FINAL EXAM

Physics 140A– WINTER 2012

Instructions: Do your best.

Constants/Conversion factors:
Bolzmann's constant $k_{\mathrm{B}} = 1.38 \times 10^{-23}$ J/°K $= 1.38 \times 10^{-16}$ erg /°K
Planck's constant $\hbar = 1.055 \times 10^{-27}$ erg-sec
1 fortnight = 14 days
3.017 grams of He^3 contain N_A atoms
Avogadro's number $N_A = 6.022 \times 10^{23}$
1 furlong = 1/8 mile = 220 yards = 660 feet = 40 rods = 10 chains

[1.] The primitive lattice vectors of a hexagonal lattice are

$$\vec{a}_1 = \frac{\sqrt{3}a}{2}\,\hat{x} + \frac{a}{2}\hat{y} \qquad \vec{a}_2 = -\frac{\sqrt{3}a}{2}\,\hat{x} + \frac{a}{2}\hat{y} \qquad \vec{a}_3 = c\,\hat{z} \quad .$$

(a) What is the volume of the unit cell V_c?
(b) Compute the reciprocal lattice vectors $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$.
(c) Describe and sketch the first Brillouin zone.

[2.] Consider a three dimensional gas of N free electrons at $T = 0$.
(a) What is the Fermi wave vector k_{F} and how is it related to the (number) density $\rho = N/V$?
(b) What is the Fermi Energy? What is its significance?
(c) Show that the kinetic energy is $U_0 = \frac{3}{5}NE_{\mathrm{F}}$
(d) The atom He^3 has spin $\frac{1}{2}$ and is a fermion. The (mass) density of liquid He^3 is 0.081 g cm^{-3} near absolute zero. Calculate E_{F} and T_{F}.

[3.] Fermion creation operators $c_l^\dagger$ and $c_j^\dagger$ obey the anticommutation relation $\{c_l^\dagger, c_j^\dagger\} = 0$. What physical principles are embodied in this mathematics? Explain.

[4.] In class we modeled a vibrating lattice of atomic nucleii as a one dimensional coupled mass (M) - spring (K) system. We showed this has normal mode frequencies ω which depend on momentum q as

$$\omega^2(q) = \frac{2K}{M}\left(1 - \cos q\right)$$

(a) Given this equation, explain why we call the lattice vibrations "phonons".
(b) Describe qualitatively (sketch) what happens to $\omega(q)$ if there are two types of masses M_1 and M_2 which alternate. Provide some names to the resulting types of phonons.

[5.] Consider a set of isolated Hydrogen nucleii (protons). The energy levels of an electron are $E_n = -13.6/n^2$ (in eV). Each level n is highly degenerate, since the electron can be placed on any of the nucleii. As the nucleii are brought closer together, what happens to these energy levels, and what do we call the resulting collection of energies?

[6.] A classical system has two energy levels E_1 and E_2.
(a) Sketch the average energy $\langle E \rangle$ as a function of temperature T.
(b) Sketch the specific heat $C = d\langle E \rangle/dT$ as a function of T. In both cases (a) and (b), label your horizontal and vertical axes with appropriate scales.
(c) What are the low T and high T behaviors of $C(T)$? What is it about the nature of the energy levels that makes $C(T)$ behave that way?

[7.] The specific heat of a classical gas of N particles is $\frac{3}{2}k_{\rm B}$ (at all temperatures). A gas of electrons has a much smaller specific heat. In fact, it *vanishes* linearly as temperature $T \to 0$. Provide a qualitative picture for why this happens. What is the essential physical principle which prevents a cloud of fermions from changing its energy as much as a cloud of classical particles when T increases?

[8.] Consider a lattice with two sites and a hopping Hamiltonian.

$$\hat{H} = -t\,(\,c_1^\dagger c_2 + c_2^\dagger c_1\,) + E\,(\,c_1^\dagger c_1 + c_2^\dagger c_2\,)$$

(a) How many states are there with one electron? List them. (Employ the usual occupation number basis from class and HW # 6.)
(b) Compute the action of $\hat{H}$ on each of the vectors. What is the matrix for $\hat{H}$?
(c) Diagonalize $\hat{H}$. What are the eigenenergies?
(d) What happens to these eigenenergies at $t = 0$? Does this problem have any connection to problem #5 of this final exam?

