Physics 420 (Prof. Hu) Final Examination Dec. 18, 2004

(Total 2 pages, 6 problems, 200 points)
—Remember to write down YOUR NAME on each of your exam books—

1A. (15 points) A marble of mass 20 g rolls back and forth with constant speed $0.8 m/s$ inside a box $12 cm$ high and $2 mm$ thick. Calculate the probability of it escaping through the wall of the box by quantum tunneling.

1B. (30 points) For a particle of mass m in a square box of length L, derive an expression for a) the eigenfunctions $\psi(x,y)$ (remember to get the amplitude function A using the normalization condition.) (15 points) b) the energy eigenvalues E_n, labeling them with the quantum numbers (n_x, n_y) and using the notation $E_0 = \frac{\hbar^2\pi^2}{2mL^2}$. (7 points) c) the degeneracy for each of the lowest four energy levels. (8 points)

2. (25 points) Calculate the probability that the electron in the ground state of hydrogen will be found inside the first Bohr radius a_0. The wave function is $\psi_{100} = (\pi a_0^3)^{-1/2} e^{-r/a_0}$. [Hint: change to variable $z = 2r/a_0$ and do the integration by parts twice, with e.g., definitions $X = z^2, dY = e^{-z}dz$]

3A. (15 points) Draw an energy diagram for an hydrogen electron in the 2s state and 1s state when the atom is immersed in a magnetic field B, assuming the electron is spinless. Draw another diagram when electron spin is included. Label the states clearly with the quantum numbers m_l, m_s. Express the energy spacing ΔE in terms the Bohr magneton $\mu_B (= 0.927 \times 10^{-23} J/T)$

3B. (15 points) The sodium double lines arise from transitions of the outermost electron from the split 3P levels due to spin-orbit coupling to the 3S level. Draw an energy diagram explaining these transitions. Label the levels with spectroscopic notations nl_j. Which j level has the lower energy?

4A. (20 points) Explain the physical origin of exchange force for an atom with two electrons. [Reason in steps how the Pauli Principle, the spin of the electron, the symmetry of the total, space, and spin wave function enter into the picture.] (10 points) Draw the energy diagrams for the ground state (1s 1s) and excited states (1s 2s) and (1s 2p) of the helium atom, a) with Coulomb force and b) with Coulomb and exchange force. Label the singlet and triplet states. Which state has the lower energy? Why? (10 points)

4B. (10 points) Write down the electronic configuration of ^6C and ^{17}Cl atoms.

5A. (15 points) Derive an expression for the density of states $\mathcal{D}(\epsilon)$ of N non-relativistic quantum particles of mass m and energy ϵ in a cubic box of length L.

5B. (15 points) For phonons, integrating the density of state function up to the Debye frequency ν_D gives 3N, the number of modes per mole. Derive an expression for ν_D in terms of N and $V = L^3$. (10 points) What is the physical meaning of Debye temperature T_D? At what temperature range (compared to T_D) will the heat capacity at constant volume C_V for an ideal gas approach $3R$? (5 points)

5C. (20 points) For fermions of mass m, integrating the density of state function up to the Fermi energy E_F gives N, the number of fermions in volume V. Derive an expression for E_F. (10 points) Calculate E_F in eV for aluminum assuming that the number density of electrons with mass m_e is $1.8 \times 10^{29}/m^3$. (10 points)

6. (20 points) a) How does the band structure of a solid arise? Describe how one can distinguish a solid to be a conductor, an insulator or a semiconductor (name two essential factors) b) What is a Brillouin zone? What is the effective mass m^* of an electron in a periodic lattice? c) What is the distinction between intrinsic and extrinsic semiconductors? d) Describe some key features of the BCS theory of superconductivity.

Note: Please show your derivations and reasoning. You won't get any credit if you just lift the expression from your formula sheet for your answer.

Some useful constants and formulas: Planck's constant $h = 6.63 \times 10^{-34} Js$
Electron mass $m_e = 9.11 \times 10^{-31}$ kg; 1 eV = $1.6 \times 10^{-19} J$.

