$

where

$$\phi \equiv -i \int |w_{p''}|^2 G_0(p''+q) G_0(-p'') \frac{d^4 p''}{(2\pi)^4} \quad (7.4)$$

Here, $q \equiv (\vec{q}, q_0) = (0, q_0)$ is the 4-momentum of the pair, that is, q_0 is the energy of the pair. By inserting the explicit form of $G_0(p)$

$$G_0(p) = \frac{-1}{p_0 - \epsilon_p + i\eta_p} \quad \eta_p = \begin{cases} 0^+ & p > p_F \\ 0^- & p < p_F \end{cases},$$

we find on integrating over p_0'' that

$$\phi(q_0) = - \left\{ \int_{|p''| > p_F} \frac{|w_{p''}|^2 d^3 p''}{q_0 - 2\epsilon_{p''} (2\pi)^3} - \int_{|p''| < p_F} \frac{|w_{p''}|^2 d^3 p''}{q_0 - 2\epsilon_{p''} (2\pi)^3} \right\} \quad (7.5)$$

If the system is in a finite box, as we have assumed, the momentum integration is actually to be replaced by a sum

$$\int \frac{d^3 p''}{(2\pi)^3} \rightarrow \sum_{p''}$$

The function $-\phi(q_0)$ is plotted below.

The poles of t give the energies of the two-particle system, that is, the energies Ω_α are given by

$$1/\lambda = -\phi(\Omega_\alpha) \quad . \quad (7.6)$$

For a repulsive potential between particles, all solutions Ω_α are real. For $\lambda < 0$ but small, two more roots are picked up, as is seen in the diagram. A critical value of coupling is reached, however, depending upon the volume of the system, beyond which the two extra real poles degenerate into a pair of purely imaginary poles $\pm i\alpha$. This indicates an instability of the system, since the amplitude for creating a pair of opposite spin and momentum will increase exponentially with time. In the limit of a large volume, λ_c goes to zero and a system with attractive interactions is then unstable regardless of how weak the interaction is. It is straightforward to show that the difficulty persists even for center-of-mass momentum not equal to zero, although the growth rate of the instability decreases with increasing q .

It is clear that the difficulty arises from our simplified choice of single-particle Green's functions, namely, $G_0(p)$, appropriate to the noninteracting system. Somehow, we must seek a G which includes the fact that the system has undergone a pair-like condensation, and the G 's describe excitations from this new stable state.

If we work at finite temperature with Green's functions defined as

$$G^\beta(p, \tau) = i \text{Tr} \left[e^{-\beta(H - \mu n)} T \left\{ c_p(\tau) c_p^\dagger(0) \right\} \right] / \text{Tr} \left[e^{-\beta(H - \mu n)} \right] \quad , \quad (7.7)$$

then the perturbation expansion involves zero-order Green's functions:

$$G_0^\beta(p, p_0) = \frac{-f_p}{p_0 - \epsilon_p - i\eta} - \frac{(1-f_p)}{p_0 - \epsilon_p + i\eta} \quad , \quad (7.8)$$

where f_p is the Fermi function

$$f_p = \frac{1}{\exp \beta \epsilon_p + 1} \quad ,$$

and we have measured ϵ_p relative to the chemical potential μ . Inserting this expression for G_0^β , we find

$$\phi^\beta(q_0) = - \sum_p \frac{|w_p|^2 \tanh\left(\frac{1}{2} \beta \epsilon_p\right)}{q_0 - 2\epsilon_p} \quad . \quad (7.9)$$

For $\beta \rightarrow \infty$, that is, $T \rightarrow 0$, we recover our expression derived for $T = 0$. For $T \neq 0$, the effect of the $\tanh$ factor is to decrease the magnitude of $\phi(q)$ for a given value of q_0 . For a particular value of $\lambda < 0$, there will be a temperature $kT_c = 1/\beta_c$ above which the instability vanishes. This critical temperature is determined by

$$\frac{1}{|\lambda|} = \sum_p \frac{|w_p|^2}{2\epsilon_p} \tanh\left(\frac{1}{2} \beta_c \epsilon_p\right) \quad (7.10)$$

It is interesting to note that the above expression for T_c is identical with that given by the BCS theory of superconductivity when applied to this simplified problem.

We shall return later to the role played by finite lifetime effects in $G(p)$, that is, taking into account the imaginary part of $\Sigma(p)$.

B. Linearized Equations of Motion

One of the simplest methods for resolving the instability problem is to consider the equation of motion for $c_{k\uparrow}^\dagger$:

$$[H, c_{k\uparrow}^\dagger] = c_k c_{k\uparrow}^\dagger + \sum_{p,q,s} c_{k-q\uparrow}^\dagger c_{p+q,s}^\dagger c_{p,s} (k-q, p+q | V | k, p) \quad (7.11)$$

We actually work with $H - \mu n$ and absorb the chemical potential μ into ϵ_k . This procedure gives us the freedom of working with states which are superpositions of components describing different numbers of particles.

We now linearize with respect to a state $|0\rangle$ which is to be obtained in a self-consistent manner by requiring it to be the vacuum for excitation created by the normal mode operators $\gamma_{ks}^\dagger$ of the linearized equations. In the linearization we will include the Hartree-like field

$$\chi_k \equiv \langle 0 | c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger | 0 \rangle \quad (7.12)$$

$$\chi_k^* = \langle 0 | c_{-k\downarrow} c_{k\uparrow} | 0 \rangle \quad .$$

A more general linearization would involve

$$h_k \equiv \langle 0 | c_{ks}^\dagger c_{ks} | 0 \rangle \quad ,$$

which we neglect for simplicity. With this linearization we find

$$[H, c_{k\uparrow}^\dagger] = \epsilon_k c_{k\uparrow}^\dagger + \sum_{k'} V_{kk'} \chi_{k'} c_{-k\downarrow}$$

and

$$[H, c_{-k\downarrow}] = -\epsilon_k c_{-k\downarrow} + \sum_{k'} V_{k'k} \chi_{k'}^* c_{k\uparrow}^\dagger$$

