

Many-body Theory

Many-body Theory:

Normal Fermi Liquid

By

Marian Apostol

With the cooperation of dr. Liviu Cristian Cune

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1 Foreword

Our usual, common world is made of bodies, or parts of bodies, consisting of many identical particles. By "many" we understand an infinite number of particles, occupying practically an infinite volume, as in macroscopic samples of matter. We call these ensembles of particles many-particle, or many-body "systems". In some particular cases, like the atomic nuclei, finite-size effects are important. Also, systems with low dimensions, like two-, or one-dimensional systems, require a particular treatment; in particular, such systems lie usually on substrates.

We may have a clear representation of independent particles, or waves at the quantum mechanical level, but such a representation is blurred out when interaction is present. We leave aside exactly soluble interacting models, which are reduced to independent particles. The genuine effects of the interaction destroy, in fact, the concept of independent particles. The interaction may be viewed as an uncertainty in the behaviour of independent particles. Apart from interaction effects, the situation is complicated by temperature effects. Usually, we need to solve first for the interaction effects, to some approximation, and then do the thermodynamics, *i.e.* the statistical physics, for the quasi-independent particles, waves, obtained by solving the interaction. The central concept of the statistical mechanics is the independent, identical subsystems. If the temperature is sufficiently high, the systems behave classically, like solids, liquids, gases, etc, and the residual effects of the interaction are small. If the interaction prevails, as for low temperature, the systems are quantum-mechanical. We seldom have a knowledge of their ground-states, but what matters are their low-lying excited states, which are the elementary excitations (either one-particle, or collective, or more complex). We owe this observation to Landau. In some special cases, the nature of the quantum-mechanical ground-state at low temperatures may change drastically,

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as a result of the interaction, by quantum-mechanical effects, like in superconductivity, or superfluidity, or ferromagnetism. Then we are in the presence of some phase transitions, and the elementary excitations become more relevant. The concept of elementary excitations can be extended to classical systems.

Without going too deep into the structure of matter, the bodies are made of atoms and electrons. The atoms are either fermions, or bosons, depending on their integer or half-integer spins. The electrons have a one-half spin, so they are fermions.

An example of bosons is the He^4 atoms. At sufficiently low temperatures these atoms condense in a macroscopic quantum-mechanical state, undergoing a phase transition towards a superfluid state; this state is related to the Bose-Einstein condensation. There exist excited states with respect to this ground-state, some are collective excitations (like sound waves), others are particle-like excitations (called rotons); the properties of these elementary excitations are governed by the interaction (which should be repulsive, for stability). At higher temperatures, the ensemble becomes normal, and tends to a classical gas of (weakly) interacting atoms.

Examples of fermion systems are atoms of He^3 , nucleons in the atomic nuclei and electrons in solids. The fermions with an attractive interaction are unstable; they form bound states of the so-called Cooper pairs, which behave like bosons, to a large extent. The condensed state of pairs in He^3 at very low temperature gives the superfluidity of this quantum-mechanical liquid, while for electrons in solids this state leads to superconductivity. Nucleon pairing is also known in the atomic nuclei, where higher-order particle correlations may also lead to a four-fermion condensate.¹ The condensed phase is characterized by an "order parameter". Collective elementary excitations of the condensed phase exist (known as phasons and amplitudons of the order parameter), as well as one-particle excitations.

In solids, the electron-phonon interaction may provide an attractive force between the electrons, leading to superconductivity. The same interaction may lead to a condensed state of electron-hole pairs, if the Fermi surface has parallel segments, as, for instance in one-dimensional

¹See, for example, M. Apostol, "Four-fermion condensate", Phys. Lett. **A110** 141 (1985).

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systems; in this case we have a charge-, or spin-density wave.² The phonons introduce a new type of interaction, carried out by definite quanta. It is similar to the electron-photon interaction in matter. Other types of interacting particles are known, for example the interaction of the magnetic moments, which leads to elementary excitations known as magnons.

The effects of the interaction in many-body systems are treated by the perturbation theory. This theory is formulated most conveniently in terms of Green functions, or propagators, by analogy with the quantum electrodynamics. A propagator is the probability amplitude of having a state contained in another state. It is related to correlation functions and the response functions to an external perturbation. The great advantage of this technique is a formal summation of the effects, by what is known as the Dyson equations, made possible by Feynman's diagrammatic representation of the propagators and the interaction. The summations lead to formulae which look like characteristic geometric-series formulae, exhibiting a pole structure. By analogy with the free-particle propagators these poles may be interpreted as particle (or wave) states, interaction effects included, either one-particle or collective. This way, we can answer the question of what the interaction effects are. The basic technique is the zero-temperature Green functions, though Green functions at non-zero temperature are also known. The latter are used especially for the phase transitions towards condensed states, though their formalism is inconvenient, in comparison with other, more direct approaches, like canonical transformations, equations of motion, the spectrum of the elementary excitations or the Ginsburg-Landau equations. All these techniques are exhaustively presented in:

L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics*, vol. 9 (E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics*, Part 2, *Theory of the Condensed State*), Pergamon, Oxford (1980); A. A. Abrikosov, L. P. Gorkov and I. Ye. Dzialoshinskii, *Quantum Field Theoretical Methods in Statistical Physics*, Pergamon, Oxford (1965); S. Raimes, *Many-Electron Theory*, North-Holland, NY (1972); A. L. Fetter and

²M. Apostol and I. Baldea, "On the charge density wave state in the quasi-one-dimensional compound $K_2[Pt(CN)_4]Br_{0.3} \times 3.2H_2O$ (KCP)", Rev. Roum. Phys. **30** 605 (1985).

