Quantum Many Body Theory

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Week 15

15 Fermions with attractive interactions (microscopic theory of superconductivity)

Consider a gas of fermions with attractive interactions $U(x) = -\lambda\delta(x-y)$, which leads to (compare with (8.1), Week 7 notes)

$$\hat{H} = \frac{1}{2m}\int dx \sum_{\alpha=\uparrow,\downarrow}\left(\frac{\partial\hat{\psi}^\dagger_\alpha}{\partial x}\frac{\partial\hat{\psi}_\alpha}{\partial x} - \mu\hat{\psi}^\dagger\hat{\psi}\right) - \lambda\int dx\, \hat{\psi}^\dagger_\uparrow(x)\hat{\psi}^\dagger_\downarrow(x)\hat{\psi}_\downarrow(x)\hat{\psi}_\uparrow(x) = \hat{H}_0 + \hat{V}. \quad (15.1)$$

Here $\hat{H}_0$ is the free part of the Hamiltonian, which in the momentum space looks like this

$$\hat{H}_0 = \sum_{p,\alpha=\uparrow,\downarrow}\left(\frac{p^2}{2m} - \mu\right)\hat{a}^\dagger_p a_p, \quad (15.2)$$

and $\hat{V}$ is the interactions, which look like

$$\hat{V} = -\frac{\lambda}{V}\sum_{p,q,q'}\hat{a}^\dagger_{\uparrow,\frac{p}{2}+q}\hat{a}^\dagger_{\downarrow,\frac{p}{2}-q}\hat{a}_{\downarrow,\frac{p}{2}-q'}\hat{a}_{\downarrow,\frac{p}{2}+q'} \quad (15.3)$$

The interaction terms was written starting with density-density term

$$-\frac{\lambda}{2}\int dx\left(\hat{\psi}^\dagger_\uparrow\hat{\psi}_\uparrow + \hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\downarrow\right)^2 \quad (15.4)$$

and taking into account that $\hat{\psi}^2_\uparrow = 0$ (obviously also for $\hat{\psi}_\downarrow$). We would like to understand how this gas behaves.

Originally this problem was addressed in the 50s using perturbation theory. The insight of Bardeen, Cooper, and Schrieffer (BCS) was that the direct perturbation theory in powers of λ breaks down and gives incorrect results, just as the direct perturbative expansion for random matrices we explored in Problem Set 5. Instead, one needs to use a "nonpertubative" approach.

The most transparent approach to this problem is by using the effective field theory. This approach is so simple and appealing, that even though we haven't developed it throughout the semester, we will try to use it here.

If the interactions are so strong that they lead to fermions forming two-body bound states, which, being bosons, Bose condense, then the solution to the problem is the Bose condensation of these fermionic pairs. BCS understood that the formation of these pairs occur even when interactions are weak. The reason for that is truly many-body. In the presence of a weak attractive potential, two fermions cannot form bound states. However, in a many-body setting, fermions fill a Fermi sea. Those fermions which sit in the low energy states cannot respond to the interaction because all states close in energy to them are also occupied. It is only fermions close to Fermi energy which can participate in interactions. And those fermions effectively live in two dimensions - the dimensionality of a Fermi surface. So they form bound states in an arbitrary weak potential.

The process of bound state formation cannot be explored in perturbation theory in powers of λ. Indeed, the energy of a bound state in a potential $-\lambda\delta(x)$ in two dimensions is known to go as $\exp(-1/\lambda)$, a function which is not Taylor-expandable in powers of λ. This explains why earlier studies of (15.1) done in the 50s missed this effect completely.

