Physics 242: Homework Problem Set 1

Due January 26, 2011

1 Ginzburg-Landau Theory: an exercise.

In the first handout (Fetter and Hohenberg, Theory of Type II Superconductors) the free energy functional for a superconductor in a magnetic field is presented in Eq. (1). It is a functional of the complex superconducting order parameter $\Psi(\vec{r})$ and the vector potential $\vec{A}(\vec{r})$. The definition of a functional derivative was discussed in class. The problem is: to carry the functional differentiation of the free energy functional with respect to $\vec{A}(\vec{r})$ to obtain the result given in Eq. (3). For this exercise, keep all constants in the equation, that is, do not use the dimensionless form of the G-L functional.

Solution.
The functional derivative of the terms that contain $\vec{A}$ are straightforward and were done correctly in the handed-in homework. There is a term that is not nearly as straightforward. The magnetic field $\vec{h} = \nabla \times \vec{A}$ is in the functional (as $h^2/8\pi \equiv \vec{h} \cdot \vec{h}/8\pi$ and involves derivatives of $\vec{A}$. How does one evaluate

$$\frac{\delta}{\delta \vec{A}(r)} \int dr' |\nabla \times \vec{A}(r')|^2 \tag{1}$$

(the 8π can be inserted later)?

First one needs to know (see Wikipedia "Functional Derivatives" which even gives the short proof) that

$$\begin{aligned} F[\rho] &\equiv \int f(r, \rho(r), \nabla\rho(r)) dr, \\ \frac{\delta F[\rho]}{\delta \rho(r)} &= \frac{\partial f}{\partial \rho} - \nabla \cdot \frac{\partial f}{\partial \nabla \rho} = \frac{\partial f}{\partial \rho} - \sum_j \frac{\partial}{\partial r_j} \frac{\partial f}{\partial (\frac{\partial \rho}{\partial r_j})} \end{aligned} \tag{2}$$

where the r.h.s. is evaluated at r and $\rho(r)$, and $r_1 = x$, etc.

Letting our $F[\vec{A}] = \int f(\{\partial_m A_n\}) = \int h^2 \equiv \int \vec{h} \cdot \vec{h}$, we see there in no dependence on $\vec{A}$ itself, but only on its first derivatives, for which the above formulae apply. So we need

$$\frac{\delta f}{\delta \vec{A}} = -\sum_j \partial_j \frac{\partial |\vec{h}|^2}{\partial(\partial_j \vec{A})} \tag{3}$$

where notation is simplified by $\partial/\partial r_j \equiv \partial_j$.

This is a vector equation (in the components of $\vec{A}$) and subscripts are about to proliferate. Let's take one component A_m as a representative. Continuing the differentiation,

$$\frac{\delta F}{\delta A_m(r)} = -\sum_j \partial_j \frac{\partial |\vec{h}|^2}{\partial(\partial_j A_m)} = -2(\sum_j \partial_j \vec{h} \cdot \frac{\partial \vec{h}}{\partial(\partial_j A_m)}). \tag{4}$$

So we need $\partial \vec{h}/\partial(\partial_j A_m)$. Writing out $\vec{h}$:

$$h_x = \partial_y A_z - \partial_z A_y, h_y = \partial_z A_x - \partial_x A_z, h_z = \partial_x A_y - \partial_y A_x, \tag{5}$$

we see that (choosing a specific component a_y of $\vec{A}$):

$$\frac{\partial \vec{h}}{\partial(\partial_x A_y)} = +(0,0,1), \quad \frac{\partial \vec{h}}{\partial(\partial_y A_y)} = (0,0,0), \quad \frac{\partial \vec{h}}{\partial(\partial_z A_y)} = -(1,0,0), \tag{6}$$

and other derivatives can be obtained by permuting indices. Then

$$\frac{\delta F}{\delta A_y(r)} = -2\sum_j \partial_j \vec{h} \cdot \frac{\partial \vec{h}}{\partial(\partial_j A_y)} = -2[\partial_x \vec{h} \cdot \frac{\partial \vec{h}}{\partial(\partial_x A_y)} + \partial_y \vec{h} \cdot \frac{\partial \vec{h}}{\partial(\partial_y A_y)} + \partial_z \vec{h} \cdot \frac{\partial \vec{h}}{\partial(\partial_z A_y)}]. \tag{7}$$

