Solution Exam TFY4210/FY8302
May 26, 2021

1a)
$$H = -J\sum_{\langle i,j\rangle}\left[S_{iz}S_{jz} + \Delta\left(S_{ix}S_{jx} + S_{iy}S_{jy}\right)\right]$$

$$= -J\sum_{\langle i,j\rangle}\left(S_{iz}S_{jz} + \Delta\, S_{i+}S_{j-}\right)$$

Now using the Holstein-Primakoff transformation, computing to quadratic order, we find

$$H = E_0 - J\sum_{\langle i,j\rangle} 2S\left[a_i^{+}a_i + b_i^{+}b_i + \Delta\left(a_i b_j + b_i^{+}a_j^{+}\right)\right]$$

Now, introducing Fourier-transformed operators, we may write

$$H = E_0 - 2JS\sum_q \left(a_q^{+}a_q + b_q^{+}b_q\right) - 2JS\sum_q \Delta\,\gamma(\vec{q})\left(a_q b_q + b_q^{+}a_q^{+}\right)$$

$$\gamma(\vec{q}) = \sum_{\vec{\delta}} e^{i\vec{q}\cdot\vec{\delta}}$$

δ: Vector connecting i to its nearest neighbors.

If we now define

$$\tilde{\gamma}(\vec{q}) = \Delta\, \gamma(\vec{q}),$$

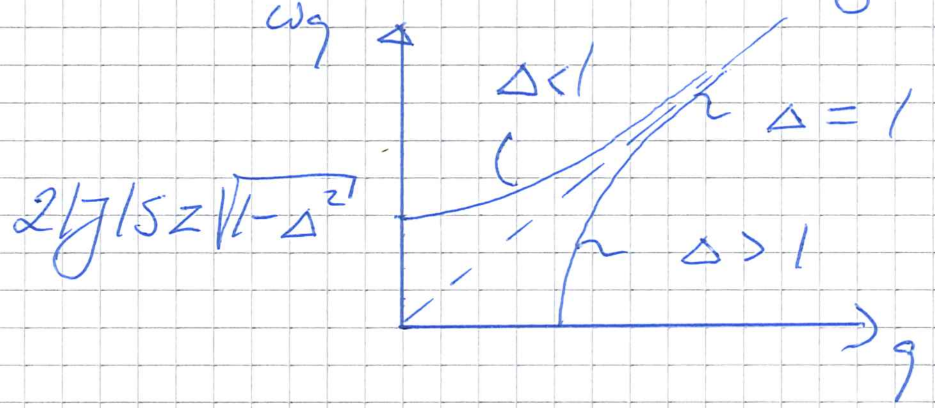
then H has exactly the same form as the $\Delta = 1$ case, and we can immediately write

$$H = 2NJz\, S(S+1) + \sum_q \hbar\omega_q \left(A_q^+ A_q + 1/2\right) + \sum_q \hbar\omega_q \left(B_q^+ B_q + 1/2\right)$$

$$\omega_q = 2|J|S \sqrt{z^2 - \tilde{\gamma}^2(q)}$$

$$= 2|J|S \left(z^2 - \Delta^2 \gamma^2(\vec{q})\right)^{1/2}$$

z = # nearest neighbors



(b) From the lecture notes, we have

$$M = S - \frac{1}{N}\sum_q v_q^2 - \frac{1}{N}\sum_{\vec{q}} \frac{u_q^2 + v_q^2}{e^{\beta\omega_q} - 1}$$

The temperature-corrections are in the third term.

At low T, the integral is completely dominated by small momenta, since the factor $e^{-\beta\omega_q}$ serves as an efficient cutoff-factor.

$$u_q^2 + v_q^2 = \frac{z}{\sqrt{z^2 - \Delta^2\gamma^2}} \quad ; \quad \Delta < 1$$

$$C(T) \equiv \frac{1}{N}\sum_q \frac{u_q^2 + v_q^2}{e^{\beta\omega_q} - 1}$$: Thermal correction to M

$$C(T) = \frac{1}{N}\sum_q e^{-\beta\omega_q} \frac{z}{\sqrt{z^2 - \Delta^2\gamma^2}} \sum_{n=0}^{\infty} e^{-n\beta\omega_q}$$

Since $\lim_{q \to 0} \omega_q \neq 0 \quad ; \quad \Delta < 1$

the integral is completely dominated

by the term $n=0$, $\beta|J|>>1$. Thus, we get

$$C(T) \simeq \frac{1}{N}\sum_q \frac{z}{(z^2-\Delta^2\gamma^2)^{1/2}}\, e^{-\beta\omega_q}$$

$$\beta\omega_q = \eta\,(z^2-\Delta^2\gamma^2)^{1/2}; \quad \eta \equiv 2S\beta|J|$$

