Contents

1 Introduction

1.1 Goals in this course

I will treat Solid State II this semester as a kind of a hybrid. On the one hand, there are students in this course who plan to do theoretical work in condensed matter physics; for you I would like to introduce the basic tools of many-body theory. On the other hand, there are some students, in particular those planning to do experimental work, for whom this may be the last condensed matter physics course they take; for you I feel obligated to provide some introduction to magnetism and superconductivity, the research areas which dominate condensed matter physics in our department. In a year or two, the revised condensed matter curriculum will divide these responsibilities into two one-semester courses, but for now my conscience is still fairly clear. I don't mind exposing experimental students to a bit of many-body theory: despite the fact that you may not end up doing calculations with Green's functions in your future research (on the other hand, you may-there are many experimentalists out there who are proficient in these methods), it is invaluable to be exposed to them at least once, so you can listen to the growing number of seminars and read the growing number of papers where the language is that of second quantization, Feynman diagrams, and field theory (of course, this last sentence could have been written in the early 1960's, but the numbers are still growing!). For the theory students, I have no qualms in exposing you to phenomenology and experimental data. My own tastes lie in this direction, and I hope to communicate to you my own prejudice that it is better to have a pedestrian theory which is right than an elegant, formal theory which is wrong.

This is not to say that I reject formalism altogether. A good deal of what is hard to teach in a course like this, but which the student entering research must learn, is how to distinguish what *is* right and what *is* wrong. In undergraduate courses, and even to a large extent in the graduate core courses you have taken up until now, homework problems are to be solved exactly. In real life, models which describe interesting physical systems are almost never exactly soluble. So we have to invent clever approximation methods, and learning which of these methods are appropriate for which problems is one of the hardest things to learn and teach. Often an interesting physical problem cannot be solved perturbatively, as there is no obvious small parameter; approximate methods can still be employed, but it becomes not only desirable but vital that such approximations respect the symmetries and analytic properties which we can understand by studying the formal structure of the theory.

I want to add to the subject matter covered by this course the quantum Hall effect, in part because this year's physics Nobel prize went to Tsui, Störmer, and Laughlin for their discovery and explanation of the (fractional) effect, in part because important work in this area is continuing at the National High Magnetic Field Laboratory, with whom many of us have some connection, and in part because methods introduced to solve this (2-dimensional) many-body problem are *not* among those taught in a traditional many-body course. I am not an expert on the quantum Hall effect, and intend to improve my own understanding through teaching it. In this area in particular, as in all others, I would appreciate suggestions from the class about references you found helpful or interesting, directions you would like to pursue, etc.

I have to do about a month's worth of formalism before starting new physics. Instead of remaining completely abstract, I will ask you to keep in mind a simple example to which I will keep returning, that of the free Fermi gas. I'll show how one can derive all the results you know for this simple problem from knowledge of the single-particle Green's function. After killing the fly with the sledgehammer, we'll study the sledgehammer itself for awhile, then use it to attack more suitable problems.

1.2 Statistical mechanics of free Fermi gas

1.2.1 $T = 0$ Fermi sea

Start with simple model of electrons in metal, neglecting $e^- - e^-$ interactions. Hamiltonian is

$$\hat{H} = -\sum_j \frac{\hbar^2 \nabla_j^2}{2m}, \quad j = 1, \dots N \text{ particles} \tag{1}$$

Eigenstates of each $-(\hbar^2\nabla^2/2m)$ are just plane waves $e^{i\mathbf{k}\cdot\mathbf{r}}$ labelled by $\mathbf{k}$, with $k_i = 2\pi n_i/L_i$ in box with periodic B.C. Recall electrons are fermions, which means we can only put one in each single-particle state. Including spin we can put two particles ($\uparrow\downarrow$) in each $\mathbf{k}$-state. At zero temperature the ground state of N-electron system is then formed by adding particles until we run out of electrons. Energy is $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$, so start with two in lowest state $k = 0$, then add two to next states, with k_x or k_y or $k_z = 2\pi/L$, etc. as shown. Energy of highest particle called "Fermi energy" ε_F, magnitude of corresponding wave vector called k_F. Typical Fermi energy for metal $\varepsilon_F \simeq 1eV \simeq 10^4 K$. At $T = 0$ only states with $k < k_F$ occupied (Fermi "sea" or Fermi sphere), so we can write density of electrons as 2*# occupied states/Volume (2 is for spin):

$$n = \frac{2}{L^3} \sum_{k=0}^{k_F} \simeq 2 \int_{k<k_F} \frac{d^3k}{(2\pi)^3} = \frac{1}{\pi^2} \int_0^{k_F} k^2 dk = \frac{k_F^3}{3\pi^2} \tag{2}$$

so

$$k_F = (3\pi^2 n)^{1/3} \quad \text{or} \quad \varepsilon_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m} \tag{3}$$

in other words, nothing but the density of electrons controls the Fermi energy.

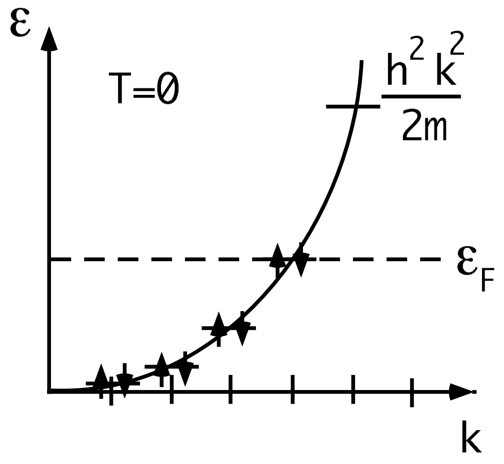


Figure 1: States of Fermi gas with parabolic spectrum, $\varepsilon = k^2/2m$.

The total ground state energy of the Fermi gas must be of order ε_F, since there is no other energy in the problem. If we simply add up the energies of all particles in states up to Fermi level get

$$\frac{E}{L^3} = \frac{1}{\pi^2}\int_0^{k_F} dk\ k^2 \left(\frac{\hbar^2 k^2}{2m}\right) = \frac{\hbar^2 k_F^5}{10\pi^2 m} \tag{4}$$

and the ground state energy per particle ($N = nL^3$ is the total number) is

$$\boxed{\frac{E}{N} = \frac{3}{5}\varepsilon_F}. \tag{5}$$

1.2.2 $T > 0$ Free energy.

