# Physics 212 - Final Exam
## Solutions

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1.) a) Let $s_i = \begin{cases} +1 & R \\ -1 & L \end{cases}$

$$\mathcal{H} = -J \sum_i \delta_{s_i, s_{i+1}}$$

$$Z = \sum_{s_i = \pm 1} \exp\left[ \beta J \sum_i \delta(s_i, s_{i+1}) \right] = \sum_{s_i = \pm 1} (\omega)^{\delta(s_i, s_{i+1})}$$

b.) To compute the partition function, use the transfer matrix method

$$Z = v_L^T \, T^{N-1} \, v_R$$

where $T = \begin{pmatrix} \omega & 1 \\ 1 & \omega \end{pmatrix}$ and $v_L, v_R$ depend on the boundary conditions. The eigenvectors of $T$ are

$$v_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \lambda_+ = (\omega + 1)$$

$$v_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \lambda_- = (\omega - 1) \qquad \omega = e^{\beta J}$$

then $$Z = v_L^T v_+ \lambda_+^{N-1} v_+^T v_R + v_L^T v_- \lambda_-^{N-1} v_-^T v_R$$

for $N \gg 1$ $$\sim (\text{const}) \cdot \lambda_+^N$$

then $$\log Z = N \log \lambda_+ + O(1)$$

using $$e^{-\beta F} = \log Z \qquad F = -TN \log(e^{\beta J} + 1)$$

c.) $$\langle R_n \rangle = v_L^T \, T^n \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} T^{N-1-n} v_R / Z$$

$\uparrow$ [projection onto $s_i = R$]*

both $T^n$ and $T^{N-n}$ are dominated by $v_+$

$$\cong v_+^T \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} v_+ = \frac{1}{2}(1\,1)\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2}$$

so $\langle R_n \rangle = \frac{1}{2}$ as expected

d.) $$\langle R_n R_{n+m} \rangle = v_L^T T^n \underline{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}} T^m \underline{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}} T^{N-1-n-m} v_R / Z$$

$$\cong v_+^T \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} T^m \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} v_+$$

$$= \frac{1}{2}(1,1)\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\left[ v_+ \lambda_+^m v_+^T + v_- \lambda_-^m v_-^T \right]\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} / \lambda_+^m$$

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* Note: it is not right to put $R_n = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and blindly copy the lecture notes.

so

$$\langle R_n R_{n+m} \rangle = \frac{1}{4} \left( 1 + 1 \cdot \left( \frac{\lambda_-}{\lambda_+} \right)^m \right)$$

$$= \frac{1}{4} \left( 1 + \left( \frac{\omega - 1}{\omega + 1} \right)^m \right)$$

or

$$\langle R_n R_{n+m} \rangle = \frac{1}{4} \left[ 1 + \left( \tanh \frac{\beta J}{2} \right)^m \right]$$

$$\longrightarrow \underline{\frac{1}{4} = \left( \frac{1}{2} \right)^2} \text{ as } m \to \infty$$

✓

e.) For $\omega \gg 1$ or $\beta \to \infty$

$$\frac{\omega - 1}{\omega + 1} \simeq 1 - \frac{2}{\omega} = 1 - 2 e^{-\beta J}$$

$$\left( \frac{\omega - 1}{\omega + 1} \right)^m = \exp \left[ - 2 m e^{-\beta J} \right]$$

so the correlation length is $\xi = \left( \frac{1}{2} e^{+\beta J} \right)$

From at R, the probability that the next link is an $T_L$ is

$$\frac{1}{\omega} = e^{-\beta J}$$

This makes sense, I think,

$M = e^{\beta J}$ to see an $T_L$

$M' = \frac{1}{2} e^{\beta J}$ to destroy the correlation, on the average.