where $V_{k,k'} = \langle k', -k' | V | k, -k \rangle$. A normal coordinate transformation to the eigenoperator $\gamma_{ks}^\dagger$ satisfying

$$[H, \gamma_{ks}^\dagger] = E_k \gamma_{ks}^\dagger \quad (7.14)$$

is straightforward. One finds

$$\begin{aligned} c_{k\uparrow}^\dagger &= u_k \gamma_{k\uparrow}^\dagger + v_k \gamma_{-k\downarrow} \\ c_{-k\downarrow}^\dagger &= u_k \gamma_{-k\downarrow}^\dagger - v_k \gamma_{k\uparrow} \end{aligned} \quad (7.15)$$

where

$$\begin{aligned} u_k^2 &= \frac{1}{2} (1 + \epsilon_k / E_k) \\ v_k^2 &= \frac{1}{2} (1 - \epsilon_k / E_k) \end{aligned} \quad (7.16)$$

and the excitation energy E_k is given by

$$E_k = +\sqrt{\epsilon_k^2 + |\Delta_k|^2} \quad (7.17)$$

The energy-gap parameter Δ_k satisfies the integral equation

$$\Delta_k = - \sum_{k'} V_{kk'} \chi_{k'} = - \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \quad (7.18)$$

where the second equality follows from inserting the normal coordinate expressions for $c_{k\uparrow}^\dagger$ and $c_{-k\downarrow}^\dagger$ in the definition of χ_k and using the property of the quasi-particle vacuum $\gamma_{ks}|0\rangle \equiv 0$ for all k, s .

There always exists the trivial solution $\Delta_k = 0$. For certain potentials there are also nontrivial solutions. Since E_k involves Δ_k , the integral equation is nonlinear and can be solved exactly only for simple potentials, for example a factorizable potential

$$V_{kk'} = \lambda w_k^* w_{k'} \quad .$$

In this case one has

$$-\frac{1}{\lambda} = \sum_{\mathbf{k}'} \frac{|w_{\mathbf{k}'}|^2}{E_{\mathbf{k}'}} \quad , \quad (7.19)$$

which has a solution only for $\lambda < 0$, that is, for an attractive interaction between particles. The minimum excitation energy is then given by $2\Delta_{\mathbf{k}_F}$ since, as in the normal state, fermion excitations are created in pairs, in that case a particle and the associated hole. Here we speak of quasi particles and cannot distinguish particles and holes, since the operator $\gamma_{\mathbf{k}s}^\dagger$ is a linear combination of particle- and hole-creation operators. The normal mode transformation was introduced independently by Bogoliubov and by Valatin and, in many respects, gives a more convenient mathematical formalism for expressing the BCS theory than that used in the original exposition of the theory, although the schemes are mathematically equivalent. It is straightforward to show that the BCS ground state

$$|0\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |\theta\rangle$$

is just the quasi-particle vacuum introduced above, where $|\theta\rangle$ is the state with no electrons in the system, rather than the Fermi sea. The BCS excited states are just

$$|k_1 s_1 k_2 s_2 \dots k_n s_n\rangle = \gamma_{k_1 s_1}^\dagger \gamma_{k_2 s_2}^\dagger \dots \gamma_{k_n s_n}^\dagger |0\rangle \quad .$$

C. Finite Temperature Linearized Equations

At finite temperature, the Hartree field will be modified since the presence of quasi-particle excitations leads to a reduction in the available phase space for virtual transitions of pairs ($k\uparrow - k\downarrow$), and hence to a reduction in the pairing energy characterized by $\Delta_{\mathbf{k}}$. Thus, rather than the ground state expectation value, we introduce

$$\chi_{\mathbf{k}} = \text{Tr} \left\{ e^{-\beta H_{\mathbf{q.p.}}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \right\} / \text{Tr} e^{-\beta H_{\mathbf{q.p.}}} \quad , \quad (7.20)$$

where the full Hamiltonian is approximated by that part which is diagonalized by the normal mode transformation

$$H_{\mathbf{q.p.}} = \sum_{\mathbf{k},s} E_{\mathbf{k}} \gamma_{\mathbf{k}s}^\dagger \gamma_{\mathbf{k}s} \quad . \quad (7.21)$$

It follows as in the zero-temperature calculation that $\Delta_{\mathbf{k}}$ satisfies the integral equation

$$\Delta_k = - \sum_{k'} \frac{V_{kk'} \Delta_{k'}}{2E_{k'}} \tanh \left(\frac{\beta E_{k'}}{2} \right) \quad (7.22)$$

The only effect of finite temperature therefore is to insert the tanh factor in the $T = 0$ gap equation. As the temperature increases, Δ_k decreases and goes to zero at a critical temperature $kT_c \equiv 1/\beta_c$ which, in the case of the factorizable potential, satisfies

$$-\frac{1}{\lambda} = + \frac{1}{|\lambda|} = \sum_k \frac{|w_k|^2}{2|\epsilon_k|} \tanh \frac{\beta |\epsilon_k|}{2} \quad (7.23)$$

in agreement with the critical temperature derived from the pair instability discussion above. Thus we see that the transition temperature calculated from the theories appropriate to the normal and superconducting states agree.

