Unconventional superconductivity — a general view, d-wave pairing etc.

§ Definition: (real space picture)

The Cooper pairing structure can be classified by its symmetry property. Let us consider a strong coupling limit such that Cooper pairs can be viewed as diatom molecule whose real space wavefunctions can be written as

$$\psi_{\alpha_1\alpha_2}(\vec{r}_1, \vec{r}_2) = \Phi(\vec{R})\, \phi(\vec{r}_1-\vec{r}_2)\, \chi_{\alpha_1\alpha_2}.$$

where $\vec{R} = \frac{\vec{r}_1+\vec{r}_2}{2}$ is the center of mass coordinate, $\vec{r} = \vec{r}_1 - \vec{r}_2$ is the relative coordinate, $\chi_{\alpha_1\alpha_2}$ is the spin-wave function. For simplicity, we assume $\Phi(\vec{R})$ = constant, i.e. momentum zero pairing. In isotropic system, we can expane $\phi(\vec{r}_1-\vec{r}_2)$ in terms of angular momentum basis. If no spin-orbit coupling. $\chi_{\alpha_1\alpha_2}$ can be classified as $\chi_s = \frac{|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}$ (spin singlet)

and $$\chi_{t,\, S_z=1,0,-1} = \begin{cases} |\uparrow_1\rangle|\uparrow_2\rangle, \\ \frac{|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}, \\ |\downarrow\rangle_1 |\downarrow_2\rangle \end{cases} \quad \text{(spin triplet)}.$$

Considering the fermionic statistics, $\psi_{\alpha_1\alpha_2}(\vec{r}_1, \vec{r}_2) = -\psi_{\alpha_2\alpha_1}(\vec{r}_2, \vec{r}_1)$, we have

$$\psi_{\alpha_1\alpha_2}(\vec{r}_1, \vec{r}_2) = \begin{cases} R_n(r)\, Y_{lm}(\vec{r})\, \chi_s & (\text{for } l = \text{even}) \\ R_n(r)\, Y_{lm}(\vec{r})\, \chi_{t,\,0,\pm1} & (\text{for } l = \text{odd}). \end{cases}$$

* $R_n(r)$ is the radial wavefunction, and n is the radial quantum number.

classification: according to symmetry.

① conventional pairing: S-wave, spin singlet. $R_{n=0}(r)$ positive definite. — Hg, Al, Pb, etc

② unconventional pairing: all other pairing symmetries except the s-wave.

example: d-wave high T_c cuprates, singlet (Nobel prize)

p-wave ^3He-A and B phases, spin triplet (Nobel prizes)
Sr_2RuO_4 (?) almost

f-wave ? UPt_3

They may be nodal or nodeless, may be topologically trivial or not.

③ Extended s-wave: paring wavefunction does not change sign as varying angular variables, but changes sign along radial direction.

(e.g. Iron-based superconducters, but not fully settled yet!)

(*) Unconventional pairing can save Coulumb repulsion energy since $\phi(\vec{r}=0)=0$. The propalbility of two electrons coinside at the same point vanishes!

§ Weak coupling (momentum space picture) — gap equation

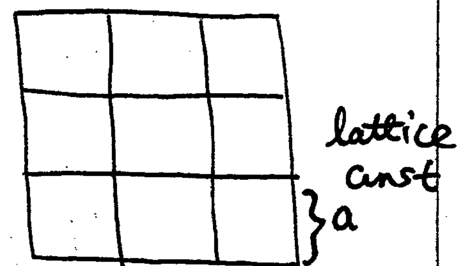
cnt.

we first consider the unconventional pairing in the singlet channel.

- The simplest and most celebrate example is the high Tc cuprates, whose physics mainly occurs in the 2D CuO plane. The lattice ~~structure~~ is square, and the rotation symmetry is only 4-fold.

$\boxed{\text{Background:}}$

The kinetic energy : tight-binding model



$$H_0 = -t \sum_{\langle ij \rangle} C^{+}_{i\sigma} C_{j\sigma} + h.c.$$

plug in Fourier component

$$C_i = \frac{1}{\sqrt{N}} \sum_{k} e^{i\vec{k}\cdot\vec{r}_i} C_k$$

N is the number of lattice sites

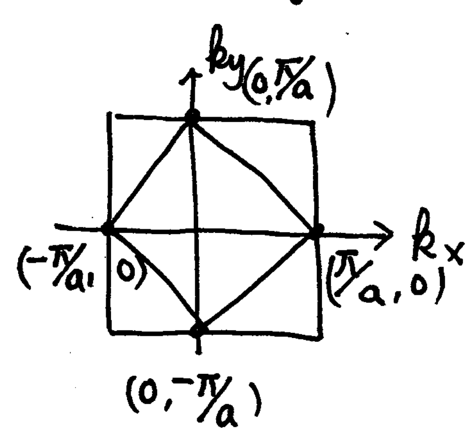
$$\Rightarrow H_0 = \sum_{k} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} \quad \text{with } \varepsilon_k = -2t(\cos k_x + \cos k_y) - \mu$$

Ex: ① please derive the H_0 in momentum space.

② prove that at half filling, i.e. $\langle n \rangle = \langle C^{+}_{i\sigma} C_{i\sigma} \rangle = 1$.

The chemical potential $\mu = 0$, and the Fermi surface has the shape of a diamond. i.e.

$$\boxed{\cos k_x + \cos k_y = 0}$$



③ please also plot Fermi surfaces for negative values of μ, say $|\mu/t| = 0.05, 0.1$, etc.

