Part II: The Hubbard Model and BCS Theory

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Goal

- Derive the theoretical relationship

$$\frac{2|\Delta(T=0)|}{k_B T_c} = 3.5278,$$

  where T_c is the critical temperature and Δ is the energy gap at $T = 0$.
- Why is this interesting?
  - Doesn't depend on material properties such as density of states, strength of electron interactions, etc.
  - *Universal*

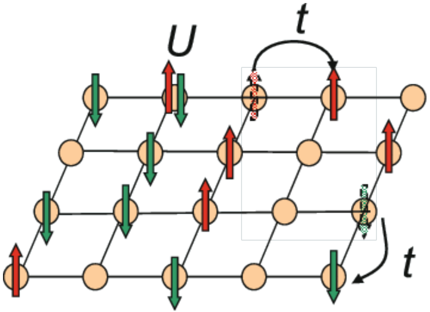
Hubbard Model Hamiltonian

$$\hat{H} = -t \sum_{\langle i,j \rangle ,\sigma} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma} \right) - U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

look at all pairs of sites

creating electron at site i and destroying electron at site j (and vice-versa)

attractive potential between electrons at the site i



The Partition Function

The Partition function is given by

$$Z = \mathrm{Tr}(e^{-\beta \hat{H}})$$

After a lot of tedious mathematics, we get

$$Z = \int \exp\left(\underbrace{-\int_0^\beta \left[\sum_i \bar{c}_{i\tau} \partial_\tau c_{i\tau} + H[\bar{c}, c] \right] \mathrm{d}\tau}_{\text{The Action } S} \right) \mathcal{D}\bar{c}\mathcal{D}c$$

The Hubbard-Stratonovich Transformation

We can write

$$e^{Un_\uparrow n_\downarrow} = e^{U\bar{c}_\uparrow \bar{c}_\downarrow c_\downarrow c_\uparrow} = \int \exp\left(-\frac{1}{U}|\Delta(T=0)|^2 - \Delta \bar{c}_\uparrow \bar{c}_\downarrow - \Delta^* c_\downarrow c_\uparrow\right) \mathrm{d}\Delta^* \, \mathrm{d}\Delta \,.$$

We can rewrite the action in terms of Δ, Δ^*. If $Z = \int e^{-S_{\text{eff}}} \mathcal{D}\Delta^* \mathcal{D}\Delta$ then

$$S_{\text{eff}} = \int_0^\beta \underbrace{\sum_i \frac{1}{U}|\Delta_{i\tau}|^2}_{\text{gaussian term}} \mathrm{d}\tau - \underbrace{\log\left\langle \exp\left(-\int_0^\beta \sum_i (\Delta_{i\tau}\bar{c}_{i\tau\uparrow}\bar{c}_{i\tau\downarrow} + h.c.)\, \mathrm{d}\tau\right)\right\rangle_0}_{\text{interaction term (between cooper pairs)}}$$

We write the interaction term as

$$\Delta S_{\text{eff}} = -\log\langle e^{-S'}\rangle_0$$

Cumulant Expansion

Recall that

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots$$

$$\log(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} + \cdots$$

Then:

$$\begin{aligned} -\log\left(\langle e^{-S'}\rangle_0\right) &= -\log\left(1 + \langle -S'\rangle_0 + \frac{1}{2}\left\langle \left(S'\right)^2\right\rangle_0 + \cdots\right) \\ &= \langle S'\rangle_0 + \frac{1}{2}\left\langle S'^2\right\rangle_0 - \frac{1}{2}\langle S'\rangle_0^2 + \cdots \end{aligned}$$

We will compute up to order 2.

Cumulant Expansion

We wish to compute

$$\Delta S_{\text{eff}} \approx \langle S' \rangle_0 + \frac{1}{2}\left\langle S'^2 \right\rangle_0 - \frac{1}{2}\langle S' \rangle_0^2$$

We compute

$$\langle S' \rangle_0 = \langle \bar{c}_{k-p,\uparrow}, \bar{c}_{p,\downarrow} \rangle_0 = 0.$$

and

$$\frac{1}{2}\langle S'^2 \rangle_0 = -\frac{1}{\beta N}\sum_k |\Delta_k|^2 \pi(\boldsymbol{k}, ik_0)$$

Effective Action

We derived

$$S_{\text{eff}} = \frac{1}{\beta N} \sum_{k} |\Delta_k|^2 \left(\frac{1}{U} - \pi(\boldsymbol{k}, ik_0) \right)$$