D. Physical Interpretation of the Superconducting State

To gain physical insight into the above solutions, it is helpful to express the ground state wave function in configuration space. As Dyson pointed out, when $|0\rangle$ is projected onto the space of n particles it is of the form

$$\begin{aligned} \psi(\vec{r}_1 s_1, \vec{r}_2 s_2, \dots, \vec{r}_n s_n) = A[\phi(\vec{r}_1 - \vec{r}_2) \uparrow_1 \downarrow_2][\phi(\vec{r}_3 - \vec{r}_4) \uparrow_3 \downarrow_4] \dots \\ \dots [\phi(\vec{r}_{n-1} - \vec{r}_n) \uparrow_{n-1} \downarrow_n] \quad (7.24) \end{aligned}$$

where A is the antisymmetrization operator and the pair function ϕ satisfies

$$\phi(\vec{r}_{12}) = \sum_k \frac{v_k}{u_k} e^{ik \cdot \vec{r}_{12}} \quad (7.25)$$

The spin functions are denoted by $\uparrow_i$ and $\downarrow_i$. Notice that each pair of electrons is in the same pair function. Antisymmetrization cancels most of the correlations, as can be seen by noticing that the Fermi sea can be expressed in the above form with

$$\phi_F(\vec{r}_{12}) = \sum_{k < k_F} e^{ik \cdot \vec{r}_{12}} \quad (7.26)$$

Except for an unimportant normalization factor, v_k/u_k differs from the value appropriate to the normal state (1 for $k < k_F$, 0 for $k > k_F$) only in a region in energy $\sim 2\Delta \sim 10^{-3} E_F$ about the Fermi surface. The superconductor function ϕ has a range in coordinate space $\sim \xi_0 \equiv \pi \Delta / \hbar v_F \sim 10^{-4}$ cm, where v_F is the electron velocity at the Fermi surface. Since only those electrons within an energy $\sim \Delta$ of the Fermi surface are affected by the transition to the

superconducting state, we can say roughly that of the order of 10^{-3} of the electrons participate in pairing correlations, or roughly in a volume ξ_0^3 there are of the order 10^6 electrons strongly affected by the transition. It is clear, therefore, that a picture of well-isolated pairs is inappropriate and that there is strong overlap of pair functions. It is, in fact, this overlap of pairs which leads to the energy gap in the excitation spectrum of the superconductor. For, if there were little overlap, there would be a dense spectrum of boson excitations just above the ground state, corresponding to drifting of individual pairs. For a system with short-range forces there is, below the gap 2Δ , a continuous boson spectrum corresponding to a density fluctuation of the particles. This spectrum gives a very low density of states and is completely absent if one introduces the long-range Coulomb interaction, in which case the density fluctuations go over into plasma oscillations of energy ~ 10 - 20 ev.

The simple picture of ψ given by the product of pair functions is not to be taken literally. More precisely, the wave function should be thought of as being constructed from normal state-like configurations in which one has included all the correlations present in the normal state which lead to a correlation energy ~ 1 ev per electron. It is only the small residual interaction between the effective fermion excitations in the normal state which introduces the superconducting correlations, giving an added correlation energy of $\sim 10^{-8}$ ev per electron. These added correlations would be uninteresting except for the fact that they strongly affect electrons which take part in electrical conductivity, the magnetic properties, and the thermodynamic properties of the system.

The attractive potential required to give the superconducting state arises from virtual exchange of phonons between the electrons, in analogy with the attractive nucleon-nucleon potential being due to virtual exchange of mesons. One can think of the effective interaction as being due to the bare Coulomb interaction being reduced by the total frequency-dependent dielectric constant of the medium which can become negative if the 4-momentum transfer q at a vertex satisfies

$$q_0 < \omega_q \quad ,$$

where ω_q is the frequency of phonons of wave vector q . Roughly speaking, a virtual transition in which an electron goes from a state with 4-momentum p to a state with $p+q$ creates a charge-density fluctuation which is dynamically screened by the ions. The response of the ions is proportional to

$$\frac{1}{q_0^2 - \omega_q^2} \quad ,$$

so that as q_0 increases toward ω_q , the ions tend to overscreen the initiating charge-density fluctuation and the second electron sees a net positive charge and is attracted to the first electron. For $q_0 > \omega_q$, the ions respond out of phase with the electron and tend to increase, rather than decrease, the

interaction between electrons. The RPA expression for the total interaction is given by summing all bubble graphs for which the interaction line is the sum of the bare Coulomb interaction and the bare phonon interaction. Thus, for the bare potential we have

$$V(q) = V_c(q) - |g_q^0|^2 D_0(q) \simeq \frac{4\pi e^2}{q^2} + |g_q^0|^2 \frac{1}{q_0^2 - \omega_q^{02} + i\eta} \quad , \quad (7.27)$$

where g_q^0 and ω_q^0 are the bare phonon-electron matrix element and the bare phonon frequency, respectively. In real crystals, one must take account of umklapp processes by proper definition of g_q^0 and ω_q^0 if q is outside the first Brillouin zone. Also, the Coulomb matrix elements will be altered by crystal-line effects.

The screened interaction is then

$$\mathcal{V}^s(q) = \frac{V(q)}{1 + iV(q)P_0(q)} \quad .$$

If we insert jellium values for g_q^0 and ω_q^0 (that is, the phonon-electron matrix elements appropriate to point ions using free electron wave functions and using the ionic plasma frequency for ω_q), one finds

$$\mathcal{V}^s(q) = \frac{V_c^s(q)}{1 - (\omega_q^2/q_0^2) + i\eta} \quad , \quad (7.28)$$

where the screened Coulomb interaction is

$$V_c^s(q) = V_c(q)/\kappa(q)$$

and the dressed phonon frequency is

$$\omega_q^2 = \omega_q^{02}/\kappa(q) \quad .$$

Here, $\kappa(q) \equiv 1 + iV_c P_0(q)$ is the electronic dielectric constant within the RPA. Since for frequencies of interest to us, $\kappa(q) \simeq \kappa(q, 0)$, we see that the effective interaction is attractive for $q_0 < \omega_q$, passes through a resonance for $q_0 = \omega_q$, and saturates at the screened Coulomb interaction for high frequencies, as shown below. The resonance is damped if we take account of the finite imaginary part of $\kappa(q)$ at $q_0 = \omega_q$, i.e., the finite lifetime of the phonon. This effect in practice is weak and we will neglect it for now.

