



Project Report

Fluctuations in Phase Disordered Superconductors

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1 Classical Statistical Mechanics

Micro-canonical Ensemble:

A system can only access the $\Omega(E)$ states which define the constrained event space. As a consequence of Entropy maximization, each state has an equal probability. The probability of a state c to have energy E is given by

$$p(c) = \frac{1}{\Omega(E)}$$

The Entropy of the system is given by

$$S = \ln(\Omega(E))$$

Ideal gas:

Let us consider an ideal box of volume L^d containing N -free particles with only the Kinetic Energy but no interactions (Ideal gas). No. of micro-states with energy upto E is

$$N(E) = V^N \left(\frac{mE}{2\pi\hbar^2} \right)^{\frac{Nd}{2}} \frac{1}{\Gamma(\frac{Nd}{2} + 1)}$$

No. of microstates with energy E and $E+dE$ is

$$\Omega(E) = \frac{V^N}{N!} E^{\frac{Nd-2}{2}} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{Nd}{2}} \frac{Nd}{2\Gamma(\frac{Nd}{2} + 1)}$$

For $d=3$ and the Entropy ($s = \frac{S}{N}$) is given by

$$s = \frac{5}{2} + \ln v \left(\frac{mE}{3\pi\hbar^2} \right)^{\frac{3}{2}}$$

This equation is called Sackur-Tetrode Equation.

Canonical Ensemble:

The probability in this ensemble is given by

$$p(c) = \frac{\exp(-\beta H(c))}{Z(\beta)}$$

The partition function is given by

$$Z(\beta) = \sum \exp(-\beta H(c))$$

The Internal Energy $E = T^2 \frac{\partial \ln Z(\frac{1}{T})}{\partial T}$

The Entropy of the ensemble is $S = \beta E + \ln(Z(\beta))$

Specific heat $C_v = \frac{\langle H^2 \rangle - \langle H \rangle^2}{T^2}$

Ideal gas:

The Partition function is given by $Z = \frac{V^N}{N!} \left(\frac{mT}{2\pi\hbar^2} \right)^{\frac{Nd}{2}}$

The Internal Energy $E = \frac{Nd}{2}T$ and $C_v = \frac{Nd}{2}$

The Entropy $s = 1 + \frac{d}{2} + \ln v \left(\frac{mE}{d\pi\hbar^2} \right)^{\frac{d}{2}}$, same as derived from the microcanonical ensemble.

Equivalence of Ensembles - If the actual system is at fixed energy E , we can do the calculations in the canonical ensemble at fixed T so that the average energy in the canonical ensemble is equal to the fixed energy in micro-canonical ensemble.

Grand Canonical Ensemble:

The probability $p(c) = \frac{\exp(-\beta[H_c - \mu N_c])}{Z(\beta, \mu)}$

The partition function $Z(\beta, \mu) = \sum \exp(-\beta[H_c - \mu N_c])$

Isothermal Compressibility is dependent on the number fluctuations and is given by $k_T = \frac{1}{n^2TV} [\langle N^2 \rangle - \langle N \rangle^2]$

2 Quantum Statistical Mechanics

We take hilbert space of Energy eigenstates and construct the event space as the probability $P(|n\rangle) = p_n$. So, the density matrix can be written as $\rho = \sum p_n |n\rangle\langle n|$.

The entropy can be defined from density matrix as

$$S = -\text{Tr} \rho \ln(\rho)$$

Microcanonical Ensemble:

$$p_n = \frac{1}{\Omega(E)} \delta(E_n - E)$$

Canonical Ensemble:

$$p_n = \frac{\exp(-\beta E_n)}{Z(\beta)}$$

$$Z(\beta) = \sum \exp(-\beta E_n) = \text{Tr} \exp(-\beta H)$$

Quantum Harmonic Oscillator:

The Hamiltonian

$$H = (a^\dagger a + \frac{1}{2})\hbar\omega$$

The Partition function

$$Z(\beta) = [Tr \exp(-\beta h\omega(n + \frac{1}{2}))]^N = (z(\beta))^N$$

The distribution is given by

$$\langle n \rangle = \frac{1}{\exp(\beta h\omega) - 1}$$

This distribution is called as Bose distribution function. It diverges as $\frac{T}{\omega}$ for ω close to 0. The function is negative for $\omega \leq 0$ and has no physical meaning. So, we consider only the $\omega > 0$ cases. The distribution decreases exponentially for large ω .