The 1st term is -$2\partial_x \vec{h} \cdot (0,0,1) = -2\partial_x h_z$. The 2nd term vanishes. The third term is $-2\partial_z \vec{h} \cdot (-1,0,0) = +2\partial_z h_x$. The sum is

$$\frac{\delta F}{\delta A_y(r)} = -2(\partial_x h_z - \partial_z h_x) = 2(\nabla \times \vec{A})_y. \tag{8}$$

Permuting the indices x, y, z, the result becomes

$$\frac{\delta F}{\delta \vec{A}(r)} = \frac{\delta}{\delta \vec{A}(r)} \int dr' |\nabla \times \vec{A}(r')|^2 = 2\ \nabla \times \nabla \times \vec{A}(r) = 2\ \nabla \times \vec{h}(r). \tag{9}$$

Comment: Since $\nabla \times \vec{A}$ is "perpendicular to" $\vec{A}$, and the functional derivative is asking for the change "along $\vec{A}(r)$," a reasonable guess would be that the derivative might vanish. It doesn't, but it does requires something "special" to be non-zero: a current (by Maxwell's equations). For a vector potential describing a system without charge currents, the functional derivative does vanish.

Putting this result together with the functional derivative of the rest of the free energy expression, the usual Ginzburg-Landau equation results.

Note. Using the succinct notation for the cross product $h_i = \sum_{j,k} \epsilon_{ijk} \partial_j A_k$, where ϵ is the antisymmetric tensor, the derivation given above becomes much simpler, and one gets the result without 'seeing' what all happens to give the result.

2 The Cooper Pair Wavefunction.

In Cooper's original paper Phys. Rev. **104**, 1189 (1956), in Eq. (6) he writes down an expression of the Cooper pair wavefunction, and makes claims about it. Your tasks (this is a mini-research project, not a "find the answer") are:

A. argue where this form came from; note that he wrote the form of the wavefunction in Eq. (2). "Argue" means to derive making appropriate approximations.

B. perform the integral, making the approximations that are consistent with Cooper's level of description. Hint: set K to zero at an earlier step than Cooper does; he was trying to be convincing about something (K=0 pairs) that is taken for granted nowadays. If you prefer to use the formalism introduced in class (somewhat more modern, more familiar), do so.

Interpret expressions that you come up with. It can be helpful to interpret expressions along the way as well.

Toward a Solution. Cooper's wavefunction is the exapnsion in plane waves (non-interacting bloch states, more generally), with the coefficients geven by his solution of the bound state problem, involving the gap $W = 2\Delta$ (or E as sometimes written). Given the Cooper pair wavefunction, which up to a normalization constant has an orbital part given by ($\vec{r} = \vec{r}_2 - \vec{r}_1$)

$$\psi(\vec{r}) = \sum_{|\vec{k}|>k_F} \frac{cos\vec{k} \cdot \vec{r}}{2\xi_k + 2\Delta},$$

do the angular integral. Then see what can be said about the behavior of the wavefunction, and of the length scales and energy scales that enter into determining the behavior of the wavefunction.

Partial Solution. Write, using μ = cosine of the angle between $\vec{k}$ and $\vec{r}$,

$$\begin{aligned}
\psi(\vec{r}) &= Re \sum_{|\vec{k}|>k_F} \frac{e^{i\vec{k}\cdot\vec{r}}}{2\xi_k + 2\Delta} = Re\frac{\Omega_c}{8\pi^2}\int_{k_F}^{\infty} k^2 dk \int_{-1}^{1} d\mu \frac{e^{ikr\mu}}{\xi_k + \Delta} \\
&= \frac{\Omega_c}{4\pi^2}\int_{k_F}^{\infty} k^2 dk \frac{sin(kr)}{kr(\xi_k + \Delta)} = \frac{\Omega_c}{4\pi^2 r}\int_{k_F}^{\infty} kdk \frac{sin(kr)}{(\hbar^2/2m)[(k^2 - k_F^2) + k_\Delta^2]} \\
&= \frac{2m\Omega_c}{4\pi^2\hbar^2 r}\int_{k_F r}^{\infty} krd(kr)\frac{sin(kr)}{(k^2r^2 - k_F^2r^2) + k_\Delta^2 r^2} = \frac{C}{r}\int_{x_F}^{\infty}\frac{xsinx}{x^2 - x_F^2 + x_\Delta^2} \\
&= F(r, k_F r, k_\Delta r).
\end{aligned} \tag{10}$$