Reminder: partition function for free fermions in grnd conical ensemble is

$$\begin{aligned} Z &= \mathrm{Tr}\ e^{-\beta(\hat{H}-\mu\hat{N})} && (6)\\ &= \sum_{n_1,n_2...n_{k_\infty}} \langle n_1, n_2...n_\infty | e^{-\beta(\hat{H}-\mu\hat{N})} | n_1, n_2...n_\infty \rangle && (7)\\ &= \sum_{n_1,n_2...n_\infty} \langle n_1, n_2...n_\infty | e^{-\beta(\sum_i[\varepsilon_i n_i - \mu n_i])} | n_1, n_2...n_\infty \rangle && (8) \end{aligned}$$

where i labels single-fermion state, e.g. $i = \mathbf{k}, \sigma$, and n_i runs from 0 to 1 for fermions. Since many-fermion state in occ. no. representation is simple product: $|n_1, n_2...n_\infty\rangle = |n_1\rangle|n_2\rangle...|n_\infty\rangle$, can factorize:

$$Z = \left(\sum_{n_1} e^{-\beta[\varepsilon_1 n_1 - \mu n_1]}\right) \cdots \left(\sum_{n_\infty} e^{-\beta[\varepsilon_\infty n_\infty - \mu n_\infty]}\right), \tag{9}$$

so

$$\boxed{Z = \Pi_{i=0}^{\infty}\left(1 + e^{-\beta(\varepsilon_i - \mu)}\right)} \tag{10}$$

Since the free energy (grand canonical potential) is $\Omega = -k_B T\ \log Z$, we get

$$\boxed{\Omega = -k_B T\, \Sigma_{i=1}^{\infty} \log\left(1 + e^{-\beta(\varepsilon_i - \mu)}\right)} \tag{11}$$

1.2.3 Avg. fermion number.

We may want to take statistical averages of quantum operators, for which we need the *statistical operator* $\hat{\rho} = Z^{-1} e^{-\beta(\hat{H} - \mu\hat{N})}$. Then any operator $\hat{\mathcal{O}}$ has an expectation value $\langle\hat{\mathcal{O}}\rangle = \mathrm{Tr}(\hat{\rho}\hat{\mathcal{O}})$. For example, avg. no. of particles

$$\begin{aligned}\langle\hat{N}\rangle &= \mathrm{Tr}(\rho\hat{N}) &(12)\\ &= \frac{\mathrm{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})}\hat{N})}{\mathrm{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})})} &(13)\end{aligned}$$

Now note this is related to derivative of Ω wrt chem. potential μ:

$$\begin{aligned}\frac{\partial\Omega}{\partial\mu} &= -k_B T \frac{\partial \log Z}{\partial\mu} = \frac{-k_B T}{Z}\frac{\partial Z}{\partial\mu} &(14)\\ &= \frac{-1}{Z}\mathrm{Tr}(\rho\hat{N}) = -\langle\hat{N}\rangle &(15)\end{aligned}$$

and using Eq. 11, we see

$$\langle\hat{N}\rangle = \sum_{i=1}^{\infty} \frac{1}{1 + e^{\beta(\varepsilon_i - \mu)}} \equiv \sum_{i=1}^{\infty} n_i^0 \tag{16}$$

where n_0^i is the avg. number of fermions in a single-particle state i in equilibrium at temperature T. If we recall i was a shorthand for $\mathbf{k}, \sigma$, but $\varepsilon_{\mathbf{k}}$ doesn't depend on σ, we get Fermi-Dirac distribution function

$$\boxed{n^0_{\mathbf{k}\sigma} = \frac{1}{1+e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}}} \tag{17}$$

1.2.4 Fermi gas at low T.

Since the Fermi energy of metals is so high ($\sim 10^4 K$), it's important to understand the limit $k_B T \ll \varepsilon_F$, where the Fermi gas is nearly degenerate, and make sure the classical limit $k_B T \gg \varepsilon_F$ comes out right too. Let's calculate, for example, the entropy and specific heat, which can be obtained from the thermodynamic potential Ω via the general thermodynamic relations

$$S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu}; \qquad C_V = T\left(\frac{\partial S}{\partial T}\right)_{V,\mu} \tag{18}$$

From (11) and (16), and including spin, we have

$$\begin{aligned}
\Omega &= -2k_B T \sum_{\mathbf{k}} \log\left(1+e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right) \\
&= 2k_B T L^3 \int d\varepsilon N(\varepsilon) \log\left(1+e^{-\beta(\varepsilon-\mu)}\right) \\
&\Rightarrow \\
c_V &\equiv \frac{C_V}{L^3} = 2\,\frac{1}{k_B T}\int_0^\infty d\varepsilon N(\varepsilon)\left(\frac{-\partial f}{\partial \varepsilon}\right)(\varepsilon-\mu)^2 \\
&= 2\,\frac{1}{k_B T}\int_{-\mu}^\infty d\xi\ N(\xi)\ \left(\frac{-\partial f}{\partial \xi}\right)\xi^2
\end{aligned} \tag{19}$$

where I introduced the *density of* $\mathbf{k}$*-states* for one spin $N(\varepsilon) = L^{-3}\sum_{\mathbf{k}}\delta(\varepsilon - \varepsilon_{\mathbf{k}})$. The Fermi function is $f(\varepsilon) = 1/(1+\exp\beta(\varepsilon-\mu))$, & I defined shifted energy variable $\xi = \varepsilon - \mu$. In general, the degenerate limit is characterized by $\mathbf{k}$ sums which decay rapidly for energies far from the Fermi surface, so the game is to assume the density of states varies slowly on a scale of the

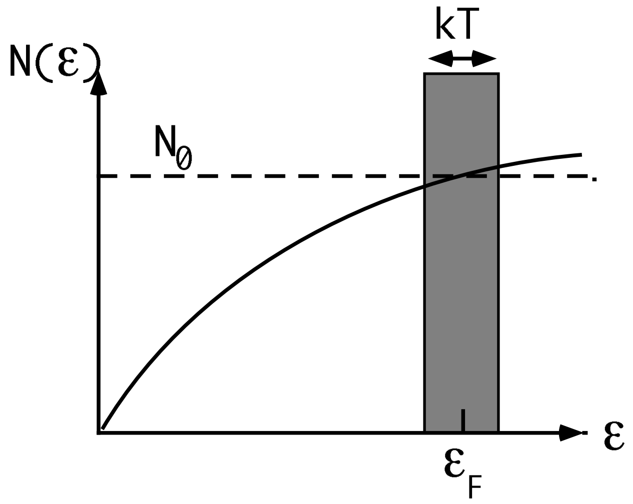


Figure 2: Density of states for parabolic spectrum, $\varepsilon = k^2/2m$

thermal energy, and replace $N(\varepsilon)$ by $N(\varepsilon_F) \equiv N_0$. This type of Sommerfeld expansion[1] assumes the density of states is a smoothly varying fctn., i.e. the thermodynamic limit $V \to \infty$ has been taken (otherwise $N(\varepsilon)$ is too spiky!). For a parabolic band, $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/(2m)$ in 3D, the delta-fctn. can be evaluated to find[2]

$$\boxed{N(\varepsilon) = \frac{3}{2}\frac{n}{\varepsilon_F}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \theta(\varepsilon).} \tag{22}$$

This can be expanded around the Fermi level:[3]

[1] If you are integrating a smooth function of ε multiplied by the Fermi function derivative $-\partial f/\partial\varepsilon$, the derivative restricts the range of integration to a region of width $k_B T$ around the Fermi surface. If you are integrating something times $f(\varepsilon)$ itself, it's convenient to do an integration by parts. The result is (see e.g. Ashcroft & Mermin appendix C)

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon)|_{\varepsilon=\mu} \tag{20}$$

where $a_n = \left(2 - 1/2^{2(n-1)}\right)\zeta(2n)$ (ζ is Riemann ζ fctn., $\zeta(2) = \pi^2/6$, $\zeta(4) = \pi^4/90$, etc.).

