PHY 770 -- Statistical Mechanics
12:00* - 1:45 PM TR Olin 107

Instructor: Natalie Holzwarth (Olin 300)
Course Webpage: http://www.wfu.edu/~natalie/s14phy770

Lecture 15

Chap. 6 – Interacting particles
- ❑ **Cluster expansions**
- ❑ **Virial coefficients for classical gas**
- ❑ **Interacting Fermi particles**

***Partial make-up lecture -- early start time**

6	Tue: 02/04/2014	Chap. 4	Phase transitions	#6	02/11/2014
7	Thur: 02/06/2014	Chap. 2	Microscopic analysis of entropy	#7	02/11/2014
8	Thur: 02/06/2014	Chap. 2	Microscopic analysis of entropy	#8	02/11/2014
9	Tue: 02/11/2014	Chap. 2	Microscopic analysis of entropy	#9	02/18/2014
	Thur: 02/13/2014		Class cancelled due to weather		
10	Tue: 02/18/2014	Chap. 5	Equilibrium Statistical Mechanics	#10	02/27/2014
11	Tue: 02/18/2014	Chap. 5	Equilibrium Statistical Mechanics	#11	02/27/2014
12	Thur: 02/20/2014	Chap. 5	The Ising model (class 12-1:45 PM)	#12	02/27/2014
	Tue: 02/25/2014		NAWH out of town -- no class		
13	Thur: 02/27/2014	Chap. 6	Grand partition function (class 12-1:45 PM)		
	Tue: 03/04/2014	*APS Meeting*	Take-home exam (no class meeting)		
	Thur: 03/06/2014	*APS Meeting*	Take-home exam (no class meeting)		
	Tue: 03/11/2014		Spring break (no class meeting)		
	Thur: 03/13/2014		Spring break (no class meeting)		
14	Tue: 03/18/2014	Chap. 6	Fermi and Bose particles (class 12-1:45 PM; Exam due)	#13	03/25/2014
15	Thur: 03/20/2014	Chap. 6	Interacting particles (class 12-1:45 PM)	#14	03/25/2014
16	Tue: 03/24/2014	Chap. 6	Interacting particles (class 12-1:45 PM)	#15	03/25/2014

Effects of interactions between particles – classical case

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i}{2m} + \sum_{i,j}^{N(N-1)} V\left(\hat{\mathbf{r}}_{ij}\right) \equiv \hat{T}^N + \hat{V}^N$$

Canonical partition function : $Z_N(T) = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \frac{1}{N!}\frac{1}{(\lambda_T)^{3N}} Q_N(T,V)$

where $Q_N(T,V) \equiv \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_N e^{-\beta\hat{V}^N}$

Grand canonical partition function :

$$Z_\mu(T) = \sum_{N=1}^{\infty} Z_N(T) e^{\beta N\mu} = \sum_{N=1}^{\infty} \frac{1}{N!}\frac{1}{(\lambda_T)^{3N}} Q_N(T,V) e^{\beta N\mu}$$

Effects of interactions between particles – classical case -- continued

$$\hat{V}^N = \sum_{i,j}^{N(N-1)} V\left(\hat{\mathbf{r}}_{ij}\right)$$

$$Q_N(T,V) \equiv \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_N e^{-\beta \hat{V}^N}$$

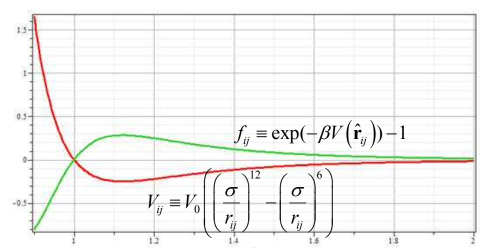
$$= \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_N e^{-\beta \sum_{i,j}^{N(N-1)} V\left(\hat{\mathbf{r}}_{ij}\right)}$$

$$\approx \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_N W_N\left(\mathbf{r}_1, \mathbf{r}_2 ... \mathbf{r}_N\right)$$

$$W_N\left(\mathbf{r}_1, \mathbf{r}_2 ... \mathbf{r}_N\right) \equiv \prod_{i,j}^{N(N-1)} (f_{ij} + 1)$$