15.1 Habbard-Stratonovich transformation and the gap equation

To make further progress, we consider the following integral

$$\int d^2z\, e^{-az^*-a^*z-\lambda zz^*} = \int d^2z\, e^{-\lambda\left(z+\frac{a}{\lambda}\right)\left(z^*+\frac{a^*}{\lambda}\right)+\frac{1}{\lambda}aa^*} = \int d^2z\, e^{-\lambda zz^*+\frac{1}{\lambda}aa^*} = \frac{\pi}{\lambda}e^{\frac{1}{\lambda}aa^*}. \quad (15.5)$$

Suppose we would like to compute the partition function of our problem

$$e^{-\frac{F}{T}} = \sum_n \langle n| \exp\left(-\frac{1}{T}\sum_{p,\alpha=\uparrow,\downarrow}\frac{p^2}{2m}\hat{a}^\dagger_{\alpha,p}\hat{a}_{\alpha,p} + \frac{\lambda}{TV}\sum_{p,q,q'}\hat{a}^\dagger_{\uparrow,\frac{p}{2}+q}\hat{a}^\dagger_{\downarrow,\frac{p}{2}-q}\hat{a}_{\downarrow,\frac{p}{2}-q'}\hat{a}_{\downarrow,\frac{p}{2}+q'}\right)|n\rangle\,. \quad (15.6)$$

We now employ (15.5)

$$e^{-\frac{F}{T}} = \int\prod_p\left[d^2\Delta_p\frac{\lambda T}{\pi V}\right]\sum_n\langle n|\, e^{-\frac{\hat{H}_0}{T}-\frac{1}{T}\sum_p\Delta_p\sum_q\hat{a}^\dagger_{\uparrow,\frac{p}{2}+q}\hat{a}^\dagger_{\downarrow,\frac{p}{2}-q}-\frac{1}{T}\sum_p\Delta^*_p\sum_q\hat{a}^\dagger_{\downarrow,\frac{p}{2}-q}\hat{a}^\dagger_{\uparrow,\frac{p}{2}+q}-\frac{V}{\lambda T}\sum_p\Delta^*_p\Delta_p}|n\rangle\,. \quad (15.7)$$

The transformation from (15.6) to (15.7) is called the Habbard-Stratonovich transformation. Notice it would not be possible to do if the interaction was repulsive.

For further clarity, we introduce the following notation

$$e^{-\frac{F}{T}} = \int\prod_p\left[d^2\Delta_p\frac{\lambda T}{\pi V}\right]e^{-\frac{F[\Delta]}{T}}, \quad (15.8)$$

where

$$F[\Delta] = -T\log\left(\sum_n\langle n|\, e^{-\frac{\hat{H}_0}{T}-\frac{1}{T}\sum_p\Delta_p\sum_q\hat{a}^\dagger_{\uparrow,\frac{p}{2}+q}\hat{a}^\dagger_{\downarrow,\frac{p}{2}-q}-\frac{1}{T}\sum_p\Delta^*_p\sum_q\hat{a}_{\downarrow,\frac{p}{2}-q}\hat{a}_{\uparrow,\frac{p}{2}+q}-\frac{V}{\lambda T}\sum_p\Delta^*_p\Delta_p}|n\rangle\right). \quad (15.9)$$

Now the idea is that $F[\Delta]$ has a sharp minimum at some value of Δ, so instead of integrating we will simply calculate $F[\Delta]$ at this minimum. This would give us an approximation to the integral and a good approximation to $F \approx F[\Delta_{\min}]$. Such an approach is called the "saddle point approximation".

To implement it, we differentiate $F[\Delta]$ with respect to Δ_p^* and set the derivative to zero. We find

$$\sum_n \langle n| e^{\frac{F-\hat{\hat{H}}}{T}} \sum_q \hat{a}_{\downarrow,\frac{p}{2}-q}\hat{a}_{\uparrow,\frac{p}{2}+q} |n\rangle + \frac{V}{\lambda T}\Delta_p = 0. \tag{15.10}$$

Here $\hat{\hat{H}}$ is given by

$$\hat{\hat{H}} = \sum_{p,\alpha=\uparrow,\downarrow} \left(\frac{p^2}{2m} - \mu\right) \hat{a}^\dagger_{\alpha,p} a_{\alpha,p} + \sum_p \Delta_p \sum_q \hat{a}^\dagger_{\uparrow,\frac{p}{2}+q}\hat{a}^\dagger_{\downarrow,\frac{p}{2}-q} + \sum_p \Delta_p^* \sum_q \hat{a}_{\downarrow,\frac{p}{2}-q}\hat{a}_{\uparrow,\frac{p}{2}+q} + \frac{V}{\lambda}\sum_p \Delta_p^*\Delta_p. \tag{15.11}$$