[9.] An x-ray scatters elastically off a crystal. What can you say about possible values of its change in momentum? Using your answer, prove that a Bragg peak can arise only if the incoming wave vector $\vec{k}$ lies on a plane bisecting one of the reciprocal lattice vectors $\vec{G}$. Since these planes are only a two dimensional subset of a three dimensional space, the chance of $\vec{k}$ satisfying this condition is incredibly small. How do experimentalists solve this problem?

[10.] The "power method" is a numerical technique to find the eigenvector of a matrix which has the largest eigenvalue. What do you do to implement it? Why does it work?

[11.] The operator $\hat{h} = c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l$ hops an electron between two sites l and $l+1$.
(a) Show that $[\hat{h}, n_l] \neq 0$. Here $n_l = c_l^\dagger c_l$ is the number operator on site l.
(b) Show that $[\hat{h}, n_l + n_{l+1}] = 0$.
(c) Explain physically whether you would expect the operator $\hat{\Delta} = c_l^\dagger c_{l+1}^\dagger$ which creates *two* fermions (one on site l and one on site $l+1$) to commute with $n_l + n_{l+1}$. (You can work out the commutator mathematically, but a correct intuitive reason will suffice.)

1.

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$\boxed{1}$ a) $V_c = \left| \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right|$

$$\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}}{2}a & \frac{1}{2}a & 0 \\ 0 & 0 & c \end{vmatrix} = \hat{x}\,\frac{1}{2}ac + \hat{y}\,\frac{\sqrt{3}}{2}ac$$

$$V_c = \left| \left(\frac{\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}\right)\cdot\left(\frac{1}{2}ac\hat{x} + \frac{\sqrt{3}}{2}ac\hat{y}\right) \right|$$

$$= \sqrt{3}/4\, a^2c + \sqrt{3}/4\, a^2 c = \sqrt{3}/2\, a^2 c$$

b) $$\vec{b}_1 = \frac{2\pi}{V_c}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\left(\frac{1}{2}ac\hat{x} + \frac{\sqrt{3}}{2}ac\hat{y}\right)$$

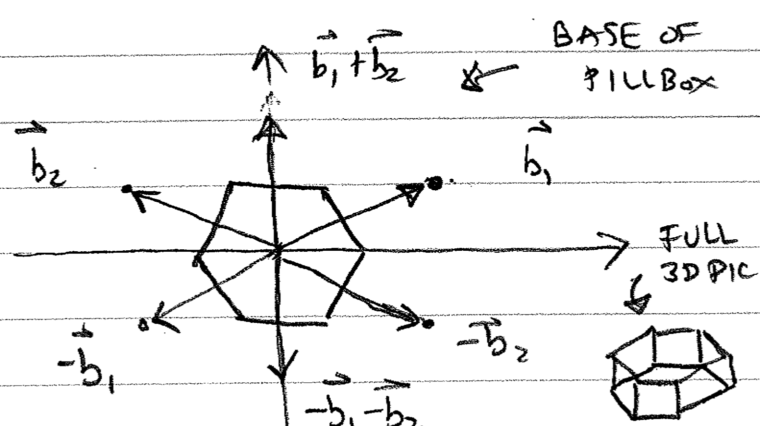
$$= \frac{2\pi}{\sqrt{3}}\frac{1}{a}\hat{x} + 2\pi\frac{1}{a}\hat{y}$$

$$\vec{b}_2 = \frac{2\pi}{V_c}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\left(-\frac{1}{2}ac\hat{x} + \frac{\sqrt{3}}{2}ac\hat{y}\right)$$

$$= -\frac{2\pi}{\sqrt{3}}\frac{1}{a}\hat{x} + 2\pi\frac{1}{a}\hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{V_c}(\vec{a}_1 \times \vec{a}_2) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\left(\frac{\sqrt{3}}{2}a^2\hat{z}\right) = \frac{2\pi}{c}\hat{z}$$

c) The first BZ is a hexagonal pill box: Draw the vectors $n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$ and their bisecting planes to see this.