f.) If we modify the partition function to

$$Z = \sum_{s_i} e^{\beta J \sum_i \delta(s_i, s_{i+1})} e^{\sum_i \phi s_i \tau}$$

then

$$\frac{\partial}{\partial \tau} \log Z = \frac{\sum_{s_i} e^{\beta J \sum_i \delta(s_i s_{i+1})} e^{\sum_i \phi \tau s_i}}{Z} \cdot \sum_i \phi_i s_i$$

$$= \langle \sum_i \phi_i s_i \rangle$$

This counts $+\phi$ for a R $-\phi$ for a L, so it gives the total twist $\Phi$

$$\langle \Phi \rangle = \frac{\partial}{\partial \tau} \log Z$$

This corresponds to modifying the transfer matrix by

$$T \rightarrow \begin{pmatrix} \omega & 1 \\ 1 & \omega \end{pmatrix} \begin{pmatrix} e^{\phi\tau} & \\ & e^{-\phi\tau} \end{pmatrix}$$

$$\text{or} \quad \begin{pmatrix} e^{\phi\tau/2} & \\ & e^{-\phi/2} \end{pmatrix} \begin{pmatrix} \omega & 1 \\ 1 & \omega \end{pmatrix} \begin{pmatrix} e^{\phi\tau/2} & \\ & e^{-\phi\tau/2} \end{pmatrix}$$

g) The torque should satisfy $\frac{\partial E}{\partial \Phi} = \mathbb{T}$

or, with an appropriate Gibbs free energy depend on $\Phi$

$$\frac{\partial G}{\partial \Phi} = \mathbb{T}$$

What we have is $\frac{\partial}{\partial \tau} \log Z = \Phi$ or $\frac{\partial}{\partial \tau} F = -T \cdot \Phi$

this would work better if we wrote $\tau = \beta \mathbb{T}$

then $\frac{\partial F}{\partial \mathbb{T}} = -\Phi$

$$G = F + \Phi \mathbb{T} \Rightarrow \frac{\partial G}{\partial \Phi} = + \mathbb{T}$$

This is just like the relation between $M = \sum s_i$ and $h$ in a magnetic system.

Again $\tau = \beta \mathbb{T}$

Now, what is should have asked you to compute was.

$$\left. \frac{\partial \Phi}{\partial \mathbb{T}} \right|_{\mathbb{T}=0}$$

To compute this, compute the free energy at finite $\mathbb{T}$:

$$F = -\frac{1}{\beta} N \log \tilde{\lambda}_+$$

where $\tilde{\lambda}_+$ is the larger eigenvalue of

$$T' = \begin{pmatrix} e^{\beta\phi\mathbb{I}/2} & 0 \\ 0 & e^{-\beta\phi\mathbb{I}/2} \end{pmatrix} \begin{pmatrix} \omega & 1 \\ 1 & \omega \end{pmatrix} \begin{pmatrix} e^{\beta\phi\mathbb{I}/2} & 0 \\ 0 & e^{-\beta\phi\mathbb{I}/2} \end{pmatrix}$$

$$= \begin{pmatrix} \omega e^{\beta\phi\mathbb{I}} & 1 \\ 1 & \omega e^{-\beta\phi\mathbb{I}} \end{pmatrix}$$

The eigenvalues of $T$ satisfy

$$\det \begin{pmatrix} \omega e^{\beta\phi\mathbb{I}} - \tilde{\lambda} & 1 \\ 1 & \omega e^{-\beta\phi\mathbb{I}} - \tilde{\lambda} \end{pmatrix} = 0$$

$$(\tilde{\lambda} - \omega e^{\beta\phi\mathbb{I}})(\tilde{\lambda} - \omega e^{-\beta\phi\mathbb{I}}) - 1 = 0$$

$$\tilde{\lambda}^2 - \tilde{\lambda}\omega\, 2\cosh\beta\phi\mathbb{I} + \omega^2 - 1 = 0$$

$$\tilde{\lambda} = \omega\cosh\beta\phi\mathbb{I} \pm \left[\omega^2\cosh^2\beta\phi\mathbb{I} - (\omega^2 - 1)\right]^{1/2}$$

$$= \omega\cosh\beta\phi\mathbb{I} \pm \left[\omega^2\sinh^2\beta\phi\mathbb{I} + 1\right]^{1/2}$$

for $\mathbb{I} = 0$ $\quad \lambda = \omega \pm 1$ $\quad$ which is what we found on p.1

$$\tilde{\lambda}_+ = \omega\cosh\beta\phi\mathbb{I} + \left[\omega^2\sinh^2\beta\phi\mathbb{I} + 1\right]^{1/2}$$

$$F = -\frac{1}{\beta} N \log\left[\omega \cosh\beta\phi\mathbb{T} + \left[\omega^2 \sinh^2\beta\phi\mathbb{T} + 1\right]^{\frac{1}{2}}\right]$$