This corresponds to the situation of doping.

Due to the strong onsite Coulomb interaction, we consider the pairing on NN bonds. (The mechanism for the gluing force remains unknown).

$$H_{int} = -\frac{V}{2} \sum_{\delta=\pm\hat{x},\pm\hat{y}} \left(C^+_{i+\delta\downarrow} C^+_{i\uparrow} - C^+_{i+\delta\uparrow} C^+_{i\downarrow}\right)\left(C_{i\uparrow} C_{i+\delta\downarrow} - C_{i\downarrow} C_{i+\delta\uparrow}\right)$$

— phenomenological interaction leading to d-wave pairing

perform Fourier transformation, and keep the pairing term

$$H_{pair} = -\frac{V}{2N} \sum_{k',k} \sum_{\vec{\delta}} e^{i\vec{k}'\cdot\vec{\delta}} \cdot e^{-i\vec{k}\cdot\vec{\delta}} \left[C^+_{-k'\downarrow} C^+_{k'\uparrow} - C^+_{-k'\uparrow} C^+_{k'\downarrow}\right] \left[C_{k\uparrow} C_{-k\downarrow} - C_{k\downarrow} C_{-k\uparrow}\right]$$

$$= -\frac{V}{2N} \sum_{k'k} 4\left(\cos k'_x \cos k_x + \cos k'_y \cos k_y\right) C^+_{-k'\downarrow} C^+_{k'\uparrow} C_{k\uparrow} C_{-k\downarrow}$$

$$= -\frac{V}{N} \sum_{k'k} \Big\{ \left(\cos k'_x + \cos k'_y\right) C^+_{-k'\downarrow} C^+_{k'\uparrow} \left(\cos k_x + \cos k_y\right) C_{k\uparrow} C_{-k\downarrow}$$

$$+ \left(\cos k'_x - \cos k'_y\right) C^+_{-k'\downarrow} C^+_{k'\uparrow} \left(\cos k_x - \cos k_y\right) C_{k\uparrow} C_{-k\downarrow} \Big\}$$

Define $\Delta_s = \frac{V}{N} \sum_k C_{k\uparrow} C_{-k\downarrow} \left(\cos k_x + \cos k_y\right)$

$$\Delta_d = \frac{V}{N} \sum_k C_{k\uparrow} C_{-k\downarrow} \left(\cos k_x - \cos k_y\right)$$

$$\frac{1}{N} H_{MF} = -\frac{V}{N} \sum_k \Delta_s^* \left(\cos k_x + \cos k_y\right) C_{k\uparrow} C_{-k\downarrow} + h.c$$

$$- \frac{V}{N} \sum_k \Delta_d^* \left(\cos k_x - \cos k_y\right) C_{k\uparrow} C_{-k\downarrow} + h.c$$

$$+ \frac{1}{V} \left(\Delta_s^* \Delta_s + \Delta_d^* \Delta_d\right)$$

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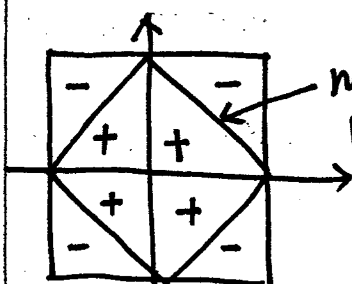
We have chosen the interaction $V(kk') = V_0(\cos k_x' \cos k_x + \cos k_y' \cos k_y)$.

This interaction can give rise to two possible singlet pairing symmetries:

the extended s-wave: gap function $\Delta_s(\cos k_x + \cos k_y)$

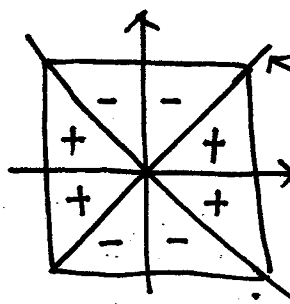
d-wave: gap function $\Delta_d(\cos k_x - \cos k_y)$.



nodal line $|k_x| + |k_y| = \pi$

extended s-wave

rotational invariant but changes sign acrossing $|k_x| + |k_y| = \pi$.



nodal line $k_x = k_y$

nodal line $k_x = -k_y$

d-wave

rotate 90°

$\Delta d \to -\Delta d$

Ex: please perform Fourier transformation back to real space.

① Δ_s corresponds to the real space pattern

$$\Delta(i, i+x) = \Delta(i, i-x) = \Delta(i, i+\hat{y}) = \Delta(i, i-\hat{y})$$

$i+\hat{y}$, $i-\hat{x}$, i, $i+x$, $i-\hat{y}$

② Δ_d corresponds to the pattern

$$\Delta(i, i+x) = \Delta(i\ i-x) = -\Delta(i, i+\hat{y}) = -\Delta(i, i-\hat{y})$$

where $\Delta(i, i+\delta) = V \langle C_{i\uparrow} C_{i+\delta\downarrow} - C_{i\downarrow} C_{i+\delta\uparrow} \rangle$.