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J. D. Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, NY (1971); G. D. Mahan, *Many-Particle Physics*, Kluwer, NY (1981); H. Bruus and K. Flensberg, *Many-body Quantum Theory in Condensed Matter Physics*, Oxford University Press, Oxford (2004); G. Rickayzen, *Green Functions and Condensed Matter*, Dover, NY (2013); Ph. Nozieres, *Theory of Interacting Fermi Systems*, Westview, NY (1964); D. Pines and Ph. Nozieres, *The Theory of Quantum Liquids*, vol. 1, Benjamin, NY (1966); Ph. Nozieres and D. Pines, *The Theory of Quantum Liquids*, vol.2, Westview, NY (1990).

For phase transitions with condensed states like superfluidity, or superconductivity, the interaction effects are comparatively easier to be derived, because the characteristics of the problem are more definite. The situation is more complicate for the so-called normal Fermi liquids, *i.e.* fermions with repulsive interaction which do not suffer a phase transition. The most known examples in this case are the electrons in solids, or the He^3 atoms slightly above the critical temperature of superfluidity. At first sight we may expect weak interaction effects, but it is difficult to maintain such an assertion when the interaction is strong, like the Coulomb interaction. The Coulomb interaction is not only a long-range interaction, it is also singular at short distances, which introduces further difficulties. In solids, where positive ions are present, the electrons screen out the ionic Coulomb interaction, an effect which may lead to the cohesion of matter.³ But even if the positive ionic background may ensure stability, the electron-electron interaction, albeit screened, is still strong and it may have long-range effects. The solution to this problem has been provided by Landau's theory of the Fermi liquid. The fermions suffer the interaction effects according to their wavelength, *i.e.* they feel the Fourier transform $V(p)$ of the interaction, where p is the fermion momentum. It follows that the fermions placed at the Fermi surface feel a weaker interaction $V(p_F)$, if the Fermi wavevector p_F is sufficiently large, *i.e.* we are in the high-density limit.⁴ This interaction effect is a blur

³L. C. Cune and M. Apostol, "Ground-state energy and geometric magic numbers for homo-atomic metallic clusters", *Phys. Lett.* **A273** 117 (2000). See also M. Apostol, *Physical Kinetics*, Cambridge Scholars Publishing, Newcastle upon Tyne (2020).

⁴The dilute limit of the fermion systems is simply an application of the perturbation theory.

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of the Fermi surface, which means a small change of the occupation number of the sharp Fermi surface. Consequently, we have a quasiparticle spectrum of the Fermi surface, where the interaction effects are localized. The free-particle properties, like mass, magnetic susceptibility, density excitations, are modified by small interaction effects, incorporated in interaction functions, which remain phenomenological. It would be desirable to derive these functions from the original interaction. This is the main task of the present book. The first eight chapters of the book deal with the formal Green-function theory of interacting fermions. The rest of the chapters deal with the Landau theory of the normal Fermi liquid. The effect of the screened interaction in the high-density limit is much larger than the temperature effects, because the liquid is in the so-called degenerate state in this case, such that we may compute the temperature effects by using the quasiparticle picture.

2 Second Quantization

2.1 Quantum states

We consider an ensemble of interacting identical particles. We prefer to denote by x the continuous position vector \mathbf{r} , or \mathbf{x} , for a particle in space. We denote by the ket vector $|x\rangle$ the quantum-mechanical state x . We say that the scalar product $\langle x' | x \rangle$ with the bra vector $\langle x' |$ is the "wavefunction" x of variable x' , defined by

$$\langle x' | x \rangle = \delta(x' - x) ; \quad (2.1)$$

we say that the state vectors are orthogonal. Moreover, since

$$\begin{aligned} \langle x' | x \rangle &= \int dy \delta(x' - y) \delta(y - x) = \\ &= \int dy \langle x' | y \rangle \langle y | x \rangle , \end{aligned} \quad (2.2)$$

we say that the set of state vectors is "complete", *i.e.*

$$\int dy |y\rangle \langle y| = 1 , \quad (2.3)$$

and the wavefunctions are orthogonal. Equation (2.2) tells that any wavefunction can be expanded in the set of wavefunctions,

$$\langle x' | x \rangle = \int dy C_{yx} \langle x' | y \rangle , \quad (2.4)$$

where $C_{yx} = \langle y | x \rangle$. This would be the superposition principle of the quantum mechanics. Also, since $|\langle x' | x \rangle|^2 dx'$ should be the localization probability, we need to add a factor \sqrt{v} to δ in equation (2.1), where v is a small volume around x (and $\delta(0) = 1/v$).