[2] Here's one way to get this:

$$N(\varepsilon) = L^{-3}\sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \to \int \frac{d^3k}{(2\pi)^3} |\frac{d\varepsilon}{dk}|^{-1} \delta(k - \frac{\sqrt{2m\varepsilon}}{\hbar}) = \int \frac{k^2 dk}{2\pi^2}\left(\frac{m}{\hbar^2 k}\right)\delta(k - \frac{\sqrt{2m\varepsilon}}{\hbar}) = \frac{3}{2}\frac{n}{\varepsilon_F}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \tag{21}$$

[3] When does the validity of the expansion break down? When the approximation that the density of states is a smooth function does, i.e. when the thermal energy $k_B T$ is comparable to the splitting between states at the Fermi level,

$$\delta\varepsilon_k|_{\varepsilon_F} \simeq \frac{\hbar^2 k_F \delta k}{m} \simeq \varepsilon_F \frac{\delta k}{k_F} \simeq \varepsilon_F \frac{a}{L}, \tag{23}$$

$$N(\xi) = N(0) + N'(0)\xi + \frac{1}{2}N''(0)\xi^2 + \dots \tag{24}$$

(In a horrible misuse of notation, $N(0)$, $N(\varepsilon_F)$, and N_0 all mean the density of states at the Fermi level). The leading order term in the low-T specific heat is therefore found directly by scaling out the factors of T in Eq. (19):

$$c_V \simeq 2k_B \frac{1}{T} N_0 \int_{-\infty}^{\infty} d\xi \left(\frac{-\partial f}{\partial \xi}\right)\xi^2 = 2k_B T \underbrace{\int_{-\infty}^{\infty} dx \left(\frac{-\partial f}{\partial x}\right) x^2}_{\pi^2/3} \tag{25}$$

So

$$c_V \simeq \frac{2\pi^2}{3} N_0 k_B T + \mathcal{O}(T^3). \tag{26}$$

This is the famous linear in temperature specific heat of a free Fermi gas. [4]

---

where a is the lattice spacing and L is the box size. At $T = 1K$, requiring $k_B T \sim \delta\varepsilon$, and taking $\varepsilon_F/k_B \simeq 10^4 K$ says that systems (boxes) of size less than $1\mu m$ will "show mesoscopic" effects, i.e. results from Sommerfeld-type expansions are no longer valid.

[4]Note in (26), I extended the lower limit $-\mu$ of the integral in Eq. (19) to $-\infty$ since it can be shown that the chemical potential is very close to ε_F at low T. Since we are interested in temperatures $k_B T \ll \varepsilon_F$, and the range in the integral is only several $k_B T$ at most, this introduces neglible error.

Why:

At T=0, the Fermi function $n^0_{\mathbf{k}} \to$ step function $\theta(\mu - \varepsilon_{\mathbf{k}})$, so we know $\mu(T = 0)$ must just be the Fermi energy $\varepsilon_F = \hbar^2(3\pi^2 n)^{2/3}/2m$.

$$\begin{aligned}
n &= \frac{N}{L^3} = 2L^{-3}\sum_{\mathbf{k}}^{\infty} n^0_{\mathbf{k}} \\
&= 2\int d\varepsilon N(\varepsilon) f(\varepsilon) \\
&\simeq \int_{-\infty}^{\mu} d\varepsilon N(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 N'(\varepsilon)|_{\varepsilon=\mu} \qquad \text{(continued on next page)} \\
&\simeq \underbrace{\int_{-\infty}^{\varepsilon_F} d\varepsilon N(\varepsilon)}_{n} + (\mu - \varepsilon_F) N(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2 N'(\varepsilon)|_{\varepsilon=\mu} \\
\Rightarrow &\quad \boxed{\mu \simeq \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{N'(\varepsilon_F)}{N(\varepsilon_F)}}
\end{aligned}$$

Since N'/N is typically of order $1/\varepsilon_F^2$, corrections are small.

1.2.5 Classical limit.

I won't calculate the classical limit. All the standard results for a Boltzman statistics gas, e.g. $c_V(T \gg \varepsilon_F) = (3/2)Nk_B$ follow immediately from noticing that the Fermi function reduces to the Boltzman distribution,

$$f(\varepsilon) \to e^{-\beta(\varepsilon-\mu)}, \qquad T \to \infty. \tag{27}$$

(You will need to convince yourself that the classical result $\mu/(k_B T) \to -\infty$ is recovered to make this argument.)

1.3 Second quantization

1.3.1 Symmetry of many-particle wavefunctions

Quantum mechanics allows for the possibility of indistinguishable particles, and nature seems to have taken advantage of this as a way to construct things. No electron can be distinguished from another electron, except by saying where it is, what quantum state it is in, etc. Internal quantum-mechanical consistency requires that when we write down a many-identical-particle state, we make that state noncommittal as to which particle is in which single-particle state. For example, we *say* that we have electron 1 and electron 2, and we put them in states a and b respectively, but exchange symmetry requires (since electrons are fermions) that a satisfactory wave-function has the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = A[(\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) - \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)]. \tag{28}$$

If we have N particles, the wavefunctions must be either symmetric or antisymmetric under exchange:[5]

$$\Psi^B(\mathbf{r}_1 \ldots \mathbf{r}_i \ldots \mathbf{r}_j \ldots \mathbf{r}_N) = \Psi^B(\mathbf{r}_1 \ldots \mathbf{r}_j \ldots \mathbf{r}_i \ldots \mathbf{r}_N) \quad \text{Bosons} \tag{29}$$

$$\Psi^F(\mathbf{r}_1 \ldots \mathbf{r}_i \ldots \mathbf{r}_j \ldots \mathbf{r}_N) = -\Psi^F(\mathbf{r}_1 \ldots \mathbf{r}_j \ldots \mathbf{r}_i \ldots \mathbf{r}_N) \quad \text{Fermions} \tag{30}$$

[5]Recently, a generalization of Bose & Fermi statistics to particles called anyons has been intensely discussed. Under exchange an anyon wavefunction behaves as $\Psi^A(\mathbf{r}_1 \ldots \mathbf{r}_i \ldots \mathbf{r}_j \ldots \mathbf{r}_N) = e^{i\theta}\Psi^A(\mathbf{r}_1 \ldots \mathbf{r}_j \ldots \mathbf{r}_i \ldots \mathbf{r}_N)$ for some $0 \le \theta \le 2\pi$.