$\boxed{2.}$ a) The "volume" associated with each $\vec{k}$ point is $\frac{(2\pi)^3}{V}$ (see class discussion or kittel)

$$\therefore \quad N = 2 \frac{1}{(2\pi)^3/V} \frac{4}{3}\pi k_F^3 = \frac{V}{3\pi^2} k_F^3$$

$\#e^- = 2(\# k \text{ points})$

spin

Volume of Indiv k point

volume of sphere radius k_F

$$\therefore \quad k_F^3 = 3\pi^2 N/V \qquad k_F = (3\pi^2 \rho)^{1/3}$$

b) $E_F = \hbar^2 k_F^2/2m$ = maximum Energy level occupied by e^- at $T=0$

c) $$u_0 = 2 \frac{1}{(2\pi)^3/V} \int_0^{k_F} \frac{\hbar^2 k^2}{2m} 4\pi k^2 \, dk$$

$$= \frac{V}{\pi^2} \frac{\hbar^2}{2m} \frac{k_F^5}{5} = \frac{V}{\pi^2} \underbrace{3\pi^2 \frac{N}{V}}_{k_F^3} \underbrace{\frac{\hbar^2 k_F^2}{2m}}_{E_F} \frac{1}{5} = \frac{3}{5} N E_F$$

d) Convert mass density to # density:

$$\underbrace{.081 \frac{g}{cm^3}}_{\text{mass density}} \cdot \frac{6 \cdot 10^{23} \text{ atoms}}{3g} = .162 \cdot 10^{23} \frac{\text{atoms}}{cm^3}$$

$\boxed{2}$ (cont'd) $\quad k_F = (3\pi^2 \rho)^{1/3} = \left(3\pi^2 (.162\cdot 10^{23})\right)^{1/3} = .78 \cdot 10^{8} \frac{1}{cm}$

$$E_F = \left(\frac{\hbar^2 k_F^2}{2m}\right) = \left[\frac{(1.055\cdot 10^{-27}\cdot .78\cdot 10^{8})^2}{2\,(3.017/6\cdot 10^{23})}\right] = \frac{(1.055)^2(.78)^2}{6.034/6}\cdot 10^{-15}$$

$$= 6.8\cdot 10^{-16} \text{ erg}$$

$$T_F = E_F/k_B = 6.8\cdot 10^{-16}/1.38\cdot 10^{-16} = 4.9\,°K$$

$\boxed{3.}$ Choosing $l = j$ $\quad c_l^+ c_l^+ + c_l^+ c_l^+ = 0 \Rightarrow \underbrace{c_l^+ c_l^+ = 0}$

PAULI: cannot put 2 e^- in same state l

Choosing $l \neq j$ $\quad c_l^+ c_j^+ + c_j^+ c_l^+ = 0$

$$c_l^+ c_j^+ = -c_j^+ c_l^+$$

Exchanging $2e^-$ $\Rightarrow$ − sign

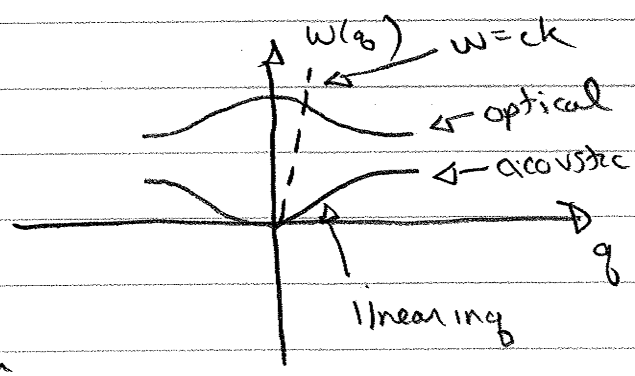
Fermion wavefunction is antisymmetric

$\boxed{4}$ $\cos q \approx 1 - \frac{1}{2} q^2$ so $\omega^2(q) \approx \frac{2K}{M}\frac{1}{2} q^2 \Rightarrow \omega(q) = \sqrt{\frac{K}{m}}\, q$