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On the other hand we have

$$\delta(x' - x) = \frac{1}{V} \sum_k e^{ik(x' - x)} , \quad (2.5)$$

where k stands for a wavevector \mathbf{k} ; we prefer to use cyclic boundary conditions over the volume V , *i.e.* $k_x = \frac{2\pi}{L_x} n_x$, n_x any integer, etc. Since

$$\langle x' | x \rangle = \sum_k \frac{1}{\sqrt{V}} e^{ikx'} \frac{1}{\sqrt{V}} e^{-ikx} , \quad (2.6)$$

we have the states $|k\rangle$ and the wavefunctions

$$\langle x | k \rangle = \frac{1}{\sqrt{V}} e^{ikx} , \quad (2.7)$$

such that

$$\langle x' | x \rangle = \sum_k \langle x' | k \rangle \langle k | x \rangle \quad (2.8)$$

and the states k are complete ($\sum_k |k\rangle\langle k| = 1$) and orthogonal ($\langle k' | k \rangle = \delta_{kk'}$). The wavefunction $\langle x | k \rangle$ given by equation (2.7) is the state k as a function of the variable x , with the localization probability dx/V .

We can add the spin σ , both as a variable and a state label, by using tensorial products like $|x\sigma\rangle = |x\rangle |\sigma\rangle$, etc; σ represents the values of the spin along a control axis, say the z -axis. Also, we can introduce many-particle states, like $|x_1 x_2 \dots\rangle = |x_1\rangle |x_2\rangle \dots$, by using tensorial products.

The whole machinery described above was introduced by Dirac.¹

2.2 Field operators

Let the particles be fermions. The state $|k\rangle$ represents a particle (with wavevector k). According to Pauli's exclusion principle, only one such state is admitted. Then, we introduce the "creation" operator

$$c_k^* |0\rangle = |k\rangle , \quad (2.9)$$

¹P. A. M. Dirac, *The Principles of Quantum Mechanics*, Clarendon Press, Oxford (1930, 1934, 1947).

2 Second Quantization

where $|0\rangle$ is the vacuum state. Similarly, we have an "annihilation" ("destruction") operator

$$c_k |k\rangle = |0\rangle . \quad (2.10)$$

Since a two-particle state $|kk'\rangle$ is antisymmetric with respect to the permutation of the two particles, we must have the anticommutation relations

$$\{c_k^*, c_{k'}^*\} = c_k^* c_{k'}^* + c_{k'}^* c_k^* = 0 , \quad \{c_k, c_{k'}\} = c_k c_{k'} + c_{k'} c_k = 0 . \quad (2.11)$$

Each time when an operator c^* (c) passes over another operator c^* (c) we get a factor -1 . This is known as the Jordan-Wigner factor $(-1)^{JW}$.

Similarly,

$$c_2^* c_1 |10\rangle = |01\rangle , \quad c_1 c_2^* |10\rangle = - |01\rangle , \quad (2.12)$$

such that

$$\{c_k^*, c_{k'}\} = c_k^* c_{k'} + c_{k'} c_k^* = \delta_{kk'} ; \quad (2.13)$$

indeed, $n_k = c_k^* c_k$ is the number of particles in state k (occupation number) and $c_k c_k^* = 1 - n_k$ is the number of "holes" in that state. We note that instead of k we may use 1, on various positions 1, 2, 3... which one-particle state can take in the multiparticle state.

The field operators are defined by

$$\psi(x) = \frac{1}{\sqrt{V}} \sum_k c_k e^{ikx} , \quad \psi^*(x) = \frac{1}{\sqrt{V}} \sum_k c_k^* e^{-ikx} , \quad (2.14)$$

with the (anti)commutation relations

$$\begin{aligned} \{\psi(x), \psi(x')\} &= 0 , \quad \{\psi^*(x), \psi^*(x')\} = 0 , \\ \{\psi(x), \psi^*(x')\} &= \delta(x - x') . \end{aligned} \quad (2.15)$$

We use to say that such commutation relations define a "second quantization".

The state $|x\rangle$ is defined as

$$|x\rangle = \psi^*(x) |0\rangle ; \quad (2.16)$$

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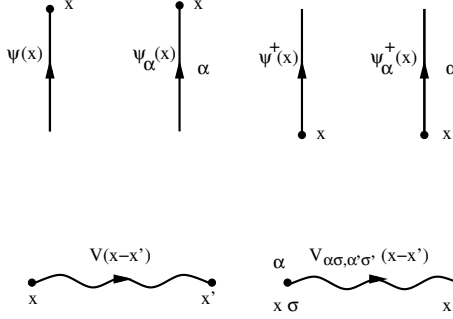


Figure 2.1: Particle and interaction lines.

we can see that it is a superposition of states $|k\rangle$, such that

$$\langle x' | x \rangle = \langle 0 | \psi(x') \psi^*(x) | 0 \rangle = \delta(x' - x) , \quad (2.17)$$

as in the definition (2.1). Similarly, a two-particle state $|x_1 x_2\rangle$ is

$$|x_1 x_2\rangle = \frac{1}{\sqrt{2!}} \psi^*(x_1) \psi^*(x_2) |0\rangle \quad (2.18)$$

and

$$\begin{aligned} & \langle x'_2 x'_1 | x_1 x_2 \rangle = \\ &= \frac{1}{2!} \langle 0 | \psi(x'_2) \psi(x'_1) \psi^*(x_1) \psi^*(x_2) | 0 \rangle = \\ &= \frac{1}{2!} [\delta(x'_1 - x_1) \delta(x'_2 - x_2) - \delta(x'_1 - x_2) \delta(x'_2 - x_1)] ; \end{aligned} \quad (2.19)$$

the second row in this equation is obtained by using the (anti)commutation relations. Similar definitions can be given for multi-particle states, whose wavefunctions are the so-called Slater determinants. The great simplification brought by the second quantization is the replacement of the symmetrized wavefunctions by the (anti)commutation relations between field operators.