The energy of a single oscillator is given by

$$\frac{E}{N} = h\omega \left[\frac{1}{2} + \frac{1}{\exp(\beta h\omega) - 1} \right]$$

Case: $T \ll \omega$ or $\beta\omega \gg 1$

The Ground state energy is given by

$$\frac{E}{N} = \frac{h\omega}{2} + h\omega \exp\left(-\frac{h\omega}{T}\right)$$

The additional term added is called 1st Excitation Boltzmann-factor. The corresponding specific heat is given by

$$C_v = \frac{\partial E}{\partial T} = \left(\frac{h\omega}{2T}\right)^2 \frac{1}{\sinh^2\left(\frac{h\omega}{2T}\right)}$$

$$C_v \sim \left(\frac{h\omega}{2T}\right)^2 \exp\left(-\frac{h\omega}{T}\right)$$

$$C_v \sim 0$$

Case: $T \gg \omega$ or $\beta\omega \ll 1$

The Ground state energy is given by

$$\frac{E}{N} \sim T + \frac{\omega^2}{12T}$$

The additional term here is the 1st Quantum Correction and the 1st term is corresponding to equipartition principle.

The specific heat is given by

$$C_v \sim 1 - \frac{1}{12} \left(\frac{h\omega}{T}\right)^2$$

$$C_v \sim 1$$

3 Lattice Vibrations and Phonons

Phonon Hamiltonian:

$$H = \sum \frac{P_i^2}{2M} + \frac{1}{2} \sum D(R_i - R_j) u_i u_j$$

By fourier transforming and by diagonalizing the D matrix we get

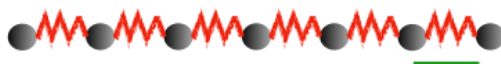
$$H = \sum \frac{P(q)P(-q)}{2M} + \frac{1}{2} \sum D(q) u(q) u(-q)$$

For each q we have a corresponding Harmonic oscillator with frequency

$$\omega(q) = \sqrt{\frac{D(q)}{M}}$$

Toy Models:

Model 1



By assuming the nearest neighbour atoms are coupled by a spring of spring constants K. The Potential is given by

$$V = \frac{K}{2} \sum [u(R_i) - u(R(i+1))]^2$$

$$V = K \sum [1 - \cos(qa)] u(q) u(-q)$$

The D operator has the form here as

$$D(q) = K[1 - \cos(qa)]$$

The frequency of the harmonic oscillator is

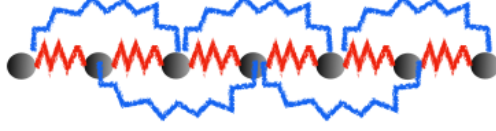
$$\omega(q) = \sqrt{\frac{K}{M}} \sqrt{1 - \cos(qa)}$$

For $qa \ll 1$,

$$\omega \sim c_s q$$

$$c_s = \sqrt{\frac{K}{M}} \frac{a}{\sqrt{2}}$$

. Model 2



The Potential is given by

$$V = \frac{K}{2} \sum [u(R_i) - u(R_{i+1})]^2 + \frac{K'}{2} \sum [u(R_i) - u(R_{i+2})]^2$$

The D operator has the form here as

$$D(q) = K[1 - \cos(qa)] + K'[1 - \cos(2qa)]$$

For $qa \ll 1$,

$$\omega \sim c_s q$$

$$c_s = \sqrt{\frac{K}{2} + 2K' \frac{a}{\sqrt{M}}}$$

We observe that the functional form of the low energy phonon dispersion $\omega \sim c_s q$ is universal and doesnot depend upon the microscopic details.