Solution to

Phys 420 704 final

Dec. 18. 2004

1.A $$U = mgy = (0.02\ \text{kg})(9.8\ \text{m/s}^2)(0.12\ \text{m}) = 0.0235\ \text{J}$$

$$E = K = \frac{1}{2}mv^2 = \frac{1}{2}(0.02\text{kg})(0.8\ \text{m/s})^2 = 0.0064\ \text{J}$$

$$\alpha = \frac{\sqrt{2m(U-E)}}{\hbar} = \frac{\sqrt{2(0.02\text{kg})(0.0171\text{J})}}{1.055\times10^{-34}\ \text{J}\cdot\text{s}} = 2.5\times10^{32}\ \text{m}^{-1}$$

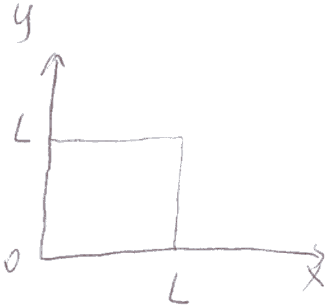
So $$T = e^{-2\alpha L} = e^{-2(2.5\times10^{32})(12\times10^{-3})} = e^{-10\times10^{29}} \sim 10^{-10^{30}}$$

very small

1. B

a) Schrödinger eqn.

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi = E\psi$$



let $\psi = f(x)\,g(y)$

$$\Rightarrow \begin{cases} -\frac{\hbar^2}{2m} f''(x) = E_x f(x) \\ -\frac{\hbar^2}{2m} g''(y) = E_y g(y) \end{cases}$$ where $E_x + E_y = E$

$$\Rightarrow \begin{cases} f(x) = A\cos k_x x + B\sin k_x x \\ g(y) = C\cos k_y y + D\sin k_y y \end{cases}$$

boundary condition at $x=0$ & $y=0$ $f(0)=0 \Rightarrow A=0$

$g(0)=0 \Rightarrow C=0$

boundary condition at $x=L$: $f(L)=0 \Rightarrow k_{nx} = \frac{n_x \pi}{L}$ $n_x = 1, 2, 3, \cdots$

at $y=L$: $g(L)=0 \Rightarrow k_{ny} = \frac{n_y \pi}{L}$ $n_y = 1, 2, 3 \cdots$

So $\psi(x,y) = N \sin\left(\frac{n_x\pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right)$

$\iint dx\,dy\, |\psi|^2 = 1 \Rightarrow N = \frac{2}{L}$

$\therefore \psi(x,y) = \frac{2}{L} \sin\left(\frac{n_x\pi}{L} x\right) \sin\left(\frac{n_y\pi}{L} y\right)$ for $n_x = 1, 2, 3 \cdots$
$n_y = 1, 2, 3 \cdots$

1. B

b) $\because H\psi(x,y) = E\psi(x,y)$

$$\therefore E_n = \frac{\hbar^2}{2m} \left[\left(\frac{n_x\pi}{L}\right)^2 + \left(\frac{n_y\pi}{L}\right)^2\right]$$

$$= \frac{\hbar^2\pi^2}{2mL^2} (n_x^2 + n_y^2)$$

$$= E_0 (n_x^2 + n_y^2)$$

c)

	n_x	n_y	E/E_0
2 degeneracy →	3 2	2 3	13
1 .. →	2	2	8
2 .. →	2 1	1 2	5
1 .. →	1	1	2

2.

$$P = \int_0^{a_0} r^2 dr \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \, |\psi_{100}|^2$$

$$= 4\pi \int_0^{a_0} r^2 dr \, (\pi a_0^3)^{-1} e^{-2r/a_0}$$

$$= \frac{4}{a_0^3}\left(\frac{a_0}{2}\right)^3 \int_0^2 dz \, z^2 e^{-z} \qquad \text{where } z = 2r/a_0$$