Creation and destruction operators can also be introduced for bosons; only that a one particle state for bosons may have an indefinite number n of particles; we get

$$a^{*n} |0\rangle = \sqrt{(n+1)!} |n+1\rangle , \quad a^* |n\rangle = \sqrt{n+1} |n+1\rangle \quad (2.20)$$

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and

$$a^n |n\rangle = \sqrt{n!} |0\rangle, \quad a |n\rangle = \sqrt{n} |n-1\rangle \quad (2.21)$$

for one state. Since the two-particle wavefunction is symmetric, we get the commutation relations

$$\begin{aligned} [a_k^*, a_{k'}^*] &= a_k^* a_{k'}^* - a_{k'}^* a_k^* = 0, \\ [a_k, a_{k'}] &= a_k a_{k'} - a_{k'} a_k = 0, \\ [a_k, a_{k'}^*] &= a_k a_{k'}^* - a_{k'}^* a_k = \delta_{kk'} \end{aligned} \quad (2.22)$$

and

$$\begin{aligned} [\psi(x), \psi(x')] &= 0, \quad [\psi^*(x), \psi^*(x')] = 0 \\ [\psi(x), \psi^*(x')] &= \delta(x - x') \end{aligned} \quad (2.23)$$

for field operators defined by equations (2.14) with the c 's replaced by a 's. The occupation number is $n_k = a_k^* a_k$ ($n_k |n\rangle = n |n\rangle$).

Second-quantization operators can be introduced for any set of single-particle states, spin included. The operators will carry then a spin label. Though most part of the formalism is the same for fermions and bosons, henceforth our identical particles will be fermions. The second quantization was introduced by Dirac² and Jordan and Wigner³.

2.3 One- and two-particle operators

Let us examine the operator

$$\rho(x) = \psi^*(x)\psi(x) = \frac{1}{V} \sum_{kk'} c_k^* c_{k'} e^{i(k'-k)x}. \quad (2.24)$$

We can see that the operator

$$N = \int dx \rho(x) = \sum_k n_k \quad (2.25)$$

²P. A. M. Dirac, "The quantum theory of the emission and absorption of radiation", Proc. Roy. Soc. London **A114** 243 (1927).

³P. Jordan and E. P. Wigner, "Ueber das Paulische Aequivalenzverbot", Z. Physik **47** 631 (1928).

2 Second Quantization

gives the number of particles N when applied on any state with N particles. Therefore, $\rho(x)$ is the particle-density operator. It follows that any one-particle operator

$$O_1 = \sum_i O_1(x_i) \quad (2.26)$$

can be written as

$$O_1 = \int dx \psi^*(x) O_1(x) \psi(x) ; \quad (2.27)$$

it is important to put $O(x)$ between the field operators in order to allow it to act upon the wavefunctions $(x | k >.$ In particular, the density

$$\rho(x) = \sum_i \delta(x - x_i) \quad (2.28)$$

becomes $\rho(x)$ given by equation (2.24). Similarly, $\rho_h(x) = \psi(x)\psi^*(x)$ is the hole density. Also, the spin density

$$\sigma(x) = \sum_i s_{zi} \delta(x - x_i) \quad (2.29)$$

becomes

$$\sigma(x) = \psi^*(x) s_z \psi(x) = \sum_{\sigma} \sigma \psi_{\sigma}^*(x) \psi_{\sigma}(x) , \quad (2.30)$$

where we represent the ψ as a column vector with spin components and the ψ^* as a line vector with spin components. $\rho_{\sigma}(x) = \psi_{\sigma}^*(x) \psi_{\sigma}(x)$ is the spin-component density.

We can check that O given by equation (2.27), when applied to any vector with N particles,

$$\begin{aligned} & O_1 | x_1 x_2 \dots > = \\ & = \frac{1}{\sqrt{N!}} \int dx \psi^*(x) O_1(x) \psi(x) \psi^*(x_1) \psi^*(x_2) \dots | 0 > = \\ & = \frac{1}{\sqrt{N!}} \int dx O_1(x_1) \psi^*(x_1) \psi^*(x_2) \dots | 0 > - \\ & - \frac{1}{\sqrt{N!}} \int dx \psi^*(x) O_1(x) \psi^*(x_1) \psi(x) \psi^*(x_2) \dots | 0 > = \dots , \end{aligned} \quad (2.31)$$

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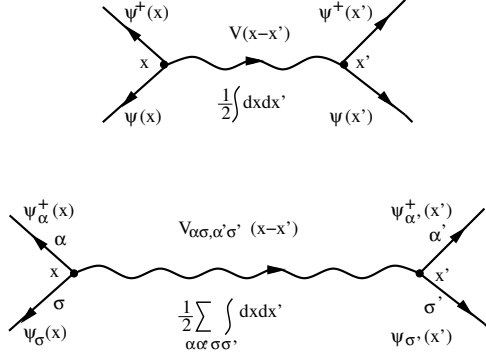


Figure 2.2: Interaction diagrams.

gives the operator in equation (2.26) applied to that state.