Here $k_\Delta \equiv (2m\Delta/\hbar^2)^{1/2}$ is the wavevector associated with the energy Δ. Now consider length/wavevector scales: $\Delta << E_F$ means $x_\Delta << x_F$. **So can x_Δ be neglected in the denominator? How do the various length scales affect the integrand?**

One can consider a standard weak-coupling case: aluminum, $T_c = 1$ K so $\Delta \sim 2$ K. $E_F \sim 3$ eV $\rightarrow$ 40000 K. Then $k_F/k_\Delta = \sqrt{20000} \sim 10^2$ (forget factors like $\sqrt{2}$).

So can x_Δ be neglected in the denominator? Well, it can't; the integral would diverge at the lower end if it is set to zero.

How to do the integral? An approximation: split the integral into two regions: $[x_F, x_f + 10x_\Delta]$ where the numerator is hardly varying and can be set to $x_F sin x_F$, and the rest of the region, where x_Δ can be neglected in the denominator. The first is just the integral of a Lorentzian

$$\begin{aligned} F_1(r, k_F r, k_\Delta r) &= C k_F sin(k_F r) \int_{x_F}^{x_F+10x_\Delta} \frac{dx}{2x_F(x-x_F)+x_\Delta^2} \\ &= C k_F \frac{sin(k_F r)}{2k_F r} \int_{x_F}^{x_F+10x_\Delta} \frac{dx}{x - x_F + x_\Delta^2/2x_F} \\ &= C k_F \frac{sin(k_F r)}{2k_F r} log \frac{10x_\Delta + x_\Delta^2/2x_F}{x_\Delta^2/2x_F} \approx 8 C k_F \frac{sin(k_F r)}{2k_F r}. \end{aligned} \tag{11}$$

The integral became independent of r, and for our aluminum example the integral was about $log(2000) \approx 8$. The constant depended only logarithmically on our choice of "cutoff" of the integral, which is good.

Then there is the remaining integral where x_Δ can be neglected in the denominator:

$$\begin{aligned} F_2(r, k_F r, k_\Delta r) &= \frac{C}{r} \int_{x_F+10x_\Delta}^{\infty} \frac{x sin x}{x^2 - x_F^2} \\ &= \frac{C}{r} \int_{x_F+10x_\Delta}^{\infty} \frac{dx\ x sin x}{2x_F} \left(\frac{1}{x - x_F} - \frac{1}{x + x_F}\right) \\ &+ \frac{C}{2k_F r^2} \left(\int_{x_\Delta}^{\infty} \frac{dx}{x} (x + x_F) sin(x + x_f) - \int_{x_F}^{\infty} \frac{dx}{x} \frac{x sin x}{x + x_F} \right). \end{aligned} \tag{12}$$

Since even $Si(x) \equiv \int_0^x dt sin(t)/t$ is not really closed form (it is used a lot and well understood by those who do) there does not seem to be hope except for numerical integration, which should not be hard, as there are no poles in the integrands. Only the lower end of the first integral needs to be watched. In addition, for very small values of r (which have no physical significance) or very large r, one might have to watch the numerical algorithms.

But what about the asymptotic behavior, when (say) $r >> 1/k_\Delta$? Then $x_\Delta >> 1$ and x_F is even larger. A worrying feature is that $Si(x) \rightarrow$ constant at $x \rightarrow \infty$, which brings into question whether the pair function defined this way is normalizable.

Disclaimer as of February 2011. I now see that the upper limit of summation/integration of the initial expression for the wavefunction should be limited to the range ε_F to $\varepsilon_F + \omega$, i.e. the thin wedge around the Fermi surface in which the pairing interaction is presumed to be non-zero. We should look into ths correction (most likely an important one) together.