E. Explanation of the Properties of Superconductors

We are now in a position to explain a number of experimental effects observed in superconductors.

a) The theory predicts a second-order phase transition at T_c in agreement with experiment.

b) Due to the approximate Gallilean invariance of the Hamiltonian for small drift velocities, there is an energy gap even if the system carries a current due to the electrons flowing as a whole relative to the ions. This gap prevents fluctuations due to scattering of the electrons by phonons or imperfections from decreasing the energy of the system and giving electrical resistance.

c) Due to the energy gap, the wave function of the superconductor is only weakly affected by a magnetic field, and diamagnetic currents build up to screen out the external magnetic field. One can think of the superconductor as a gigantic diamagnetic "molecule" in a manner first emphasized by London. The long-range order in coordinate space due to the pair-pair correlations ensures the Meissner effect.

d) The observed exponential electronic specific heat and the absence of absorption of sound and infrared radiation of energy $\hbar\omega < 2\Delta$ at temperatures $T \ll T_c$ is accounted for naturally by the energy gap.

e) Coherence effects in the electromagnetic and acoustic absorption and the nuclear magnetic relaxation rate first predicted theoretically have been well established experimentally and give strong support for the pairing scheme introduced in the BCS theory.

Many other effects have been calculated, and agreement between theory and experiment is generally surprisingly good considering the simple models upon which the calculations are based. The reader is referred to the review article of Bardeen and Schrieffer for a more detailed discussion of the comparison of theory and experiment.

F. Green's Function Approach to Superconductivity

To obtain corrections to the BCS approximation, it is convenient to go over to a Green's function scheme. An elegant formalism has been introduced by Nambu. As suggested by Gar'kov, one is interested in studying functions of the form

$$\begin{aligned}
 G_{11}(p, \tau) &= i \langle 0_N | T \{ c_{p\uparrow}(\tau) c_{p\uparrow}^\dagger(0) \} | 0_N \rangle \\
 G_{22}(p, \tau) &= i \langle 0_N | T \{ c_{-p\downarrow}^\dagger(\tau) c_{-p\downarrow}(0) \} | 0_N \rangle \\
 G_{12}(p, \tau) &= i \langle 0_{N-2} | T \{ c_{+p\uparrow}(\tau) c_{-p\downarrow}(0) \} | 0_N \rangle \\
 G_{21}(p, \tau) &= i \langle 0_{N+2} | T \{ c_{-p\downarrow}^\dagger(\tau) c_{p\uparrow}^\dagger(0) \} | 0_N \rangle
 \end{aligned} \tag{7.29}$$

The subscript N refers to the number of particles in the state. The first two are the Green's functions for particles of spin up and holes in states of down spin. The G_{12} and G_{21} functions are of prime interest in the pairing problem and are closely related to the gap Δ_k , as we will see. The function $G_{21}(p, 0)$ may be thought of as the amplitude for a pair of bare electrons created in states of opposite spin and momentum going into the bound state which is macroscopically occupied in $|0_N\rangle$. Since we expect each of the Green's functions $G_{\alpha\beta}$ to be slowly varying with the number of particles N , we introduce an ensemble-averaged ground state $|0\rangle$, given by a superposition of ground state eigenfunctions $|0_N\rangle$ with weights sharply peaked about an average number N_0 . The four functions $G_{\alpha\beta}(p, \tau)$ can then be written in terms of a pseudo-spinor field

$$\begin{aligned}
 \Psi_p &= \begin{pmatrix} c_{p\uparrow} \\ c_{-p\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} \Psi_{p,1} \\ \Psi_{p,2} \end{pmatrix} \\
 \text{Thus} \quad G_{\alpha\beta}(p, \tau) &= i \langle 0 | T \Psi_p(\tau) \alpha \Psi_p^\dagger(0) \beta | 0 \rangle
 \end{aligned} \tag{7.30}$$

Nambu introduces the Pauli matrices 1 , τ_1 , τ_2 , and τ_3 , to express the Hamiltonian in terms of the Ψ_p :

$$\begin{aligned}
 H &= \sum_p \epsilon_p \Psi_p^\dagger \tau_3 \Psi_p + \frac{1}{2} \sum_{q \neq 0, p, p'} (p+q, p'-q | V | p, p') (\Psi_{p+q}^\dagger \tau_3 \Psi_p) (\Psi_{p'-q}^\dagger \tau_3 \Psi_{p'}) \\
 &+ \text{constant}
 \end{aligned} \tag{7.31}$$

The τ_3 enters due to the spin-down terms entering with the wrong sign unless it is included. If $H_0 \equiv \sum_p \epsilon_p \Psi_p^\dagger \tau_3 \Psi_p$, then the zero-order Green's function is given by

$$G_0(p) = \frac{-1}{p_0 1 - (\epsilon_p - i\eta p) \tau_3} = -\frac{(p_0 1 + \epsilon_p \tau_3)}{p_0^2 - \epsilon_p^2 + i\eta} \quad \eta_p = \begin{cases} 0^+ & p > p_F \\ 0^- & p < p_F \end{cases} \quad \eta = 0^+ \quad , \quad (7.32)$$

where we measure ϵ_p from the Fermi energy, i.e., $\epsilon_{p_F} = 0$. The full Green's function satisfies a Dyson's equation

$$G^{-1}(p) = G_0^{-1}(p) + \Sigma(p) \quad ,$$

where G , G_0 , and Σ are matrices in the pseudo-spin space. The self-energy operator is constructed by using the usual rules for calculations in momentum space with the exception that at each 3-vertex one must insert τ_3 due to the τ_3 's in the interaction Hamiltonian. To obtain the BCS solution, we approximate $\Sigma(p)$ by

$$\Sigma(p) = \text{---} \overbrace{\text{---}}^{\text{---}} \text{---} = -i \int \tau_3 G(p') \tau_3 (p' p | V | p p') \frac{d^4 p'}{(2\pi)^4} \quad . \quad (7.33)$$

where $G(p')$ is given self-consistently by inserting this value of Σ into $G^{-1} = G_0^{-1} + \Sigma$. We now expand Σ in the full set of Pauli matrices:

$$\Sigma(p) = (1 - z_p) p_0 1 + \chi_p \tau_3 + \Delta_p \tau_1 \quad . \quad (7.34)$$

