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Advanced Condensed Matter Theory — SS10

Exercise 3

1.0. In-Class Exercise: The Momentum Distribution

As you know from your solid state physics lecture, (free) Fermi systems possess a Fermi surface, i.e., at $T = 0$ the occupation number $\langle n_{\mathbf{k}\sigma}\rangle$ jumps discontinuously at $\epsilon_{\mathbf{k}} = \mu$. This discontinuity is the origin of many physical properties of solids.

a) Show that $\langle n_{\mathbf{k}\sigma}\rangle$ can be expressed via

$$\langle n_{\mathbf{k}\sigma}\rangle \;=\; \int_{-\infty}^{\infty} d\omega\, f(\omega)\, A_{\mathbf{k}\sigma}(\omega) \;\stackrel{T\to 0}{=}\; \int_{-\infty}^{0} d\omega\, A_{\mathbf{k}\sigma}(\omega), \quad \text{with } f(\omega) \;=\; \frac{1}{e^{\beta\omega}+1}. \tag{1}$$

Hint: To derive Eq. (1) rewrite the expectation value $\langle n_{\mathbf{k}\sigma}\rangle = \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle$ in its spectral representation and compare the result the expression for the spectral function as given in class.

b) Reminding yourself of the expression for the renormalized energy $\tilde{\xi}_k$ from the previous exercise sheet, what can you say about the discontinuity at $\tilde{\xi}_{\mathbf{k}} = \mu$?

1.1. Wick's Theorem for $T \neq 0$ (7 points)

Recall from the lecture (or from the Quantum Field Theory of Condensed Matter lecture last semester) that the perturbation expansion for the Matsubara Green's function is very similar to that for the zero-temperature Green's function. In that case, the expansion could be greatly simplified by the use of Wick's theorem, which provided a prescription for relating a time-ordered product of interaction-picture operators to the normal-ordered product of the same operators. The ground state expectation value of the normal products vanished identically, so that the time-ordered product contained *only* fully contracted terms. Unfortunately, no such simplification occurs at finite temperature, because the ensemble average of the normal product is zero only at zero temperature. Nevertheless, as first proven by Matsubara[1], there exists a *generalized* Wick's theorem that allows a diagrammatic expansion of the temperature Green's functions. This exercise will guide you through a similar proof of the generalized Wick's theorem.

The generalized Wick's theorem can be written down directly as follows:

$$\langle \hat{T}_\tau[\hat{A}\hat{B}\hat{C}\ldots\hat{F}]\rangle_0 = [\hat{A}^\bullet\hat{B}^\bullet\hat{C}^{\bullet\bullet}\cdots\hat{F}^{\bullet\bullet\bullet}] + [\hat{A}^\bullet\hat{B}^{\bullet\bullet}\hat{C}^\bullet\cdots\hat{F}^{\bullet\bullet\bullet}] + \ldots \tag{2}$$

$$= \text{sum of all possible contractions} \tag{3}$$

where $\hat{A}, \hat{B}, \ldots$ are operators in the interaction picture $\psi(x,\tau)$ (or $\psi^\dagger(x,\tau)$), and the notation for *contraction* is defined as

$$\hat{A}^\bullet\hat{B}^\bullet \equiv \langle \hat{T}_\tau[\hat{A}\hat{B}]\rangle_0 = \mathrm{Tr}\{e^{-\beta \mathrm{H}_0}\mathrm{T}_\tau[\hat{A}\hat{B}]\}$$

[1] T. Matsubara, *Prog. Theoret. Phys. (Kyoto)*, **14**:351 (1955)