The extended s-wave and d-wave compete, and the d-wave pairing wins. The reason is that the nodallines of Δ_s coincide with the Fermi surface at half-filling (For high Tc cuprates, the filling is very close to half-filling), thus the gap function is suppressed on Fermi surface. Now let us only keep the d-wave channal.

$$\frac{H}{N} = \frac{1}{N}\sum_k \left(C_{k\uparrow}^{+} \quad C_{-k\downarrow}\right)\begin{pmatrix} \varepsilon_k-\mu & \Delta_d(\cos k_x-\cos k_y) \\ \Delta_d^{*}(\cos k_x-\cos k_y) & -(\varepsilon_k-\mu)\end{pmatrix}\begin{pmatrix} C_{k\uparrow} \\ C_{-k\downarrow}^{+}\end{pmatrix}$$

$$+ \frac{1}{N}\sum_k(\varepsilon_k-\mu) + \frac{1}{V}\Delta_d^{*}\Delta_d$$

Introducing Bogoliubov transformation, and assum Δ_d is real

$$\begin{pmatrix} C_{k\uparrow} \\ C_{-k\downarrow}^{+}\end{pmatrix} = \begin{pmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k\end{pmatrix}\begin{pmatrix} \alpha_{k\uparrow} \\ \beta_{-k\downarrow}^{+}\end{pmatrix}$$

we have

$$\rightarrow (\alpha_{k\uparrow}^{+} \quad \beta_{-k\downarrow})\underbrace{\begin{pmatrix} \cos\theta_k & \sin\theta_k \\ -\sin\theta_k & \cos\theta_k\end{pmatrix}\begin{pmatrix} \xi_k & \Delta(k) \\ \Delta(k) & -\xi_k\end{pmatrix}\begin{pmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k\end{pmatrix}}\begin{pmatrix} \alpha_{k\uparrow} \\ \beta_{-k\downarrow}^{+}\end{pmatrix}$$

$$\Downarrow$$

$$= \begin{bmatrix} \xi_k\cos2\theta_k+\Delta(k)\sin2\theta_k, & -\xi_k\sin2\theta_k+\Delta(k)\cos2\theta_k \\ -\xi_k\sin2\theta_k+\Delta(k)\cos2\theta_k, & -\xi_k\cos2\theta_k-\Delta(k)\sin2\theta_k\end{bmatrix}$$

$$(\xi_k = \varepsilon_k-\mu, \quad \Delta(k) = \Delta_d(\cos k_x - \cos k_y))$$

Set $\tan 2\theta_k = \dfrac{\Delta(k)}{\xi_k}$ $\quad \cos2\theta_k = \dfrac{\xi_k}{E_k}$, $\sin2\theta_k = \dfrac{\Delta_k}{E_k}$

with $E_k = \sqrt{\xi_k^2+\Delta^2(k)}$

$$\Rightarrow \frac{H}{N} = \frac{1}{N}\sum_k E_k \left[(\alpha^+_{k\uparrow}\alpha_{k\uparrow} - 1/2) + (\beta^+_{-k\downarrow}\beta_{-k\downarrow} - 1/2) \right]$$

$$+ \frac{1}{N}\sum_k (\varepsilon_k - \mu) + \frac{1}{V}|\Delta_d|^2 ,$$

$$\cos^2\theta_k = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right), \quad \sin^2\theta_k = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right).$$

§ Self-consistency.

$$\frac{F}{N} = \frac{1}{N}\sum_k -\frac{2}{\beta}\ln\left(e^{\frac{\beta}{2}E_k} + e^{-\frac{\beta}{2}E_k}\right) + \frac{1}{N}\sum_k (\varepsilon_k - \mu) + \frac{\Delta_d^2}{V}$$

$$= -\frac{2}{\beta}\int_{FBZ}\frac{d^2k}{(2\pi)^2}\ln 2\cosh\frac{\beta}{2}E_k + \frac{\Delta_d^2}{V} + \text{const}$$

$$\frac{\partial F}{\partial \Delta_d} = -\frac{2}{\beta}\int_{FBZ}\frac{d^2k}{(2\pi)^2}\frac{\sinh\frac{\beta}{2}E_k}{\cosh\frac{\beta}{2}E_k}\cdot\frac{\beta}{2}\,\frac{\Delta_d(\cos k_x - \cos k_y)^2}{E_k} + \frac{2\Delta_d}{V} = 0$$

$$\Rightarrow \boxed{\Delta_d = V\int_{FBZ}\frac{d^2k}{(2\pi)^2}\frac{\Delta_d(\cos k_x - \cos k_y)^2}{2E_k}\tanh\frac{\beta}{2}E_k .}$$

Gap equation "d-wave".

$$n = -\frac{1}{N}\frac{\partial F}{\partial \mu} \Rightarrow \frac{1}{N}\frac{\partial F}{\partial \mu} = -\frac{2}{\beta}\int_{FBZ}\frac{d^2k}{(2\pi)^2}\tanh\frac{\beta}{2}E_k\cdot\frac{\beta}{2}\,\frac{-\xi_k}{E_k} - 1 = -n$$

$$\Rightarrow \boxed{1 - n = \int_{FBZ}\frac{d^2k}{(2\pi)^2}\tanh\frac{\beta}{2}E_k\cdot\frac{\xi_k}{E_k}}$$

particle number

Gap equation: cf. the general form of gap equation:

$$\boxed{\Delta(k) = \int\frac{d^dk'}{(2\pi)^d}V(k,k')\frac{\Delta(k')}{2\sqrt{\xi^2 + \Delta^2(k')}}\tanh\frac{\beta}{2}\sqrt{\xi^2 + \Delta^2(k')}}$$

plug in $\Delta(k) = \Delta_d(\cos k_x - \cos k_y)$, $V(k,k') = V(\cos k_x - \cos k_y)(\cos k_x' - \cos k_y')$.