$$f_{ij} \equiv \exp(-\beta V\left(\hat{\mathbf{r}}_{ij}\right)) - 1$$

Effects of interactions between particles – classical case -- continued



Effects of interactions between particles – classical case -- continued

$$Z_\mu(T,V) = \sum_{N=0}^{\infty} \frac{1}{N!} \frac{1}{\lambda_T^{3N}} e^{\beta N \mu} \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_N W_N\left(\mathbf{r}_1, \mathbf{r}_2 ... \mathbf{r}_N\right)$$

$$W_N\left(\mathbf{r}_1, \mathbf{r}_2 ... \mathbf{r}_N\right) \equiv \prod_{i,j}^{N(N-1)} (f_{ij} + 1)$$

$$f_{ij} \equiv \exp(-\beta V\left(\hat{\mathbf{r}}_{ij}\right)) - 1$$

Note that:

$W_1 = 1 \qquad W_2\left(\mathbf{r}_1, \mathbf{r}_2\right) = 1 + f_{12}$

$W_3\left(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\right) = \left(1 + f_{12}\right)\left(1 + f_{13}\right)\left(1 + f_{23}\right)$

Effects of interactions between particles – classical case -- continued

$$Z_\mu(T,V) = \sum_{N=0}^{\infty} \frac{1}{N!}\frac{1}{\lambda_T^{3N}} e^{\beta N\mu} \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_N W_N(\mathbf{r}_1,\mathbf{r}_2...\mathbf{r}_N)$$

In terms of cumulant expansion:

$$Z_\mu(T,V) = \exp\left(\sum_{\nu=0}^{\infty} \frac{1}{\nu!}\frac{1}{\lambda_T^{3\nu}} e^{\beta\nu\mu} \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_\nu U_\nu(\mathbf{r}_1,\mathbf{r}_2...\mathbf{r}_\nu)\right)$$

Typical cluster functions:

$$U_1(\mathbf{r}_1) = W_1(\mathbf{r}_1)$$

$$U_2(\mathbf{r}_1,\mathbf{r}_2) = W_2(\mathbf{r}_1,\mathbf{r}_2) - W_1(\mathbf{r}_1)W_1(\mathbf{r}_2)$$

Cluster integrals:

$$b_\nu(V,T) \equiv \frac{1}{V\nu!}\int ... \int d\mathbf{r}_1 d\mathbf{r}_2 ... d\mathbf{r}_\nu U_\nu(\mathbf{r}_1,\mathbf{r}_2...\mathbf{r}_\nu)$$

Effects of interactions between particles – classical case -- continued

$$Z_\mu(T,V) = \exp\left(\sum_{\nu=0}^{\infty} \frac{1}{\nu!}\frac{1}{\lambda_T^{3\nu}} e^{\beta\nu\mu} \int d\mathbf{r}_1 \int d\mathbf{r}_2 .... \int d\mathbf{r}_\nu U_\nu(\mathbf{r}_1,\mathbf{r}_2...\mathbf{r}_\nu)\right)$$

$$= \exp\left(V\sum_{\nu=0}^{\infty} \frac{1}{\lambda_T^{3\nu}} e^{\beta\nu\mu} b_\nu(V,T)\right)$$

Grand potential: $\Omega(V,T,\mu) = -kT\ln(Z_\mu(T,V))$

$$= -kTV\sum_{\nu=0}^{\infty}\frac{1}{\lambda_T^{3\nu}} e^{\beta\nu\mu} b_\nu(V,T)$$

Derived functions: $P = -\frac{\Omega(V,T,\mu)}{V} = kT\sum_{\nu=0}^{\infty}\frac{1}{\lambda_T^{3\nu}} e^{\beta\nu\mu} b_\nu(V,T)$

$$\frac{\langle N\rangle}{V} = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial\mu}\right)_{V,T} = \sum_{\nu=0}^{\infty}\frac{\nu}{\lambda_T^{3\nu}} e^{\beta\nu\mu} b_\nu(V,T)$$

Effects of interactions between particles – classical case -- continued

Virial expansion of the equation of state for a (weakly) interacting gas:

$$\frac{P}{kT} = \sum_{\nu=1}^{\infty} B_\nu(T)\left(\frac{\langle N\rangle}{V}\right)^\nu$$