4 Debye Model

Momentum Integrals

$$\sum F(q) = V \int \frac{d^d q}{(2\pi)^d} F(q)$$

The single particle density of states

$$g(\epsilon) = \frac{1}{V} \sum \delta(\epsilon - \hbar\omega(q)) = V \int \frac{d^d q}{(2\pi)^d} \delta(\epsilon - \hbar\omega(q))$$

$$g(\epsilon) = \frac{d\Omega_d}{2\pi\hbar c_s} \epsilon^{d-1}$$

Specific heat is given by

$$\frac{E}{V} \sim \frac{d\Omega_d}{(2\pi\hbar c_s)^d} T^{d+1} \int_0^{\frac{\hbar\omega_D}{T}} x^d \frac{1}{\exp(x) - 1} dx$$

$$x = \frac{\hbar\omega}{T}$$

For $T \ll h\omega_D$

$$\frac{E}{V} \sim T^{d+1}$$

$$C_v \sim T^d$$

For $T \gg h\omega_D$

$$\frac{E}{V} \sim NT$$

$$C_v \sim N$$

We see that at very low temperatures we need to follow the debye model and for very high temperatures we need to follow Einsteins model. In between the range of T we cannot have a linear dispersive relation.

5 Thermodynamics of Free Bose gas

The number density of the states is given by

$$\rho = \rho_0 + AT^{\frac{3}{2}}\Gamma(\frac{3}{2})Li_{\frac{3}{2}}(z)$$

Where,

$$Li_k(z) = \sum_0^\infty \left(\frac{z}{k}\right)^n$$

$$A = \frac{2}{\sqrt{\Pi}} \left[\frac{m}{2\Pi h^2} \right]^{\frac{3}{2}}$$

For $T \gg T_c$,

$$Li_k(z) \sim z$$

$$z \sim \zeta[\frac{3}{2}] \left[\frac{T_c}{T} \right]^{\frac{3}{2}}$$

For $T \rightarrow T_c^+$,

$$z \sim 1 - \left[\frac{\zeta(3/2)}{2\sqrt{\Pi}} \right]^2 \left[1 - \left(\frac{T_c}{T} \right)^{\frac{3}{2}} \right]^2$$

Internal Energy

$$u = \frac{E}{N} = AT^{\frac{5}{2}}\Gamma(\frac{5}{2})Li_{\frac{5}{2}}(z)$$

For $T > T_c$

$$\frac{E}{N} = \frac{3}{2}T \frac{Li_{\frac{5}{2}}(z)}{Li_{\frac{3}{2}}(z)}$$

For large T:

$$\frac{E}{N} = \frac{3T}{2} - \frac{3\zeta(\frac{3}{2})}{8\sqrt{2}} \frac{T_c^{\frac{3}{2}}}{T^{\frac{1}{2}}}$$

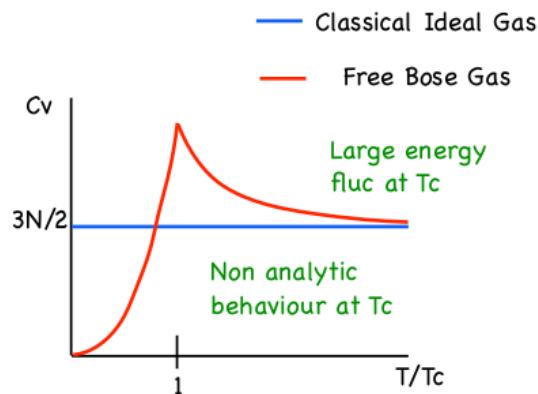
The first term is the classical answer and the second term is the Quantum correction for bosons.

