Due at noon on May 4, Monday

PHSX 545 Condensed Matter - FINAL EXAM

No collaboration; Open books; Open notes; Please write neatly or type.

Problem 1 2D electrons

Consider low-energy electronic hamiltonian of graphene at half-filling:

$$\mathcal{H} = \sum_{\mathbf{k},s=\pm 1} \varepsilon_{\mathbf{k}s} a^\dagger_{\mathbf{k}s} a_{\mathbf{k}s}$$

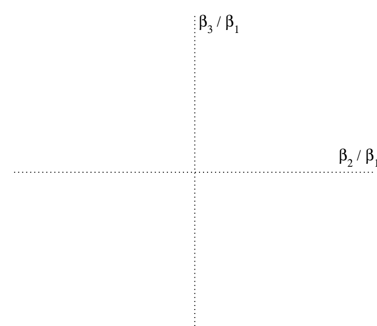
with $\mathbf{k} = (k_x, k_y)$, $\varepsilon_{\mathbf{k}s} = s v_f |\mathbf{k}|$, and zero-temperature chemical potential $\mu(0) = 0$.
(a) Sketch the energy dispersion of excitations and determine the low-energy density of states $N(\varepsilon)$;
(b) Show that the chemical potential remains zero for finite T;
(c) Find the specific heat at low temperature.

Problem 2 Two-component superconductor

A superconductor in tetragonal crystal is described by a two-component order parameter $\boldsymbol{\eta} = (\eta_1, \eta_2)$ that can be treated as a vector in two-dimensional plane. The Ginzburg-Landau functional for this superconductor is given by

$$F[\boldsymbol{\eta}] = \alpha(\boldsymbol{\eta}\cdot\boldsymbol{\eta}^*) + \frac{\beta_1}{2}(\boldsymbol{\eta}\cdot\boldsymbol{\eta}^*)^2 + \frac{\beta_2}{2}|\boldsymbol{\eta}\cdot\boldsymbol{\eta}|^2 + \frac{\beta_3}{2}\left(|\eta_1|^4 + |\eta_2|^4\right)$$

where $\alpha(T) = a(T - T_c)$ and β_i are coefficients (assume $\beta_1 > 0$). Determine the structure of the order parameter, $\eta_{1,2}$, depending on the values of β_3/β_1 and β_2/β_1. Consider phases $\boldsymbol{\eta} \propto (1,0) = (0,1), (1,1), (1,i)$ and on the attached diagram indicate stability region of each.



Problem 3 Magnetic susceptibility

Calculate the spin magnetization in a superconducting state.
(a) Diagonalize the BCS Hamiltonian with spin-singlet isotropic order parameter in the presence of Zeeman magnetic field:

$$\mathcal{H} = \sum_{\mathbf{k},\alpha=\pm 1} (\xi_\mathbf{k} - \mu_B H \alpha) a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} - \sum_\mathbf{k} \left(\Delta\, a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} + \Delta^*\, a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\right)$$

(b) Then find the expectation value

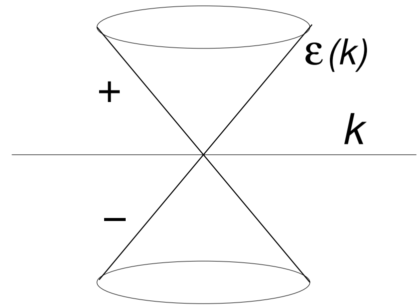
$$M = \sum_{\mathbf{k},\alpha=\pm} \langle a^\dagger_{\mathbf{k}\alpha}\, (\mu_B \alpha)\, a_{\mathbf{k}\alpha}\rangle = \mu_B \sum_\mathbf{k} \langle a^\dagger_{\mathbf{k}\uparrow}\, a_{\mathbf{k}\uparrow} - a^\dagger_{\mathbf{k}\downarrow}\, a_{\mathbf{k}\downarrow}\rangle = \chi(T) H$$

and write down expression for susceptibility $\chi(T)$.
(c) find limiting behavior of $\chi(T)/\chi_N$ near T_c and in $T \to 0$ limit. χ_N is the normal state magnetic susceptibility of Fermi gas. Discuss your results physically.