Using: $P = -\frac{\Omega(V,T,\mu)}{V} = kT\sum_{\nu=0}^{\infty}\frac{1}{\lambda_T^{3\nu}} e^{\beta\nu\mu} b_\nu(V,T)$

$$\frac{\langle N\rangle}{V} = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial\mu}\right)_{V,T} = \sum_{\nu=0}^{\infty}\frac{\nu}{\lambda_T^{3\nu}} e^{\beta\nu\mu} b_\nu(V,T)$$

$$B_1(T) = b_1(T) = 1$$

$$B_2(T) = -b_2(T)$$

$$b_2(V,T) = \frac{1}{2V}\int\int d\mathbf{r}_1 d\mathbf{r}_2 U_2(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{2}\int d\mathbf{r}_{12}\left(e^{-\beta V(r_{12})} - 1\right)$$

Effects of interactions between particles – classical case -- continued

Virial expansion of the equation of state for a (weakly) interacting gas:

$$\frac{P}{kT} = \frac{\langle N \rangle}{V} + B_2(T)\left(\frac{\langle N \rangle}{V}\right)^2 + \ldots$$

$$B_2(V,T) = -\frac{1}{2}\int d\mathbf{r}_{12}\left(e^{-\beta V(r_{12})} - 1\right)$$

Example: Lennard-Jones interaction

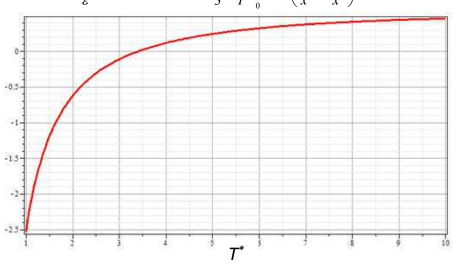
$$V(r) = -4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

Let $\mathrm{T}^* \equiv \frac{kT}{\varepsilon}$ $\qquad B_2(T^*) = \frac{2\pi\sigma^3}{3}\frac{4}{T^*}\int_0^\infty x^2 dx\left(\frac{12}{x^{12}} - \frac{6}{x^6}\right)e^{-\frac{4}{T^*}\left(\frac{1}{x^{12}} - \frac{1}{x^6}\right)}$

Effects of interactions between particles – classical case – continued
Virial coefficient for Lennard-Jones potential

Lennard-Jones interaction: $V(r) = -4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$

Let $T^* \equiv \frac{kT}{\varepsilon}$ $\qquad B_2(T^*) = \frac{2\pi\sigma^3}{3}\frac{4}{T^*}\int_0^\infty x^2 dx\left(\frac{12}{x^{12}} - \frac{6}{x^6}\right)e^{-\frac{4}{T^*}\left(\frac{1}{x^{12}} - \frac{1}{x^6}\right)}$



Effects of interactions between particles – classical case – continued

Virial expansion of the equation of state for a (weakly) interacting gas:

$$\frac{P}{kT} = \frac{\langle N \rangle}{V} + B_2(T)\left(\frac{\langle N \rangle}{V}\right)^2 + \ldots$$

Relationship to van der Waals equation of state:

$$\left(P + a\left(\frac{\langle N \rangle}{V}\right)^2\right)\left(1 - b\left(\frac{\langle N \rangle}{V}\right)\right) = \left(\frac{\langle N \rangle}{V}\right)kT$$

$$\frac{P}{kT} = \frac{\langle N \rangle}{V}\frac{1}{1 - b\left(\langle N \rangle / V\right)} - \frac{a}{kT}\left(\frac{\langle N \rangle}{V}\right)^2 = \frac{\langle N \rangle}{V} + \left(b - \frac{a}{kT}\right)\left(\frac{\langle N \rangle}{V}\right)^2 + \ldots$$

Interacting Fermi fluid

BCS (Bardeen, Schrieffer, and Cooper) model

Superconducting phase transition

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Theory of Superconductivity*

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(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_c$ at $T=0°$K to zero at T_c. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