Given a set of single-particle wave functions $\phi_{E_i}(\mathbf{r})$, where E_i is a quantum number, e.g. energy, we can easily construct wave fctns. which satisfy statistics, e.g.

$$\Psi^{\substack{B\\F}}_{n_1\ldots n_\infty}(\mathbf{r}_1,\ldots\mathbf{r}_N) = \left(\frac{n_1!n_2!\cdots n_\infty!}{N!}\right)^{1/2} \sum_{\mathcal{P}\in\{E_1,E_2\ldots E_N\}} (\pm 1)^{\;\mathrm{sgn}\mathcal{P}}\; \mathcal{P}\;\Pi_{i=1}^{N}\;\phi_{E_i}(\mathbf{r}_i) \quad (31)$$

Remarks on Eq. (31):

- sum all permutations of the E_i's in product $\phi_{E_1}(\mathbf{r}_1)\phi_{E_2}(\mathbf{r}_2)\ldots\phi_{E_N}(\mathbf{r}_N)$.[6]
- # distinct E_i's occuring may be less than N, some missing because of multiple occupation in boson case. Example:

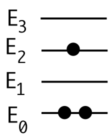


Fig. 2. Possible state of 3 noninteracting Bose particles

$$\begin{aligned} &\Psi^{B}_{20100\ldots 0}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \\ = \;&\frac{1}{\sqrt{3}}\{\phi_{E_1}(\mathbf{r}_1)\phi_{E_1}(\mathbf{r}_2)\phi_{E_3}(\mathbf{r}_3) + \\ &+\phi_{E_3}(\mathbf{r}_1)\phi_{E_1}(\mathbf{r}_2)\phi_{E_1}(\mathbf{r}_3) + \\ &+\phi_{E_1}(\mathbf{r}_1)\phi_{E_3}(\mathbf{r}_2)\phi_{E_1}(\mathbf{r}_3)\} \end{aligned}$$

- Completely antisymmetric Fermionic wavefunction called Slater determinant:

$$\Psi_{n_1\ldots n_\infty}(\mathbf{r}_1,\ldots\mathbf{r}_N) = \left(\frac{1}{N!}\right)^{1/2} \begin{vmatrix} \phi_{E_{min}}(\mathbf{r}_1) & \ldots & \phi_{E_{max}}(\mathbf{r}_1) \\ \vdots & & \vdots \\ \phi_{E_{min}}(\mathbf{r}_N) & \ldots & \phi_{E_{max}}(\mathbf{r}_N) \end{vmatrix} \quad (32)$$

  where there are N eigenvalues which occur between E_{min} and E_{max}, inclusive, corresponding to N occupied states.

[6] You might think the physical thing to do would be to sum all permutations of the particle labels. This is correct, but actually makes things harder since one can double count if particles are degenerate (see example of 3 bosons below.) The normalization factor is chosen with the sum over all permutation of the E_i's in mind.

1.3.2 Field operators

2nd quantization is alternative way of describing many body states. We describe a particle by a *field operator*

$$\hat{\psi}(\mathbf{r}) = \sum_i a_i \phi_{E_i}(\mathbf{r}) \tag{33}$$

where i runs over the quantum numbers associated with the set of eigenstates ϕ, a_i is a "coefficient" which is an operator (I'm going to neglect the hats ($\hat{}$) which normally denote an operator for the a's and $a^\dagger$'s), and ϕ_{E_i} is a "1st-quantized" wavefunction, i.e. a normal Schrödinger wavefunction of the type we have used up to now, such that (for example) $H\phi_{E_i} = E_i\phi_{E_i}$. Now we *impose* commutation relations

$$\left[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right]_\pm = \delta(\mathbf{r} - \mathbf{r}') \tag{34}$$

$$\left[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')\right]_\pm = \left[\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right]_\pm = 0, \tag{35}$$

which implies

$$[a_i, a_j^\dagger]_\pm = \delta_{ij} \quad ; \quad [a_i, a_j]_\pm = [a_i^\dagger, a_j^\dagger]_\pm = 0. \tag{36}$$

The upper sign is for fermions and the lower for bosons in Eqs. (35) and (36).

Now construct many-body states from vacuum (no particles) $|0\rangle$. a called *annihilation* operator, $a^\dagger$ *creation operator* (see below).

Examples & comments (*all properties follow from commutation relations*):

<u>Bosons</u>:

- one particle in state i: $a_i^\dagger|0\rangle \equiv |1\rangle_i$
- annihilate vacuum $a_i|0\rangle = 0$
- (Bosons)[7] $a_i^\dagger a_i^\dagger|0\rangle \equiv |2\rangle_i$

[7] Analogous state for fermions is zero, by commutation relations-check!

- (Bosons) two in i and one in j: $a_i^\dagger a_i^\dagger a_j^\dagger|0\rangle \equiv |2\rangle_i|1\rangle_j$
- $a_i^\dagger a_i \equiv \hat{n}_i$ is *number operator* for state i.

  Proof: (bosons)

$$\begin{aligned}
(a_i^\dagger a_i)|n\rangle_i &= (a_i^\dagger a_i)(a_i^\dagger)^n|0\rangle \\
&= a_i^\dagger(1 + a_i^\dagger a_i)(a_i^\dagger)^{n-1}|0\rangle = |n\rangle_i + (a_i^\dagger)^2 a_i (a_i^\dagger)^{n-1}|0\rangle \\
&= 2|n\rangle_i + (a_i^\dagger)^3 a_i (a_i^\dagger)^{n-2}|0\rangle \ldots = n|n\rangle_i
\end{aligned}$$

Similarly show (bosons):[8]

- $\boxed{a_i^\dagger|n\rangle_i = (n+1)^{1/2}|n+1\rangle_i}$
- $\boxed{a_i|n\rangle_i = n^{1/2}|n-1\rangle_i}$
- many-particle state

$$\left(\frac{1}{n_1!n_2!\ldots n_\infty!}\right)^{1/2}(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots|0\rangle \equiv |n_1, n_2 \ldots n_\infty\rangle \tag{37}$$

$\star$ occupation numbers specify state completely, exchange symmetry included due to commutation relations! (normalization factor left for problem set)

Fermions

- Anticommutation relations complicate matters, in particular note

$$a^2 = (a^\dagger)^2 = 0 \quad \Rightarrow n_i = \begin{matrix}1\\0\end{matrix} \quad \text{(Pauli principle)} \tag{38}$$

[8] By now it should be clear that the algebra for the bosonic case is identical to the algebra of simple harmonic oscillator *ladder operators*.

- so

$$\boxed{\begin{array}{cc} a^\dagger|0\rangle = |1\rangle & a|1\rangle = |0\rangle \\ a^\dagger|1\rangle = 0 & a|0\rangle = 0 \end{array}} \tag{39}$$

- many-particle state

$$(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots|0\rangle \equiv |n_1, n_2 \ldots n_\infty\rangle \tag{40}$$

$\star$ note normalization factor is 1 here.