Similarly, a two-particle operator

$$O_2 = \frac{1}{2} \sum_{i \neq j} O_2(x_i - x_j) \quad (2.32)$$

can be written as

$$O_2 = \frac{1}{2} \int dx dx' \psi^*(x) \psi^*(x') O_2(x - x') \psi(x') \psi(x) , \quad (2.33)$$

where we see that the "ultraviolet" contributions $O_2(0)$ are excluded. If spin is included, we have

$$O_2 = \frac{1}{2} \sum_{\alpha\alpha'\sigma\sigma'} \int dx dx' \cdot \psi_\alpha^*(x) \psi_{\alpha'}^*(x') O_{2\alpha\sigma, \alpha'\sigma'}(x - x') \psi_{\sigma'}(x') \psi_\sigma(x) . \quad (2.34)$$

An interaction operator is a two-particle operator. The particle identity requires

$$O_{2\alpha\sigma, \alpha'\sigma'} = O_{2\alpha'\sigma', \alpha\sigma} ; \quad (2.35)$$

the spin reversal symmetry requires

$$O_{2\alpha\sigma, \alpha'\sigma'} = O_{2\overline{\alpha}\overline{\sigma}, \overline{\alpha'}\overline{\sigma'}} , \quad (2.36)$$

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where the upper bars indicate the reversed spins; and the spin conservation requires $\sigma + \sigma' = \alpha + \alpha'$; which means that the interaction carries a spin β , such that $\alpha = \sigma + \beta$ and $\alpha' = \sigma' - \beta$. A general form of spin-dependent interaction is

$$O_{2\alpha\sigma,\alpha'\sigma'}(x-x') = V(x-x')\delta_{\alpha\sigma}\delta_{\alpha'\sigma'} + U(x-x')\sigma_{\alpha\sigma}\sigma'_{\alpha'\sigma'} \quad , \quad (2.37)$$

where σ, σ' are spin operators.

Following Feynman, we attach particle lines and interaction lines to the field operators and the interaction, as shown in Fig. 2.1; the interaction diagrams are shown in Fig. 2.2.⁴

2.4 Interacting fermions

The kinetic hamiltonian of free fermions with mass m

$$H_0 = \sum_i \frac{p_i^2}{2m} \quad (2.38)$$

is

$$H_0 = \sum_i \left(-\frac{\hbar^2}{2m} \Delta_i \right) \quad , \quad (2.39)$$

where \hbar ($\simeq 10^{-27} \text{erg} \cdot \text{s}$) is Planck's constant and $p = -i\hbar \text{grad}$ is the one-particle momentum. The wavefunctions are the plane waves $\frac{1}{\sqrt{V}} e^{ikx}$, the states are labelled by the wavevector k (and spin), where $p = \hbar k$ is the momentum. The one-particle energy is $\varepsilon_k = \hbar^2 k^2 / 2m$, the ground-state is the Fermi sea, filled up to the Fermi wavevector k_F , given by the number of particles

$$N = 2 \sum_k 1 = \frac{2V}{(2\pi)^3} \int_0^{k_F} d\mathbf{k} = \frac{V}{3\pi^2} k_F^3 \quad , \quad (2.40)$$

⁴R. P. Feynman, "The theory of positrons", Phys. Rev. **76** 749 (1949); "Space-time approach to quantum electrodynamics", *ibid.* 769 (1949): "wouldn't it be funny if these diagrams were to become really useful...?".

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where V is the volume and we take the spin $1/2$. In the second quantization the kinetic (free) hamiltonian reads

$$H_0 = \int dx \psi^*(x) \left(-\frac{\hbar^2}{2m} \Delta_i \right) \psi(x) = \sum_k \varepsilon_k c_k^* c_k . \quad (2.41)$$

The particle number is given by

$$N = \int dx \psi^*(x) \psi(x) = \sum_k c_k^* c_k ; \quad (2.42)$$

it commutes with the free hamiltonian.

It is customary to introduce the inter-particle spacing a ($a \simeq 1/k_F$), through $N \cdot \frac{4\pi}{3} a^3 = V$, and to measure it in Bohr radii $a_H = \hbar^2/m_e^2 \simeq 0.53 \text{\AA}$, where $e = -4.8 \times 10^{-10} \text{esu}$ is the electron charge and $m \simeq 10^{-27} g$ is the electron mass ($\hbar \simeq 10^{-27} \text{erg} \cdot s$), such that $a = a_H r_s$ and $k_F = (9\pi/4)^{1/3}/r_s a_H$. We get the ground-state (kinetic) energy per particle $\varepsilon_{kin} \simeq 2.21/r_s^2$ (ry), where the rydberg is $1 \text{ry} = e^2/2a_H \simeq 13.6 \text{eV}$.