Answer of exercise 1

(a) Determine the low-energy density of states $N(\varepsilon)$;

$$\mathcal{H} = \sum_{\mathbf{k},s=\pm1} \varepsilon_{\mathbf{k}s} a^\dagger_{\mathbf{k}s} a_{\mathbf{k}s}$$



This hamiltonian can be considered as a two-band system, with one postive, conduction, band $+v_f k$, and the valence band $-v_f k$. The bands have linear dispersion, forming a cone, and the Fermi surface is just a single point in 2-dimensional momentum space.

The DOS per spin is

$$N(\varepsilon) = \sum_{\mathbf{k},s} \delta(\varepsilon - \varepsilon_{\mathbf{k}s}) = \int \frac{d^2k}{(2\pi\hbar)^2} \delta(\varepsilon - s v_f k) = \int \frac{k dk}{2\pi\hbar^2} \delta(|\varepsilon| - v_f k) = \frac{|\varepsilon|}{2\pi\hbar^2 v_f^2}$$

(b) Show that the chemical potential remains zero for finite T as well; The distribution of the particles over states is given by the Fermi-Dirac distribution, where temperature enters through chemical potential deviation $\delta\mu(T)$ and overall $\beta = 1/T$:

$$f_{\mathbf{k}s} = \frac{1}{e^{[\varepsilon_{\mathbf{k}s} - \delta\mu(T)]/T} + 1}$$

Temperature variation of the chemical potential can be evaluated from the invariance of the particle number:

$$n = \sum_{\mathbf{k},s} f_{\mathbf{k}s} = 2\int d\varepsilon N(\varepsilon) f(\varepsilon, T) \qquad \Rightarrow \qquad \delta n = 0 = 2\int d\varepsilon N(\varepsilon)\delta f(\varepsilon, T) = 2\int_{-\infty}^{+\infty} d\varepsilon \frac{N(\varepsilon)}{4\cosh^2\frac{\varepsilon - \delta\mu}{2T}} \left(\frac{\varepsilon - \delta\mu}{T^2} + \frac{1}{T}\frac{\partial\delta\mu}{\partial T}\right)\delta T$$

In the energy integral we put infinite limits since at low temperature the integrals are fast converging. We use substitution $\xi = \varepsilon - \delta\mu$ to rewrite:

$$0 = \int_{-\infty}^{+\infty} d\xi \frac{N(\xi + \delta\mu)}{4\cosh^2(\xi/2T)} \left(\frac{\xi}{T^2} + \frac{1}{T}\frac{\partial\delta\mu}{\partial T}\right)$$

To find the variation of chemical potential with temperature, we need to evaluate two itegrals with $\delta\mu$ as a parameter and find the differential equation on $\delta\mu$. This requires some work. We can, however, easily check that $\delta\mu = 0$ is a solution. Setting $\delta\mu = 0$ in the density of states we get:

$$\delta\mu = 0 \qquad \Rightarrow \qquad 0 = \int_{-\infty}^{+\infty} d\xi \frac{\xi\, N(\xi)}{4T^2\cosh^2(\xi/2T)} + \frac{1}{T}\frac{\partial\delta\mu}{\partial T}\int_{-\infty}^{+\infty} d\xi \frac{N(\xi)}{4T^2\cosh^2(\xi/2T)}$$

The first integral is zero due to perfect particle-hole symmetry: $N(\xi) = N(-\xi) \propto |\xi|$, and the second integral is finite. From this equation then it follows that $\frac{\partial}{\partial T}\delta\mu = 0$ and $\delta\mu(T) = const = 0$.