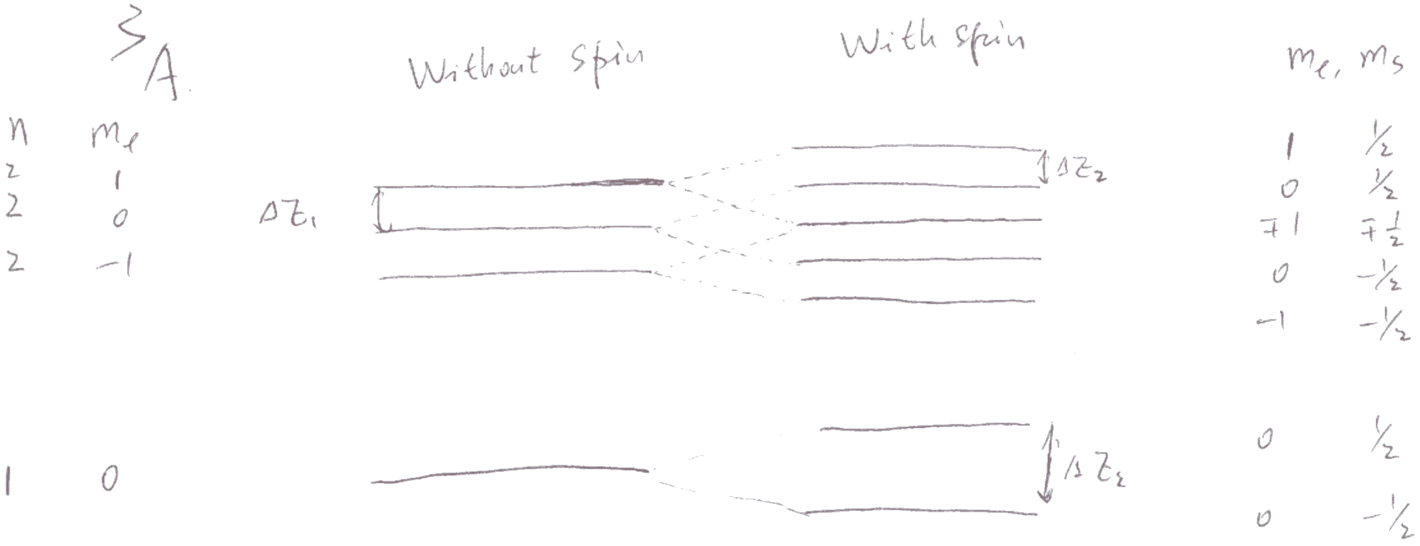
$$= \frac{1}{2}\left[(-1)e^{-z}z^2\Big|_0^2 + \int_0^2 e^{-z}\, 2\cdot z \, dz\right]$$

$$= -\frac{1}{2}e^{-2}\cdot 4 + (-1)e^{-z}z\Big|_0^2 + \int_0^2 e^{-z}dz$$

$$= -2e^{-2} - 2e^{-2} + (-e^{-z})\Big|_0^2$$

$$= 1 - 5e^{-2}$$

3 A.



$$U_1 = -\vec{\mu}_l \cdot B = \frac{e}{2m_e} B (L_z) = \mu_B B m_l \qquad m_l = 1, 0, -1$$

$$\therefore \Delta Z_1 = \mu_B B$$

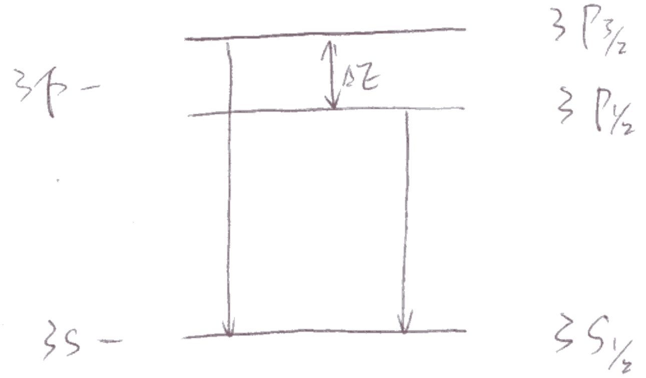
$$U_z = -\vec{\mu}_s \cdot \vec{B} = \frac{e}{2m_e} B g S_z$$

$$= \frac{e}{m_e} B \hbar m_s \qquad (m_s = \pm \tfrac{1}{2})$$

$$= 2\mu_B B m_s$$

$$\Delta E_z = \mu_B B$$

3.B.



The $j = \frac{1}{2}$ $l = 1$ state has the lower energy than $3P_{3/2}$ state.

4.A Exchange Force

- Pauli Principle: no two electrons can occupy the same quantum state.