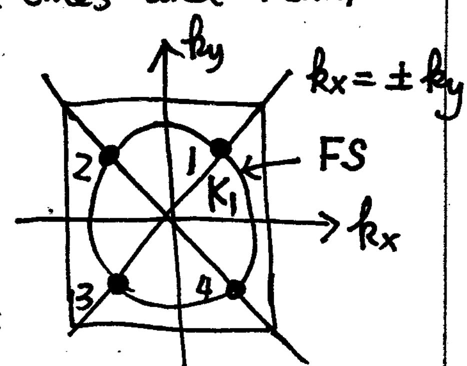
we will get the d-wave gap equation.

⊛ Dirac spectra (nodal quasi-particle)

$$\pm E_k = \pm\sqrt{\xi_k^2 + \Delta^2(k)} \quad : \quad \xi_k = 0 \text{ (Fermi surface)}$$

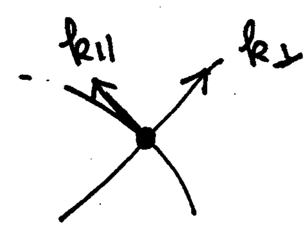
$$\Delta(k) = 0 \text{ gap nodal line}$$

zeros of E_K: crossing points of gap nodal lines and Fermi surface. There are nodal points.



"d"-wave superconductivity is NOT fully gapped, but gapless. The nodal quasi-particles dominates over the low energy thermodynamic properties!

Let us linearize the d-wave Hamiltonian around one of the nodes, say, node 1.



$$\begin{cases} \xi_K = \hbar v_F \delta k_\perp \\ \Delta(k) = \Delta_d \delta k_{\parallel} a \end{cases}$$

where $\begin{cases} \delta k_\perp = \dfrac{\delta k_x + \delta k_y}{\sqrt{2}} \\ \delta k_{\parallel} = \dfrac{-\delta k_x + \delta k_y}{\sqrt{2}} \end{cases}$ and $\delta \vec{k} = \vec{k} - \vec{K}_1$

$$\boxed{H(k) = \begin{pmatrix} \xi_K & \Delta(k) \\ \Delta(k) & -\xi_K \end{pmatrix} = \hbar v_F \delta k_\perp \tau_z + \Delta_d \delta k_{\parallel} \tau_x}$$

Thermodynamics of nodal superconductors (singlet)

2D-d-wave

In this lecture, we will study new features associated with the nodal quasi-particles of the d-wave superconductors. The d-wave gap equation can be solved analytically in the continuum approximation:

① Assum ξ_k is isotropic, i.e. independent of the azimuthal angle φ_k

$$\int \frac{d^2k}{(2\pi)^2} \longrightarrow \int \frac{d\varphi}{2\pi} \int_{-\omega_0}^{\omega_0} d\xi \; \rho_0(\xi)$$, where $\rho_0(\xi)$ is the density of states. If $\rho_0(\xi)$ doesnot have sigularity, it can be replace by N_F, i.e. the DOS right at Fermi surface. ω_0 is the cut off, which plays the role of Debye frequency in conventional SC. In high T_c, the origin of ω_0 is still in debate, most probably, it arises from antiferromagnetic fluctuations.

② We replace the lattice version of the angular form factor $\cos k_x - \cos k_y$ by $\cos 2\varphi_k$, which has the same $d_{x^2-y^2}$ symmetry. An issue is the normalization, which can absorbed in the definition of Δ_d and V. Say, $\cos k_x - \cos k_y \sim C \cdot \cos 2\varphi_k$

$$\Rightarrow \int_0^{2\pi} \frac{d\varphi}{2\pi} \int_0^{\omega_0} d\xi \; \frac{C^2 \cos^2 2\varphi_k}{\sqrt{\xi^2 + \Delta_d^2 C^2 \cos^2 2\varphi_k}} \tanh \frac{\beta}{2} \sqrt{\xi^2 + \Delta_d^2 C^2 \cos^2 2\varphi_k} = \frac{1}{N_F V}$$

we can define $\frac{1}{VC^2} \rightarrow \frac{1}{V}$ and $\Delta_d^2 C^2 \rightarrow \Delta_d^2$, we have

$$\boxed{\int_0^{2\pi} \frac{d\varphi}{2\pi} \int_0^{\omega_0} d\xi \; \frac{\cos^2 2\varphi}{\sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}} \tanh \frac{\beta}{2} \sqrt{\xi^2 + \Delta_d^2 \cos^2 \varphi} = \frac{1}{N_F V}}$$

* Solve T_c

we have around T_c, $\underbrace{}_{\Delta=0}$ $\Rightarrow$ $\displaystyle\int_0^{\frac{\omega_0}{2k_BT_c}} dx \, \frac{\tanh x}{x} = \frac{2}{N_F V}$

($x = \frac{\beta_c}{2}\xi$, the "2" factor on RHS comes from $\int \frac{d\varphi}{2\pi} \gamma_\varphi^2 = \frac{1}{2}$).

Integral by part $\Rightarrow$ LHS= $\ln \frac{\omega_0}{2k_BT_c} \tanh \frac{\omega_0}{2k_BT_c} - \displaystyle\int_0^{\frac{\omega_0}{2k_BT_c}} dx \, \ln x \, \mathrm{sech}^2 x$

we can set $\frac{\omega_0}{2k_BT_c} \to \infty$ converge!

define $C_0 = \frac{1}{2} \exp\left[-\displaystyle\int_0^\infty dx \, \frac{\ln x}{\cosh^2 x}\right]$

$= 1.134$

$$\Rightarrow \boxed{k_B T_c \approx C_0 \omega_0 e^{-\frac{2}{N_F V}}}$$

Because ω_0, V are difficult to know, this equation does not tell much useful information!