$$C_v = \frac{3N}{2} + N \frac{3\zeta(\frac{3}{2})}{16\sqrt{2}} \frac{T_c^{\frac{3}{2}}}{T^{\frac{3}{2}}}$$

For $T < T_c$:

$$\frac{E}{N} = \frac{3}{2} T * 0.514 * \left[\frac{T}{T_c}\right]^{\frac{3}{2}}$$

$$C_v = \frac{3}{2} N * 0.514 * \left[\frac{T}{T_c}\right]^{\frac{3}{2}}$$



6 Free Fermi gas

Many body Hamiltonian is given by

$$H = \sum \epsilon_{\alpha} c^{\dagger}_{\alpha} c_{\alpha}$$

The partition function is given by

$$Z = \sum \exp(-\beta \sum [\epsilon_{\alpha} - \mu] n_{\alpha}) = \prod_{\alpha} Z_{\alpha}$$

$$n_{\alpha} = \frac{1}{1 + \exp(\beta(\epsilon_{\alpha} - \mu))}$$

This distribution is called fermi distribution. Single spin Density of states at Fermi Energy is given by

$$\rho = 2 \frac{g(\epsilon_F)}{\sqrt{\epsilon_F}} \frac{2}{3} \epsilon_F^{\frac{3}{2}}$$

The ground state energy is given by

$$E = \frac{3}{5} N \epsilon_F$$

There exists a finite ground state due to occupation of Fermi states as a consequence of Pauli Exclusion principle. **Low T Thermodynamics of Free Fermi Gas**

From Sommerfield Expansion at low T:

$$\int_0^\infty F(\epsilon) f(\epsilon - \mu) = \int_0^\mu d\epsilon F(\epsilon) + \frac{\Pi^2}{6} T^2 F'(\mu) + O\left(\left(\frac{T}{\mu}\right)^4\right)$$

The Density is given by

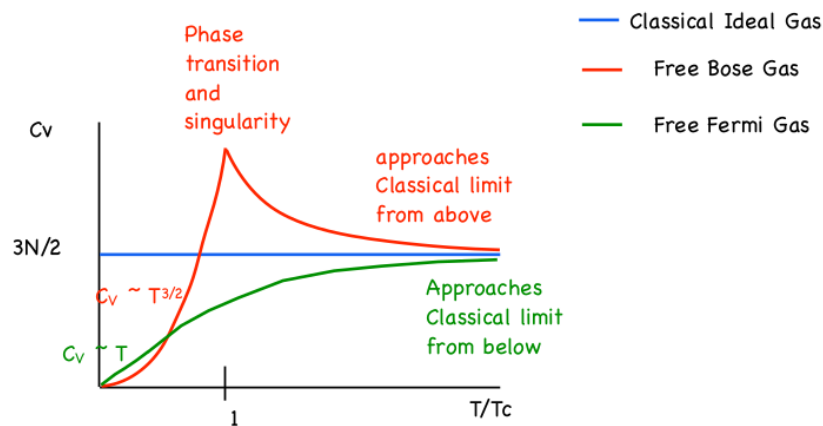
$$\rho = \int d\epsilon g(\epsilon) f(\epsilon - \mu) = A \frac{\epsilon_F^{\alpha+1}}{\alpha+1}$$

The Internal Energy is given by

$$\frac{E}{V} = \int d\epsilon g(\epsilon) f(\epsilon - \mu) = A \frac{\epsilon_F^{\alpha+2}}{\alpha+2} \left[1 + \frac{\Pi^2}{6} (\alpha+2) \frac{T^2}{\epsilon_F^2} \right]$$

$$C_v = g(\epsilon_F) \frac{\Pi^2}{3} T$$

Comparing classical, Bose and Fermi gas:



7 Weakly Repulsive Bose gas

The Hamiltonian for a large number of bosonic particles (spin=0) interacting with each other by pair-wise contact interaction.

$$H = \sum_k \frac{k^2}{2m} a^\dagger_k a_k + \frac{g}{2V} \sum_{k,k',q} a^\dagger_{k+q} a^\dagger_{k'-q} a_k a_{k'}$$

For weakly interacting system we expect the occupation of $k=0$ mode be macroscopically large $\langle a_0^\dagger a_0 \rangle = N_0 \sim N$. We can replace a_0 as an expectation value as a complex number Φ with $N_0 = |\Phi|^2$.

