FINAL EXAM
Physics 140A—WINTER 2012

Instructions: Do your best.

Constants/Conversion factors:
Boltzmann’s constant \( k_B = 1.38 \times 10^{-23} \) J/°K = 1.38 x 10^{-16} erg /°K
Planck’s constant \( \hbar = 1.055 \times 10^{-27} \) erg-sec
1 fortnight = 14 days
3.017 grams of He³ 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

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

(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 \( U_0 = \frac{3}{8} N E_F \)
(d) The atom He³ has spin \( \frac{1}{2} \) and is a fermion. The (mass) density of liquid He³ is 0.081 g cm\(^{-3}\) near absolute zero. Calculate \( E_F \) and \( T_F \).

[3.] Fermion creation operators \( c^\dagger \) and \( c_j^\dagger \) obey the anticommutation relation \( \{ c^\dagger_j, c^\dagger_k \} = 0 \). 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 \( \omega \) 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 nuclei. 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 $\frac{3}{2} k_B$ (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. a) \[ \mathbf{V}_c = \frac{\mathbf{q}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}{\sqrt{a^2 + \frac{\sqrt{3}}{2} ac}} \]

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

\[ \mathbf{V}_c = \left| \left( \frac{\sqrt{3}}{2} a \hat{x} + \frac{1}{2} a \hat{y} \right) \cdot \left( \frac{1}{2} ac \hat{x} + \frac{\sqrt{3}}{2} ac \hat{y} \right) \right| \]

\[ = \sqrt{3/4} a^2 c + \sqrt{3/4} a^2 c = \sqrt{3/2} a^2 c \]

b) \[ \mathbf{b}_1 = \frac{2\pi}{\mathbf{V}_c} \left( \mathbf{a}_2 \times \mathbf{a}_3 \right) = \frac{2\pi}{\sqrt{3} a^2 c} \left( \frac{1}{2} ac \hat{x} + \frac{\sqrt{3}}{2} ac \hat{y} \right) \]

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

\[ \mathbf{b}_2 = \frac{2\pi}{\mathbf{V}_c} \left( \mathbf{a}_3 \times \mathbf{a}_1 \right) = \frac{2\pi}{\sqrt{3} a^2 c} \left( -\frac{1}{2} ac \hat{x} + \frac{\sqrt{3}}{2} ac \hat{y} \right) \]

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

\[ \mathbf{b}_3 = \frac{2\pi}{\mathbf{V}_c} \left( \mathbf{a}_1 \times \mathbf{a}_2 \right) = \frac{2\pi}{\sqrt{3} a^2 c} \left( \frac{\sqrt{3}}{2} a \hat{z} \right) = \frac{2\pi}{a} \hat{z} \]

c) The first Bz is a hexagonal pill box. Draw the vectors \( n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3 \) and their bisecting planes to see two.
2. a) The "volume" associated with each \( k \) point is \( \frac{(2\pi)^3}{V} \) (see class discussion or Kittel).

\[
N = 2 \frac{1}{(2\pi)^3/V} \frac{1}{3} \pi k_F^3 = \frac{V}{3\pi^2} k_F^3
\]

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

Volume of sphere radius \( k_F \)

Volume of indiv \( k \) point

\[
k_F^3 = 3\pi^2 N/V
\]

\[
k_F = (3\pi^2 N/V)^{1/3}
\]

b) \( E_F = k_F^2 / 2m = \text{maximum energy level occupied by } e^- \text{ at } T = 0 \)

c) \( U_0 = \frac{1}{2} \frac{1}{(2\pi)^3} \int_0^{k_F} \frac{1}{2m} \frac{k^4}{4\pi^2} 4\pi k^2 dk \)

\[
= \frac{V}{\pi^2} \frac{h^2}{2m} \frac{K_F^5}{5} = \frac{V}{\pi^2} \frac{3\pi^2 N}{V} \frac{k_F^2 k_F^2}{2m} \frac{1}{5} = \frac{3}{5} N E_F
\]

\[
k_F^3 = E_F
\]

d) Convert mass density to \# density:

\[
0.081 \text{ g/cm}^3 \cdot \frac{6 \cdot 10^{23} \text{ atoms}}{3 \text{ g}} = 0.162 \cdot 10^{23} \text{ atoms/cm}^3
\]
(2) (cont'd) \[ k_F = \left( \frac{3\pi^2 n}{2} \right)^{1/3} = \left( \frac{3\pi^2 \cdot (1.12 \cdot 10^{-23})}{2} \right)^{1/3} = 0.78 \cdot 10^8 \text{ cm} \]

\[ E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{(1.055 \cdot 10^{-27} \cdot 0.78 \cdot 10^{-8})^2}{2 \cdot (3.017/6 \cdot 10^{23})} = \frac{(1.055 \cdot 778)^2}{6.039/6} \cdot 10^{-15} \]