So for 2 electron atoms, the total electronic wave function is antisymmetric with respect to interchange of 1↔2

- Total wave function = Space wave function × Spin Wavefunction
  Ψ $\qquad\qquad\qquad\qquad$ Φ $\qquad\qquad\qquad\qquad$ $\chi_{S m_s}$

you don't need to show this

- Spin Wave function $s_1 = \frac{1}{2},\ s_2 = \frac{1}{2} \rightarrow$ combined spin $S = 0,\ m_s = 0$ Singlet or $1,\ m_s = \begin{smallmatrix}+1\\0\\-1\end{smallmatrix}\Big\}$ Triplet

$\chi_{S m_s}$: $\chi_{00} = \frac{1}{\sqrt{2}}(\chi_1^+ \chi_2^- - \chi_1^- \chi_2^+)$ antisymmetric wrt 1↔2

$$S = 1,\ m_s = \begin{cases} 1 : \chi_{11} = \chi_1^+ \chi_2^+ \\ 0 : \chi_{10} = \frac{1}{\sqrt{2}}(\chi_1^+ \chi_2^- + \chi_1^- \chi_2^+) \\ -1 : \chi_{1-1} = \chi_1^- \chi_2^- \end{cases} \Bigg\} \text{ Symmetric wrt } 1 \leftrightarrow 2$$

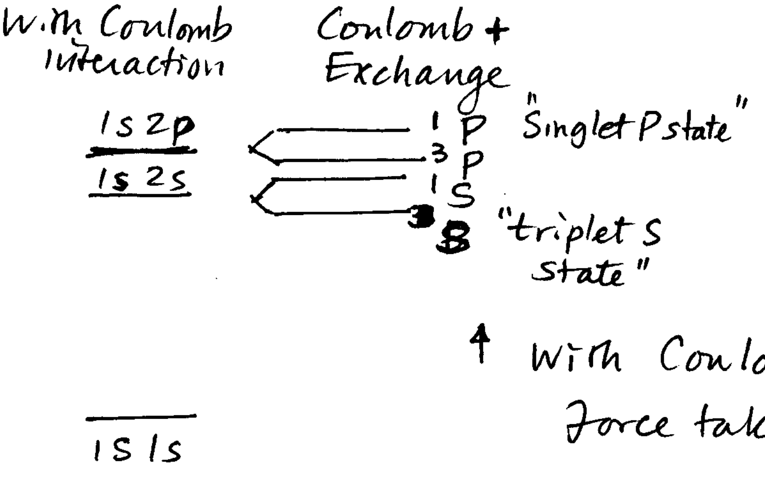
A symmetric spin wavefunction (Triplet state) is joint with an antisymmetric spatial wavefunction

⇒ 2 electrons are farther apart ⇒ weaker Coulomb repulsion

⇒ Triplet state has lower energy than singlet state

4 B. He Atom

Schematic energy level diagram



↑ With Coulomb and Exchange force taken into consideration, Triplet states are lower in energy for reasons given in 4A.

↑ With Coulomb interaction 1s2p is split from 1s2s. 1s2s is lower in energy because the 2e⁻ are more widely separated ⇒ weaker repulsion

$\boxed{4B}$ ${}^{6}C$: $1s^2 2s^2 2p^2$

${}^{17}Cl$: $1s^2 2s^2 2p^6 3s^2 3p^5$

$\boxed{6}$ All from class notes.

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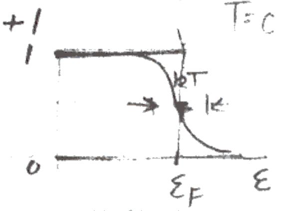
spin ½ parti

2 spin orientat

$\boxed{5C}$

$$\mathcal{D}(\varepsilon)\,d\varepsilon = \frac{\overset{②\ \text{electron spin } \frac{1}{2}}{2}\pi V}{h^3}(2m)^{3/2}\varepsilon^{1/2}\,d\varepsilon \qquad n(\epsilon) = \frac{1}{e^{(\epsilon-\epsilon_F)/kT}+1}$$

$$N = \int_0^{\infty} \mathcal{D}(\varepsilon)\,n(\varepsilon)\,d\varepsilon \cong \frac{4\pi V}{h^3}(2m)^{3/2}\cdot\frac{\varepsilon^{1/2}\,d\varepsilon}{e^{(\varepsilon-\varepsilon_F)/kT}+1}$$



when $\underline{kT \ll \varepsilon_F}$, approximate by $n(\epsilon) \approx \begin{cases} 1 & \text{for } \varepsilon < \varepsilon_F \\ 0 & \text{for } \varepsilon > \varepsilon_F \end{cases}$

$$\boxed{N = \int_0^{\varepsilon_F} \mathcal{D}(\varepsilon)\,d\varepsilon} = \frac{8\pi V(2m)^{3/2}}{3h^3}\varepsilon_F^{3/2}$$