We observe that for reasons of translational invariance, $\Delta_p = 0$ for all $p \neq 0$. Denoting $\Delta = \Delta_0$, we find the only nontrivial equation

$$\sum_n \langle n| e^{\frac{F-H_{\mathrm{BCS}}}{T}} \sum_q \hat{a}_{\downarrow,-q}\hat{a}_{\uparrow,q} |n\rangle + \frac{V}{\lambda T}\Delta = 0, \tag{15.12}$$

where

$$\hat{H}_{\mathrm{BCS}} = \sum_{p,\alpha=\uparrow,\downarrow} \left(\frac{p^2}{2m} - \mu\right) \hat{a}^\dagger_p a_p + \Delta \sum_q \hat{a}^\dagger_{\uparrow,q}\hat{a}^\dagger_{\downarrow,-q} + \Delta^* \sum_q \hat{a}_{\downarrow,-q}\hat{a}_{\uparrow,q} + \frac{V}{\lambda}\Delta^*\Delta. \tag{15.13}$$

H_{BCS} is called the BCS Hamiltonian. (15.12) is called the BCS gap equation, whose unknown is Δ.

15.2 The Dyson equation

We observe that we need to calculate

$$\langle n| e^{\frac{F-H_{\mathrm{BCS}}}{T}} \sum_q \hat{a}_{\downarrow,-q}\hat{a}_{\uparrow,q} |n\rangle . \tag{15.14}$$

To do so, we introduce the normal and anomalous temperature Green's functions

$$\begin{aligned}
G_\alpha(\tau,x) &= -\sum_n \langle n| e^{\frac{F-\hat{H}_{\mathrm{BCS}}}{T}} T\hat{\psi}_\alpha(x_f,\tau_f)\hat{\bar{\psi}}_\alpha(x_i,\tau_i) |n\rangle , \\
F(\tau,x) &= -\sum_n \langle n| e^{\frac{F-\hat{H}_{\mathrm{BCS}}}{T}} T\hat{\psi}_\downarrow(x_f,\tau_f)\hat{\psi}_\uparrow(x_i,\tau_i) |n\rangle , \\
\bar{F}(\tau,x) &= -\sum_n \langle n| e^{\frac{F-\hat{H}_{\mathrm{BCS}}}{T}} T\hat{\bar{\psi}}_\uparrow(x_f,\tau_f)\hat{\bar{\psi}}_\downarrow(x_i,\tau_i) |n\rangle
\end{aligned} \tag{15.15}$$

where $\alpha = \uparrow$ or $\downarrow$, and $\tau = \tau_f - \tau_i$, $x = x_f - x_i$. Then the expression (15.14) is given by

$$\sum_n \langle n| e^{\frac{F - H_{\rm BCS}}{T}} \sum_q \hat{a}_{\downarrow,-q} \hat{a}_{\uparrow,q} |n\rangle = \sum_q F(\tau = +0, q). \tag{15.16}$$

Now we would like to calculate G and F for a BCS Hamiltonian, with a given Δ. We do it by analogy with (11.7) and (11.8) of the Week 10 notes, which were the Dyson equations for a superfluid Bose gas. We notice however that the self-energy corrections due to the presence of the Δ, Δ^* terms, are known exactly (ultimately because these terms are quadratic in creation and annihilation operators), so the Dyson equations will lead to exact Green's functions of $\hat{H}_{\rm BCS}$ (however, keep in mind that $\hat{H}_{\rm BCS}$ is itself of course but an approximation).