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

\[ T_F = \frac{E_F}{k_B} = \frac{6.8 \cdot 10^{-16}}{1.38 \cdot 10^{-16}} = 4.9 \text{ K} \]

3. Choosing \( l = 0 \)
\[ \phi_0 \phi_0^* + \phi_e \phi_e^* = 0 \Rightarrow \phi_e \phi_e^* = 0 \]

Pauli:
cannot put \( 2 \) \( e^- \)
in same state \( l \)

Choosing \( l \neq 0 \)
\[ \phi_0 \phi_0^* + \phi_e \phi_e^* = 0 \]

\[ \phi_e \phi_e^* = -\phi_0 \phi_0^* \]

Exchanging \( 2e^- \Rightarrow -\text{sgn} \)
Fermion wavefunction is antisymmetric

4. \( \cos q \approx 1 - \frac{1}{2} q^2 \)
so \( w^2(q) \approx \frac{2k}{M} \cdot \frac{1}{2} q^2 \), \( \Rightarrow \omega(q) = \sqrt{k/M} \cdot q \)

Energy \( \omega \) like a photon \( \Rightarrow E = cp \).

\[ \text{Photon } w = ck \]

Energy \( \omega \) very large
would intense optical branch
but not acoustic.
The energy levels which are highly degenerate broaden into energy "bands". See also problem #8:

\[
\begin{pmatrix}
E_n + t \\
E_n
\end{pmatrix}
\]

The matrix has eigenvalues \( E_n + t \) and \( E_n - t \).

\[E_3\]  \[\rightarrow\] \[E_n\] (x2)  \[\rightarrow\] \[E_{n-t}\]

\[E_2\]  \[\rightarrow\] \[\text{Energy band}\]

\[E_1\]  \[\rightarrow\] \[\text{\(N\)}\text{A fold degenerate discrete atom levels}\]

\[\langle E_2(T) \rangle\]

\[\frac{1}{2}(E_1 + E_2)\]

\[E_1\]

\[E_2 - E_1\]

\[\langle C(T) \rangle\]

\[\frac{1}{2}(E_2 - E_1)\]

\[\rightarrow\] \[T\]

\[\rightarrow\] \[\text{C(T)}\]

\[\rightarrow\] \[\text{\(E_2 - E_1\)}\]

\[\rightarrow\] \[\text{\(E_1\)}\]

\(c)\) \(C(T)\) \(\rightarrow\) 0 \(\text{at high T because there is a maximal energy level.}\)

\(\text{C(T)}\) \(\rightarrow\) 0 \(\text{exponentially at low T because there is a gap between ground and first excited states.}\)
7. Pauli principle prevents two $\text{e}^-$ from having same momentum (ignoring spin). Only $\text{e}^-$ with $k_BT$ of Fermi surface away empty momentum states in which to move when $T$ increases (Most) when $\text{e}^-$ deep inside Fermi sphere cannot change their momentum. classical result

\[
\begin{align*}
\theta & \sim N k_B \frac{k_BT}{E_F} \\
\Rightarrow \quad \text{Pauli blocking} \\
\text{reduction factor}
\end{align*}
\]

8. \[H |10\rangle = E |10\rangle - t |01\rangle \quad \Rightarrow \quad H = \begin{pmatrix} E - t & -t \\ -t & E \end{pmatrix} \]

\[H |10\rangle = -t |10\rangle + E |01\rangle \]

\[\begin{align*}
\text{two states} \\
\text{with } 1 \text{ e}^- \\
\text{c) } (E - \lambda)^2 - t^2 = 0 \\
\Rightarrow \lambda = E \pm t
\end{align*} \]

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 bond
An x-ray scattering off a crystal will have its momentum changed by \( \mathbf{k} + \mathbf{G} \) where \( \mathbf{G} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3 \).

is a reciprocal lattice vector. For elastic scattering \( |\mathbf{k}'| = |\mathbf{k}| \)

\[
\mathbf{k}' = \mathbf{k} + \mathbf{G}
\]

\[
k'^2 = k^2 + 2\mathbf{k} \cdot \mathbf{G} + \mathbf{G}^2 \Rightarrow \mathbf{k} \cdot \mathbf{G} = \frac{1}{2} |\mathbf{G}|
\]

equal

if elastic

Experimental sal/s is unlikeliness of satisfying Bragg condition

(1) nonmonochromatic x-rays

so \( |\mathbf{k}| \) has many values

(2) Robte crystal, increasing

no. of \( \mathbf{G} \) values.