Energy ~ q like a photon
(E = cp.)

photon $\omega = ck$
$\uparrow$ very large

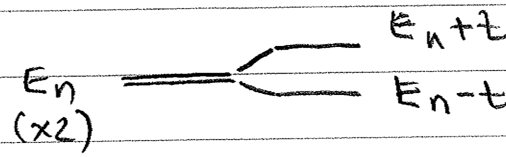
would intersect optical branch
but not acoustic

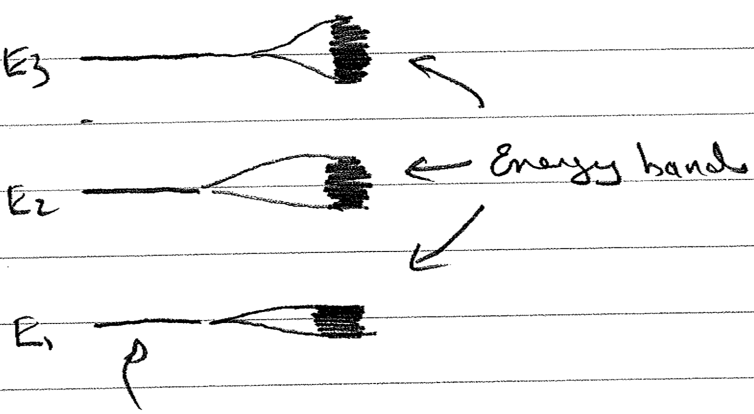


4.

$\boxed{5}$ The energy levels which are highly degenerate broaden into energy "bands". See also problem # 8 :

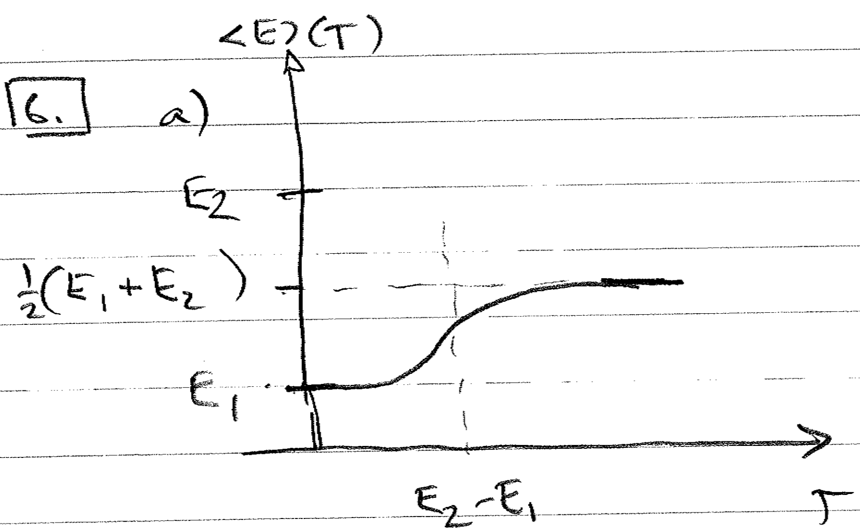
a matrix $\begin{pmatrix} E_n & t \\ t & E_n \end{pmatrix}$ has eigenvalues $E_n \pm t$

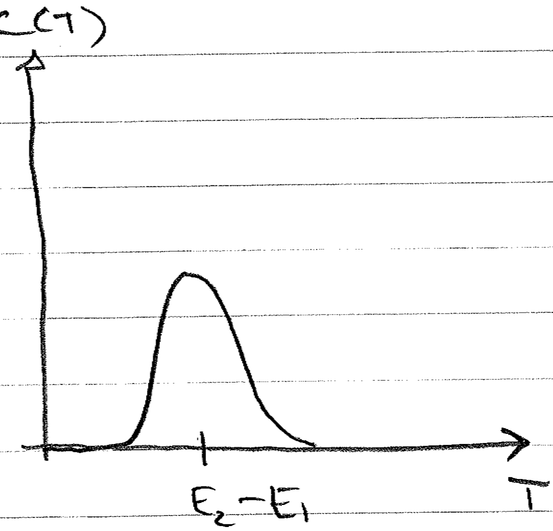




$\sim N_A$ fold degenerate discrete atomic levels

$\boxed{6.}$ a) b)