Interacting Fermi fluid

BCS (Bardeen, Schrieffer, and Cooper) model

Superconducting phase transition

Model Hamiltonian expressed terms of eigenstates of non-interacting Fermi gas of wavevector **k** and spin σ:

$$\hat{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow}$$

Electron creation operator: $a^\dagger_{\mathbf{k}\sigma}$

Electron annihilation operator: $a_{\mathbf{k}\sigma}$

Single particle energy: $\varepsilon_{\mathbf{k}} = \dfrac{\hbar^2 k^2}{2m}$

Interaction potential: $V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V_0 & |\mu - \varepsilon_{\mathbf{k}}| < \Delta\varepsilon \text{ and } |\mu - \varepsilon_{\mathbf{k}'}| < \Delta\varepsilon \\ 0 & \text{otherwise} \end{cases}$

$$\left[a_{\mathbf{k}\sigma}, a^\dagger_{\mathbf{k}'\sigma'}\right]_+ = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'} \qquad \left[a_{\mathbf{k}\sigma}, a_{\mathbf{k}'\sigma'}\right]_+ = 0 \qquad \left[a^\dagger_{\mathbf{k}\sigma}, a^\dagger_{\mathbf{k}'\sigma'}\right]_+ = 0$$

Interacting Fermi fluid -- BCS model -- continued

$$\hat{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow}$$

Mean field approximation:

$$\hat{H}_{MF} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta^* a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} + \sum_{\mathbf{k}} \Delta a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}$$

$$\Delta_{\mathbf{k}}^* \equiv -V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left\langle a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} \right\rangle \qquad \Delta_{\mathbf{k}} \equiv -V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right\rangle$$

$$\left\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right\rangle \equiv \mathrm{Tr}\left[\hat{\rho} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\right] \qquad \hat{N} \equiv \sum_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}$$

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}_{MF} - \mu\hat{N})}}{\mathrm{Tr}\left[e^{-\beta(\hat{H}_{MF} - \mu\hat{N})}\right]}$$

Interacting Fermi fluid -- BCS model -- continued

$$\hat{H}_{MF} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta^{*} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} + \sum_{\mathbf{k}} \Delta a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow}$$

Define: $\xi_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu$

$$\hat{K} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \left(a^{\dagger}_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} - a_{-\mathbf{k}\downarrow} a^{\dagger}_{-\mathbf{k}\downarrow} \right) + \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^{*} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow}$$

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}_{MF} - \mu\hat{N})}}{\mathrm{Tr}\left[e^{-\beta(\hat{H}_{MF} - \mu\hat{N})} \right]} = \frac{e^{-\beta\hat{K}}}{\mathrm{Tr}\left[e^{-\beta\hat{K}} \right]}$$

Introduce two component basis vectors:

$$\boldsymbol{\alpha}_{\mathbf{k}} \equiv \begin{pmatrix} a_{\mathbf{k}\uparrow} \\ a^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \qquad \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \equiv \begin{pmatrix} a^{\dagger}_{\mathbf{k}\uparrow} & a_{-\mathbf{k}\downarrow} \end{pmatrix} \qquad \mathbf{K}_{\mathbf{k}} \equiv \begin{pmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^{*} & -\xi_{\mathbf{k}} \end{pmatrix}$$

$$\hat{K} = \sum_{\mathbf{k}} \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \mathbf{K}_{\mathbf{k}} \boldsymbol{\alpha}_{\mathbf{k}}$$

Interacting Fermi fluid -- BCS model -- continued

$$\boldsymbol{\alpha}_{\mathbf{k}} \equiv \begin{pmatrix} a_{\mathbf{k}\uparrow} \\ a^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \qquad \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \equiv \begin{pmatrix} a^{\dagger}_{\mathbf{k}\uparrow} & a_{-\mathbf{k}\downarrow} \end{pmatrix} \qquad \mathbf{K}_{\mathbf{k}} \equiv \begin{pmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^{*} & -\xi_{\mathbf{k}} \end{pmatrix}$$

$$\hat{K} = \sum_{\mathbf{k}} \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \mathbf{K}_{\mathbf{k}} \boldsymbol{\alpha}_{\mathbf{k}}$$