- action of creation & annilation operators (suppose $n_s = 1$):

$$\begin{aligned} a_s|\ldots n_s \ldots\rangle &= (-1)^{n_1+n_2+\ldots n_{s-1}}(a_1^\dagger)^{n_1}\cdots a_s a_s^\dagger \cdots (a_\infty^\dagger)^{n_\infty}|0\rangle \\ &= (-1)^{n_1+n_2+\ldots n_{s-1}}(a_1^\dagger)^{n_1}\cdots(1-\underbrace{a_s^\dagger a_s}_{=0})\cdots(a_\infty^\dagger)^{n_\infty}|0\rangle \\ &= (-1)^{n_1+n_2+\ldots n_{s-1}}|\ldots n_s - 1\ldots\rangle \end{aligned}$$

also

$$a_s|\ldots 0 \ldots\rangle = 0 \tag{41}$$

and similarly

$$a_s^\dagger|\ldots n_s \ldots\rangle = \begin{cases} (-1)^{n_1+n_2+\ldots n_{s-1}}|\ldots n_s+1\ldots\rangle & n_s = 1 \\ 0 & n_s = 0 \end{cases} \tag{42}$$

1.3.3 2nd-quantized Hamiltonian

$\star$ Point: Now "it can be shown"[9] that state vector

$$|\Psi(t)\rangle = \sum_{n_1,n_2\ldots n_\infty} f(n_1, n_2 \ldots n_\infty, t)|n_1, n_2 \ldots n_\infty\rangle \tag{43}$$

[9]Normally I hate skipping proofs. However this one is so tedious I just can't resist. And my conscience is clear: Rickayzen couldn't resist either. The bravehearted can look, e.g. in chapter 1 of Fetter and Wallecka.

satisfies the Schrödinger equation (our old friend)

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \tag{44}$$

if we take the "2nd-quantized" form of $\hat{H}$

$$\begin{aligned}\hat{H} &= \sum_{ij} a_i^\dagger\langle i|T|j\rangle a_j + \frac{1}{2}\sum_{ijk\ell} a_i^\dagger a_j^\dagger\langle ij|V|k\ell\rangle a_\ell a_k &(45)\\ &= \int d^3r\hat{\psi}^\dagger(\mathbf{r})T(\mathbf{r},\nabla_\mathbf{r})\hat{\psi}(\mathbf{r}) &(46)\\ &+\frac{1}{2}\int\int d^3r\ d^3r'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) &(47)\end{aligned}$$

where the 1st quantized Hamiltonian was $H = T + V$.

Translationally invariant system

It may be more satisfying if we can at least verify that this formalism "works" for a special case, e.g. translationally invariant systems. For such a system the momentum $\mathbf{k}$ is a good quantum number, so choose single-particle plane wave states

$$\phi_i(\mathbf{r}) = \phi_{\mathbf{k}\sigma}(\mathbf{r}) = L^{-3/2}e^{i\mathbf{k}\cdot\mathbf{r}}u_\sigma, \tag{48}$$

where u_σ is a spinor like $u_\downarrow = \binom{0}{1}$, etc. 1st quantized T is $-\nabla^2/(2m)$,[10] so 2nd-quantized kinetic energy is

$$\boxed{\hat{T} \equiv \sum_{ij} a_i^\dagger\langle i|T|j\rangle a_j = \sum_{\mathbf{k}\sigma}\left(\frac{\mathbf{k}^2}{2m}\right)a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}}. \tag{49}$$

Since we showed $a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$ is just number operator which counts # of particles in state $\mathbf{k}\sigma$, this clearly just adds up the kinetic energy of all the occupied states, as it should. For general two-particle interaction V, let's assume $V(\mathbf{r},\mathbf{r}') = V(\mathbf{r}-\mathbf{r}')$ only, as must be true if we have transl. invariance. In terms of the Fourier transform

$$V(\mathbf{q}) = \frac{1}{L^3}\int d^3\mathbf{r}\ e^{i\mathbf{q}\cdot\mathbf{r}}\ V(\mathbf{r}) \tag{50}$$

[10]I'll set $\hbar = 1$ from here on out, unless required for an honest physical calculation.

we have (steps left as exercise)

$$\boxed{\hat{V} = \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} a^\dagger_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} V(\mathbf{q}) a_{\mathbf{k}'\sigma} a_{\mathbf{k}+\mathbf{q}\sigma}} \tag{51}$$

1.3.4 Schrödinger, Heisenberg, interaction representations

Here we just give some definitions & reminders on different (equivalent) representations of quantum mechanics. In different reps., *time dependence* is associated with states (Schrödinger), operators (Heisenberg), or combination (interaction).

- **Schrödinger picture**

$$\begin{aligned} \text{state } \ |\hat{\psi}_S(t)\rangle, \qquad &\text{operators } \ \hat{\mathcal{O}}_S \neq \hat{\mathcal{O}}_S(t) \\ i\frac{\partial}{\partial t}|\hat{\psi}_S(t)\rangle \ &= \ \hat{H}|\hat{\psi}_S(t)\rangle \end{aligned}$$

  has formal solution

$$\boxed{|\hat{\psi}_S(t)\rangle = e^{-i\hat{H}(t-t_0)}|\hat{\psi}_S(t_0)\rangle} \tag{52}$$

  Note $\hat{H}$ hermitian $\Rightarrow$ *time evolution operator* $\boxed{\hat{U} \equiv e^{i\hat{H}(t-t_0)}}$ is unitary.

- **Interaction picture** (useful for pert. thy.)

$$\hat{H} = \hat{H}_0 + \hat{H}' \qquad\qquad \text{(where } \hat{H}_0 \text{ usually soluble)}$$

  Def. in terms of Schr. picture:

$$\begin{aligned} |\hat{\psi}_I(t)\rangle \ &= \ e^{i\hat{H}_0 t}|\hat{\psi}_S(t)\rangle \\ \hat{\mathcal{O}}_I(t) \ &= \ e^{i\hat{H}_0 t}\hat{\mathcal{O}}_S e^{-i\hat{H}_0 t} \end{aligned}$$

$$\Rightarrow i\frac{\partial}{\partial t}|\hat{\psi}_I(t)\rangle \ = \ \hat{H}'(t)|\hat{\psi}_I(t)\rangle$$

$$\text{with} \quad \hat{H}'(t) \;=\; e^{i\hat{H}_0 t}\hat{H}' e^{-i\hat{H}_0 t}$$

Remarks:

– states and ops. t-dependent in interaction picture, but time dependence of operators very simple, e.g.

$$\begin{aligned} \hat{H}_0 &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \\ i\frac{\partial}{\partial t} a_{\mathbf{k}I}(t) &= e^{i\hat{H}_0 t}[a_{\mathbf{k}}, \hat{H}_0] e^{-i\hat{H}_0 t} \\ &= \varepsilon_{\mathbf{k}} a_{\mathbf{k}I}(t) \end{aligned}$$

$$\Rightarrow a_{\mathbf{k}I}(t) = a_{\mathbf{k}} e^{-i\varepsilon_{\mathbf{k}} t}$$

– Time evolution operator determines state at time t:

$$|\hat{\psi}_I(t)\rangle = \hat{U}(t, t_0)|\hat{\psi}_I(t_0)\rangle$$

From Schrödinger picture we find

$$\boxed{\hat{U}(t, t_0) = e^{i\hat{H}_0 t} e^{-i\hat{H}(t-t_0)} e^{-i\hat{H}_0 t_0}} \tag{53}$$

(Note ($[\hat{H}, \hat{H}_0] \neq 0$!)