For small q: $z^2-\Delta^2\gamma^2 \simeq z^2-\Delta^2\left(z-\frac{1}{2}q^2\right)^2$

$$= z^2(1-\Delta^2)+\Delta^2 z q^2 = a+bq^2$$

$$a \equiv z^2(1-\Delta^2); \quad b \equiv \Delta^2 z$$

Converting the q-sum to an integral:

$$C(T) = \frac{1}{2\pi}\cdot z\int_0^\infty \frac{dq\, q}{\sqrt{a+bq^2}}\, e^{-\eta\sqrt{a+bq^2}}$$

$$= \frac{z}{4\pi}\int_0^\infty \frac{dx}{\sqrt{a+bx}}\, e^{-\eta\sqrt{a+bx}}$$

$$= \frac{z}{4\pi}\,\frac{2}{b\eta}\, e^{-\eta\sqrt{a}}$$

$$C(T) = \frac{1}{4\pi}\,\frac{1}{\Delta^2 S}\,\frac{k_B T}{|J|}\, e^{-z\sqrt{1-\Delta^2}\,2S\beta|J|}$$

Note the drastic suppression of $C(T)$ with increasing z and S, at a given low temperature $k_B T \ll |J|$.

When $\Delta = 1$, the thermal corrections

corrections to M is a power-law in (T/J), $\sim \left(\frac{T}{J}\right)^{d-1}$, $d>2$

When $\Delta < 1$, the corrections are exponentially small in J/T.

This drastic change is due to the gap in the spin-wave spectrum as $q \to 0$ when $\Delta < 1$.

1(c) We assume to begin with spin-ordering along z-axis in spin-space. When $\Delta < 1$ this makes sense, since it is more energetically favorable to order spins along z-axis than along (x, y)-axes in spin space.

This is reflected in the fact that when $q \to 0$, $\omega_q \neq 0$ for $\Delta < 1$.

This is the typical situation in an Ising-model, which does not have low-energy spin-waves.

When $\Delta > 1$, it is energetically favorable to order spins along (x, y)-directions in spin-space, Thus the z-axis ordering presumed in the H-P-transformation makes little sense.

For $\Delta > 1$

$$\omega_q = 2|J|S\left(z^2 - \Delta^2 \gamma^2\right)^{1/2}$$

becomes imaginary for low q.

This reflects an instability from a spin-state ordered along z-axis to a spin-state ordered in the (x,y)-plane in spin-space. Our starting point with spin-ordering along z-axis + small assumed fluctuations (H-P-transformation) is just not the correct starting point. We should have assumed spin-ordering in the (x,y)-plane and considered a modified spin-wave theory around such a starting point.

Problem 2

a) i) Scattering of electrons on opposite sides of the Fermi-surface $(k,-k)$ to $(\vec{k}',-k')$ within a thin energy shell around Fermi-surface

ii) Electrons that interact are in opposite spin-states, such that the electron-pair forms a spin-singlet.

b) The BCS gap-equation:

$$\Delta(\vec{k}) = -\sum_{k'} V_{k,k'}\, \Delta(k')\, \chi_{k'}$$

$$\chi_{k'} = \frac{1}{2E_{k'}} \tanh\left(\frac{\beta E_{k'}}{2}\right)$$

$$E_{k'} = \left((\varepsilon_{k'}-\mu)^2 + |\Delta(k')|^2\right)^{1/2}$$

$$\beta = \frac{1}{k_B T}$$

c) For this particular form of $V_{k,k'}$:

$$\Delta(k) = V g(\vec{k}) \underbrace{\sum_{k'} g(k') \Delta(k') \chi_{k'}}_{\vec{k}\text{-independent}}$$