Bogoliubov transformation to decouple interactions using unitary transformation

$$\mathbf{U}_{\mathbf{k}} \equiv \begin{pmatrix} u^{*}_{\mathbf{k}} & v_{\mathbf{k}} \\ -v^{*}_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \qquad \mathbf{U}^{\dagger}_{\mathbf{k}} \equiv \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v^{*}_{\mathbf{k}} & u^{*}_{\mathbf{k}} \end{pmatrix} \qquad \text{where } |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$$

$$\mathbf{U}^{\dagger}_{\mathbf{k}} \mathbf{K}_{\mathbf{k}} \mathbf{U}_{\mathbf{k}} = \mathbf{E}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} \qquad \text{where } E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^{2} + |\Delta_{\mathbf{k}}|^{2}}$$

Interacting Fermi fluid -- BCS model -- continued

$$\hat{K} = \sum_{\mathbf{k}} \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \mathbf{K}_{\mathbf{k}} \boldsymbol{\alpha}_{\mathbf{k}} = \sum_{\mathbf{k}} \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \mathbf{U}_{\mathbf{k}} \mathbf{U}^{\dagger}_{\mathbf{k}} \mathbf{K}_{\mathbf{k}} \mathbf{U}_{\mathbf{k}} \mathbf{U}^{\dagger}_{\mathbf{k}} \boldsymbol{\alpha}_{\mathbf{k}} = \sum_{\mathbf{k}} \boldsymbol{\alpha}^{\dagger}_{\mathbf{k}} \mathbf{U}_{\mathbf{k}} \mathbf{E}_{\mathbf{k}} \mathbf{U}^{\dagger}_{\mathbf{k}} \boldsymbol{\alpha}_{\mathbf{k}}$$

Define: $\boldsymbol{\Gamma}_{\mathbf{k}} = \mathbf{U}^{\dagger}_{\mathbf{k}} \boldsymbol{\alpha}_{\mathbf{k}} = \begin{pmatrix} \gamma_{\mathbf{k},0} \\ \gamma^{\dagger}_{\mathbf{k},1} \end{pmatrix}$

$$\hat{K} = \sum_{\mathbf{k}} \boldsymbol{\Gamma}^{\dagger}_{\mathbf{k}} \mathbf{E}_{\mathbf{k}} \boldsymbol{\Gamma}_{\mathbf{k}} \qquad \mathbf{E}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} \qquad \text{where } E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^{2} + |\Delta_{\mathbf{k}}|^{2}}$$

Self-consistency condition:

$$\Delta_{\mathbf{k}}^{*} \equiv -V_0 \sum_{\mathbf{k};(|\mu - \varepsilon_{\mathbf{k}}| < \Delta\varepsilon)} \left\langle a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \right\rangle \qquad \Delta_{\mathbf{k}} \equiv -V_0 \sum_{\mathbf{k};(|\mu - \varepsilon_{\mathbf{k}}| < \Delta\varepsilon)} \left\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right\rangle$$

$$\left\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right\rangle \equiv \mathrm{Tr}\left[\hat{\rho} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right] \qquad \hat{\rho} = \frac{e^{-\beta\hat{K}}}{\mathrm{Tr}\left[e^{-\beta\hat{K}} \right]}$$

Interacting Fermi fluid -- BCS model -- continued

Self-consistency condition $\Leftrightarrow$ Gap equation (according to textbook):

$$1 = V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_\mathbf{k}|<\Delta\varepsilon)} \frac{1}{2E_\mathbf{k}} \tanh\left(\frac{E_\mathbf{k}}{2kT}\right) \quad \text{where } E_\mathbf{k} = \sqrt{\xi_\mathbf{k}^2 + |\Delta_\mathbf{k}|^2}$$

Derivation of gap equation -- noting that:

$$\left\langle \boldsymbol{\alpha}_\mathbf{k} \boldsymbol{\alpha}^\dagger_\mathbf{k} \right\rangle = \begin{pmatrix} 1-\left\langle a^\dagger_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} \right\rangle & -\left\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right\rangle \\ -\left\langle a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} \right\rangle & \left\langle a^\dagger_{-\mathbf{k}\downarrow} a_{-\mathbf{k}\downarrow} \right\rangle \end{pmatrix}$$

$$= \mathbf{U}_\mathbf{k} \begin{pmatrix} 1-\left\langle \gamma^\dagger_{\mathbf{k}0} \gamma_{\mathbf{k}0} \right\rangle & 0 \\ 0 & \left\langle \gamma^\dagger_{\mathbf{k}1} \gamma_{\mathbf{k}1} \right\rangle \end{pmatrix} \mathbf{U}^\dagger_\mathbf{k}$$