We have used the invariance of H with respect to rotations in the pseudo-spin space about the z axis to set the coefficient of τ_2 equal to 0. This is simply a phase transformation of no interest to us. Then G is given in terms of the three functions z , χ , and Δ by

$$G(p) = \frac{-1}{z_p p_0 1 - \tilde{\epsilon}_p \tau_3 - \Delta_p \tau_1} = \frac{-(z_p p_0 + \tilde{\epsilon}_p \tau_3 + \Delta_p \tau_1)}{(z_p p_0)^2 - \tilde{\epsilon}_p^2 - \Delta_p^2 + i\eta} \quad , \quad (7.35)$$

where $\tilde{\epsilon}_p = \epsilon_p + \chi_p$. For simplicity, we neglect χ_p and set $z_p = 1$, which corresponds to choosing a free-particle approximation for the normal state. The parameter Δ_p is given by the τ_1 component of the self-energy equation:

$$\Delta_p = i \int \frac{\Delta_{p'}}{p_0'^2 - E_{p'}^2 + i\eta} (p'p | V | pp') \frac{d^4 p'}{(2\pi)^4} \quad , \quad (7.36)$$

where $E_{p'} \equiv \sqrt{\epsilon_{p'}^2 + \Delta_{p'}^2}$. By carrying out the p_0' integral, we have

$$\Delta_p = - \int \frac{V_{pp'} \Delta_{p'}}{2E_{p'}} \frac{d^3 p'}{(2\pi)^3} \quad (7.37)$$

where $V_{pp'} \equiv (p'p | V | pp') = (p', -p' | V | p, -p)$. This is just the energy-gap equation we found earlier, and we note that the quasi-particle energy given by the pole of G is again

$$E_p = \sqrt{\epsilon_p^2 + \Delta_p^2}$$

G. Collective Boson Excitations in Superconductors

The collective modes which occur in the energy gap can be obtained in many different manners. Anderson and Bogoliubov derived the spectrum of the longitudinal density fluctuations by schemes closely related to the linearized equations of motion discussed above; however, one must study the time evolution of products of fermion operators in this case, that is, $c_{k+q\uparrow}^\dagger c_{k\uparrow}$, $c_{k+q\downarrow}^\dagger c_{-k\downarrow}^\dagger$, and $c_{-k-q\downarrow} c_{k\uparrow}$. We shall derive the collective excitation from the poles of the two-particle Green's function.

The collective modes may be thought of as a bound state of a pair of quasiparticles. Since the interaction conserves momentum, the boson wave function will be the product of a plane wave describing the center-of-mass motion multiplied by a relative coordinate wave function $\chi(\vec{r})$. For small center-of-mass momentum, the function χ will be of the form

$$\chi(\vec{r}_{12}) = \tilde{\chi}(|\vec{r}_{12}|) Y_\ell^m(\theta_{12}, \phi_{12}) \quad , \quad (7.38)$$

where $\vec{r}_{12} \equiv \vec{r}_1 - \vec{r}_2$ is the relative coordinate between the 2 quasi particles. If the ground state has s state pairing (i.e., u_k and v_k are independent of angle in k space), then the $\ell = 0, m = 0$ collective mode corresponds to a density fluctuation of the system. In the absence of Coulomb forces the energy of this excitation is proportional to q , the center-of-mass momentum, as shown below. The higher angular momentum states $\ell = 1, 2 \dots$ are bound if the ℓ -wave part of the potential is finite.

As we shall see, if the $\ell (\neq 0)$ wave part of the potential is greater than the s-wave part, a new instability arises and the ground state must be formed with ℓ -state pairs. Presumably, if He^3 were a superconductor the presence of the hard core repulsion would lead to the $\ell = 2$ state being the most stable configuration.

Since the exciton (i.e., collective mode) wave function must be antisymmetric upon interchange of the quasi-particle coordinates, even ℓ states have singlet spin functions while odd ℓ states have triplet spin functions and may be thought of as spin waves.

To obtain the excitons we must treat residual interactions neglected within the BCS approximation, i.e., interactions between particles in states other than $(k\uparrow, -k\uparrow)$. A simple scheme is to sum the ladder diagrams shown below.

To obtain spin-zero excitons, we consider interactions between electrons of opposite spin, or, in the Nambu scheme, between a 2-component particle line and a 2-component hole line. The lines are labelled by the 4-momentum p which includes the pseudo-spin $\alpha = 1, 2$. The series is summed by the t matrix:

$$(p'+q, -p' | t | p+q, -p) = -(p'+q, -p' | V | p+q, -p) \tau_3^a \tau_3^b \quad (7.39)$$

$$-i \int (p'+q, -p' | V | p''+q, -p'') \tau_3^a G^a(p'+q) \tau_3^b G^b(p'') (p''+q, -p'' | t | p+q, -p) \frac{d^4 p''}{(2\pi)^4}.$$

The indices a and b refer to the "particle" and "hole" lines, respectively, and summation over the pseudo-spin indices has been suppressed. The matrix element of V is assumed to be a function of the momentum transfer alone:

$$(p'+q, -p' | V | p+q, -p) = V(|p'-p|) \quad (7.40)$$

We expand the matrix element into its partial wave components:

$$V(|p'-p|) = \sum_{\ell=0}^{\infty} V_{\ell}(|p'|, |p|) \sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta', \phi')^* Y_{\ell m}(\theta, \phi) \quad (7.41)$$

where (θ, ϕ) and (θ', ϕ') are the angles associated with p and p' , respectively, in spherical coordinates.