Thus, we have

$$\Delta(\vec{k}) = \Delta_0 \, g(\vec{k})$$

$$\underline{\underline{F(\vec{k}) = g(\vec{k})}}$$

$$\Delta_0 \equiv V \sum_{k'} g(k') \underbrace{\Delta(k')}_{= \Delta_0 g(k')} \chi_{k'}$$

$$\Delta_0 = V \Delta_0 \sum_{k'} \left(g(\vec{k}')\right)^2 \chi_{k'}$$

Equation determining Δ_0:

$$\underline{\underline{1 = V \sum_{k'} \left(g(\vec{k}')\right)^2 \chi_{k'}}}$$

$$\underline{E_{k'} = \left((\varepsilon_{k'} - \mu)^2 + \Delta_0^2 \left(g(k')\right)^2\right)^{1/2}}$$

d) $\Delta(\vec{k}) = \Delta_0(T)\, g(\vec{k})$

In addition, the pairing amplitude

$b_k \equiv \langle C^{+}_{k\uparrow} C^{+}_{-k\downarrow} \rangle$

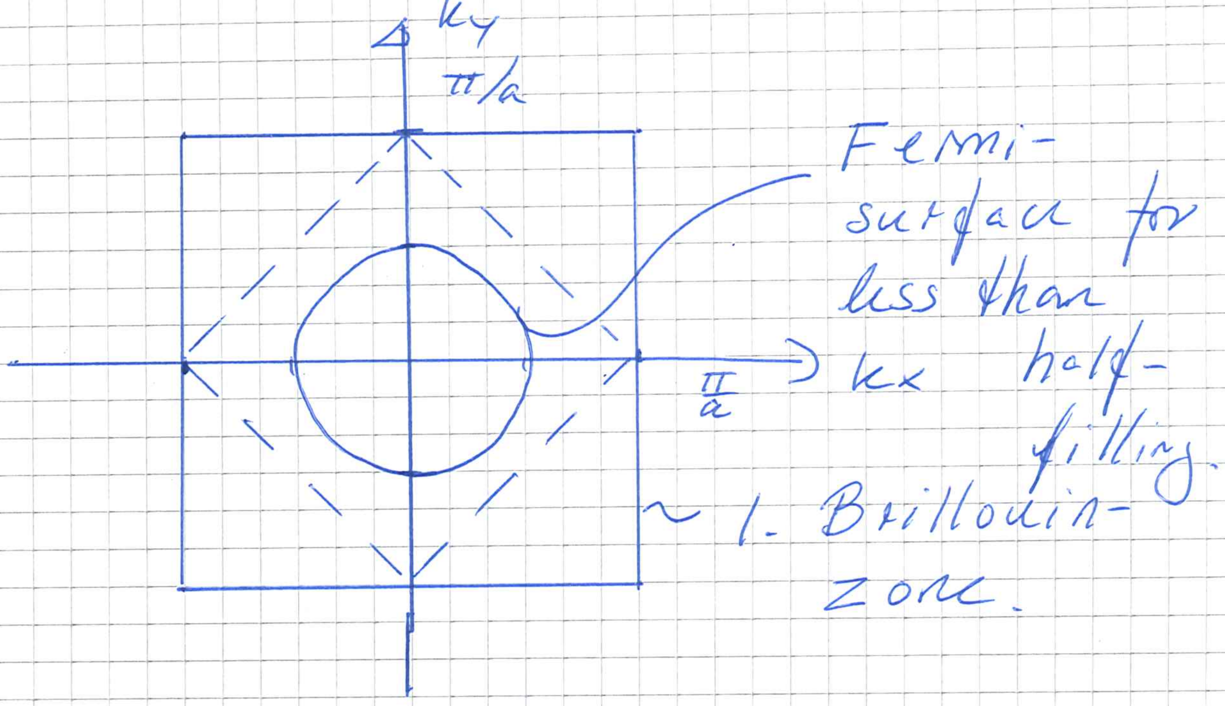
is spin-singlet. This state is antisymmetric under interchange of two electrons, and the spin-part of the pairing state is antisymmetric (spin singlet)

Therefore, the $\vec{k}$-dependent part of the pairing state must be symmetric under interchange of two electrons, i.e. symmetric when $\vec{k} \to -\vec{k}$.

The first two functions $g(\vec{k})$ are odd when $\vec{k} \to -\vec{k}$, and are therefore <u>not</u> permissible.