, with $p_F \Rightarrow \lambda_{\text{dB}} \simeq d$

Energy of Particles

$$\Rightarrow \quad \varepsilon_F = \frac{h^2}{2m}\left(\frac{3N}{8\pi V}\right)^{2/3} \cong \frac{p_F^2}{2m}$$

for metal. valid for $\gtrsim 10^5\,°K$

So Room temp is "low temp" for cond. e

$E_A \gg$ degenerate electron

Average energy of electron. $\bar{E} = \frac{1}{N}\int \mathcal{D}(\varepsilon)\,\varepsilon\,n(\varepsilon)\,d\varepsilon = \frac{3}{5}\varepsilon_F$:

This is why Conduction electrons do not contribute to the specific heat of metals at ordinary temp.

lattice elec.

electrons classical behavior manifest only at $T \gg T_F$

expect Classical : $C_R = (3 + \frac{3}{2})R$

but actual value $C_R = 3R$ at high temp.

no equipartition of energy between electrons and lattice

At low temp. (few °K) $C_{\text{electron}} > C_{\text{lattice}}$

you don't need to answer this

For aluminum, $n = 1.8 \times 10^{29}/m^3$ yields $\epsilon_F = 11.63\,eV$

[Serway Problem 10.15]

$\boxed{5A}$ Density of State :

$\mathcal{D}(\epsilon)$ number of states per unit energy interval

1) For non-relativistic particle in 1-D box of length L

$$\epsilon = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{h^2n^2}{8mL^2}, \quad \text{so } n = \left(\frac{8mL^2}{h^2}\right)^{1/2}\epsilon^{1/2}$$

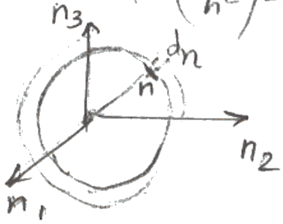
$(p = \frac{h}{\lambda})$

$$2L = n\lambda \text{ or } n = \frac{2L}{\lambda} = \frac{2L\nu}{v}$$

(speed of sound

$$dn = \left(\frac{8mL^2}{h^2}\right)^{1/2}\frac{1}{2}\epsilon^{-1/2}d\epsilon$$

in 3-D $\quad n^2 = \sum_{i=1}^{3} n_i^2$



2) Volume of n space with positive $n_1\ n_2\ n_3$

Classical Standing wave

$$\mathcal{D}(n)dn = \frac{4\pi n^2 dn}{⑧}, \quad \mathcal{D}(\nu)d\nu = \left(\frac{\pi}{2}\right)\left(\frac{2L}{v}\right)^3\nu^2 d\nu$$

quantum :

phonon (quanta of sound) : ③ vibrational dof

photon (" of light) : ② polarization

So $\mathcal{D}(\nu)d\nu = \frac{8\pi V}{v_s}\nu^2 d\nu$ for phonon

$\quad\quad c$ for photon

Assume this form applies

3) For photons or phonons, each normal mode has $\epsilon_n = nh\nu$

n photons of freq ν

And $\mathcal{D}(\epsilon)d\epsilon$

$$= \left(\frac{\pi}{2}\right)\left(\frac{8mL^2}{h^2}\right)\epsilon\left(\frac{8mL^2}{h^2}\right)^{1/2}\frac{1}{2}\epsilon^{-1/2}d\epsilon = \frac{\pi}{4}\left(\frac{8mL^2}{h^2}\right)^{3/2}\epsilon^{1/2}d\epsilon$$

$$= \frac{2\pi V}{h^3}(2m)^{3/2}\epsilon^{1/2}d\epsilon$$

$\boxed{5B}$

(phonon ① 1 longitudinal wave plus 2 transverse

② Sum over frequency up to ν_{max}

Debye Approx : number of modes = $3N$ per mole

3 translational degree of freedom

where N is the number of atoms in a mole

note: Brillouin [illegible]

$\mathcal{D}_{Debye}(\nu) = ③\mathcal{D}(\nu)$ [illegible]

Lattice [illegible]

① optical (trans?) | ② [illegible]

$$\int_0^{\nu_D} \underset{\text{1 pola}}{\mathcal{D}(\nu)}d\nu = 3N \Rightarrow \nu_D = v_s\left(\frac{9N}{4\pi V}\right)^{1/3}$$

3, if counting 3 polarization

1 acoustic +2 optical

upper limit of frequency def Debye frequency

Def : Debye temp $\boxed{h\nu_D/k = T_D}$

For ideal gas $C_V \to 3R$ when $T \gg T_D$