Concentrating on the limit $q \rightarrow 0$, if t is expanded into its partial wave components,

$$(p'+q, -p' | t | p+q, -p) = \sum_{\ell=0}^{\infty} t_{\ell}(|p'|, |p|, q_0) \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\theta', \phi') Y_{\ell m}(\theta, \phi) \quad (7.42)$$

and the ℓ -wave part of t satisfies

$$t_{\ell}(|p'|, |p|, q_0) = -V_{\ell}(|p'|, |p|) \tau_3^a \tau_3^b - i \int V_{\ell}(|p'|, |p''|) |Y_{\ell m}(\theta'', \phi'')|^2 \tau_3^a G^a(p''+q) \tau_3^b G^b(p'') t_{\ell}(|p''|, |p|, q_0) \frac{d^4 p''}{(2\pi)^4} \quad (7.43)$$

An exact solution for t_{ℓ} is obtained if one replaces V_{ℓ} by a separable potential:

$$V_{\ell}(|p'|, |p|) = \lambda_{\ell} w_{\ell}(|p'|)^* w_{\ell}(|p|) \quad (7.44)$$

In this limit of long wavelength, we find

$$t_{\ell}(|p'|, |p|, q_0) = -\lambda_{\ell} w_{\ell}(p) w_{\ell}^*(p') \tau_3^a \tau_3^b [1 + \lambda_{\ell} \phi_{\ell}(q_0)]^{-1} \quad (7.45)$$

where the matrix $\phi_{\ell}(q)$ is given by

$$\phi_{\ell}(q) = i \int |w_{\ell}(p)|^2 G^a(p+q) \tau_3^a G^b(p) \tau_3^b \frac{d^4 p}{(2\pi)^4} \quad (7.46)$$

The matrix $\phi_{\ell}(q)$ has matrix structure with respect to both the two component "particle" and "hole" lines. Thus, $[1 + \lambda_{\ell} \phi_{\ell}(q)]^{-1}$ is to be thought of as the inverse of a 4×4 matrix in the product space of the two pseudo-spin variables.

The poles of t reflect collective states of the system. Therefore, since a pole of any matrix element of t is equivalent to a zero of the determinant of $1 + \lambda_{\ell} \phi_{\ell}(q)$, the energy of the $\vec{q} = 0$ collective excitation of angular momentum ℓ satisfies

$$\det[1 + \lambda_{\ell} \phi_{\ell}(q_0)] = 0 \quad . \quad (7.47)$$

If the interaction $|w_{\ell}(p)|^2$ is symmetric with respect to the Fermi surface, the determinant factors into two 2×2 determinants for $q_0 \equiv 0$, and one finds for $q_0 \ll \Delta$ the energy of the collective state is given by

$$\frac{1}{-\lambda_{\ell}} = \sum_p |w_{\ell}(p)|^2 \frac{2\Delta^2}{E_p} \frac{1}{4E_p^2 - q_0^2} \quad . \quad (7.48)$$

Correction for $q_0 \sim \Delta$ are discussed by Bardasis and Schrieffer. For there to be a bound state of angular momentum ℓ , q_0 must be less than the gap energy $2\Delta_{p_F}$. Thus, λ_{ℓ} must be negative or the ℓ -wave part of the particle-particle interaction must be attractive. If the ground state pairing is through the ℓ_0 potential, it is straightforward to show that $q_0 = 0$ as $\vec{q} \rightarrow 0$ for the ℓ_0 boson. This excitation is just a sound wave or density fluctuation of the system and, in the absence of long-range Coulomb interactions, has a frequency of the form

$$q_0 = sq \quad ,$$

where (7.49)

$$s = v_F / \sqrt{3} \text{ for } q \xi_0 \ll 1 \quad .$$

For other ℓ 's not equal to ℓ_0 , q_0 will be finite as $q \rightarrow 0$, so that there is a finite energy to create these long wavelength "excitons."

References to Chapter VII

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APPENDIX A

ELECTRONS IN THE CRYSTAL LATTICE

We now touch briefly on the one-particle Green's function formalism for interacting electrons in real crystals, confining the discussion to a few features involved in extending the treatment presented in the text. We consider a system of spin-up electrons interacting with each other through two-body forces and moving in a one-body external potential⁽¹⁾ which is static and is spatially periodic. The Hamiltonian (2.12) is no longer translationally invariant, because $V_1(x)$ is periodic.

For formal purposes we need not specify completely the one-particle basis functions in which the electron wave field $\psi(x)$ is expanded. We let α stand for a complete set of quantum numbers labeling the eigenfunctions of the unperturbed Hamiltonian and write

$$\begin{aligned}\psi(x) &= \sum_{\alpha} u_{\alpha}(x) c_{\alpha}(t) \\ H^{(0)} &= \sum_{\alpha} \epsilon_{\alpha} c_{\alpha}^{\dagger}(t) c_{\alpha}(t)\end{aligned}\quad (A.1)$$

The corresponding zero-order Green's operator in the coordinate and the α representation is given by

$$\begin{aligned}G^{(0)}(x, x'; \tau) &= \sum_{\alpha} u_{\alpha}^*(x') u_{\alpha}(x) G^{(0)}(\alpha; \tau) \\ G^{(0)}(\alpha, \tau) &\equiv G_{\alpha\alpha}^{(0)}(\tau) = i \langle 0 | T \{ c_{\alpha}(\tau) c_{\alpha}^{\dagger}(0) \} | 0 \rangle \\ G^{(0)}(\alpha, p_0) &= (-) \left\{ p_0 + i \epsilon_0 - \epsilon_{\alpha} \right\}^{-1} \quad \gamma_{\alpha} = \begin{cases} 0^{+} & \epsilon_{\alpha} < \epsilon_F^{(0)} \\ 0^{-} & \epsilon_{\alpha} > \epsilon_F^{(0)} \end{cases},\end{aligned}\quad (A.2)$$

where $|0\rangle$ is the ground state of the unperturbed system. The function $G^{(0)}(x, x'; \tau)$ depends on x and x' separately but is invariant under the translation and point groups of the crystal lattice.

If in $H^{(0)}$ we include all the one-body terms, then the basis is formed from the Bloch function solutions u_{k_n} of standard band theory. The wave vector k lies within the first Brillouin zone and n stands for all other quantum numbers including band index and symmetry type with respect to point group operations.⁽²⁾ This choice of $H^{(0)}$ has been made in many important formal derivations,⁽³⁾ but the prospect of using the u_{k_n} basis to go beyond the Hartree-Fock approximation is not enticing.