Bogoliubov Theory of weakly Repulsive BEC

The finite Bosons with k mode interact with themselves as well as with the condensate. This theory only considers the Boson interaction with the condensate and neglects the Boson-Boson interactions.

After replacing the operators with Φ and neglect the second order terms we obtain

$$H = \sum_k \left[\frac{k^2}{2m} + g\rho \right] a^\dagger_k a_k + \frac{\rho g}{2} \sum_k a^\dagger_k a^\dagger_{-k} + a_{-k} a_k$$

The Hamiltonian is quadratic in creation and annihilation operator and not diagonal. By using the transformations

$$\gamma_{\alpha k}^\dagger = u_k^\alpha a^\dagger_k + v_k^\alpha a_{-k}$$

$$\gamma_{\alpha -k}^\dagger = u_k^\alpha a_{-k} + v_k^\alpha a^\dagger_k$$

The Hamiltonian transforms to

$$H = \frac{1}{2} \sum_k E_k (\gamma_{\alpha k}^\dagger \gamma_{\alpha k} + \gamma_{\alpha -k}^\dagger \gamma_{\alpha -k}) + \frac{1}{2} E_k - \frac{k^2}{2m} - \rho g$$

The Ground state energy is given by

$$\frac{U}{V} = \frac{1}{2} \sum_k E_k - \frac{k^2}{2m} - \rho g$$

Validity of Bogoliubov Theory

If the number of particles in mode k are given by $N' = \sum_k \langle a^\dagger_k a_k \rangle$ and their density is represented by ρ' then the ratio is given by

$$\frac{\rho'}{\rho} = \frac{8}{3\sqrt{\pi}} (\rho a_s^3)^{\frac{1}{2}}$$

The scattering length given by

$$g = \frac{4\pi a_s}{m}$$

The theory is only valid when

$$\rho a_s^3 \ll 1$$

8 Interacting Fermions

The Hamiltonian for the system is given by

$$H = \sum_{k\sigma} (\epsilon_k - E_F) c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'q\alpha} V^{\alpha\beta}_{\gamma\delta}(q) c^\dagger_{k\alpha} c^\dagger_{k'\beta} c'_{k+q} c_{k-q} \gamma$$

Coulomb gas

$$H = \sum_{k\sigma} (k^2 - 1) c^\dagger_{k\sigma} c_{k\sigma} + r_s \sum_{kk'q\sigma\sigma'} \frac{1}{q^2} c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c'_{k+q} c_{k-q} \sigma'$$

Where, $r_s = \frac{e^2}{\epsilon_0 v_F}$

Coulomb gas:1st Order Perturbation Theory

The Interaction term in the Hamiltonian causes the particle-hole excitations. There exist number conserving excitations, a fermion inside the fermi sea is pushed to a momentum state outside the fermi sea.