$$-\frac{\partial F}{\partial \mathbb{T}} = \Phi = N\phi \cdot \frac{\omega \sinh\beta\phi\mathbb{T} + \dfrac{\omega^2 \sinh\beta\phi\mathbb{T}\cosh\beta\phi\mathbb{T}}{\left[1+\omega^2\sinh^2\beta\phi\mathbb{T}\right]^{\frac{1}{2}}}}{\left(\omega\cosh\beta\phi\mathbb{T} + \left[1+\omega^2\sinh^2\beta\phi\mathbb{T}\right]^{\frac{1}{2}}\right)}$$

expand to first order in $\mathbb{T}$

$$= N\phi \cdot \frac{\omega\beta\phi\mathbb{T} + \omega^2\beta\phi\mathbb{T} + O(\mathbb{T}^3)}{\omega + 1 \quad + O(T^2)}$$

$$= N\phi \ \omega\beta\phi\mathbb{T} \ \frac{1+\omega}{1+\omega} + O(\mathbb{T}^3)$$

$$= N\phi^2\beta\omega\mathbb{T} + \cdots$$

so $$\left.\frac{\partial\Phi}{\partial\mathbb{T}}\right|_{T=0} = +\frac{N}{\beta}\phi^2 e^{\beta J} \qquad \underbrace{\left.\frac{\partial\Phi}{\partial\tau}\right|_{\mathbb{T}=0}}_{\text{a less meaningful quantity}} = N\phi^2\omega$$

h.) First, in the formalism from p. 5

$$dF = -S\,dT - \Phi\,d\mathbb{T}$$

$$dE = T\,dS - \Phi\,d\mathbb{T}$$

Then

$$\frac{\partial^2 E}{\partial S\,\partial \Pi} = \left(\frac{\partial T}{\partial \Pi}\right)\Big|_S = -\left(\frac{\partial \Phi}{\partial S}\right)\Big|_\Pi$$

now $\left(\frac{\partial S}{\partial \Phi}\right)\Big|_\Pi$ should be $< 0$ ; the larger the twist, the more predominant R is over L, the lower the entropy. Then

$$\left(\frac{\partial T}{\partial \Pi}\right)_S > 0$$

This is reasonable; we do work on the chain by torquing it, adding energy. This should be reflected in a temperature rise.

2.) a.) $H\psi_n = -\frac{\hbar^2}{2ma^2}\left[(\psi_{n+1}-\psi_n) - (\psi_n - \psi_{n-1})\right]$

$\psi_n = A e^{ikna}$

$H\psi_n = -\frac{\hbar^2}{2ma^2}\left(e^{ika} - 2 + e^{-ika}\right) \cdot A e^{ikna}$

$= \frac{\hbar^2}{ma^2}\left(1 - \cos ka\right) \cdot A e^{ika}$

the energies are then

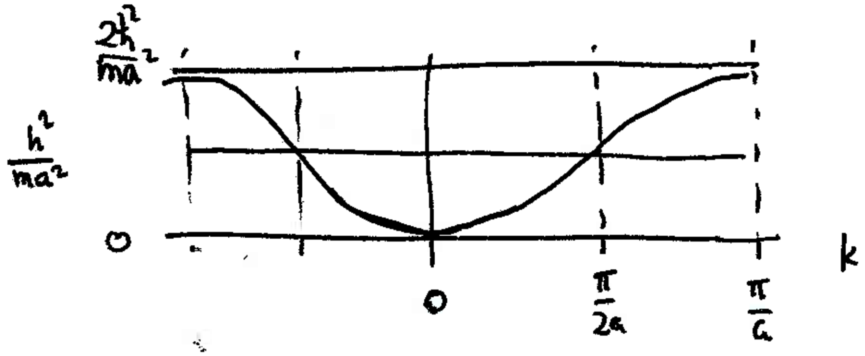
$$E(k) = \frac{\hbar^2}{ma^2}(1-\cos ka)$$

as. $E(k) \sim \frac{\hbar^2 k^2}{2m}$ as $k \to 0$

in a finite volume w. periodic b.c. $k_n = \frac{2\pi n}{L}$

but we can just write $g\sum_{k_n} = g\frac{L}{2\pi}\int dk$

Since these are electrons, $g = 2$ for spin ½.