- **Heisenberg picture**

$$\begin{aligned} \text{state} \quad |\hat{\psi}_H\rangle & \qquad t\text{-independent}, \\ \text{operators} \quad \hat{\mathcal{O}}_H(t) &= e^{i\hat{H}t}\hat{\mathcal{O}}_S e^{-i\hat{H}t} \end{aligned}$$

so operators evolve according to *Heisenberg eqn. of motion*

$$\boxed{i\frac{\partial}{\partial t}\hat{\mathcal{O}}_H(t) = [\hat{\mathcal{O}}_H(t), H]} \tag{54}$$

⋆ Note–compare three reps. at $t = 0$:

$$|\hat{\psi}_H\rangle \;= |\hat{\psi}_S(0)\rangle \;= |\hat{\psi}_I(0)\rangle \tag{55}$$

$$\hat{\mathcal{O}}_S \;= \hat{\mathcal{O}}_H(0) \;= \hat{\mathcal{O}}_I(0) \tag{56}$$

1.4 Green's function for free Fermi gas

We will now start discussing quantum amplitudes like $\langle 0|\hat{\psi}(\mathbf{r},t)\hat{\psi}^\dagger(\mathbf{r}',t')|0\rangle$, which means the probability amplitude for a particle at $\mathbf{r}'$ at time t', to propagate to a time t and be measured at $\mathbf{r}$. The idea is to do a relatively simple example (the free Fermi gas again) to give you some intuition for what this means, and what information one can gain from knowledge of this object. Instead of the amplitude given above, I'll consider instead the following strange combination of such amplitudes, which turns out to be convenient when we start discussing perturbation theory and Wick's theorem in Sec. xxx:

$$\boxed{G(\mathbf{r},t,\mathbf{r}',t') \equiv -i\langle 0|\mathcal{T}\hat{\psi}(\mathbf{r},t)\hat{\psi}^\dagger(\mathbf{r}',t')|0\rangle} \tag{57}$$
$$\equiv -i\langle 0|\hat{\psi}(\mathbf{r},t)\hat{\psi}^\dagger(\mathbf{r}',t')|0\rangle\theta(t-t') \pm i\langle 0|\hat{\psi}^\dagger(\mathbf{r}',t')\hat{\psi}(\mathbf{r},t)|0\rangle\theta(t'-t). \tag{58}$$

Note the convention regarding the order of the arguments. Here $|0\rangle$ is the Heisenberg ground state of the many-particle system (not necessarily the particle-free Fock space vacuum!), and the *time-ordering symbol* $\mathcal{T}$ is defined by

$$\boxed{\mathcal{T}\hat{A}(t)\hat{B}(t') = \hat{A}(t)\hat{B}(t')\theta(t-t') \pm \hat{B}(t')\hat{A}(t)\theta(t'-t)} \tag{59}$$

and the upper (lower) sign is for bosons (fermions). Note $\mathcal{T}$ doesn't care about $\mathbf{r},\mathbf{r}'$.

If we're considering a translationally invariant system,

$$G(\mathbf{r},t,\mathbf{r}',t') = G(\mathbf{r}-\mathbf{r}',t-t') \tag{60}$$
$$= \sum_{\mathbf{k}}\int\frac{d\omega}{2\pi}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}e^{-i\omega(t-t')}G(\mathbf{k},\omega). \tag{61}$$

<u>Example: Free Fermi gas</u>

$$\hat{H}_0 = \sum_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} \tag{62}$$

Time dependence of operators rather simple:

$$a_{\mathbf{k}\sigma}(t) = e^{i\hat{H}_0 t}a_{\mathbf{k}\sigma}e^{-i\hat{H}_0 t} \tag{63}$$

The ground state for the problem is the Fermi sea; start with the true 0-particle vacuum $|\emptyset\rangle$, and apply the creation operator N times:

$$\begin{aligned}|0\rangle &= \left\{\Pi_{\mathbf{k}} \text{ s.t. } _{k<k_F,\sigma} a^\dagger_{\mathbf{k}\sigma}\right\}|\emptyset\rangle & (64)\\ &= a^\dagger_{\mathbf{k}_1\uparrow}a^\dagger_{\mathbf{k}_1\downarrow}a^\dagger_{\mathbf{k}_2\uparrow}a^\dagger_{\mathbf{k}_2\downarrow}\dots a^\dagger_{\mathbf{k}_F\uparrow}a^\dagger_{\mathbf{k}_F\downarrow}|\emptyset\rangle & (65)\end{aligned}$$

Now consider the state when we create one more particle (state has $N+1$ fermions!)

$$\begin{aligned}a^\dagger_{\mathbf{k}\sigma}(t)|0\rangle &= e^{i\hat{H}_0 t}a_{\mathbf{k}\sigma}e^{-i\hat{H}_0 t}|0\rangle \\ &= e^{i\hat{H}_0 t}a_{\mathbf{k}\sigma}e^{-iE_0 t}|0\rangle = e^{i\hat{H}_0 t}e^{-iE_0 t}\theta(k-k_F)|0\rangle|\mathbf{k}\sigma\rangle \\ &= e^{-iE_0 t}\theta(k-k_F)e^{i(E_0+\varepsilon_{\mathbf{k}})t}|0\rangle|\mathbf{k}\sigma\rangle = e^{i\varepsilon_{\mathbf{k}}t}\theta(k-k_F)|0\rangle|\mathbf{k}\sigma\rangle \\ &= e^{i\varepsilon_{\mathbf{k}}t}\theta(k-k_F)a^\dagger_{\mathbf{k}\sigma}|0\rangle & (66)\end{aligned}$$

and similarly the $N-1$ particle state

$$a_{\mathbf{k}\sigma}|0\rangle = e^{-i\varepsilon_{\mathbf{k}}t}\theta(k_F-k)a_{\mathbf{k}\sigma}|0\rangle. \tag{67}$$