Interacting Fermi fluid -- BCS model -- continued

Note that:

$$\left\langle \gamma^\dagger_{\mathbf{k}0} \gamma_{\mathbf{k}0} \right\rangle = \frac{e^{-\beta E_\mathbf{k}}}{e^{-\beta E_\mathbf{k}} + e^{\beta E_\mathbf{k}}} = \frac{1}{2}\left(\frac{e^{-\beta E_\mathbf{k}} + e^{\beta E_\mathbf{k}}}{e^{-\beta E_\mathbf{k}} + e^{\beta E_\mathbf{k}}} + \frac{e^{-\beta E_\mathbf{k}} - e^{\beta E_\mathbf{k}}}{e^{-\beta E_\mathbf{k}} + e^{\beta E_\mathbf{k}}} \right)$$

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

$$\left\langle \gamma_{\mathbf{k}1} \gamma^\dagger_{\mathbf{k}1} \right\rangle = \frac{e^{\beta E_\mathbf{k}}}{e^{\beta E_\mathbf{k}} + e^{-\beta E_\mathbf{k}}} = \frac{1}{2}\left(\frac{e^{\beta E_\mathbf{k}} + e^{-\beta E_\mathbf{k}}}{e^{\beta E_\mathbf{k}} + e^{-\beta E_\mathbf{k}}} + \frac{e^{\beta E_\mathbf{k}} - e^{-\beta E_\mathbf{k}}}{e^{\beta E_\mathbf{k}} + e^{-\beta E_\mathbf{k}}} \right)$$

$$= \frac{1}{2}\left(1 + \tanh\left(\beta E_\mathbf{k}\right)\right) = 1 - \left\langle \gamma^\dagger_{\mathbf{k}1} \gamma_{\mathbf{k}1} \right\rangle$$

(Note: results not quite identical to textbook.

Interacting Fermi fluid -- BCS model -- continued

Continuing analysis:

$$\left\langle \boldsymbol{\alpha}_\mathbf{k} \boldsymbol{\alpha}^\dagger_\mathbf{k} \right\rangle = \begin{pmatrix} 1-\left\langle a^\dagger_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} \right\rangle & -\left\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \right\rangle \\ -\left\langle a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} \right\rangle & \left\langle a^\dagger_{-\mathbf{k}\downarrow} a_{-\mathbf{k}\downarrow} \right\rangle \end{pmatrix}$$

$$= \mathbf{U}_\mathbf{k} \begin{pmatrix} 1-\left\langle \gamma^\dagger_{\mathbf{k}0} \gamma_{\mathbf{k}0} \right\rangle & 0 \\ 0 & \left\langle \gamma^\dagger_{\mathbf{k}1} \gamma_{\mathbf{k}1} \right\rangle \end{pmatrix} \mathbf{U}^\dagger_\mathbf{k} \qquad \left\langle \gamma^\dagger_{\mathbf{k}0} \gamma_{\mathbf{k}0} \right\rangle = \frac{1}{2}\left(1 - \tanh\left(\beta E_\mathbf{k}\right)\right)$$

$$\left\langle \gamma^\dagger_{\mathbf{k}1} \gamma_{\mathbf{k}1} \right\rangle = \frac{1}{2}\left(1 - \tanh\left(\beta E_\mathbf{k}\right)\right)$$

$$= \mathbf{U}_\mathbf{k} \begin{pmatrix} \frac{1}{2} + \frac{1}{2}\tanh\left(\beta E_\mathbf{k}\right) & 0 \\ 0 & \frac{1}{2} - \frac{1}{2}\tanh\left(\beta E_\mathbf{k}\right) \end{pmatrix} \mathbf{U}^\dagger_\mathbf{k}$$