b.) For the distorted chain,

using the ansatz $\psi = \begin{cases} A e^{ik2ma} & n = 2m \\ B e^{ik(2m+1)a} & n = 2m+1 \end{cases}$

$$H\psi_{2m} = -\frac{\hbar^2}{2ma^2}\left((1+\alpha)(Be^{ika} - A) - (1-\alpha)(A - Be^{-ika})\right)e^{ik2ma}$$

$$H\psi_{2m+1} = -\frac{\hbar^2}{2ma^2}\left((1\,\text{[illegible]}\,\alpha)(Ae^{ika} - B) - (1+\alpha)(B - Ae^{-ika})\right)e^{ik(2m+1)a}$$

so for an eigenstate we require:

$$\mathcal{E}\cdot\begin{pmatrix} A \\ B \end{pmatrix} = \frac{\hbar^2}{2ma^2}\begin{pmatrix} 2A - 2B\cos ka - 2i\alpha B\sin ka \\ 2B - 2A\cos ka + 2i\alpha A\sin ka \end{pmatrix}$$

or

$$\mathcal{E}\begin{pmatrix} A \\ B \end{pmatrix} = \frac{\hbar^2}{2ma^2}\cdot 2\cdot\begin{pmatrix} 1 & (-\cos ka + i\alpha\sin ka) \\ -(\cos ka - i\alpha\sin ka) & 1 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$$

the eigenvalues of this matrix are given by

$$(\lambda - 1)^2 - (\cos ka + i\alpha\sin ka)(\cos ka - i\alpha\sin ka) = 0$$

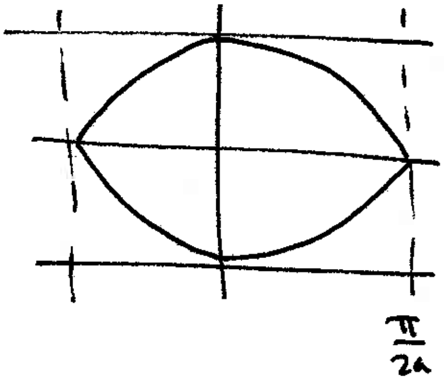
$$(\lambda - 1)^2 - (\cos^2 ka + \alpha^2\sin^2 ka) = 0$$

$$\lambda = 1 \pm \left[\cos^2 ka + \alpha^2\sin^2 ka\right]^{\frac{1}{2}}$$

For $\alpha \to 0$ this is

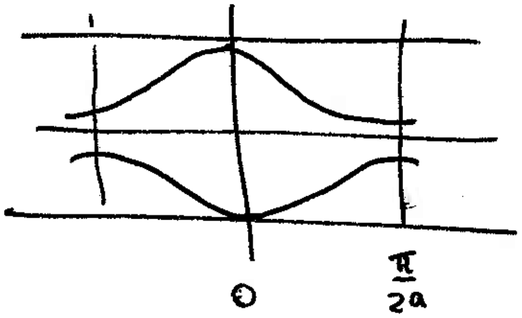
$$\mathcal{E}(k) = \left(\frac{\hbar^2}{ma^2}\right)(1 \pm \cos ka)$$

agrees w. p.9



← this piece was $\frac{\pi}{2a} < |k| < \frac{\pi}{a}$ in the previous problem

For $\alpha \neq 0$



$$\mathcal{E}(k) = \frac{\hbar^2}{ma^2}(1 \pm \alpha^2)$$

at $k = \frac{\pi}{2a}$

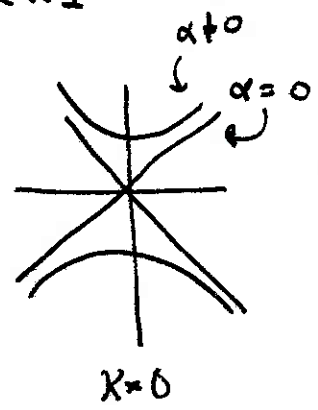
write $\kappa = k - \pi/2a$

$$\sin^2 ka = \cos^2 \kappa a \qquad \cos^2 ka = \sin^2 \kappa a$$

then

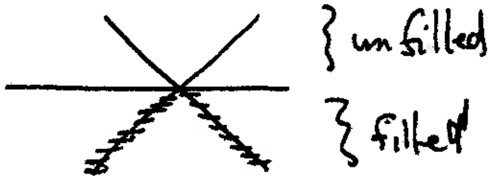
$$\partial = 1 \pm [(\kappa a)^2 + \alpha^2]^{\frac{1}{2}} \qquad \kappa a \ll 1$$

$$\mathcal{E}(\kappa) = \frac{\hbar^2}{ma^2}\left(1 \pm [\alpha^2 + (\kappa a)^2]^{\frac{1}{2}}\right)$$



c.) In the undistorted lattice $k = \pi/2a$ corresponds to $E(k) = \frac{\hbar^2}{ma^2}$