We find

$$G(\omega, p) = G_0(\omega, p) - \bar{F}(\omega, p) \Delta G_0(\omega, p), \bar{F}(\omega, p) = G(\omega, p) \Delta^* G_0(-\omega, -p). \tag{15.17}$$

Solving these equations give

$$G(\omega, p) = \frac{G_0^{-1}(-\omega, -p)}{G_0^{-1}(-\omega, -p) G_0^{-1}(\omega, p) + \Delta\Delta^*}, \ \bar{F}(\omega, p) = -\frac{\Delta^*}{G_0^{-1}(-\omega, -p) G_0^{-1}(\omega, p) + \Delta\Delta^*}. \tag{15.18}$$

Recall that

$$G_0(\omega, p) = \frac{1}{i\omega - \frac{p^2}{2m} + \mu}. \tag{15.19}$$

Thus we find

$$G(\omega, p) = \frac{-i\omega - \frac{p^2}{2m} + \mu}{\omega^2 + \left(\frac{p^2}{2m} - \mu\right)^2 + \Delta\Delta^*}, \tag{15.20}$$

and

$$\bar{F}(\omega, p) = \frac{\Delta^*}{\omega^2 + \left(\frac{p^2}{2m} - \mu\right)^2 + \Delta\Delta^*}. \tag{15.21}$$

Analogously, from writing the corresponding equation for F,

$$F(\omega, p) = G(-\omega, -p) \Delta G_0, \tag{15.22}$$

we find

$$\bar{F}(\omega, p) = \frac{\Delta}{\omega^2 + \left(\frac{p^2}{2m} - \mu\right)^2 + \Delta\Delta^*}. \tag{15.23}$$

15.3 The gap equation

Now we are in the position to compute the BCS gap equation (15.12), which takes the form

$$\frac{T}{V}\sum_{q,\omega_n}\frac{\Delta}{\omega_n^2+\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}=\frac{\Delta}{\lambda}. \tag{15.24}$$

Here $\omega_n=(2n+1)\pi T$ are the Matsubara frequencies.

One solution to this equation is $\Delta=0$. However, there may also be another solution, which solves

$$\frac{T}{V}\sum_{q,\omega_n}\frac{1}{\omega_n^2+\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}=\frac{1}{\lambda}. \tag{15.25}$$

The sum over the Matsubara frequencies can be computed in many ways. In one of them, we convert the sum into the integral

$$T\sum_{\omega_n}\frac{1}{\omega_n^2+\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}=-\oint\frac{d\omega}{2\pi}\frac{1}{\left(\omega_n^2+\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*\right)\left(e^{\frac{i\omega}{T}}+1\right)}. \tag{15.26}$$

Here the integral is taken over the contour which encloses the real axis and goes in the counterclockwise direction. However, we can deform this contour into two contours, each enclosing the poles $\omega=\pm i\sqrt{\left(\frac{p^2}{2m}-\mu\right)^2+\Delta\Delta^*}$ in the clockwise directions. There result is

$$T\sum_{\omega_n}\frac{1}{\omega_n^2+\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}=\frac{\tanh\left[\frac{\sqrt{\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}}{2T}\right]}{2\sqrt{\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}}. \tag{15.27}$$

Substituting it into (15.25) gives

$$\frac{1}{V}\sum_{q}\frac{\tanh\left[\frac{\sqrt{\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}}{2T}\right]}{2\sqrt{\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}}=\frac{1}{\lambda}, \tag{15.28}$$

Finally, converting sum over momenta into the integral gives

$$\int\frac{d^3q}{(2\pi)^3}\frac{\tanh\left[\frac{\sqrt{\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}}{2T}\right]}{2\sqrt{\left(\frac{q^2}{2m}-\mu\right)^2+\Delta\Delta^*}}=\frac{1}{\lambda}. \tag{15.29}$$

15.4 Solution to the gap equation at $T = 0$

If the temperature $T = 0$, then the gap equation simplifies further

$$\int \frac{d^3q}{(2\pi)^3} \frac{1}{2\sqrt{\left(\frac{q^2}{2m} - \mu\right)^2 + \Delta\Delta^*}} = \frac{1}{\lambda}. \tag{15.30}$$

We observe, first of all, that the integral over momenta is divergent at large momenta. Makes sense to cut it off at $q = \Lambda$, where, as usual, Λ specifies the inverse range of the interactions. This gives

$$\int \frac{d^3q}{(2\pi)^3} \left[\frac{1}{2\sqrt{\left(\frac{q^2}{2m} - \mu\right)^2 + \Delta\Delta^*}} - \frac{m}{q^2} \right] = \frac{1}{\lambda} - \frac{m\Lambda}{2\pi^2}. \tag{15.31}$$

Here the integral in the square brackets can be extended to infinity because it is convergent.