* Solve gap value at $T=0$,

$\beta \to \infty$, $\tanh \frac{\beta}{2}E \to 1$. we have

$$\int_0^{2\pi} \frac{d\varphi}{2\pi} \int_0^{\omega_0} d\xi \, \frac{\cos^2 2\varphi}{\sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}} = \frac{1}{N_F V}$$

$$\int dx \, \frac{1}{\sqrt{x^2+a^2}} = \ln(x + \sqrt{x^2+a^2}) + C$$

$$\Rightarrow \int_0^{\omega_0} d\xi \, \frac{1}{\sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}} = \ln\left(\xi + \sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}\right)\Big|_0^{\omega_0} = \ln \frac{\omega_0 + \sqrt{\omega_0^2 + \Delta_d^2 \cos^2 2\varphi}}{\Delta_d |\cos 2\varphi|}$$

$$\Rightarrow \int_0^{\pi} d\varphi \, \cos^2 2\varphi \, \ln \frac{\omega_0 + \sqrt{\omega_0^2 + \Delta_d^2 \cos^2 2\varphi}}{\Delta_d |\cos 2\varphi|} = \frac{\pi}{N_F V}$$

Consider the case of $\omega_0 \gg \Delta_d$, we can approximate the integral as

$$\int_0^{\pi} d\varphi \cos^2 2\varphi \ln \frac{2\omega_0}{\Delta_d |\cos 2\varphi|} \simeq \frac{\pi}{N_F V}$$

$$\Rightarrow \frac{\pi}{2} \ln \frac{2\omega_0}{\Delta_d} = \frac{\pi}{N_F V} + \int_0^{\pi} d\varphi \cos^2 2\varphi \ln |\cos 2\varphi|$$

$$2\int_0^{\pi/2} d\varphi \cos^2\varphi \ln \cos\varphi$$

$$\Rightarrow \frac{2\omega_0}{\Delta_d} = \frac{2}{N_F V} + \frac{4}{\pi}\int_0^{\pi/2} d\varphi \cos^2\varphi \ln\cos\varphi$$

$$\Rightarrow \boxed{\Delta_d = C_1 \omega_0 e^{-\frac{2}{N_F V}}}, \quad \text{where } C_1 = 2\cdot\exp\left[-\frac{4}{\pi}\int_0^{\pi/2} d\varphi \cos^2\varphi \ln\cos\varphi\right]$$

$$\simeq 2.426$$

we arrive the relation between gap and T_c.

$$\boxed{\frac{2\Delta_d}{k_B T_c} \simeq 4.28},$$

which is slightly higher than the s-wave value 3.53.

§ DOS in d-wave superconductor

$$\rho(\omega) = \frac{2}{Vol}\sum_k \left(u_k^2 \delta(\omega - E_k) + v_k^2 \delta(\omega + E_k)\right)$$

$$= 2\int \frac{d^2k}{(2\pi)^2} \frac{1}{2}\left[\left(1 + \frac{\xi_k}{E_k}\right)\delta(\omega - E_k) + \left(1 - \frac{\xi_k}{E_k}\right)\delta(\omega + E_k)\right]$$

$$= \int \frac{d\varphi}{2\pi}\int d\xi \frac{N_F}{2}\left[\left(1 + \frac{\xi}{E}\right)\delta(\omega - E) + \left(1 - \frac{\xi}{E}\right)\delta(\omega + E)\right]$$

← odd function

consider $\omega > 0 \Rightarrow \rho(\omega) = \int \frac{d\varphi}{2\pi}\int d\xi \, N_F \left(1 + \frac{\xi}{E}\right)\delta(\omega - E)$

$$= \int \frac{d\varphi}{2\pi}\int_0 d\xi \frac{N_F}{2}\delta\left(\omega - \sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}\right)$$

The solution of $\omega^2 = \xi^2 + \Delta_d^2 \cos^2 2\varphi \Rightarrow \xi = \pm\sqrt{\omega^2 - \Delta_d^2 \cos^2 2\varphi}$

$$\Rightarrow \delta(\omega - E) = \frac{\delta(\xi - \sqrt{\omega^2 - \Delta^2\cos^2 2\varphi}) + \delta(\xi + \sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi})}{|\xi| / \sqrt{\xi^2 + \Delta_d^2 \cos^2\varphi}}$$

$$\delta(\omega - E) = \frac{\omega}{\sqrt{\omega^2 - \Delta^2\cos^2 2\varphi}}\left[\delta\left(\xi - \sqrt{\omega^2-\Delta^2\cos^2 2\varphi}\right) + \delta\left(\xi + \sqrt{\omega^2-\Delta^2\cos^2 2\varphi}\right)\right]$$

$$\rho(\omega) = \frac{N_F}{2}\int\frac{d\varphi}{2\pi}\int d\xi \, \frac{\omega}{\sqrt{\omega^2-\Delta^2\cos^2 2\varphi}}\left[\delta\left(\xi - \sqrt{\omega^2-\Delta^2\cos^2 2\varphi}\right) + \delta\left(\xi+\sqrt{\omega^2-\Delta^2\cos^2 2\varphi}\right)\right]$$

$$= N_F \int_0^{2\pi}\frac{d\varphi}{2\pi}\frac{\omega}{\sqrt{\omega^2-\Delta^2\cos^2 2\varphi}}\,\theta(\omega > |\Delta\cos 2\varphi|)$$

$$= N_F\,\frac{1}{2}\int^{4\pi}\frac{d\varphi'}{2\pi}\frac{\omega}{\sqrt{\omega^2-\Delta^2\cos^2\varphi'}}\,\theta(\omega>|\Delta\cos 2\varphi|) = \frac{2N_F}{\pi}\int_0^{\pi/2} d\varphi' \frac{\omega}{\sqrt{\omega^2-\Delta^2\cos^2\varphi'}}\,\theta(\cdots)$$