Within the past few years it has been found that the energy-band structure within the Hartree-Fock approximation for valence and conduction electrons in many covalent crystals can be obtained from a model

system in which the crystal lattice potential is replaced by an effective one-body interaction which can readily be treated by low-order perturbation theory.⁽⁴⁾ The unperturbed Hamiltonian in the model system is just the kinetic energy plus a constant potential, and its appropriate eigenfunctions are symmetrized combinations of plane waves $S_p(x)$. Accordingly one can treat the lattice potential and the two-body interaction jointly by a perturbation expansion based on zero-order Green's functions appropriate to symmetrized plane waves.⁽⁵⁾

In the presence of both V_1 and the two-body interaction V_2 , the full Green's operator is not diagonal in a representation based on one-electron functions. For example, in the nk representation the matrix elements of V_2 lead to diagrams which are nondiagonal in the band indices n , and in a plane-wave representation V_1 allows the 3-momentum $\underline{k} + \underline{h} = \underline{p}$ to change by any reciprocal lattice vector $\underline{h}'$. Diagrams are always diagonal in p_0 and k . The matrix elements of the Green's operator are

$$G_{\alpha'\alpha}(\tau) = i \langle 0 | T \left\{ c_{\alpha'}(\tau) c_{\alpha}^{\dagger}(0) \right\} | 0 \rangle, \quad (A.3)$$

where α stands for a complete set of quantum numbers labeling the basis functions and $|0\rangle$ is now the exact ground state of the interacting system. The discussion of Section IV-E leading to (4.24) can be repeated to show that the diagonal elements $G_{\alpha\alpha}(\tau)$ again give the probability amplitude that, if the system was in a one-particle excitation state at time 0, it is in the same state at time τ . Quasi-particle energies and lifetimes are then given by poles of the diagonal terms $G_{\alpha\alpha}(p_0)$.

For the diagonal elements, the diagram analysis of V-D leading to Dyson's equation (5.24) or (5.25) can be repeated and gives

$$G_{\alpha\alpha}(p_0) = G_{\alpha\alpha}^{(0)}(p_0) \left[1 + \Sigma_{\alpha\alpha}(p_0 | \alpha) G_{\alpha\alpha}^{(0)}(p_0) \right]^{-1}. \quad (A.4)$$

Here $G_{\alpha\alpha}^{(0)}(p_0)$ is the Green's function of the unperturbed system, and $\Sigma_{\alpha\alpha}(p_0 | \alpha)$ is the irreducible self-energy for the state α . As before, we define $(1/i) \Sigma_{\alpha\alpha}(p_0 | \alpha)$ to be the contribution of all distinct diagonal self-energy diagrams which cannot be separated into two parts by breaking a single particle line carrying the label α . The reason for slight difference in notation will become clear shortly.

Let us now consider a general matrix element of the operator $G(p_0)$. The diagrams contributing to $G_{\alpha'\alpha}(p_0)$ have the general structure indicated in Figure (A-1).

Figure (A-1)

The circles represent proper self-energy parts, i.e., parts which cannot be split in two by breaking a single fermion line whatever the label on that line. The proper self-energy operator $\Sigma(p_0)$ is defined by its matrix elements by taking $(1/i) \Sigma_{\alpha'\alpha}(p_0)$ to be the contribution from all distinct proper self-energy parts with initial and final states α and α' . We get $G_{\alpha'\alpha}(p_0)$ by summing the diagrams of the figure over all proper self-energy insertions in the circles, then over all intermediate particle lines $(\alpha_1, \dots, \alpha_{n-1})$, and lastly over all $n \geq 1$.

$$\begin{aligned}
 -i G_{\alpha'\alpha}(p_0) &= \sum_{n=1}^{\infty} \sum_{\alpha_{n-1}, \dots, \alpha_1} (-i)^{2n-1} G_{\alpha'\alpha'}^{(0)}(p_0) \Sigma_{\alpha'\alpha_{n-1}}(p_0) \dots \\
 &\quad \dots G_{\alpha_1\alpha_2}^{(0)}(p_0) \sum_{\alpha_2\alpha_1} (p_0) G_{\alpha_1\alpha_1}^{(0)}(p_0) \sum_{\alpha_1\alpha} (p_0) G_{\alpha\alpha}^{(0)}(p_0) \\
 &= -i \sum_1^{\infty} (-1)^{n-1} \left\{ G^{(0)}(p_0) \left[\Sigma(p_0) G^{(0)}(p_0) \right]^{n-1} \right\}_{\alpha'\alpha} \\
 &= -i \left\{ G^{(0)}(p_0) \left[1 + \Sigma(p_0) G^{(0)}(p_0) \right]^{-1} \right\}_{\alpha'\alpha} \quad (A.5)
 \end{aligned}$$

Consequently, we have the operator equation

$$G(p_0) = G^{(0)}(p_0) \left[1 + \Sigma(p_0) G^{(0)}(p_0) \right]^{-1} \quad (A.6)$$

This is perhaps the most natural and certainly the most compact generalization to the present case of equation (5.24) of the text. The poles of $G_{\alpha\alpha}(p_0)$ are roots of

$$\det | G^{(0)}(p_0)^{-1} + \Sigma(p_0) | = 0 \quad (A.7)$$

and hence solutions of secular equations.