Now remarkably the expression on the right hand side is nothing but $m/(4\pi a)$, where a is the scattering length (see (2.23) of Week 2 notes, where one needs to remember that our λ is defined with the opposite sign (attraction) compared to λ of (2.23), which corresponded to repulsion, as in (2.26). Also, m in (2.23) should be replaced with $m/2$, that is, the reduced mass of two fermions). Thus we find

$$\int \frac{d^3q}{(2\pi)^3} \left[\frac{1}{2\sqrt{\left(\frac{q^2}{2m} - \mu\right)^2 + \Delta\Delta^*}} - \frac{m}{q^2} \right] = -\frac{m}{4\pi a}. \tag{15.32}$$

The integral here can be computed in a variety of ways. Here is one especially simple approach, which however only finds the leading asymptotics of Δ as a function of a, for a very small (and negative, as the interactions are repulsive). If a is very small, the integral is large. That means, Δ has to be small. If $\Delta = 0$, the integral is divergent logarithmically at $q^2/(2m) = \mu$. To find it at finite Δ, introduce the variable ξ,

$$\xi = q^2/(2m) - \mu. \tag{15.33}$$

At q close to $\sqrt{2m\mu}$, $d^3q/(2\pi)^3 \approx \nu d\xi$, where ν was introduced in (12.36), Week 12 (with μ playing the role of ω). So we estimate the integral by

$$\int_{-\mu}^{\mu} \nu d\xi \left[\frac{1}{2\sqrt{\xi^2 + \Delta\Delta^*}} - \frac{m}{q^2} \right] = -\frac{m}{4\pi a}. \tag{15.34}$$

This gives with logarithmic accuracy

$$\frac{\nu}{2} \log \frac{\mu}{\Delta\Delta^*} = -\frac{m}{4\pi a}. \tag{15.35}$$

Finally, this leads to

$$|\Delta|^2 = \mu \, e^{\frac{m}{2\pi a \nu}}. \tag{15.36}$$

Remember that a is small and negative. Thus Δ is given by an exponentially suppressed factor (which also happens to be nonperturbative in powers of a).

It is easy to see that this is a minimum of $F[\Delta]$ introduced in (15.9). Thus $\Delta = 0$ solution is the maximum and should be discarded.

15.5 Excitation spectrum

The spectrum of excitations is given by the poles of the Green's function (15.20), or

$$\omega = \sqrt{\left(\frac{p^2}{2m} - \mu\right)^2 + \Delta\Delta^*}. \tag{15.37}$$

Thus the spectrum is *gapped*. The quasiparticles with this spectrum are called the Bogoliubov quasiparticles.

15.6 Finite temperature

As the temperature is increased, we go back to (15.29). The higher the temperature, the smaller is Δ which solves the gap equation. At some critical T_c where Δ vanishes, we find

$$\frac{1}{2} \int \frac{d^3q}{(2\pi)^3} \tanh \left[\frac{\frac{q^2}{2m} - \mu}{2T_c}\right] \left(\frac{1}{\frac{q^2}{2m} - \mu} - \frac{2m}{q^2}\right) = -\frac{m}{4\pi a}. \tag{15.38}$$

The "honest" calculation of T_c requires some algebra as the integral here, while convergent, is not simple. However, we can estimate that

$$T_c \sim |\Delta(T = 0)|^2. \tag{15.39}$$

This is the temperature at which superconductivity vanishes, together with Δ, is of the order of Δ at zero temperature, which is given by (15.36).