Effect of the interaction term :

$$c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c'_{k+q} c_{k-q} \sigma'$$

This interaction term creates a 2 pair of different spins σ and σ' but the net momentum to the state is zero. The energy of the state measured from the ground state energy is given by

$$E = \epsilon_k + \epsilon'_k - \epsilon_{k-q} - \epsilon'_{k+q}$$

The hamiltonian of the free fermi gas is given by

$$H_0 = \sum_{k\sigma} (k^2 - 1) c^\dagger_{k\sigma} c_{k\sigma}$$

and the additional term is

$$H_1 = r_s \sum_{kk'q\sigma\sigma'} c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c'_{k+q} c_{k-q} \sigma'$$

The ground state is given by

$$|\Psi\rangle = \prod_{\sigma, |k| < k_F} c^\dagger_{k\sigma} |0\rangle$$

The first order energy shift is given by

$$\Delta E^1 = \langle \Psi | H_1 | \Psi \rangle = r_s \sum_{kk'q\sigma\sigma'} \frac{1}{q^2} \langle \Psi | c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c'_{k+q} c_{k-q} \sigma' | \Psi \rangle$$

Direct or Hartree contribution(q=0):

The first order energy shift with q=0 gives us

$$\Delta E_1 = V(q=0) \sum_{kk'} n_k n'_k$$

$$n_k = \sum_{\sigma} \langle \Psi | c_{k\sigma}^\dagger c_{k\sigma} | \Psi \rangle$$

The problem with $q = 0$ is that the coulomb potential diverges as it has an inverse dependence of q . The interactions in the calculations considered only the repulsions between the electrons. There exist additional attractions between the electron and the nuclei. Since the metal is neutral the overall average density of the electrons and the ions are equal and the Hartree contributions vanish in the metals.

The Exchange or Fock Contribution:

We consider the interactions between the two electrons in same spin $\sigma = \sigma'$

$$\begin{aligned} \langle \Psi | c_{k\sigma}^\dagger c_{k'\sigma}^\dagger c_{k+q\sigma} c_{k-q\sigma} | \Psi \rangle &= \langle \Psi | c_{k\sigma}^\dagger [\delta_{kk'} - c_{k\sigma} c_{k'\sigma}^\dagger] c_{k+q\sigma} c_{k-q\sigma} | \Psi \rangle \\ &= n_{k\sigma} \delta_{kk'} - n_{k\sigma} n_{k'\sigma} \end{aligned}$$

The first order Energy shift is given by

$$\Delta E^1 = \langle \Psi | H_1 | \Psi \rangle = -r_s \sum_{k,q,\sigma} \frac{1}{q^2} n_{k\sigma} n_{k+q\sigma}$$

We see that the Exchange contribution to the energy is negative, which tells there exist attractive interactions between the electrons of same spin.

$$\Delta E^1 = -r_s \sum_{k,q,\sigma} \frac{1}{q^2} n_{k\sigma} n_{k+q\sigma}$$

$$\Delta E^1 = \sum_k \Sigma(k) n_{k\sigma}$$

$$\Sigma(k) = -\frac{r_s}{\Pi^2} \left[\frac{1}{2} + \frac{1-k^2}{4k} \ln \frac{|1+k|}{|1-k|} \right]$$

The Energy is given by

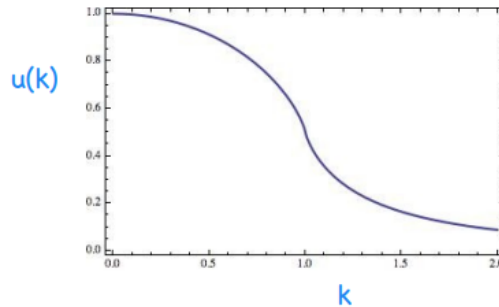
$$E = \sum_{k\sigma} E_k n_{k\sigma}$$

$$E_k = k^2 - \frac{r_s}{\Pi^2} \left[\frac{1}{2} + \frac{1-k^2}{4k} \ln \frac{|1+k|}{|1-k|} \right]$$

The term $u(k)$ is called as Effective Dispersion and given by

$$\frac{1}{2} + \frac{1-k^2}{4k} \ln \frac{|1+k|}{|1-k|}$$

The variation of effective dispersion with modes k is given by



9 References

- 1)<https://theory.tifr.res.in/~sensarma/>
- 2)Quantum Many Particle Sysytem by John.W.Negele and Henri Orland