With an eye to obtaining roots of (A.7) by low-order perturbation theory, we can introduce an operator $\Sigma(p_0|\alpha)$ whose diagonal elements are the irreducible self-energies for the state α we have defined in the text

and in (A.4). We define $(1/i) \Sigma_{\alpha' \alpha''}(p_0 | \alpha)$ to be the contribution from all distinct self-energy diagrams in which none of the intermediate single-particle excitation states $\alpha_1, \dots, \alpha_{n-1}$ is α . Either, neither, or both of α' and α'' may be the "excluded" state α . An intermediate single line (p_0, α_ν) now contributes the factor $-i G_{\alpha_\nu \alpha_\nu}^{(0)}(p_0) \cdot (1 - \delta_{\alpha_\nu, \alpha})$. We obtain the relationship between $\Sigma(p_0 | \alpha)$ and $\Sigma(p_0)$ by removing the external lines in Figure (A.1) and summing contributions. On introducing a projection operator for the state α ,

$$\left. \begin{aligned} \mathcal{P}_\alpha &= | \alpha \rangle \langle \alpha | \\ [G^{(0)}(p_0), \mathcal{P}_\alpha] &= 0 \end{aligned} \right\}, \quad (\text{A.8})$$

we find:

$$\Sigma(p_0 | \alpha) = \Sigma(p_0) \left\{ 1 + G^{(0)}(p_0) (1 - \mathcal{P}_\alpha) \Sigma(p_0) \right\}^{-1} \quad (\text{A.9})$$

By substituting the solution of (A.9) for $\Sigma(p_0 | \alpha)$ into (A.6), we can express $G(p_0)$ in terms of $\Sigma(p_0 | \alpha)$. The diagonal elements $G_{\alpha\alpha}(p_0)$ are, as announced, given by the numerical equation (A.4), but the off-diagonal elements are rather more complicated. We find

$$\begin{aligned} G_{\alpha' \alpha''}(p_0) &= \delta_{\alpha' \alpha''} G_{\alpha' \alpha'}^{(0)}(p_0) - G_{\alpha' \alpha'}^{(0)}(p_0) \Sigma_{\alpha' \alpha''}(p_0 | \alpha) G_{\alpha'' \alpha''}^{(0)}(p_0) \\ &\quad + G_{\alpha' \alpha'}^{(0)}(p_0) \Sigma_{\alpha' \alpha}(p_0 | \alpha) G_{\alpha \alpha}(p_0) \Sigma_{\alpha \alpha''}(p_0 | \alpha) G_{\alpha'' \alpha''}^{(0)}(p_0) . \end{aligned} \quad (\text{A.10})$$

When the Hamiltonian is translationally invariant, $\Sigma(p_0 | \alpha) = \Sigma(p_0)$, as is shown by (A.9). In the present case $\Sigma(p_0 | \alpha)$ gives, e.g., the energy shift as a perturbation expansion in the proper self-energy. The numerical equation (A.4) is just the result of solving (A.7) by perturbation theory. As usual in perturbation theory, one state at a time is singled out for accurate treatment, and our notation indicates explicitly which state is so distinguished.

All this becomes more familiar if the perturbation Hamiltonian is only an external field, whose interaction with a fermion is represented by Figure (A.2a).

Figure (A.2)

The only proper self-energy diagram is (b), and $\Sigma(p_0)$ is just the external perturbation, but in $\Sigma(p_0|\alpha)$ we must include improper "scattering" diagrams such as (c). On using (A.9) in (A.4), we can see that the poles of $G_{\alpha\alpha}(p_0)$ are given by the Brillouin-Wigner expansion. On further replacing the pole ϵ_{α} by a perturbation expansion $\epsilon_{\alpha}^{(0)} + \epsilon_{\alpha}^{(1)} + \epsilon_{\alpha}^{(2)} + \dots$, we recover the Rayleigh-Schrödinger expansion for the eigenvalue ϵ_{α} in the form in which it commonly first appears in elementary quantum mechanics courses. The improper diagrams of (A-2c) provide the contributions from virtual transitions.

The ground state energy may be given in terms of $G(p_0)$ by the same derivation used in Section (V.E) so long as only two-body interactions occur in the perturbation. Choosing $H^{(0)}$ to be the one-body part H_1 of the Hamiltonian, we find

$$E_0 = \frac{(-1)}{2\pi i} \int_{-\infty}^{+\infty} dp_0 e^{ip_0\eta} \text{trace} \left\{ \left[H_1 + \frac{1}{2} \Sigma(p_0) \right] G(p_0) \right\} \quad (\text{A.11})$$

In the nk-representation we have

$$\begin{aligned} \text{trace} \left\{ H_1 + \frac{1}{2} \Sigma(p_0) \right\} G(p_0) &= \sum_{nk} \left\{ \epsilon_{nk} G_{nk,nk}(p_0) + \frac{1}{2} \left[\Sigma(p_0) G(p_0) \right]_{nk,nk} \right\} \\ &= \sum_{nk} \left\{ \epsilon_{nk} + \frac{1}{2} \Sigma_{nk,nk}(p_0|nk) \right\} G_{nk,nk}(p_0) \end{aligned} \quad (\text{A.12})$$

If for $H^{(0)}$ we choose the kinetic energy plus a constant V_0 , then the derivation of the ground state energy proceeds as before, but leads to a slightly different result because one-body interactions are included in the perturbation. In terms of the proper self-energy, one finds

$$E_0 = \frac{(-1)}{2\pi i} \int_{-\infty}^{+\infty} dp_0 e^{ip_0\eta} \text{trace} \left\{ \left[H^{(0)} + \frac{1}{2} (V_1 - V_0 + \Sigma(p_0)) \right] G(p_0) \right\} \quad (\text{A.13})$$

In terms of the irreducible self-energy we have

$$\begin{aligned} \text{trace} \left\{ \left[H^{(0)} + \frac{1}{2} (V_1 - V_0 + \Sigma(p_0)) \right] G(p_0) \right\} &= \sum_{\alpha} \left\{ \epsilon_{\alpha} + \frac{1}{2} \left[V_1 - V_0 + \Sigma(p_0|\alpha) \right]_{\alpha\alpha} \right. \\ &\quad \left. - \frac{1}{2} \left[(V_1 - V_0)(1 - \mathbb{P}_{\alpha}) G^{(0)}(p_0) \Sigma(p_0|\alpha) \right]_{\alpha\alpha} \right\} G_{\alpha\alpha}(p_0) \end{aligned} \quad (\text{A.15})$$

References for Appendix A

Only a few references relevant to the material of Appendix A are cited here, and they may be consulted for more complete lists.

1. Bogoliubov and Shirkov, Introduction to the Theory of Quantized Fields, Interscience (1959), Section 21.4.
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