Physics 195 / Applied Physics 195 — Assignment #1

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Due: 12:45pm + 10 min grace period, Sep. 20, 2017 at the dropbox outside Maxwell-Dworkin Rm 131.

Problem 1 (60 pt): Electron sharing lowers energy and creates attraction.

Using a hydrogen molecular ion (2 protons + 1 electron), Lecture #1 showed that electron sharing lowers energy and creates attraction. Particle sharing to create attraction is an important concept encountered in many contexts of physics; in this course it is the basis of covalent and metallic bonding. The associated approximation method used in Lecture #1, named tight binding, will be also important in several key parts of this course. Given the importance, I wish you to work through the problem, now using 3 protons + 1 electron. Let the 3 protons be lined up in one dimension with any two neighboring protons separated by distance d. Let $|n\rangle$ ($n = 1, 2, 3$) be the ground state of the electron (energy: ϵ_0) if the electron were only with the n-th proton with the associated potential energy being denoted as V_n. That is: $\left[p^2/(2m) + V_n\right]|n\rangle = \epsilon_0|n\rangle$ ($n = 1, 2, 3$). The energy eigenstates $|\psi\rangle$ and eigenvalues E of the electron with all 3 protons together then satisfy $H|\psi\rangle = E|\psi\rangle$ where $H = p^2/(2m) + \sum_{n=1}^{3} V_n$.

(a) Using $|n\rangle$'s ($n = 1, 2, 3$) as an approximate orthonormal basis set, express H as a matrix in this basis; assume only nearest-neighbor tunneling (hopping) with the tunneling strength denoted as δ (> 0). Find the energy eigenstates as linear combinations of $|1\rangle$, $|2\rangle$, and $|3\rangle$ and the corresponding energy eigenvalues. Considering the distribution of energy eigenvalues in comparison to ϵ_0, their manner of change with decreasing d, and the manner of delocalization of the electron wave function in each eigenstate, explain how sharing an electron lowers the system energy and creates cohesive (attractive) force.

(b) Describe the temporal change of the electronic quantum state $|\psi(t)\rangle$ when the initial condition is $|\psi(t = 0)\rangle = |2\rangle$ (or roughly speaking, the electron is initially localized at the 2nd proton). Show that the electron periodically returns to the initial state after intervening hopping (tunneling) episodes. What is this period? Do you see that the tunneling strength δ dictates this period? (and thus do you understand why δ is called tunneling strength?) Repeat this problem with the initial condition of $|\psi(t = 0)\rangle = |1\rangle$.

Problem 2 (60 pt): Van der Waals attraction

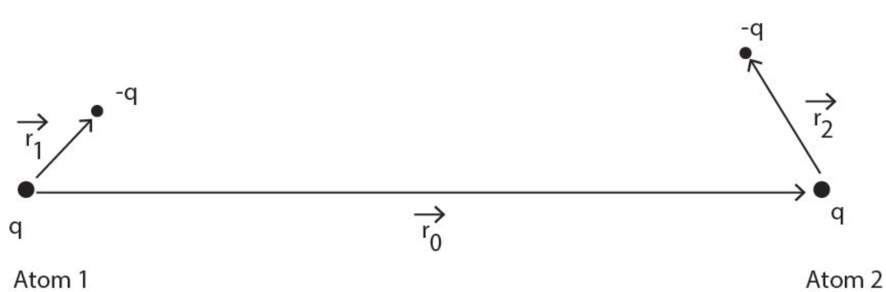

Figure 1:

Consider two model atoms shown in Fig. 1. They are substantially separated: $r_0 \gg r_1, r_2$ ($r_0 \equiv |\vec{r}_0|$, $r_1 \equiv |\vec{r}_1|$, $r_2 \equiv |\vec{r}_2|$). Let H_1 be the Hamiltonian of the mobile negative charge $-q$ in Atom 1 alone:

$$H_1 = \frac{p_1^2}{2m} - \frac{q^2}{4\pi\epsilon_0}\frac{1}{r_1}. \tag{1}$$

Similarly, H_2 is the Hamiltonian of the mobile negative charge $-q$ in Atom 2 alone:

$$H_2 = \frac{p_2^2}{2m} - \frac{q^2}{4\pi\epsilon_0}\frac{1}{r_2}. \tag{2}$$

The system Hamiltonian is then $H = H_1 + H_2 + H_d$ where

$$H_d \equiv \frac{q^2}{4\pi\epsilon_0}\left[\frac{1}{r_0} - \frac{1}{|\vec{r}_0 - \vec{r}_1|} - \frac{1}{|\vec{r}_0 + \vec{r}_2|} + \frac{1}{|\vec{r}_0 - \vec{r}_1 + \vec{r}_2|}\right] \tag{3}$$

is due to the dipolar interaction between the two atoms, and acts as a weak perturbation. Given the substantial separation of the two atoms, assume zero overlap between wave functions of Atom 1 and Atom 2.