11. Power method: Apply matrix \( M \) many times to initial vector \( \mathbf{v} \) project out \( \mathbf{v}_n \) with largest \( \lambda_n \)

Initial vector cannot be \( \perp \) to \( \mathbf{v}_{\text{max}} \). May need to normalize during iteration to prevent overflow.

Why it works:

\[
M^p \mathbf{v} = M^p \sum \alpha_n \mathbf{v}_n = \sum \alpha_n \lambda_n^p \mathbf{v}_n
\]

\[
= \left( \lambda_{\text{max}} \right)^p \sum \alpha_n \left( \frac{\alpha_n}{\lambda_{\text{max}}} \right)^p \mathbf{v}_n
\]

\( \rightarrow \) nonzero \( \forall n \) except max.
(11) a) \[ c_x^t c_{e+1}^t c_e^t c_e = -c_x^t c_e^t c_{e+1}^t c_e = 0 \]

\[ c_x^t c_e^t c_{e+1}^t c_e = c_x^t (1 - c_e^t c_e) c_{e+1}^t = c_x^t c_{e+1}^t \]

\[ \left[ c_x^t c_{e+1}^t, c_e^t c_e \right] = -c_x^t c_{e+1}^t \]

Like wise \[ c_{e+1}^t c_e^t c_e^t c_e = c_{e+1}^t (1 - c_e^t c_e) c_e = c_{e+1}^t c_e \]

\[ c_{e+1}^t c_e^t c_{e+1}^t c_e = -c_x^t c_{e+1}^t, c_e c_e = 0 \]

So \[ \hat{[h, n_e]} = c_{e+1}^t c_e - c_x^t c_{e+1}^t \]

Like a "current operator"?

b) \[ c_{e+1}^t c_{e+1}^t c_{e+1}^t c_e = c_x^t (1 - c_{e+1}^t c_{e+1}^t) c_{e+1}^t = c_x^t c_{e+1}^t \]

\[ c_{e+1}^t c_{e+1}^t, c_{e+1}^t c_{e+1}^t = 0 \]

\[ c_{e+1}^t c_e c_{e+1}^t c_{e+1}^t = 0 \]

\[ c_{e+1}^t c_{e+1}^t c_{e+1}^t c_e = c_{e+1}^t c_e \]

\[ \hat{[h, n_{e+1}]} = c_{e+1}^t c_{e+1}^t - c_{e+1}^t c_e = -\hat{[h, n_e]} \]

So \[ \hat{[h, n_e + n_{e+1}]} = 0 \]
**cont'd** Since $\hat{A} = c^+_e c_{e+1}$ creates 2 electrons

We would not expect it to commute with $n_e n_{e+1}$.

We can compute it if we like:

$$c^+_e c^+_e c^+_e c_e = -c^+_e c^+_e c_{e+1} c_e = \emptyset$$

$$c^+_e c_e c^+_e c_{e+1} = c^+_e (1-c^+_e c_e) c_{e+1} = c^+_e c_{e+1}$$

$$\therefore [\hat{A}, n_e] = -c^+_e c_{e+1},$$

$$c^+_e c_{e+1} c^+_e c_{e+1} = \emptyset$$

$$c^+_e c_{e+1} e c_{e+1} = -c^+_e c_{e+1} e c_{e+1} c^+_e c_{e+1}$$

$$\therefore [\hat{A}, n_{e+1}] = -c^+_e c_{e+1}$$

Another way:

$$c^+_e c^+_e |00\gamma = |11\gamma$$

$$\Rightarrow (n_e + n_{e+1}) c^+_e c^+_e |00\gamma = 2 |11\gamma \quad \{\text{so do not commute}\}$$

$$c^+_e c^+_e c_{e+1} (n_e + n_{e+1}) |00\gamma = \emptyset$$