We can first of all assume that the operators are already in the proper time ordering, as the operators may be reordered on both sides of (2) without introducing any additional changes of sign. Therefore we want to prove the identity

$$\langle[\hat{A}\hat{B}\hat{C}\dots\hat{F}]\rangle_0 = [\hat{A}^{\bullet}\hat{B}^{\bullet}\hat{C}^{\bullet\bullet}\cdots\hat{F}^{\bullet\bullet\bullet}] + [\hat{A}^{\bullet}\hat{B}^{\bullet\bullet}\hat{C}^{\bullet}\cdots\hat{F}^{\bullet\bullet\bullet}] + \dots \tag{4}$$

where we have assumed the time ordering of $\tau_A > \tau_B > \tau_C > \cdots > \tau_F$. We next simplify our notation by introducing the arbitrary operator α_j defined by

$$\psi(x,\tau) \text{ or } \psi^{\dagger}(x,\tau) = \sum_j \chi_j(x,\tau)\alpha_j \tag{5}$$

a) Rewrite the left-hand side of (4) in the new notation (5).

b) Taking your result in (a), start with an arbitrary operator under the trace, say α_a (the first operator in the product). Commute α_a successively to the right until you reach the end of the product of operators (in our notation above, that would be to the right of α_f). You will obtain a sum of traces containing commutators. (Hint: Keep track of sign changes!)

c) We look at the final term in the sum you obtained in (b). Using the cyclic property of the trace you can replace it by the following:

$$\mathrm{Tr}\{e^{-\beta \mathrm{H}_0}\alpha_b\alpha_c\dots\alpha_f\alpha_a\} \rightarrow \mathrm{Tr}\{\alpha_a e^{-\beta \mathrm{H}_0}\alpha_b\alpha_c\dots\alpha_f\} \tag{6}$$

Using the Baker-Hausdorff-Campbell formula, prove that

$$e^{\beta \mathrm{H}_0}\alpha_a e^{-\beta \mathrm{H}_0} = \alpha_a e^{\lambda_a \beta \varepsilon_a} \tag{7}$$

where $\lambda_a = 1$ if α_a is a creation operator, and $\lambda_a = -1$ if α_a is a destruction operator, while ε_a is the kinetic energy corresponding to the α_a

d) Using the result in (c), write down an expression for $\mathrm{Tr}\{e^{-\beta \mathrm{H}_0}\alpha_a\alpha_b\alpha_c\dots\alpha_f\}$ based on the expression you obtained in (b)

e) Define a contraction as

$$\alpha_a^{\bullet}\alpha_b^{\bullet} \equiv \frac{[\alpha_a,\alpha_b]_{\pm}}{1 \mp e^{\lambda_a\beta\varepsilon_a}}$$

where the upper (lower) signs refer to bosons (fermions). Prove the generalized Wick's theorem (4).

1.2. Matsubara Feynman Diagrams: 1st Order Perturbation Theory (9 points)

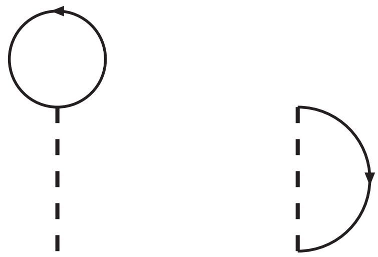
Analogously to zero-temperature Green's functions, pertubative calculations via Feynman diagrams can be done in the Matsubara formalism. In this exercise and the next one we will see how the calculations are done based on the Matsubara Feynman rules. For this purpose we consider the Hamiltonian $\mathcal{H}$ of interacting electrons,

$$\mathcal{H} \equiv \mathcal{H}_0 + V = \sum_{\mathbf{k},\sigma}(\varepsilon(\mathbf{k})-\mu)c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}} V_{\mathbf{q}}^{\sigma,\sigma'} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}$$

We want to calculate the single-particle Matsubara Green's function $G_{\mathbf{k}\sigma}(\mathrm{i}\omega)$ by treating the potential V as a perturbation. According to Dyson's equation,

$$G_{\mathbf{k}\sigma}(\mathrm{i}\omega) = G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega) + G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega)\Sigma_{\mathbf{k}\sigma}(\mathrm{i}\omega)G_{\mathbf{k}\sigma}(\mathrm{i}\omega),$$

we have to calculate the self energy $\Sigma_{\mathbf{k}\sigma}(\mathrm{i}\omega)$. Restricting to 1^{st} order in V this corresponds to the evaluation of the two Feynman diagrams