(c) Find the specific heat at low temperature. From the expression for the fermionic entropy we get the specific heat

$$S = -\sum_{\mathbf{k},s}[f_{\mathbf{k}s}\ln f_{\mathbf{k}s} + (1 - f_{\mathbf{k}s})\ln(1 - f_{\mathbf{k}s})] \qquad \Rightarrow \qquad C = T\frac{\partial S}{\partial T} = \sum_{\mathbf{k},s} \varepsilon_{\mathbf{k}s}\frac{\partial f_{\mathbf{k}s}}{\partial T} = 2\int_{-\infty}^{+\infty} d\varepsilon\, N(\varepsilon)\, \varepsilon \frac{\varepsilon}{4T^2\cosh^2(\varepsilon/2T)}$$

where we used the zero-μ property found before. Prefactor 2 is from spin. Using expression for $N(\varepsilon)$ we have the final answer:

$$C = \frac{(2T)^2}{2\pi\hbar^2 v_f^2} 4 \underbrace{\int_0^{+\infty} \frac{x^3 dx}{\cosh^2 x}}_{9\zeta(3)/8} = \frac{9\zeta(3)}{\pi(\hbar v_f)^2} T^2$$

Answer of exercise 2

The first two term in the Ginzburg-Landau functional

$$F[\boldsymbol{\eta}] = \alpha(\boldsymbol{\eta}\cdot\boldsymbol{\eta}^*) + \frac{\beta_1}{2}(\boldsymbol{\eta}\cdot\boldsymbol{\eta}^*)^2 + \frac{\beta_2}{2}|\boldsymbol{\eta}\cdot\boldsymbol{\eta}|^2 + \frac{\beta_3}{2}\left(|\eta_1|^4 + |\eta_2|^4\right)$$

are symmetric with respect to continuous rotations in the (η_1, η_2) plane and with respect to the relative phase between the two components.

The β_3 term breaks the rotational symmetry, but still independent on the relative phase between η_1 and η_2.

The β_2 term fixes the relative phase.

Let's see how this comes about. One can just compare the free energies of the typical phases $\boldsymbol{\eta} \propto (1,0) = (0,1), (1,1), (1,i)$ and select the lowest energy state. But let's start from a general formulation and let's find how one can determine the structure of the order parameter and the regions of phases stability in paramter space. Look for the order parameter in the form

$$\boldsymbol{\eta} = (\eta_1, \eta_2) = \eta(\cos\theta, e^{i\varphi}\sin\theta)$$

With this substitution the free energy becomes

$$F[\boldsymbol{\eta}] = \alpha\eta^2 + \frac{\beta_1}{2}\eta^4 + \frac{\beta_2}{2}\eta^4|\cos^2\theta + e^{2i\varphi}\sin^2\theta|^2 + \frac{\beta_3}{2}\eta^4\left(\cos^4\theta + \sin^4\theta\right)$$

which we can re-write with single $\beta\eta^4$ term that depends on the angles θ, φ

$$F[\boldsymbol{\eta}] = \alpha\eta^2 + \frac{\beta}{2}\eta^4 \qquad \textit{with} \qquad \beta(\theta,\varphi) = \beta_1 + \beta_2(\cos^4\theta + \sin^4\theta + 2\cos 2\varphi\cos^2\theta\sin^2\theta) + \beta_3\left(\cos^4\theta + \sin^4\theta\right)$$

The angle-dependent terms we re-write using identity $\cos^4\theta + \sin^4\theta = 1 - 2\cos^2\theta\sin^2\theta$

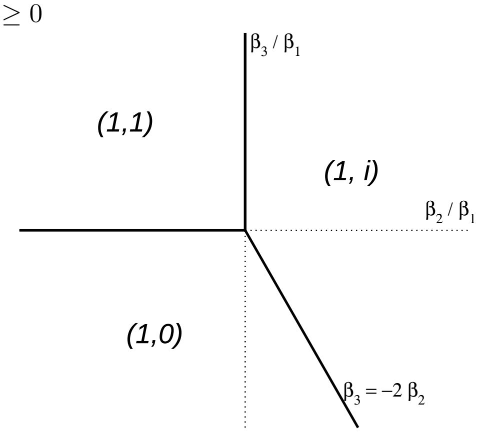
$$\beta(\theta,\varphi) = \beta_1 + \beta_2 + \beta_3 - \frac{1}{2}\sin^2 2\theta\,(\beta_3 + \beta_2 - \beta_2\cos 2\varphi)$$