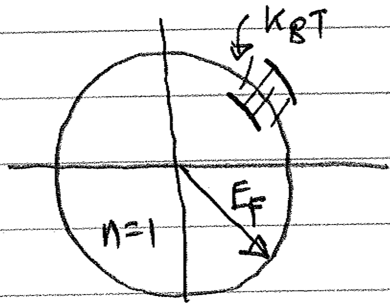


c) $C(T) \to 0$ at high T because there is a maximal energy level.

$C(T) \to 0$ exponentially at low T because there is a gap between ground and first excited states.

5.

[7] Pauli principle prevents two e^- from having same momentum (ignoring spin). Only e^- within k_BT of Fermi surface have empty momentum states in which to move when T increases. (Most) other e^- deep inside Fermi sphere cannot change their momentum.



classical result

$$C \sim N k_B \frac{k_BT}{E_F}$$

Pauli blocking reduction factor

[8] a,b

$$H|10\rangle = E|10\rangle - t|01\rangle$$
$$H|01\rangle = -t|10\rangle + E|01\rangle$$

$$\Rightarrow H = \begin{pmatrix} E & -t \\ -t & E \end{pmatrix}$$

Two states with 1 e^-

c) $(E-\lambda)^2 - t^2 = 0$

$\Rightarrow \lambda = E \pm t$

d) at $t=0$ $\lambda = E$ (degenerate)

When two levels/states "touch" via t their degeneracy is broken. This is a simple way of understanding how N_A degenerate atomic levels $\Rightarrow$ Energy band

$\boxed{9}$ An x ray scattering off a crystal will have its momentum changed by $\hbar\vec{G}$ where $\vec{G} = n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3$ is a reciprocal lattice vector. For elastic scattering $|\vec{k}'| = |\vec{k}|$

$$\vec{k}' = \vec{k} + \vec{G}$$

$$\underbrace{k'^2 = k^2}_{\text{equal if elastic}} + 2\vec{k}\cdot\vec{G} + G^2 \Rightarrow \underbrace{\underbrace{\vec{k}\cdot\hat{G}}_{\text{component of } \vec{k} \text{ along } \hat{G}} = \underbrace{\tfrac{1}{2}|\vec{G}|}_{\frac{1}{2} \text{ length of } \vec{G}}}_{\vec{k} \text{ lies on plane bisecting } \vec{G}}$$

Experimental sol'ns to unlikeliness of satisfying Bragg condition

(1) nonmonochromatic x rays so $|\vec{k}|$ has many values

(2) rotate crystal, increasing the # of $\vec{G}$ values

$\boxed{10}$ Power method: Apply matrix M many times to initial vector to project out $|e_n\rangle$ with largest λ_n. Initial vector cannot be $\perp$ to $|e_{max}\rangle$. May need to normalize during iteration to prevent overflow.

Why it works:

$$M^p |v\rangle = M^p \sum_n \alpha_n |e_n\rangle = \sum \alpha_n \lambda_n^p |e_n\rangle$$

$$= (\lambda_{max})^p \sum_n \alpha_n \left(\frac{\lambda_n}{\lambda_{max}}\right)^p |e_n\rangle$$

$\rightarrow \phi \; \forall n$ except max

11 a) $c_\ell^\dagger c_{\ell+1} c_\ell^\dagger c_\ell = -c_\ell^\dagger c_\ell^\dagger c_{\ell+1} c_\ell = 0$

$c_\ell^\dagger c_\ell c_\ell^\dagger c_{\ell+1} = c_\ell^\dagger (1 - c_\ell^\dagger c_\ell) c_{\ell+1} = c_\ell^\dagger c_{\ell+1}$