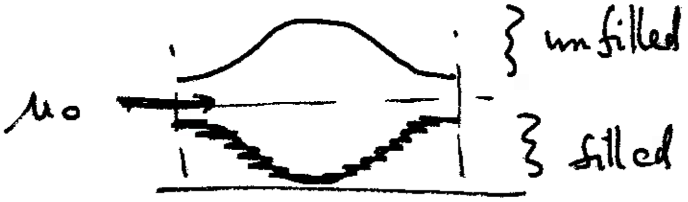
filling up to this level gives $\mu_0 = \frac{\hbar^2}{ma^2}$ at $T=0$



Half of the k states are filled, with g=2, so the density of electrons is

$$n = 1 / \text{lattice site} = 1/a$$

Similarly, in the distorted lattice with $\mu = \mu_0$ and $T=0$



so $n = 1/a$

The energy difference between the two states is

$$\Delta E = g \frac{L}{2\pi} \int_{-\pi/2a}^{\pi/2a} dk \; \left[ E(k,\alpha) - E(k, \alpha=0) \right]$$

since $E(k,\alpha) - E(k,\alpha=0)$ is large only near $k = \pi/2a$, it is natural to shift the integral to one about $K=0$. The functions $E(k,\alpha)$ are symmetrical so

$$\Delta E = g\frac{L}{2\pi}\cdot 2\int_0^{\pi/2a} dK\,\left[E(K,\alpha) - E(K,\alpha=0)\right]$$

$$\cong \frac{gL}{\pi}\int_0^{\pi/2a} dK\,\left[-\left[(Ka)^2+\alpha^2\right]^{1/2} + |Ka|\right]\cdot\frac{\hbar^2}{ma^2}$$

$\rho = Ka$
$$= -\frac{gL}{\pi a}\cdot\frac{\hbar^2}{ma^2}\int_0^{\pi/2} d\rho\,\left[\left[\alpha^2+\rho^2\right]^{1/2} - |\rho|\right]$$

Now, let $c$ be a number of order 1:

$$\int_0^c d\rho\ \rho = \frac{1}{2}c^2$$

$$\int_0^c d\rho\ \left[\rho^2+\alpha^2\right]^{1/2} = \frac{1}{2}\left[\rho\left[\rho^2+\alpha^2\right]^{1/2} + \alpha^2\log\left(\rho + \left[\rho^2+\alpha^2\right]^{1/2}\right)\right]\Big|_0^c$$

$$= \frac{1}{2}\left[c^2\left(1+\frac{\alpha^2}{c^2}\right)^{1/2} + \alpha^2\log\left(\frac{c+(c^2+\alpha^2)^{1/2}}{\alpha}\right)\right]$$

$$= \frac{1}{2}c^2 + \frac{1}{4}\alpha^2 + \frac{1}{2}\alpha^2\log\frac{2c}{\alpha} + \cdots$$

so

$$\int_0^c d\rho\,\left[\left[\alpha^2+\rho^2\right]^{1/2} - \rho\right] = \underbrace{\frac{1}{2}\alpha^2\log\frac{1}{\alpha}} + \alpha^2\cdot(\text{finite}) + \cdots$$

for the purpose of the exam, keep just this leading term.