The interaction can be written as

$$\begin{aligned} H_1 &= \frac{1}{2} \int dx dx' \psi^*(x) \psi^*(x') V(x-x') \psi(x') \psi(x) = \\ &= \frac{1}{2} \sum_{kk'} V(q) c_{k+q}^* c_{k'-q}^* c_{k'} c_k , \end{aligned} \quad (2.43)$$

where $V(q)$,

$$V(q) = \int dx V(x) e^{-iqx} , \quad V(x) = \frac{1}{V} \sum_q V(q) e^{iqx} , \quad (2.44)$$

is the Fourier transform of the interaction (potential). Usually, we assume $V(q=0) = 0$. We can check that N commutes with H_1 , and with the whole hamiltonian $H = H_0 + H_1$, which means that N is conserved. Spin labels can be attached to the c -operators, according to the rule given in equation (2.34).

Similar expressions in the second quantization can be written for the total momentum and the total angular momentum (which are conserved). For instance, the total momentum is

$$\begin{aligned} P &= \int dx \psi^*(x) (-i\hbar \text{grad}) \psi(x) = \\ &= \sum_k \hbar k c_k^* c_k ; \end{aligned} \quad (2.45)$$

2 Second Quantization

on the ground-state (Fermi sea) it gives zero, $P | \Phi \rangle = 0$, and on one-particle states it gives the momentum of those states,

$$P c_k^* | \Phi \rangle = \hbar k c_k^* | \Phi \rangle , \quad P c_k | \Phi \rangle = -\hbar k c_k | \Phi \rangle . \quad (2.46)$$

Finally, we note an interesting particularity of the many-particle hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V(x_i - x_j) . \quad (2.47)$$

By introducing the relative coordinates

$$\xi_{ij} = x_i - x_j \quad (2.48)$$

and the center-of-mass coordinate

$$X = \frac{1}{N} \sum_i x_i , \quad (2.49)$$

we get

$$x_i = X + \frac{1}{N} \sum_j \xi_{ij} \quad (2.50)$$

and

$$p_i/m = \dot{x}_i = \dot{X} + \frac{1}{N} \sum_j \dot{\xi}_{ij} , \quad (2.51)$$

or

$$p_i/m = P/M + \frac{1}{M} \sum_j (p_i - p_j) , \quad p_i = \frac{m}{M} P + \frac{1}{N} \sum_j (p_i - p_j) , \quad (2.52)$$

where $M = Nm$ is the total mass and P is the center-of-mass momentum (total momentum). By inserting this p_i into equation (2.47), we get

$$H = P^2/2M + \frac{1}{2} \sum_{ij} p_i (\mu^{-1})_{ij} p_j + \frac{1}{2} \sum_{i \neq j} V(\xi_{ij}) , \quad (2.53)$$

where the reciprocal mass matrix is

$$(\mu^{-1})_{ij} = \frac{1}{m} \delta_{ij} - \frac{1}{M} . \quad (2.54)$$

In equation (2.53) the roles of the free hamiltonian and the interaction hamiltonian are reversed.

3 One-Particle Green Function

3.1 Chronological product

Another great simplification brought by the many-body theory is the interaction and Heisenberg representations. This way, the time dependence is transferred from the wavefunctions to the operators. An operator O in the Heisenberg representation is written as

$$O(t) = e^{\frac{i}{\hbar}Ht} O e^{-\frac{i}{\hbar}Ht} , \quad (3.1)$$

where t denotes the time and H is the hamiltonian. The equation of motion is

$$\dot{O} = \frac{i}{\hbar} [H, O(t)] . \quad (3.2)$$

In the interaction representation the Heisenberg representation is used with the free hamiltonian H_0 (which may include an external field, besides the kinetic part). For instance, in the interaction representation the particle operators read $c_k(t) = c_k e^{-\frac{i}{\hbar}\varepsilon_k t}$, $c_k^*(t) = c_k^* e^{\frac{i}{\hbar}\varepsilon_k t}$, where ε_k denotes the one-particle energy; such relations are obtained by using $[AB, C] = A\{B, C\} - \{A, C\}B$ for any three operators A, B, C (also $[AB, C] = A[B, C] + [A, C]B$).

Another important element of the many-body theory is the chronological product, defined as

$$T(A(t)B(t')) = \begin{cases} A(t)B(t') , & t > t' , \\ -B(t')A(t) , & t < t' \end{cases} \quad (3.3)$$

for a pair of fermion operators (for bosons the minus sign is missing). It can also be written as

$$T(A(t)B(t')) = A(t)B(t')\theta(t - t') - B(t')A(t)\theta(t' - t) , \quad (3.4)$$

where θ is the step function.

3.2 One-particle Green function

The one-particle Green function is defined as

$$iG(xt, x't') = \langle \tilde{\Phi} | T(\psi(xt)\psi^*(x't')) | \tilde{\Phi} \rangle / \langle \tilde{\Phi} | \tilde{\Phi} \rangle, \quad (3.5)$$

where $|\tilde{\Phi}\rangle$ is the ground-state vector of the ensemble with interaction (as distinct from the Fermi sea $|\Phi\rangle$).¹ This Green function is the amplitude of propagation in time of a particle ($t > t'$) or a hole ($t' > t$), the latter being the propagation of a particle backwards in time (according to Feynman). This is why such a function is called a (particle) propagator. It may carry a spin label.