$\therefore \quad [c_\ell^\dagger c_{\ell+1}, c_\ell^\dagger c_\ell] = -c_\ell^\dagger c_{\ell+1}$

Likewise $c_{\ell+1}^\dagger c_\ell c_\ell^\dagger c_\ell = c_{\ell+1}^\dagger (1 - c_\ell^\dagger c_\ell) c_\ell = c_{\ell+1}^\dagger c_\ell$

$c_\ell^\dagger c_\ell c_{\ell+1}^\dagger c_\ell = -c_\ell c_{\ell+1}^\dagger c_\ell c_\ell = \phi$

So $[\hat{h}, n_\ell] = \underbrace{c_{\ell+1}^\dagger c_\ell - c_\ell^\dagger c_{\ell+1}}_{\text{like a "current operator" !}}$

b) $c_\ell^\dagger c_{\ell+1} c_{\ell+1}^\dagger c_{\ell+1} = c_\ell^\dagger (1 - c_{\ell+1}^\dagger c_{\ell+1}) c_{\ell+1} = c_\ell^\dagger c_{\ell+1}$

$c_{\ell+1}^\dagger c_{\ell+1} c_\ell^\dagger c_{\ell+1} = \phi$

$c_{\ell+1}^\dagger c_\ell c_{\ell+1}^\dagger c_{\ell+1} = \phi$

$c_{\ell+1}^\dagger c_{\ell+1} c_{\ell+1}^\dagger c_\ell = c_{\ell+1}^\dagger c_\ell$

$[\hat{h}, n_{\ell+1}] = c_\ell^\dagger c_{\ell+1} - c_{\ell+1}^\dagger c_\ell = -[\hat{h}, n_\ell]$

So $[\hat{h}, n_\ell + n_{\ell+1}] = \phi$.

$\boxed{11}$ cont'd Since $\hat{\Delta} = c_\ell^\dagger c_{\ell+1}^\dagger$ creates 2 electrons

we would not expect it to commute with $n_\ell + n_{\ell+1}$.

We can compute it if we like:

$$c_\ell^\dagger c_{\ell+1}^\dagger c_\ell^\dagger c_\ell = -c_\ell^\dagger c_\ell^\dagger c_{\ell+1}^\dagger c_\ell = \emptyset$$

$$c_\ell^\dagger c_\ell c_\ell^\dagger c_{\ell+1}^\dagger = c_\ell^\dagger (1 - c_\ell^\dagger c_\ell) c_{\ell+1}^\dagger = c_\ell^\dagger c_{\ell+1}^\dagger$$

$$\therefore \quad [\hat{\Delta}, n_\ell] = -c_\ell^\dagger c_{\ell+1}^\dagger$$

$$c_\ell^\dagger c_{\ell+1}^\dagger c_{\ell+1}^\dagger c_{\ell+1} = \emptyset$$

$$c_{\ell+1}^\dagger c_{\ell+1} c_\ell^\dagger c_{\ell+1}^\dagger = -c_{\ell+1}^\dagger c_{\ell+1} c_{\ell+1}^\dagger c_\ell^\dagger$$

$$= -c_{\ell+1}^\dagger (1 - c_{\ell+1}^\dagger c_{\ell+1}) c_\ell^\dagger = -c_{\ell+1}^\dagger c_\ell^\dagger = +c_\ell^\dagger c_{\ell+1}^\dagger$$

$$\therefore \quad [\hat{\Delta}, n_{\ell+1}] = -c_\ell^\dagger c_{\ell+1}^\dagger$$

$$\therefore \quad [\hat{\Delta}, n_\ell + n_{\ell+1}] \neq \emptyset$$

Another way:

$$c_\ell^\dagger c_{\ell+1}^\dagger |00\rangle = |11\rangle$$

$$\left.\begin{array}{l} (n_\ell + n_{\ell+1}) c_\ell^\dagger c_{\ell+1}^\dagger |00\rangle = 2|11\rangle \\ c_\ell^\dagger c_{\ell+1}^\dagger (n_\ell + n_{\ell+1}) |00\rangle = \emptyset \end{array}\right\} \text{so do not commute}$$