The magnitude of the order parameter and the free energy is

$$\eta^2 = -\frac{\alpha}{\beta(\theta,\varphi)} \qquad \Rightarrow \qquad F = -\frac{\alpha^2}{2\beta(\theta,\varphi)}$$

The minimal negative value for F is obtained when $\beta(\theta,\varphi)$ is minimal positive. We choose values of θ and φ to minimize $\beta(\theta,\varphi)$ for given $\beta_{2/1} = \beta_2/\beta_1, \beta_{3/1} = \beta_3/\beta_1$:

$$\sin^2 2\theta\left(\beta_{3/1} + 2\beta_{2/1}\sin^2\varphi\right) \to max \geq 0$$



The phase $\boldsymbol{\eta} = (1,1)$ $\quad(\sin^2 2\theta = \sin^2 2(\pi/2) = 1,\ \varphi = 0)$ is most favorable when

$$\boldsymbol{\eta} = (1,1) \qquad \beta_{2/1} < 0 \qquad \beta_{3/1} > 0$$

The phase $\boldsymbol{\eta} = (1,i)$ $\quad(\sin^2 2\theta = \sin^2 2(\pi/2) = 1,\ \varphi = \pi/2)$

$$\boldsymbol{\eta} = (1,i) \qquad \beta_{2/1} > 0 \qquad \beta_{3/1} + 2\beta_{2/1} > 0$$

The phase $\boldsymbol{\eta} = (1,0)$ $\quad(\sin^2 2\theta = 0)$

$$\boldsymbol{\eta} = (1,0) \qquad \beta_{3/1} < 0 \qquad \beta_{3/1} + 2\beta_{2/1} < 0$$

Answer of exercise 3

(a) To diagonalize the BCS Hamiltonian with magnetic field included we write it in a matrix form:

$$\mathcal{H} = \sum_{\mathbf{k},\alpha=\pm1} (\xi_{\mathbf{k}} - \mu_B H\alpha) a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} - \sum_{\mathbf{k}} \left(\Delta\, a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} + \Delta^*\, a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right)$$

$$= E_0 + \sum_{\mathbf{k}} \left(\begin{array}{cc} a^\dagger_{\mathbf{k}\uparrow} & a_{-\mathbf{k}\downarrow} \end{array} \right) \underbrace{\left(\begin{array}{cc} \xi_{\mathbf{k}\uparrow} & -\Delta \\ -\Delta^* & -\xi_{\mathbf{k}\downarrow} \end{array} \right)}_{\hat{\mathcal{H}}_k} \left(\begin{array}{c} a_{\mathbf{k}\uparrow} \\ a^\dagger_{-\mathbf{k}\downarrow} \end{array} \right)$$

where E_0 is part of the ground state energy that we are not calculating. We also introduced shorthand for quasiparticle energies in magnetic field

$$\xi_{\mathbf{k}\uparrow,\downarrow} = \xi_{\mathbf{k}} \mp \mu_B H$$

Then we introduce new fermionic operators

$$\left(\begin{array}{c} a_{\mathbf{k}\uparrow} \\ a^\dagger_{-\mathbf{k}\downarrow} \end{array} \right) = \underbrace{\left(\begin{array}{cc} u_k & v_k \\ v^*_{-k} & u^*_{-k} \end{array} \right)}_{U_k} \left(\begin{array}{c} b_{\mathbf{k}\uparrow} \\ b^\dagger_{-\mathbf{k}\downarrow} \end{array} \right)$$

The transformation matrix indices include both momentum and spin states: $k = (\mathbf{k}, \uparrow)$ and $-k = (-\mathbf{k}, \downarrow)$, for convenience. Since the new operators have to obey fermionic anti-commutation relations, we can put some constraints on the matrix entries: requiring

$$[b_k, b_p]_+ = 0 \qquad\qquad [b_k, b^\dagger_p]_+ = \delta_{kp}$$

we have

$$[a_k, a_p]_+ = 0 \qquad \Rightarrow \qquad v_k u_{-k} = -v_{-k} u_k \qquad ; \qquad [a_k, a^\dagger_p]_+ = \delta_{kp} \qquad \Rightarrow \qquad |u_k|^2 + |v_k|^2 = 1$$