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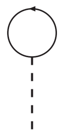
a) General case:

Use the Feynman rules to show that the first diagram  (Hartree term) yields

$$\Sigma^{(\mathrm{H})}_{k\sigma}(\mathrm{i}\omega) \;=\; \left(V^{\sigma,\sigma}_{\mathbf{q}=0} + V^{\sigma,-\sigma}_{\mathbf{q}=0}\right)\sum_{\mathbf{k}'} f(\epsilon(\mathbf{k}') - \mu)$$

and the second one  (Fock term) yields

$$\Sigma^{(\mathrm{F})}_{k\sigma}(\mathrm{i}\omega) \;=\; -\sum_{\mathbf{q}} V^{\sigma,\sigma}_{\mathbf{q}} f(\epsilon(\mathbf{k}-\mathbf{q}) - \mu).$$

Hint: Recall that for a holomorphic function $F(z)$

$$\frac{1}{\beta}\sum_{\omega} F(\mathrm{i}\omega) \;=\; -\oint_{C_1} \frac{dz}{2\pi\mathrm{i}} f(z)\,F(z) \;=\; \oint_{C_2} \frac{dz}{2\pi\mathrm{i}} f(z)\,F(z),$$

where C_1 encloses only the poles of $f(z)$ and C_2 only those of $F(z)$.

b) Coulomb interaction:
Consider the concrete example of a Coulomb interaction of a gas of free electrons in three dimensions. The Fourier transform of the Coulomb potential is

$$V^{\sigma,\sigma'}_{\mathbf{q}} \;=\; \begin{cases} 0 & , \quad \mathbf{q} = 0 \\ \frac{1}{V}\frac{4\pi e_0^2}{q^2} & , \quad \mathbf{q} \neq 0 \end{cases} \qquad (e_0\text{: elementary electric charge}).$$

Use the result from a) to obtain

$$\Sigma_{k\sigma}(\mathrm{i}\omega) \;=\; -\sum_{\mathbf{q}} V^{\sigma\sigma}_{\mathbf{k}-\mathbf{q}} f(\epsilon(\mathbf{q}) - \mu) \overset{T\to 0}{=} \frac{e_0^2}{2\pi} k_{\mathrm{F}} \left(2 + \frac{k_{\mathrm{F}}^2 - k^2}{k k_{\mathrm{F}}} \ln\left|\frac{k_{\mathrm{F}} + k}{k_{\mathrm{F}} - k}\right|\right).$$

Hint:

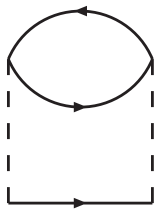
$$\int_0^x dy\, y\, \ln\left|\frac{y-1}{y+1}\right| \;=\; -x - \frac{1}{2}\left(1 - x^2\right)\ln\left|\frac{x-1}{x+1}\right|$$

1.3. The Spectral Weight: A Physical Picture, Part II (9 points)

As we have seen in the previous exercise sheet, the power of the Landau Fermi Liquid Theory is dependent on the validity of the quasiparticle picture. In order for the Fermi Liquid Theory to be valid we would expect a large value of the lifetime. In this exercise, we will discuss a perturbative proof of this quasiparticle concept. For that purpose, consider an electron gas with a local (Hubbard) interaction

$$\mathcal{H} \;\equiv\; \mathcal{H}_0 + V \;=\; \sum_{\mathbf{k},\sigma}(\epsilon(\mathbf{k}) - \mu)\, c^\dagger_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} \;+\; U \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow}\, c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow}\, c_{\mathbf{k}'\downarrow}\, c_{\mathbf{k}\uparrow}.$$