① if $\omega > \Delta \Rightarrow$ $\rho(\omega) = \frac{2N_F}{\pi}\int_0^{\pi/2} d\varphi' \frac{1}{\sqrt{1-(\Delta/\omega)^2\cos^2\varphi'}} = \frac{2N_F}{\pi}\int_0^{\pi/2} d\varphi' \frac{1}{\sqrt{1-\left(\frac{\Delta}{\omega}\right)^2\sin^2\varphi'}}$

This is the complete Elliptic integral of 1st kind.

as $\boxed{\begin{array}{ll} \Delta/\omega \to 1, \text{ we have} & \rho(\omega) \simeq \frac{N_F}{\pi}\ln\frac{8}{1-\Delta/\omega} \\ \Delta/\omega \to \infty & \rho(\omega) = N_F \end{array}}$

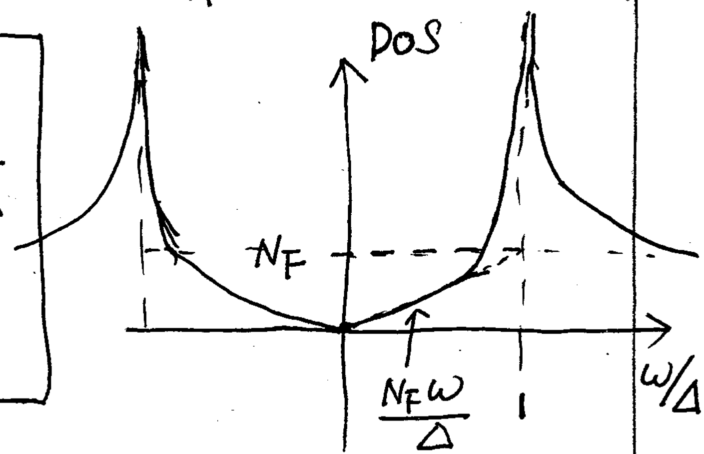
② if $\omega < \Delta$ define $\cos\phi = \frac{\Delta}{\omega}\cos\varphi'$ $\Rightarrow$ $\sin\phi \, d\phi = \frac{\Delta}{\omega}\sin\varphi' \, d\varphi'$

$$\rho(\omega) = \frac{2N_F}{\pi}\int_0^{\pi/2}\left(\frac{\Delta}{\omega}\right)^{-1}\frac{\sin\phi}{\sin\varphi'}\,d\phi \cdot \frac{1}{\sqrt{1-\cos^2\phi}}$$

$$= \frac{\omega}{\Delta}\,\frac{2N_F}{\pi}\int_0^{\pi/2}\frac{d\phi}{\sin\varphi'} \leftarrow \sin\varphi' = \sqrt{1-\cos^2\varphi'} = \sqrt{1-\left(\frac{\omega}{\Delta}\right)^2\cos^2\phi}$$

$$= \frac{\omega}{\Delta}\,\frac{2N_F}{\pi}\int_0^{\pi/2}d\phi\,\frac{1}{\sqrt{1-\left(\frac{\omega}{\Delta}\right)^2\cos^2\phi}} = \frac{\omega}{\Delta}\,\frac{2N_F}{\pi}\int_0^{\pi/2}d\phi\,\frac{1}{\sqrt{1-\left(\frac{\omega}{\Delta}\right)^2\sin^2\phi}}$$

$$\boxed{\begin{array}{l} \text{as } \omega \to \Delta \\ \qquad \rho(\omega) \to \frac{N_F\,\omega}{\pi\,\Delta}\ln\frac{8}{1-\omega/\Delta} \\ \text{as } \omega \to 0 \quad \rho(\omega) \to \frac{N_F\,\omega}{\Delta} \end{array}}$$



§ Specific heat

$\leftarrow \mathrm{Vol} = N a^2$

a: lattice constant

The free energy density $\frac{F(T)}{\mathrm{Vol}} = -k_B T \ln Z$

$$\frac{F(T)}{\mathrm{Vol}} = -k_B T \frac{1}{\mathrm{Vol}} \sum_k 2 \ln \left(e^{-\frac{1}{2}\beta E_k} + e^{\frac{1}{2}\beta E_k} \right) + \frac{\Delta_d^2}{V}$$

$$= -k_B T \int_{FBZ} \frac{d^2k}{(2\pi)^2}\, 2 \ln 2\cosh \frac{\beta}{2} E_k + \frac{\Delta_d^2}{V}$$