Since the order parameter is real we can take u_k, v_k real as well. Moreover, to satisfy these normalization conditions we assume symmetry and parametrization of these functions to be

$$u_{-k} = u_k = \cos\theta_k \qquad\qquad v_{-k} = -v_k = \sin\theta_k$$

The product of three matrices give

$$U^\dagger_k \hat{\mathcal{H}}_k U_k = \left(\begin{array}{c|c} \xi_k |u_k|^2 - \xi_{-k} |v_{-k}|^2 - \Delta u^*_k v^*_{-k} - \Delta^* u_k v_{-k} & \xi_k u^*_k v_k - \xi_{-k} u^*_{-k} v_{-k} - \Delta u^*_k u^*_{-k} - \Delta^* v_k v_{-k} \\ \hline \xi_k u_k v^*_k - \xi_{-k} u_{-k} v^*_{-k} - \Delta^* u_k u_{-k} - \Delta v^*_k v^*_{-k} & \xi_k |v_k|^2 - \xi_{-k} |u_{-k}|^2 - \Delta u^*_{-k} v^*_k - \Delta^* u_{-k} v_k \end{array} \right)$$

and we require the off-diagonal terms to vanish which gives us equation for θ_k using our assumptions about reality and symmetry of u, v-functions:

$$(\xi_k + \xi_{-k}) u_k v_k - \Delta(u_k^2 - v_k^2) = 0 \qquad \Rightarrow \qquad \tan 2\theta_k = \frac{2\Delta}{\xi_k + \xi_{-k}} = \frac{\Delta}{\xi_{\mathbf{k}}}$$

- spin independent value, that gives the same expressions for transformation matrix as in case of no magnetic field! The u-function is symmetric with respect to spin and momentum, and the v-function can be taken to be symmetric in momentum and odd in spin index:

$$u_k = u_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} \qquad v_k = v_{\mathbf{k}\uparrow} = \sqrt{\frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} \qquad v_{-k} = v_{-\mathbf{k}\downarrow} = v_{\mathbf{k}\downarrow} = -\sqrt{\frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)}$$

and the transformations between old and new operators can be written in a compact way

$$a_{\mathbf{k}\alpha} = u_{\mathbf{k}} b_{\mathbf{k}\alpha} + \alpha v_{\mathbf{k}} b^\dagger_{-\mathbf{k},-\alpha}$$

The Hamiltonian matrix thus becomes diagonal with elements

$$U_k^\dagger \hat{\mathcal{H}}_k U_k = \begin{pmatrix} E_{\mathbf{k}} - \mu_B H & 0 \\ 0 & -E_{\mathbf{k}} - \mu_B H \end{pmatrix} \qquad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$$

that gives final answer in terms of new quasiparticle operators

$$\mathcal{H} = E_0 + \sum_{\mathbf{k}} \begin{pmatrix} b_{\mathbf{k}\uparrow}^\dagger & b_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} E_{\mathbf{k}} - \mu_B H & 0 \\ 0 & -E_{\mathbf{k}} - \mu_B H \end{pmatrix} \begin{pmatrix} b_{\mathbf{k}\uparrow} \\ b_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} = E_{gs} + \sum_{\mathbf{k},\alpha=\pm 1} \underbrace{(E_{\mathbf{k}} - \mu_B H\alpha)}_{E_{\mathbf{k}\alpha}} b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha}$$

(b) To find the observables, we note that the new diagonal Hamiltonian results in the usual Fermion distribution function for the quasiparticles:

$$\langle b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} \rangle \equiv f(E_{\mathbf{k}\alpha}) = \frac{1}{e^{\beta E_{\mathbf{k}\alpha}} + 1}$$