Now let's look at the probability amplitude for a fermion to propagate from time t' to t and stay in the state $\mathbf{k}\sigma$. First we need Fourier transform wrt $\mathbf{r}-\mathbf{r}'$

$$G_0(\mathbf{r}-\mathbf{r}', t-t') = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}G_0(\mathbf{k}, t-t') \tag{68}$$

which turns out to be,[11] using the def. of field operators (33) and the Green's function itself (58):

$$G_0(\mathbf{k}, t-t') = -i\langle 0|\mathcal{T}a_{\mathbf{k}\sigma}(t)a^\dagger_{\mathbf{k}\sigma}(t')|0\rangle \tag{69}$$

Now we use def. of $\mathcal{T}$ and what we learned above:

$$\begin{aligned}G_0(\mathbf{k}, t-t') &= -i\langle 0|a_{\mathbf{k}\sigma}(t)a^\dagger_{\mathbf{k}\sigma}(t')|0\rangle\theta(t-t') + i\langle 0|a^\dagger_{\mathbf{k}\sigma}(t')a_{\mathbf{k}\sigma}(t)|0\rangle\theta(t'-t) \\ &= -ie^{-i\varepsilon_{\mathbf{k}}(t-t')}\Big(\theta(t-t')\langle 0|a_{\mathbf{k}\sigma}a^\dagger_{\mathbf{k}\sigma}|0\rangle\theta(k-k_F) - \theta(t'-t)\langle 0|a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}|0\rangle\theta(k_F-k)\Big) \\ &= -ie^{-i\varepsilon_{\mathbf{k}}(t-t')}\left(\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right) & (70)\end{aligned}$$

The easiest object to interpret turns out to be the completely Fourier transformed Green's fctn.

$$\begin{aligned}G_0(\mathbf{k},\omega) &= \int d(t-t')e^{i\omega(t-t')}G_0(\mathbf{k}, t-t') \\ &= -i\int d(t-t')e^{i(\omega-\varepsilon_{\mathbf{k}})(t-t')}\left(\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right) & (71)\end{aligned}$$

[11] Notation: I don't use a different symbol for the Fourier transform of a function, although formally it is a different function. The F.T. is indicated by the use of a different argument, and from context it should be clear that, e.g. $G(t)$ is a different function of t than $G(\omega)$ is of ω.

To make further progress, we use a useful integral representation of the θ-fctn.:

$$\theta(t-t') = -\int \frac{d\omega'}{2\pi i}\,\frac{e^{-i\omega'(t-t')}}{\omega' + i0^+}, \tag{72}$$

where 0^+ is a positive infinitesimal. This relation is important enough to prove:

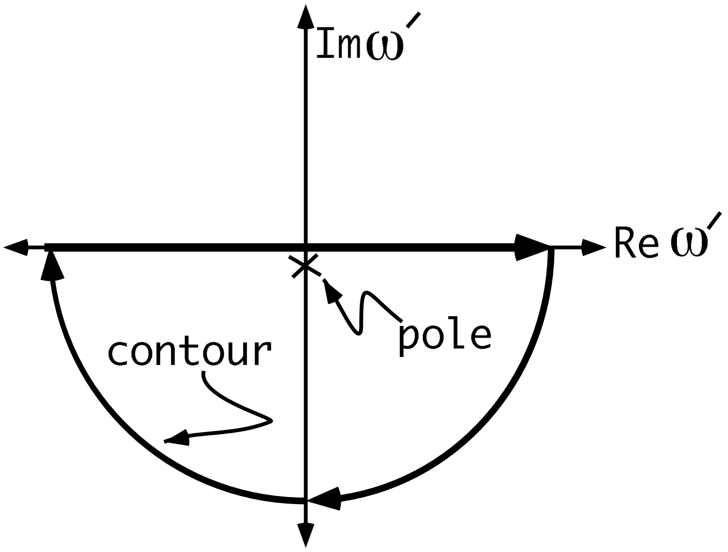


Figure 3: Contour for integral representation of θ function.

<u>a) $t > t'$</u>

Consider integrand in complex ω'-plane. Exponential blows up along + Im axis, so close contour in lower half-plane, pick up pole at $\omega = -i0^+$. Cauchy's thrm. says integral is $2\pi i \cdot$ Residue, pick up a $-$ sign from wrong sense of contour, so find integral $=e^{-i0^+} \to 1$.

<u>b) $t' > t$</u>

Exponential blows up along – Im axis, so close contour in upper half-plane, no pole enclosed $\Rightarrow$ Cauchy says integral =0!

Back to our calculation of G_0: using (72) in (71) we find

$$\begin{aligned} G_0(\mathbf{k},\omega) &= \int \frac{d\omega'}{2\pi} \underbrace{\int d(t-t') e^{i(-\varepsilon_{\mathbf{k}}+\omega-\omega')(t-t')}}_{2\pi\delta(-\varepsilon_k+\omega-\omega')} \left[\frac{\theta(k-k_F)}{\omega'+i0^+} + \frac{\theta(k_F-k)}{\omega'-i0^+}\right] \\ &= \underbrace{\frac{\theta(k-k_F)}{\omega-\varepsilon_k+i0^+}}_{\text{“}particles\text{”}} + \underbrace{\frac{\theta(k_F-k)}{\omega-\varepsilon_k-i0^+}}_{\text{“}holes\text{”}} \end{aligned} \tag{73}$$

which may be written succinctly as

$$\boxed{G_0(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + i0^+\mathrm{sgn}(k-k_F)}} \tag{74}$$

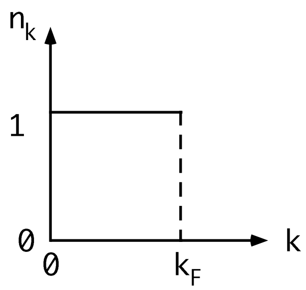
Notice that $\star$ the poles of $G_0(\mathbf{k},\omega)$ are at $\omega = \varepsilon_{\mathbf{k}} \pm i0^+$, where the + sign is for holes, i.e. states below the Fermi energy, and the – sign is for particles. Ignoring the infinitesimal imaginary part, these are just the energies of the elementary single-particle-like excitations of this many-particle system; the poles of the Green's function in the complex ω-plane generally give these energies. If you trace back through the derivation where the $\pm i0^+$ came from, you'll find they they came from the $\theta(t-t')$ and $\theta(t'-t)$, i.e. they were *required to preserve causality*: they make sure, e.g. that a particle doesn't get to its final point $\mathbf{r}$ at a time earlier than it left its initial point $\mathbf{r}'$. The *mathematical formulation* of this causality condition is opposite for particles and holes, hence Feynman's[12] famous observation that holes can be thought of as particles travelling backwards in time.