$$\frac{S}{\mathrm{Vol}} = \frac{-\partial F}{\mathrm{Vol}\,\partial T} = k_B \int \frac{d^2k}{(2\pi)^2}\, 2\ln 2\cosh \frac{\beta}{2}E_k + k_B T \int \frac{d^2k}{(2\pi)^2}\, 2 \tanh \frac{\beta}{2} E_k \frac{\partial}{\partial T}\left(\frac{\beta E_k}{2}\right)$$

$$- \frac{2\Delta_d}{V} \frac{\partial \Delta_d}{\partial T}$$

gap Eq: $$\frac{\Delta_d}{V} = \int \frac{d^2k}{(2\pi)^2}\, \Delta_d \frac{(\cos k_x - \cos k_y)^2}{2E_k} \tanh \frac{\beta}{2} E_k$$

$$\frac{\partial}{\partial T}\left(\frac{\beta}{2} E_k\right) = \frac{-1}{2k_B T^2} E_k + \frac{\beta}{2} \frac{\Delta_d (\cos k_x - \cos k_y)^2}{E_k} \frac{\partial \Delta}{\partial T}$$

$$\Rightarrow \frac{S}{\mathrm{Vol}} = 2k_B \int \frac{d^2k}{(2\pi)^2} \ln\left(2\cosh \frac{\beta}{2} E_k\right) - 2k_B \int \frac{d^2k}{(2\pi)^2} \tanh \frac{\beta}{2} E_k \frac{\beta E_k}{2}$$ (other term cancels)

Ex: check $\frac{S}{\mathrm{Vol}}$ can also be written as

$$\frac{S}{\mathrm{Vol}} = -2k_B \sum_k \left[(1-f_k) \ln (1-f_k) + f_k \ln f_k \right]$$

with $f_k = \frac{1}{e^{\beta E_k} + 1}$. Check it's consistent with the above Eq.

$$\frac{C}{\mathrm{Vol}} = T \frac{\partial S}{\partial T} = -\beta \frac{\partial S}{\partial \beta} = 2\beta k_B \frac{1}{\mathrm{Vol}} \sum_k \frac{\partial f_k}{\partial \beta} \ln \frac{f_k}{1-f_k} = -2\beta^2 k_B \frac{1}{\mathrm{Vol}} \sum_k E_k \frac{\partial f_k}{\partial \beta}$$

$$= -2\beta^2 k_B \frac{1}{\mathrm{Vol}} \sum_k E_k \frac{d f_k}{d(\beta E_k)} \left(\frac{d(\beta E_k)}{d\beta} \right) \leftarrow \frac{d\beta E_k}{d\beta} = E_k + \beta \frac{dE_k}{d\beta}$$

$$= 2\beta k_B \frac{1}{\mathrm{Vol}} \sum_k \left(\frac{-\partial f_k}{\partial E_k} \right) \left(E_k^2 + \frac{1}{2} \beta \frac{d E_k^2}{d\beta} \right)$$

$$\frac{C}{Vol} = 2k_B \int \frac{d^2k}{(2\pi)^2} \frac{e^{\beta E_K}}{(e^{\beta E_K}+1)^2} \left(\frac{E_K^2}{k_B^2 T^2} - \frac{1}{2} \frac{dE_k^2}{k_B^2 T dT} \right)$$

① Next we consider low T limit.

Now we use continuum approx: $E_k^2 = \xi^2 + \Delta_d^2 \cos^2 2\varphi_k$

$$\frac{E_k^2}{k_B^2 T^2} = \frac{\xi^2 + \Delta_d^2(T) \cos^2 2\varphi_K}{k_B^2 T^2}$$

$$\frac{E_K dE_K}{k_B^2 T dT} = \frac{\Delta_d(T)}{k_B T} \frac{d\Delta_d(T)}{k_B dT} \cos^2 2\varphi_K = \frac{\Delta^2(T)}{(k_B T)^2} \cos^2 2\varphi_K \left(\frac{k_B T}{\Delta_d(T)} \right)^3$$

because at $T << \Delta(T)$, $\frac{d\Delta(T)}{k_B dT} \simeq \frac{k_B^2 T^2}{\Delta_d^2(T)}$ (for d-wave),

we can neglect the contribution from the second term.

$\Rightarrow$ at $T<<\Delta$, $$\frac{C}{k_B} = \frac{1}{k_B^2 T^2} N_F \int \frac{d\varphi}{2\pi} \int d\xi \frac{e^{\beta E}}{(e^{\beta E}+1)^2} E^2$$

$$= \frac{N_F}{4 k_B^2 T^2} \int \frac{d\varphi}{2\pi} \int_{-\infty}^{+\infty} d\xi \frac{E^2}{\cosh^2(E/2T)}$$

The factor $\cosh^2 E/2T$ suppresses the contribution except from the nodal region:

$$|\xi| > |\Delta| |\cos 2\varphi| \Rightarrow \Delta\varphi \sim |\varphi - \pi/4| < \frac{|\xi|}{2|\Delta|}$$

consider there're four nodes,

$$\frac{C}{k_B} = \frac{N_F}{k_B^2 T^2} \int_{-\infty}^{+\infty} d\xi \frac{\xi^2}{\cosh^2(\xi/2T)} \int_{-\frac{|\xi|}{2|\Delta|}}^{\frac{|\xi|}{2\Delta}} d\Delta\varphi + o(e^{-\Delta/T})$$

$$\approx \frac{N_F}{k_B^2 T^2} \frac{1}{\Delta} \int_{-\infty}^{+\infty} d\xi \frac{|\xi|^3}{\cosh^2 \xi/2Tk_B}$$ defin $X = \frac{\xi}{2Tk_B}$

$$\frac{C}{k_B} \approx \frac{2^5 N_F k_B^2 T^2}{\Delta} \int_0^{+\infty} dx \frac{x^3}{\cosh^2 x} \simeq \text{const.} \frac{N_F (k_B T)^2}{\Delta}$$