Expectation value for particle operators:

$$\langle a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} \rangle = \langle (u_{\mathbf{k}} b_{\mathbf{k},\alpha}^\dagger + \alpha v_{\mathbf{k}} b_{-\mathbf{k},-\alpha})(u_{\mathbf{k}} b_{\mathbf{k},\alpha} + \alpha v_{\mathbf{k}} b_{-\mathbf{k},-\alpha}^\dagger) \rangle = u_{\mathbf{k}}^2 \langle b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} \rangle - v_{\mathbf{k}}^2 \langle b_{-\mathbf{k},-\alpha}^\dagger b_{-\mathbf{k},-\alpha} \rangle + v_{\mathbf{k}}^2$$

and the magnetization is

$$M = \mu_B \sum_{\mathbf{k},\alpha=\pm} \alpha \, \langle a_{\mathbf{k}\alpha}^\dagger \, a_{\mathbf{k}\alpha} \rangle = \mu_B \sum_{\mathbf{k},\alpha=\pm} \left[u_{\mathbf{k}}^2 \alpha \langle b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} \rangle - \alpha v_{\mathbf{k}}^2 \langle b_{-\mathbf{k},-\alpha}^\dagger b_{-\mathbf{k},-\alpha} \rangle \right] = \mu_B \sum_{\mathbf{k},\alpha=\pm} (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) \alpha \langle b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} \rangle$$

$$\boxed{M = \mu_B \sum_{\mathbf{k}} \left[f(E_{\mathbf{k}\uparrow}) - f(E_{\mathbf{k}\downarrow}) \right]}$$

Susceptibility in the limit of small magnetic field is

$$\boxed{\chi(T) = -2\mu_B^2 \sum_{\mathbf{k}} \frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}} = 2\mu_B^2 \sum_{\mathbf{k}} \frac{1}{4T \cosh^2 \frac{E_{\mathbf{k}}}{2T}}} \qquad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$$

(c) To evaluate this function we can use isotropic property of the gap and make the sum into energy integral:

$$\chi(T) = 2\mu_B^2 \sum_{\mathbf{k}} \frac{1}{4T \cosh^2 \frac{E_{\mathbf{k}}}{2T}} = 2\mu_B^2 N_f \int_{-\infty}^{+\infty} \frac{d\xi}{4T \cosh^2 \frac{\sqrt{\xi^2+\Delta^2}}{2T}} = \chi_N \int_0^{+\infty} \frac{d\xi}{2T \cosh^2 \frac{\sqrt{\xi^2+\Delta^2}}{2T}}$$

$\chi_N = 2\mu_B^2 N_f$ is the normal state magnetic susceptibility of Fermi gas. If we substitute self-consistently determined gap $\Delta(T)$ we get a function known as Yosida function:

$$\frac{\chi(T)}{\chi_N} = \int_0^{+\infty} \frac{dx}{\cosh^2 \sqrt{x^2 + [\Delta(T)/T]^2}} \equiv Y(T)$$

At low temperatures $T \ll \Delta_0$ this function is exponentially small due to absence of quasiparticles inside the energy gap:

$$Y(T \to 0) = \int_0^{+\infty} \frac{dx}{\cosh^2 \sqrt{x^2 + [\Delta_0/T]^2}} \approx 4 \int_0^{+\infty} dx e^{-2\sqrt{x^2+[\Delta_0/T]^2}} \approx 4 \int_0^{+\infty} dx e^{-2\Delta_0/T} \, e^{-x^2/[\Delta_0/T]} = \sqrt{\frac{4\pi\Delta_0}{T}} e^{-2\Delta_0/T}$$

Near transition temperature the gap is vanishing $\Delta^2(T) \propto (T_c - T)$ so we can do expansion of the integrand:

$$Y(T \to T_c^-) = \int_0^{+\infty} \frac{dx}{\cosh^2 \sqrt{x^2 + [\Delta(T)/T_c]^2}} \approx \int_0^{+\infty} dx \left[\frac{1}{\cosh^2 x} - \frac{\sinh x}{x \cosh^3 x} \frac{\Delta^2(T)}{T_c^2} \right] = 1 - 0.85 \frac{\Delta^2(T)}{T_c^2}$$

- linearly drops from 1 as the number of quasiparticles near Fermi level starts to drop with opening of the gap.