$$\Delta E(\alpha) = -\frac{\hbar^2}{ma^2}\cdot\frac{L}{\pi a}\,\alpha^2\log\frac{1}{|\alpha|} \qquad \text{with } g=2$$

d.) Now add the lattice energy: $N = \frac{L}{a}$

$$E_{tot} = E_\ell(\alpha) + \Delta E(\alpha) = N\left\{\tfrac{1}{2}A\alpha^2 + \tfrac{1}{4}B\alpha^4 - \frac{\hbar^2}{ma^2}\frac{1}{\pi}\alpha^2\log\frac{1}{\alpha}\right\}$$

look for a minimum:

$$\frac{\partial}{\partial\alpha}E_{tot} = N\left[A\alpha + B\alpha^3 - \frac{2\hbar^2}{ma^2}\frac{1}{\pi}\alpha\left(\log\frac{1}{\alpha}\ \text{[illegible]}\ 1\right)\right]$$

small $\alpha$

$$= N\alpha\left(A - \frac{2}{\pi}\frac{\hbar^2}{ma^2}\log\frac{1}{|\alpha|}\right)$$

so there is always a solution at small $\alpha$

$$|\alpha| = \exp\left[-\frac{A}{\left(\frac{2}{\pi}\hbar^2/ma^2\right)}\right]$$

since $\alpha^2\log\frac{1}{\alpha}$ always grows very slightly faster than $\alpha^2$ close to $\alpha = 0$. $\alpha$ at the minimum can be <u>positive</u> or <u>negative</u>. ($\alpha \leftrightarrow -\alpha$ symmetry)

This instability of a 1-dimensional electron lattice near half-filling is called the <u>Peierls instability</u>.

e.) Go back to the integral on p.13. When $D \gg \alpha$

$$\int_D^C d\rho \left( [\rho^2 + \alpha^2]^{1/2} - \rho \right) = \int_D^C d\rho \, \frac{\alpha^2}{2\rho} = \frac{\alpha^2}{2} \log \frac{C}{D}$$

then

$$\Delta E(\alpha) = - N \frac{1}{\pi} \frac{\hbar^2}{2ma^2} \alpha^2 \log \frac{\pi/2}{D}$$

if the Fermi level corresponds to filling to $ka = D$

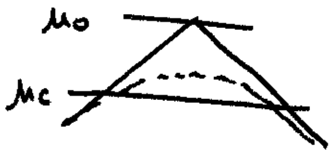
when

$$- N \cdot \frac{2}{\pi} \frac{\hbar^2}{2ma^2} \log \frac{\pi/2}{D} + N A = 0$$

there is a well-defined coefficient of $\alpha^2$ in $E_{tot}(\alpha)$ that becomes positive, and the instability goes away.

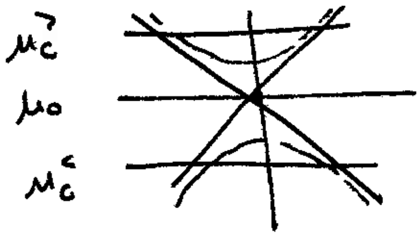
An estimate of D derived from this equation is

$$K_c a \cong \exp\left[ - \frac{A}{\frac{2}{\pi} \hbar^2 / 2ma^2} \right]$$

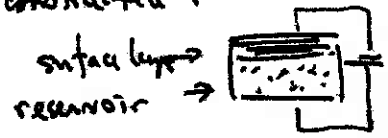


$$\mu_c = \frac{\hbar^2}{ma^2} \left( 1 - (K_c a) \right)$$

Similarly, when $\mu$ goes above $\mu_0$ there is another $\mu_c'$ where the raising of the upper set of electron states as a function of $\alpha$ balances the lowering of the lower set



f.) A real material must be locally electrically neutral, so to vary $\mu$, we must find a place to put the extra electrons. In a semiconductor, we can do this by doping or by varying the relative amounts of different transition metals in the material. Or, constructed a layered material & change the bias voltage:



g.) In an electron gas at low temperature, we expect

$$C_V \sim T^1$$

In a material with an energy gap of size $2\alpha$,

$$C_V \sim e^{-2\alpha/T} \quad \text{(dominated by } T^3 \text{ from phonons)}$$

so $$C_V \sim e^{-2\alpha/T} \text{ for } \mu_0-\alpha < \mu < \mu_0+\alpha$$

and $$C_V \sim T \text{ otherwise}$$

near $T_c$ there will be soft modes corresponding to thermal fluctuations of $\alpha$; however, these will give contributions to $C_v \sim T^3$, and those will be dominated by the electron contribution

h) When $T \gg 2\alpha \frac{\hbar^2}{ma^2}$, electrons will populate the upper and lower states and wash out the advantage of the distortion. So we expect a phase diagram