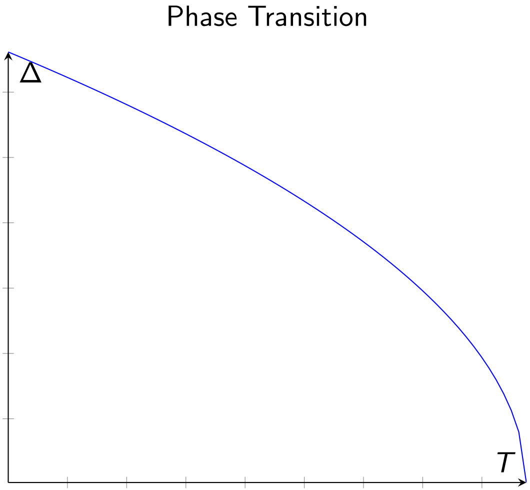
A transition occurs when the coefficient of $|\Delta_k|^2$ changes sign. Can analytically determine when $\boldsymbol{k} = k_0 = 0$. We get from complex analysis,

$$\pi(0,0) = \rho \log \left(\frac{2\beta D}{\pi} e^{\gamma} \right)$$

Gives a formula for the critical temperature

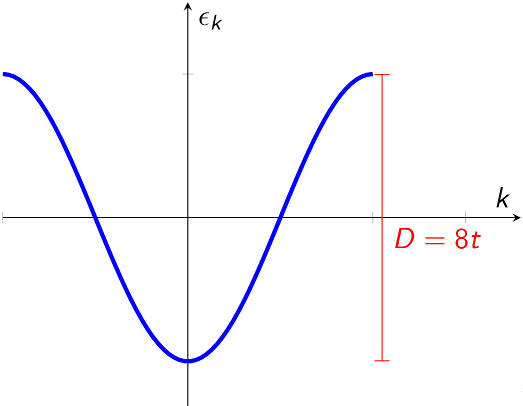
$$\boxed{T_c \sim \frac{2De^{\gamma}}{\pi k_B} e^{-1/(\rho U)}}$$

The Big Picture



Some More Assumptions

- Δ is a constant in space and time.
- $D \gg |\Delta(T = 0)|$
- $\rho(\xi) = \begin{cases} \rho_0 & |\xi| < D \\ 0 & \text{else} \end{cases}$
- Analytically analyze as $T \to 0$ (at the very end)



Action Minimization

Going back a bit... The action (as a functional)

$$S_{\text{eff}}[\Delta^*, \Delta] = \underbrace{\int_0^\beta \sum_i \frac{1}{U} |\Delta_{i\tau}|^2 \, \mathrm{d}\tau}_{\text{gaussian term}} - \underbrace{\log \left\langle \exp \left(- \int_0^\beta \sum_i (\Delta_{i\tau} \bar{c}_{i\tau\uparrow} \bar{c}_{i\tau\downarrow} + h.c.) \, \mathrm{d}\tau \right) \right\rangle_0}_{\text{interaction term}}$$

becomes a regular function,

$$S_{\text{eff}}(\Delta^*, \Delta) = \frac{\beta N |\Delta(T=0)|^2}{U} - \log \left\langle \exp \left(- \int_0^\beta \sum_i (\Delta \bar{c}_{i\tau\uparrow} \bar{c}_{i\tau\downarrow} + h.c.) \, \mathrm{d}\tau \right) \right\rangle_0$$

which we can minimize with respect to Δ^* which gives

$$\Delta = -\frac{U}{\beta N} \sum_k \langle c_{-k,\downarrow} c_{k,\uparrow} \rangle$$

Diagonalization

Assuming Δ is constant allows us to write the action as

$$S_{\text{eff}}(\Delta^*, \Delta) = \frac{\beta N |\Delta(T=0)|^2}{U} + \sum_{\boldsymbol{k},\omega} \begin{pmatrix} \bar{c}_{k,\uparrow} & c_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} -i\omega + \xi_{\boldsymbol{k}} & \Delta \\ \Delta^* & -i\omega - \xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ \bar{c}_{-k,\downarrow} \end{pmatrix}$$

We can diagonalize this, using the action minimization condition, and the assumptions above, after (a lot of) work, we get

$$|\Delta(T=0)| = 2De^{-1/\rho U}$$

Finishing Up

We have

$$T_c = \frac{2De^{\gamma}}{\pi k_B} e^{-1/(\rho U)}, \qquad |\Delta(T=0)| = 2De^{-1/\rho U}$$

so dividing through, we get

$$\frac{2|\Delta(T=0)|}{k_B T_c} = 2\pi e^{-\gamma} = 3.5278$$

	Δ_0 [a,b]	U_0 [b]	δ [c]	ω_c/ω_D	$2\Delta(0)/k_B T_c$ [d]
Zn	1.19 (1.20)	6840	1.50	0.167	3.63 (3.20)
Cd	0.26 (0.75)	5040	1.20	0.245	3.70 (3.20)
Hg	0.81 (8.25)	4900	0.44	0.124	4.76 (4.60)
Al	1.37 (1.70)	6300	1.81	0.183	3.54 (3.30)
Ga	3.96 (1.65)	5960	1.51	0.096	3.51 (3.50)
In	0.25 (5.25)	5420	0.62	0.203	3.92 (3.60)
Tl	0.23 (3.68)	5260	0.48	0.164	3.92 (3.57)
Sn	1.26 (5.75)	5440	1.25	0.158	3.70 (3.50)
Pb	0.70 (13.7)	5670	0.60	0.160	4.56 (4.38)
V	14.0 (8.00)	7930	1.20	0.068	3.95 (3.40)
Nb	4.90 (15.3)	7270	1.04	0.107	4.25 (3.80)
Ta	3.36 (7.00)	8110	0.90	0.095	3.95 (3.60)