For a time-translationally invariant system, let's set t'=0, so t is the time difference between creation and annihilation of the extra particle. A reverse Fourier transform on (74) now yields (check!)

$$G_0(\mathbf{k},t) = \begin{cases} in_{\mathbf{k}}e^{-i\varepsilon_{\mathbf{k}}t} & t \le 0 \\ -i(1-n_{\mathbf{k}})e^{-i\varepsilon_{\mathbf{k}}t} & t > 0 \end{cases} \tag{75}$$

where

$$n_{\mathbf{k}} = \begin{cases} 1 & k < k_F \\ 0 & k > k_F \end{cases} \tag{76}$$



So G_0 describes hole propagation (nonzero only for $k < k_F$) for $t < 0$ and particle propagation (nonzero only for $k > k_F$) for $t > 0$.

1.5 Observables from 1-particle Green's function

From the definition (57), several *exact* relations follow (exact means, for any many-body system, not just noninteracting particles). From knowledge of G one can obtain

[12] R.P. Feynman, Phys. Rev. 76, 749 (1949).

- **expectation values** of any "single particle operator", i.e. one which can be written

$$\hat{A} = \sum_i a_i^\dagger a_i. \tag{77}$$

Examples: (check!)

1. *density*

$$\boxed{n = \langle \hat{n}(\mathbf{r}) \rangle = \pm i G(\mathbf{r}, t; \mathbf{r}, t^+)} \tag{78}$$

where the $\pm$ prefactor is for $\substack{\text{bosons}\\\text{fermions}}$. Here t^+ means $\lim T \to 0^+$. Why is this "+" important? Because time-ordering $\mathcal{T}$ puts the operators in the order $\psi^\dagger\psi$ if 2nd time argument is greater than first, in order $\psi\psi^\dagger$ otherwise. Only $\psi^\dagger\psi$ gives the correct counting (check by operating with both on a state with, e.g. 1 particle in it).

2. *spin density*

In principle G is a matrix in spin space if one includes spin indices of field operators, $G_{\sigma\sigma'}(\mathbf{r}, t; \mathbf{r}', t') \equiv -i\langle 0|\psi_\sigma(\mathbf{r}, t)\psi^\dagger_{\sigma'}(\mathbf{r}', t')|0\rangle$. So spin density is given by

$$\boxed{\langle \hat{\sigma}_i(\mathbf{r}) \rangle = \pm i \mathrm{Tr}[\sigma_i G(\mathbf{r}, t; \mathbf{r}, t^+)]} \tag{79}$$

3. *kinetic energy*

$$\boxed{\langle \hat{T} \rangle = \pm i \int d^3r \lim_{\mathbf{r}' \to \mathbf{r}} \left[\frac{-\nabla^2}{2m} \mathrm{Tr} G(\mathbf{r}, t; \mathbf{r}', t^+) \right]} \tag{80}$$

- **ground state energy**

Simple case where $\hat{V}$ ind. of spin:

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \frac{-\nabla^2}{2m} \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \tag{81}$$

then you find[13]

$$\boxed{\langle \hat{H} \rangle = \langle \hat{T} + \hat{V} \rangle = \pm \frac{1}{2} i \int d^3r \lim_{\mathbf{r}' \to \mathbf{r}} \lim_{t' \to t^+} \left[i\frac{\partial}{\partial t} + \frac{-\nabla^2}{2m} \right] G(\mathbf{r}, t; \mathbf{r}', t')} \tag{86}$$

[13] Hints to show this: 1) use Heisenberg eqn. of motion for $\hat{\psi}$:

$$\frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = [\hat{\psi}(\mathbf{r}, t), \hat{H}] = e^{i\hat{H}t} [\hat{\psi}(\mathbf{r}), \hat{H}] e^{-i\hat{H}t} \tag{82}$$

Then calculate

$$[\hat{\psi}(\mathbf{r}), \hat{H}] = \frac{-\nabla^2}{2m} \hat{\psi}(\mathbf{r}) + \int d^3r' \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \tag{83}$$

It's frequently useful to have these results in Fourier-transformed form for a translationally invariant system:

a) *number*

$$\boxed{N = \int d^3r \langle \hat{n}(\mathbf{r})\rangle = \pm i \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} e^{i\omega 0^+} \mathrm{Tr} G(\mathbf{k},\omega)} \tag{87}$$

b) *energy*

$$\boxed{E = \pm \frac{1}{2} i \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi}\, e^{i\omega 0^+} \left(\frac{k^2}{2m} + \omega\right) \mathrm{Tr} G(\mathbf{k},\omega)} \tag{88}$$

Note here $e^{i\omega 0^+}$ is a "convergence factor" defining the appropriate contour to take in the complex ω-plane, ensuring causality.

As an example, let's apply formulae to our canonical concrete example:

Example: free fermion number:

$$N = -2i \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi}\, e^{i\omega 0^+} \left(\frac{1}{\omega - \varepsilon_{\mathbf{k}} + i0^+ \mathrm{sgn}(k - k_F)}\right) \tag{89}$$

Now imagine trying to close contour in either upper or lower half-plane. Can't apply Cauchy's theorem at all for closing in lower half-plane, since $i\omega 0^+$ will then have a positive real part s.t. $e^{i\omega 0^+}$ will diverge as $\mathrm{Im}\omega \to -\infty$. Everything is well-behaved in upper half-plane, though, so we can complete the contour. We pick up the residue from a pole in the upper half-plane *only* if $k < k_F$, therefore

$$\begin{aligned} N &= \frac{-2i}{2\pi}\, 2\pi i \sum_{\mathbf{k}} \theta(k_F - k)\ \mathrm{Res}\left(\frac{e^{i\omega 0^+}}{\omega - \varepsilon_{\mathbf{k}} + i0^+}, \omega \to \varepsilon_{\mathbf{k}} - i0^+\right) \\ &= 2 \sum_{k<k_F} 1 \qquad \text{OK} \end{aligned}$$

since this is our old result, counting once (2 for spin) each k-state inside the Fermi sphere.[14]

---

to find full eqn. of motion

$$\left[i\frac{\partial}{\partial t} - \frac{-\nabla^2}{2m}\right]\hat{\psi}(\mathbf{r},t) = \int d^3r' \hat{\psi}^\dagger(\mathbf{r}',t) V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}',t)\hat{\psi}(\mathbf{r},t) \tag{84}$$

Multiply by $\hat{\psi}^\dagger(\mathbf{r}',t')$ on left, take exp. val. $\langle 0|\ldots|0\rangle$, and $\lim_{\mathbf{r}'\to\mathbf{r}}$, $\lim_{t'\to t^+}$, then integrate $\int d^3r$, yielding

$$\langle \hat{V}\rangle = \pm i \int d^3r \lim_{\mathbf{r}'\to\mathbf{r}} \lim_{t'\to t^+} \left[i\frac{\partial}{\partial t} - \frac{-\nabla^2}{2m}\right] G(\mathbf{r},t;\mathbf{r}',t') \tag{85}$$

and combine this with (80) to get desired result for $\langle \hat{H}\rangle$.

[14]Note in the intermediate step I let $0^+ \to 0$, $e^{i\omega 0^+} \to 1$ since the contour integral had been performed; this is the general prescription.