It is easy to see that the mean value on the ground state for a one-particle operator

$$O = \int dx \psi^*(x) O(x) \psi(x) \quad (3.6)$$

is given by

$$\langle O \rangle = -i \int dx \lim_{y \rightarrow x} \text{tr} [O(x) G(xt, yt^+)] , \quad (3.7)$$

where tr refers to spin labels. In particular, the mean values of the particle and spin densities are

$$\begin{aligned} \langle \rho(x) \rangle &= -i \text{tr} G(xt, xt^+) , \\ \langle \sigma(x) \rangle &= -i \text{tr} [s_z G(xt, xt^+)] , \end{aligned} \quad (3.8)$$

and the mean value of the free hamiltonian is

$$\langle H_0 \rangle = -i \int dx \lim_{y \rightarrow x} \text{tr} [h(x) G(xt, yt^+)] , \quad (3.9)$$

¹V. M. Galitskii and A. B. Migdal, "Application of quantum field theory methods to the many body problem", ZhETF **34** 139 (1958) (Sov. Phys.-JETP **7** 96 (1958)); A. Klein and R. Prange, "Perturbation theory for an infinite medium of fermions", Phys. Rev. **112** 994 (1958); P. C. Martin and J. Schwinger, "Theory of many-particle systems. I.", Phys. Rev. **115** 1342 (1959).

3 One-Particle Green Function

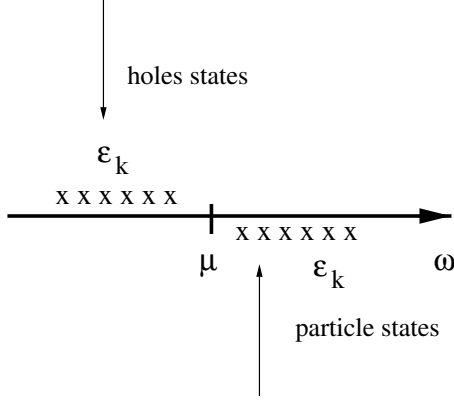


Figure 3.1: Pole structure of $G_0(k, \omega)$.

where

$$H_0 = \int dx \psi^*(x) h(x) \psi(x) . \quad (3.10)$$

By making use of the anticommutation relations and equation (3.4), we get the equation of motion of the free Green function

$$\left(i \frac{\partial}{\partial t} - \frac{1}{\hbar} h(x) \right) G_0(xt, x't') = \delta(x - x') \delta(t - t') \quad (3.11)$$

(hence the name Green function).

Similarly, the equation of motion of the field operator is

$$\begin{aligned} & \left(i \hbar \frac{\partial}{\partial t} - h(x) \right) \psi_\alpha(x, t) = \\ & = \sum_{\beta \alpha' \beta'} \int dx' \psi_{\alpha'}^*(x't) V_{\alpha \beta, \alpha' \beta'}(x - x') \psi_{\beta'}(x't) \psi_\beta(xt) , \end{aligned} \quad (3.12)$$

such that the ground-state interaction energy is given by

$$\begin{aligned} & \langle H_1 \rangle = \\ & = -\frac{i}{2} \int dx \lim_{y \rightarrow x} \text{tr} \left\{ \left[i \hbar \frac{\partial}{\partial t} - h(x) \right] G(xt, yt^+) \right\} \end{aligned} \quad (3.13)$$

3 One-Particle Green Function

and, by using equation (3.9), the total energy is

$$E = \langle H_0 + H_1 \rangle = -\frac{i}{2} \int dx \lim_{y \rightarrow x} \text{tr} \left\{ \left[i\hbar \frac{\partial}{\partial t} + h(x) \right] G(xt, yt^+) \right\} . \quad (3.14)$$

We can highlight a coupling constant g , and write $H = H_0 + gH_1$ and $dE(g)/dg = \langle H_1 \rangle_g$; then, the energy shift of the ground state is

$$\Delta E = E - E_0 = -\frac{i}{2} \int_0^1 \frac{dg}{g} \int dx \lim_{y \rightarrow x} \text{tr} \left\{ \left[i\hbar \frac{\partial}{\partial t} - h(x) \right] G_g(xt, yt^+) \right\} . \quad (3.15)$$

3.3 Free Green function

By using the expansion of the field operators in particle operators, the free Green function can be written as

$$G_0(xt, x't') = -\frac{i}{V} \sum_k (1 - n_k) e^{ik(x-x')} e^{-\frac{i}{\hbar} \varepsilon_k (t-t')} \theta(t-t') + \frac{i}{V} \sum_k n_k e^{ik(x-x')} e^{-\frac{i}{\hbar} \varepsilon_k (t-t')} \theta(t'-t) , \quad (3.16)$$

where we recognize the Fourier transform

$$iG_0(k, t-t') = [(1 - n_k) \theta(t-t') - n_k \theta(t'-t)] e^{-\frac{i}{\hbar} \varepsilon_k (t-t')} , \quad (3.17)$$

n_k being the occupation number. Here, we use the representation

$$\theta(t) = \frac{1}{2\pi i} \int d\omega \frac{e^{i\omega t}}{\omega - i\eta} \quad (3.18)$$

for the step function, where $\eta \rightarrow 0^+$, and get the time Fourier transform

$$G_0(k\omega) = \frac{1 - n_k}{\omega - \varepsilon_k/\hbar + i\eta} + \frac{n_k}{\omega - \varepsilon_k/\hbar - i\eta} \quad (3.19)$$

of the free Green function. We note the definition of the Fourier transforms

$$G_0(kt) = \frac{1}{2\pi} \int d\omega G_0(k\omega) e^{-i\omega t} , \quad G_0(k\omega) = \int dt G_0(kt) e^{i\omega t} \quad (3.20)$$