The low ~~temperature~~ specific heat in 2D nodal SC

$$\frac{C}{k_B} \simeq \text{const.} \frac{N_F (k_B T)^2}{\Delta_d},$$ which is

Consistent with the low energy DOS $\simeq N_F \frac{\omega}{\Delta_d}$

Paramagnetic susceptibility / Knight shift

consider the pairing sector $k\uparrow$ and $-k\downarrow$. The Hilbert space is 4-dimensional: $|\Omega\rangle$, $\alpha^\dagger_{k\uparrow}|\Omega\rangle$, $\beta^\dagger_{-k\downarrow}|\Omega\rangle$ $\alpha^\dagger_{k\uparrow}\beta^\dagger_{-k\downarrow}|\Omega\rangle$.

The partition function $1+e^{-\beta E_k}+e^{-\beta E_k}+e^{-2\beta E_k} = (1+e^{-\beta E_k})^2$

if adding external field, $E_{\alpha k\uparrow} = E_k - \mu_B H$

$E_{\beta -k\downarrow} = E_k + \mu_B H$

$$\Rightarrow M = \mu_B \sum_k \frac{e^{-\beta(E_k-\mu_B H)}}{(1+e^{-\beta E_k})^2} - \frac{e^{-\beta(E_k+\mu_B H)}}{(1+e^{-\beta E_k})^2}$$

we neglect the dependence on H in the denominator at the linear order of H

$$\Rightarrow \chi = \frac{\partial M}{\partial H} = \mu_B^2 \sum_k \frac{e^{-\beta E_k}}{(1+e^{-\beta E_k})^2}(2\beta)$$

$$\Rightarrow \frac{\chi}{Vol} = \beta\mu_B^2 N_F \int d\xi \int \frac{d\varphi}{2\pi} \frac{1}{(e^{-\beta E/2}+e^{\beta E/2})^2}$$

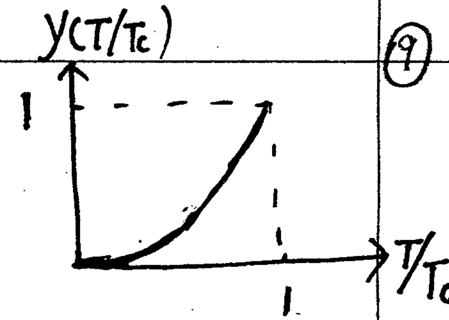
$$\frac{2}{Vol}\sum_k \to N_F \int d\xi \int \frac{d\varphi}{2\pi}$$

Define Yoshida function $Y(\varphi,T) = \frac{\beta}{4}\int_{-\infty}^{+\infty} \frac{d\xi}{\left(\cosh\frac{E(\varphi)}{2T}\right)^2}$

$$\Rightarrow \frac{\chi}{Vol} = \mu_B^2 N_F \int \frac{d\varphi}{2\pi} Y(\varphi,T)$$

For the s-wave case, $\frac{\chi}{\chi_n} = \frac{\beta}{4}\int_{-\infty}^{+\infty} \frac{d\xi}{\left[\cosh\left(\frac{[\xi^2+\Delta^2]^{1/2}}{2T}\right)\right]^2} = \frac{\beta}{2}\int_0^{+\infty} d\xi\, \mathrm{sech}^2\frac{\beta E}{2}$

$= Y(T)$ isotropic case



at $T = T_c$, $y(1) = \int_0^{+\infty} \mathrm{sech}^2 x \, dx = 1$

$T \ll \Delta$, $y(T/\Delta)$ is suppressed exponentially.
$\sim e^{-\Delta/T}$

Now let us consider the d-wave case:

$$\frac{\chi}{\chi_n} = \int_0^{+\infty} d\xi \, \frac{\beta}{2} \, \frac{1}{\cosh^2\left(\frac{\xi}{2T}\right)} \int_{-\frac{\xi}{2\Delta}}^{\frac{\xi}{2\Delta}} d\Delta\varphi + O\left(e^{-\Delta/T}\right)$$

← the low T contribution from $\xi > \Delta \cos 2\varphi$
$\Rightarrow |\Delta\varphi| < \frac{\xi}{2\Delta}$

$$\simeq \int_0^{+\infty} d\xi \, \frac{1}{2k_B T} \, \frac{\xi}{\Delta} \, \frac{1}{\cosh^2\left(\frac{\xi}{2k_B T}\right)}$$

define $x = \frac{\xi}{2k_B T}$

$$\Rightarrow \boxed{\frac{\chi}{\chi_n} \sim \frac{2k_B T}{\Delta} \int_0^{+\infty} dx \, \frac{x}{\cosh^2(x)} \simeq \text{const.} \, \frac{k_B T}{\Delta}}$$

This is also consistent with the low T DoS $\sim N_F \frac{\omega}{\Delta}$.

χ can be measured through NMR knight shift. The NMR frequency of nuclear in solids is different from that in vaccum: $B_{eff} = B_{ex} + B_{mol}$; and $B_{mol} \propto M = B_{ex}\chi$.

From the frequency shift (Kight shift), we can infer the magnetic susceptibility of the envinment, i.e. electronic structure.