$$= \frac{1}{2}\mathbf{1} + \frac{1}{2E_\mathbf{k}}\tanh\left(\beta E_\mathbf{k}\right)\, \mathbf{U}_\mathbf{k} \begin{pmatrix} E_\mathbf{k} & 0 \\ 0 & -E_\mathbf{k} \end{pmatrix} \mathbf{U}^\dagger_\mathbf{k} = \frac{1}{2}\mathbf{1} + \frac{1}{2E_\mathbf{k}}\tanh\left(\beta E_\mathbf{k}\right)\mathbf{K}_\mathbf{k}$$

where $\mathbf{K}_\mathbf{k} = \begin{pmatrix} \xi_\mathbf{k} & \Delta_\mathbf{k} \\ \Delta^*_\mathbf{k} & -\xi_\mathbf{k} \end{pmatrix}$

Interacting Fermi fluid -- BCS model -- continued

Continuing analysis:

$$\left\langle \boldsymbol{\alpha}_{\mathbf{k}}\boldsymbol{\alpha}^{\dagger}_{\mathbf{k}}\right\rangle = \begin{pmatrix} 1-\left\langle a^{\dagger}_{\mathbf{k}\uparrow}a_{\mathbf{k}\uparrow}\right\rangle & -\left\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\right\rangle \\ -\left\langle a^{\dagger}_{\mathbf{k}\uparrow}a^{\dagger}_{-\mathbf{k}\downarrow}\right\rangle & \left\langle a^{\dagger}_{-\mathbf{k}\downarrow}a_{-\mathbf{k}\downarrow}\right\rangle \end{pmatrix}$$

$$= \frac{1}{2}\mathbf{1} + \frac{1}{2E_{\mathbf{k}}}\tanh\left(\beta E_{\mathbf{k}}\right)\begin{pmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta^{*}_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{pmatrix}$$

$$\Rightarrow -\left\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\right\rangle = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\left(\beta E_{\mathbf{k}}\right)$$

Self-consistency condition:

$$\Delta_{\mathbf{k}} \equiv -V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\right\rangle = V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left(\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\left(\beta E_{\mathbf{k}}\right)\right)$$

Recall that $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$

Interacting Fermi fluid -- BCS model -- continued

Approximate evaluation of Gap equation:

$$\Delta_{\mathbf{k}} \equiv -V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\right\rangle = V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left(\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\left(\beta E_{\mathbf{k}}\right)\right)$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$

Your textbook argues that the temperature at which $\Delta_{\mathbf{k}} \to 0$ can be approximated by (apart from factors of 2)

$$1 = V_0 g\left(\varepsilon_F\right)\int_0^{\Delta\varepsilon} d\xi_{\mathbf{k}} \frac{\tanh\left(\beta_c \xi_{\mathbf{k}}\right)}{\xi_{\mathbf{k}}} \approx V_0 g\left(\varepsilon_F\right)\ln\left(\frac{2.26773\ \Delta\varepsilon}{kT_c}\right)$$

$$\Rightarrow T_c \approx \frac{2.26773\ \Delta\varepsilon}{k} e^{-1/\left(V_0 g(\varepsilon_F)\right)}$$

Interacting Fermi fluid -- BCS model -- continued

Approximate evaluation of Gap equation -- for $T \to 0,\ \Delta_{\mathbf{k}} \to \Delta_0$

$$\Delta_{\mathbf{k}} \equiv -V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\right\rangle = V_0 \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left(\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\left(\beta E_{\mathbf{k}}\right)\right)$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$

$$1 = \sum_{\mathbf{k};(|\mu-\varepsilon_{\mathbf{k}}|<\Delta\varepsilon)} \left(\frac{1}{2\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_0|^2}}\right) \approx V_0 g(\varepsilon_F)\int_0^{\Delta\varepsilon} d\xi_{\mathbf{k}} \left(\frac{1}{2\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_0|^2}}\right)$$

$$= \frac{V_0 g(\varepsilon_F)}{2}\sinh^{-1}\left(\frac{\Delta\varepsilon}{\Delta_0}\right)$$

$$\Rightarrow \Delta_0 = \frac{\Delta\varepsilon}{\sinh\left(\frac{2}{V_0 g(\varepsilon_F)}\right)}$$

Interacting Fermi fluid -- BCS model -- continued

Approximate behavior of gap as a function of T