3 One-Particle Green Function

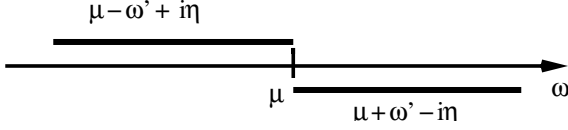


Figure 3.2: Pole structure of $G(k\omega)$.

and

$$G_0(xt) = \frac{1}{V} \sum_k G_0(kt) e^{ikx}, \quad G_0(kt) = \int dx G_0(xt) e^{-ikx}. \quad (3.21)$$

A particle is created on a hole state, where $n_k = 0$; therefore, for particle states the free Green function has poles in the lower half-plane. A hole is created on a particle state, where the poles are in the upper half-plane.

The Fermi sea has a volume V_F and a Fermi surface S_F , defined by $\varepsilon_{k_F} = \varepsilon_F$ (where k_F is viewed as a wavevector). The number of particles can be written as

$$\begin{aligned} N &= \sum_{k\sigma} n_{k\sigma} = \frac{2V}{(2\pi)^3} \int_{V_F} dk = \\ &= \frac{2V}{(2\pi)^3} \int_0^{\varepsilon_F} d\varepsilon \oint_S dS / |grad \varepsilon_k| = \int_0^{\varepsilon_F} d\varepsilon \mathcal{D}(\varepsilon), \end{aligned} \quad (3.22)$$

where

$$\mathcal{D}(\varepsilon) = \frac{2V}{(2\pi)^3} \oint_S dS / |grad \varepsilon_k| \quad (3.23)$$

is the density of energy states (spin 1/2); the surface S is defined by $\varepsilon_k = \varepsilon$. The ground-state energy is given by

$$E_0 = \int_0^{\varepsilon_F} d\varepsilon \mathcal{D}(\varepsilon), \quad (3.24)$$

such that

$$\delta N = \mathcal{D}(\varepsilon_F) \delta \varepsilon_F, \quad \delta E_0 = \varepsilon_F \mathcal{D}(\varepsilon_F) \delta \varepsilon_F. \quad (3.25)$$

We define the chemical potential

$$\mu = \frac{\partial E_0}{\partial N} = \varepsilon_F, \quad (3.26)$$

3 One-Particle Green Function

such that equation (3.19) becomes

$$G_0(k\omega) = \frac{1}{\omega - \varepsilon_k/\hbar + i0^+ \text{sgn}(\varepsilon_k - \mu)} \quad (3.27)$$

(by using $n_k = \theta(\mu - \varepsilon_k)$). The poles of the free Green function are shown in Fig. 3.1.

For $\varepsilon_k = \hbar^2 k^2 / 2m$ the density of states is $D(\varepsilon) = \frac{2V}{\pi^2} (2m/\hbar^2)^{3/2} \varepsilon^{1/2}$.

3.4 Lehmann representation

Let us introduce the energy of $N + 1$ -states (with momentum $\hbar k$)

$$E_{nk} = E + \mu + \xi_{nk} \quad (3.28)$$

and the energy of $N - 1$ -states (with momentum $\hbar \bar{k} = -\hbar k$)

$$E_{m\bar{k}} = E - \mu + \xi_{m\bar{k}} , \quad (3.29)$$

where E is the ground-state energy and ξ_{nk} , $\xi_{m\bar{k}}$ are the excitation energies. We define the density functions

$$\begin{aligned} A(k\omega) &= \sum_n \frac{|\langle nk | c_k^* | \tilde{\Phi} \rangle|^2}{\langle \Phi | \Phi \rangle} \delta(\omega - \xi_{nk}/\hbar) , \\ B(k\omega) &= \sum_m \frac{|\langle m\bar{k} | c_k | \tilde{\Phi} \rangle|^2}{\langle \Phi | \Phi \rangle} \delta(\omega - \xi_{m\bar{k}}/\hbar) , \end{aligned} \quad (3.30)$$

which lead to

$$\begin{aligned} iG(xt, x't') &= \\ &= \frac{1}{V} \sum_k e^{ik(x-x')} [\sum_n \theta(t-t') e^{-\frac{i}{\hbar}(E_{nk}-E)(t-t')} \cdot \\ &\cdot \langle \tilde{\Phi} | c_k | nk \rangle \langle nk | c_k^* | \tilde{\Phi} \rangle / \langle \tilde{\Phi} | \tilde{\Phi} \rangle - \\ &- \sum_m \theta(t'-t) e^{-\frac{i}{\hbar}(E_{m\bar{k}}-E)(t'-t)} \cdot \\ &\cdot \langle \tilde{\Phi} | c_k^* | m\bar{k} \rangle \langle m\bar{k} | c_k | \tilde{\Phi} \rangle / \langle \tilde{\Phi} | \tilde{\Phi} \rangle ; \end{aligned} \quad (3.31)$$