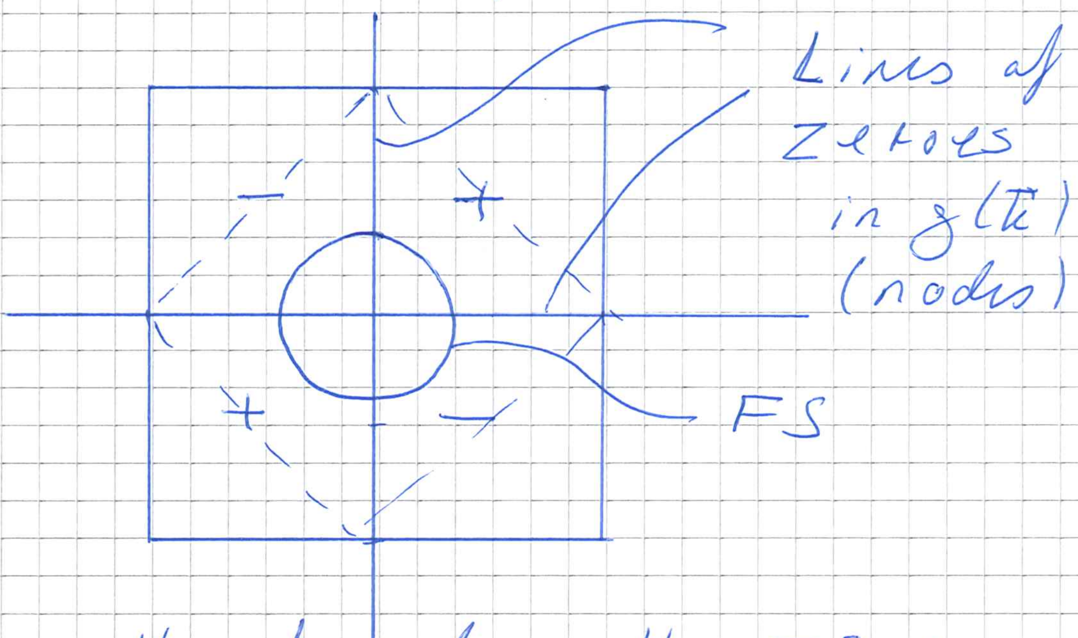
The other 3 are permissible

e)



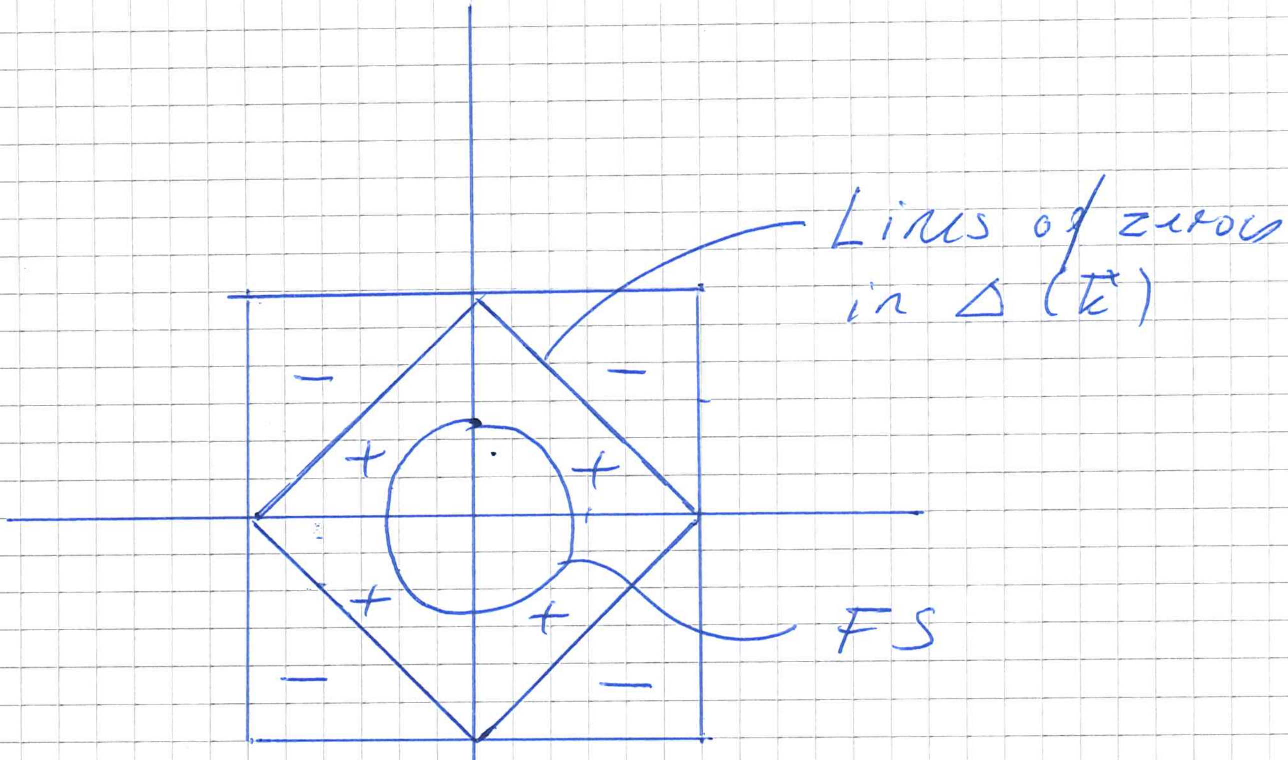
Take the three permissible functions and consider their signs on the 1. B-zone:

i) $\underline{g(\vec{k}) = \sin k_x \sin k_y}$



No matter how large the FS is (for less than half-filling) the gap changes sign four times on the FS.