a) The lifetime of a single-particle excitation is related to the imaginary part of $\Sigma_{\mathbf{k}\sigma}(\omega)$ (see exercise 2). In 1st order perturbation theory the self energy is real (exercise 3.2). Thus, we have to consider the 2nd order diagram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Use the Feynman rules to show ($\tilde{\epsilon}(\mathbf{k}) \equiv \epsilon(\mathbf{k}) - \mu$)

$$\Sigma_{\mathbf{k}\sigma}(\omega) \;=\; -U^2 \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \Big(f(\tilde{\epsilon}(\mathbf{k}_2)) - f(\tilde{\epsilon}(\mathbf{k}_3))\Big) \frac{f(\tilde{\epsilon}(\mathbf{k}_1)) + b(\tilde{\epsilon}(\mathbf{k}_3) - \tilde{\epsilon}(\mathbf{k}_2))}{\tilde{\epsilon}(\mathbf{k}_1) + \tilde{\epsilon}(\mathbf{k}_2) - \tilde{\epsilon}(\mathbf{k}_3) - \mathrm{i}\omega} \times$$
$$\times\, \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}).$$

Assuming the self energy to be strongly localized in position space to show that

$$\Sigma_{\mathbf{k}\sigma}(\omega) \;\approx\; -U^2 \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \Big(f(\tilde{\epsilon}(\mathbf{k}_2)) - f(\tilde{\epsilon}(\mathbf{k}_3))\Big) \frac{f(\tilde{\epsilon}(\mathbf{k}_1)) + b(\tilde{\epsilon}(\mathbf{k}_3) - \tilde{\epsilon}(\mathbf{k}_2))}{\tilde{\epsilon}(\mathbf{k}_1) + \tilde{\epsilon}(\mathbf{k}_2) - \tilde{\epsilon}(\mathbf{k}_3) - \mathrm{i}\omega}.$$

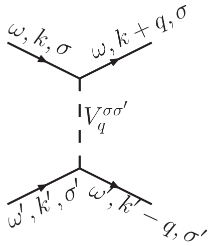
b) Assume that the density of states is bounded and slowly varying, $\sum_{\mathbf{k}} = N_0 \int d\tilde{\epsilon}(\mathbf{k})$, use $b(\tilde{\epsilon}(\mathbf{k}_3) - \tilde{\epsilon}(\mathbf{k}_2)) \approx -f(\tilde{\epsilon}(\mathbf{k}_3) - \tilde{\epsilon}(\mathbf{k}_2))$, and make the analytic continuation $\mathrm{i}\omega \to \omega + \mathrm{i}0^+$ to calculate

$$\mathrm{Im}\Sigma^R_{\mathbf{k}\sigma}(\omega) \;\overset{T\to 0}{\approx}\; -\frac{\pi}{2} N_0^3 U^2 \omega^2 \;\sim\; \omega^2.$$

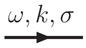
It can be shown that the contribution from n-th order pertubation theory yields $\mathrm{Im}\Sigma^R_{\mathbf{k}\sigma}(\omega) \sim \omega^n$. Why does this result mean that quasiparticles with (inverse) lifetime $\tau_{\mathbf{k}}^{-1} \ll \epsilon^*(\mathbf{k}) - \mu$ exist close to the Fermi level? What follows for the existence of a Fermi surface?

Feynman rules: (Matsubara representation)

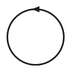
1) Draw all connected, topologically distinct diagrams of order n.

2) Each vertex corresponds to 

$= -\frac{1}{\beta} V_{\mathbf{q}}^{\sigma,\sigma'}$.

3) Each line 

corresponds to $-G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega) = \dfrac{-1}{\mathrm{i}\omega - \epsilon(\mathbf{k}) + \mu}$.

4) Each non-propagating line,  and  , gets a factor $e^{\mathrm{i}\omega 0^+}$.

5) Each closed fermion loop gets an additional factor (-1).

6) All internal indices (momenta, spins, energies, ...) have to be summed.