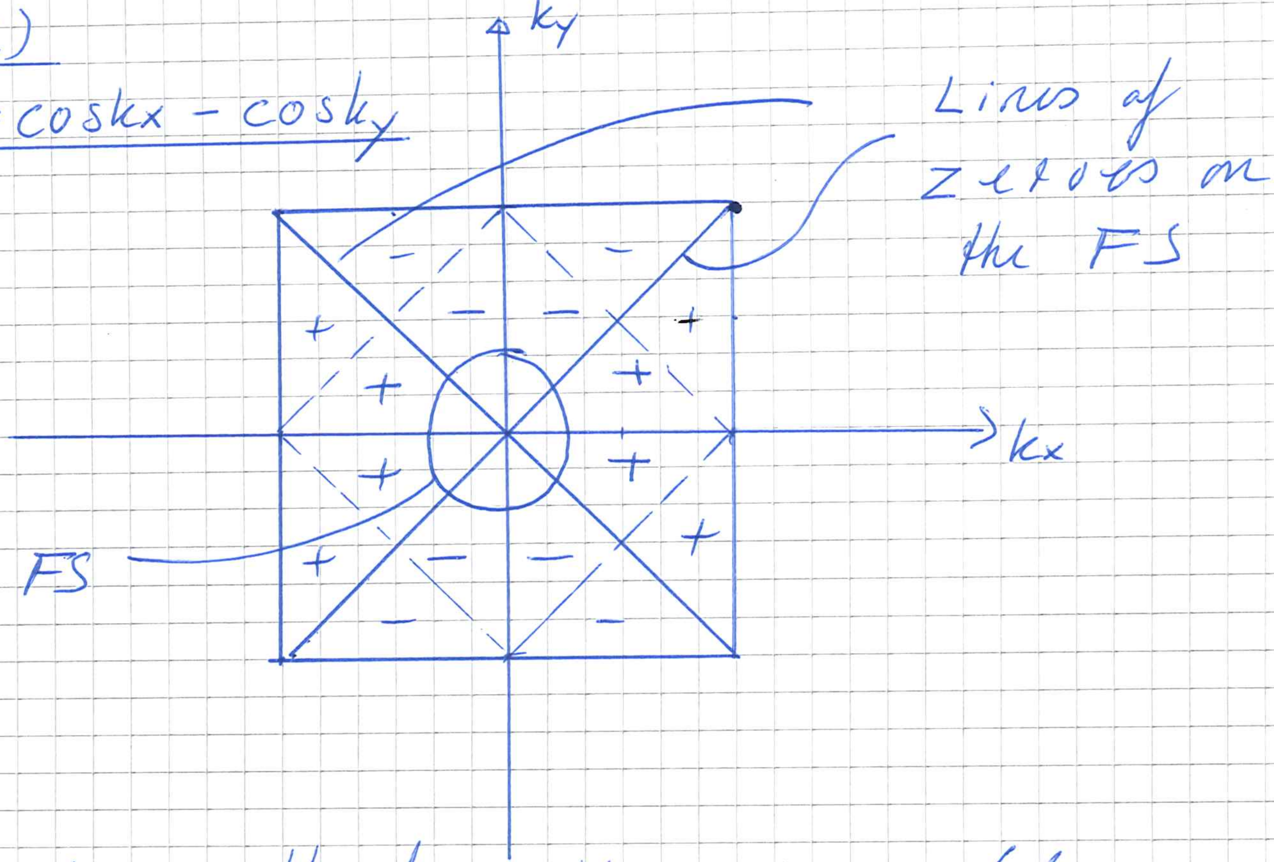
ii) $g(\vec{k}) = \cos k_x + \cos k_y$



This gap now changes sign on the Fermi-surface. This is just an anisotropic version of the $\vec{k}$-independent „s-wave" gap we find when $g(\vec{k}) = 1$. It is often referred to as „anistropic s-wave gap".

iii)

$g(\vec{k}) = \cos k_x - \cos k_y$



No matter where the FS is (less than half-filling) the gap always changes sign four times on the FS.

This form of the gap is believed to be the essentially correct form of the gap-function $\Delta(\vec{k})$ in high-T_c cuprates.