(a) Show that expansion of H_d up to the leading non-vanishing orders of r_1/r_0 and r_2/r_0 yields

$$H_d \approx \frac{q^2}{4\pi\epsilon_0}\frac{\vec{r}_1 \cdot \vec{r}_2 - 3(\vec{r}_1 \cdot \hat{r}_0)(\vec{r}_2 \cdot \hat{r}_0)}{r_0^3} \tag{4}$$

where $\hat{r}_0$ is the unit vector in the direction of $\vec{r}_0$.

(b) Prove that the first-order correction to the ground state energy of $H_1 + H_2$ due to H_d vanishes.

(c) Show that the second-order correction to the ground state energy of $H_1 + H_2$ due to H_d is proportional to r_0^{-6} and is negative. This gives the van der Waals attraction.

Problem 3 (60pt): Free electron Fermi gas: 3D

(a) Estimate v_F, ϵ_F, and T_F for sodium, copper, gold, silver, and aluminum.

(b) By directly integrating individual electron kinetic energies, show that the total energy of the Fermi gas of N free electrons at $T = 0$ K is given by $U = (3/5)N\epsilon_F$. Show then that the pressure exerted by the electron gas at $T = 0$ K is given by $P = 2U/3V$ where V is the volume of the Fermi gas. Calculate the total energy U of the Fermi gas of N free electrons at non-zero temperature T up to the lowest non-vanishing order of k_BT.

Problem 4 (50pt): Free electron Fermi gas: 2D

Consider a Fermi gas of N free electrons in area A in two dimensions. Calculate the density of states $D(\epsilon)$. Relate n_0 (electron density per unit area) with k_F and with ϵ_F. Calculate the total energy U at $T = 0$ K by direct integration. Show exactly that the chemical potential μ at temperature T is related to ϵ_F by

$$\mu = k_BT \ln\left[\exp\left(\frac{\epsilon_F}{k_BT}\right) - 1\right]. \tag{5}$$

Problem 5 (50pt): White dwarf as a relativistic Fermi gas

Material contents of white dwarf stars are mostly helium. Since $T \sim 10^7$ K, the helium atoms are completely ionized. Then a white dwarf may be modeled as a Fermi gas consisting of N electrons—where the number of helium atoms is $N/2$—in a spherical volume V. Since $T_F \gg T$ (specifically, $T_F \sim 10^{11}$ K and $T \sim 10^7$ K), treatment of the Fermi gas with $T \sim 10^7$ K ≈ 0 K will work well. In equilibrium, the outward Pauli pressure is balanced by the inward gravitational pull, where the gravitational pull is due to the star mass M, which is dominated by the helium nuclei: concretely, $M = Nm_e + (N/2) \times 4m_p \approx 2Nm_p$. Here m_e is electron mass and m_p is proton mass. Since the white dwarf is immensely dense (10^{30} electrons per cm^3), the Fermi momentum $p_F = \hbar k_F$ is high and we should treat the Fermi gas relativistically.

(a) The energy of an individual electron with a momentum $\vec{p} = \hbar\vec{k}$ is given by

$$\epsilon = [(pc)^2 + (m_e c^2)^2]^{1/2} = [(\hbar ck)^2 + (m_e c^2)^2]^{1/2} \tag{6}$$

where $k \equiv |\vec{k}|$ and $p \equiv |\vec{p}|$. The total energy U at $T \sim 10^7$ K ≈ 0 K (note once again that $T_F \gg T$) is then given by

$$U = 2 \times \frac{V}{(2\pi)^3} \int_0^{k_F} \epsilon(k) d^3\vec{k} \tag{7}$$

while k_F is connected to N via

$$N = 2 \times \frac{V}{(2\pi)^3} \int_0^{k_F} d^3\vec{k}. \tag{8}$$

We define a unit-less quantity a_F as

$$a_F \equiv \frac{\hbar k_F}{m_e c} \tag{9}$$

and we consider the strongly relativistic case of $a_F \gg 1$. Show that with $a_F \gg 1$, U of Eq. (7) can be approximated as

$$U \approx \frac{V m_e^4 c^5}{4\pi^2\hbar^3}(a_F^4 + a_F^2). \tag{10}$$

(b) Show that the Pauli pressure $P = -\partial U/\partial V$ is then given by

$$P \approx \frac{m_e^4 c^5}{12\pi^2\hbar^3}(a_F^4 - a_F^2). \tag{11}$$

(c) Let R be the radius of the white dwarf. The balance between the Pauli pressure P and the gravitational pull may be written out as

$$4\pi R^2 P = \alpha \frac{GM^2}{R^2} \tag{12}$$

The exact gravitational pull depends on the detailed inner stellar structure (*e.g.*, atomic density distribution). Instead of calculating it exactly (and while it is doable), we have smoothened it over with the undetermined constant α on the right hand side above, where α is on the order of unity. By plugging Eq. (11) into Eq. (12), the R vs. M relation is obtained. Show that R decreases with increasing M (*i.e.*, if the star is more massive, the gravitational pull becomes stronger, and the star settles in equilibrium with a smaller radius). Furthermore, show that $R \to 0$ for $M \to M_0$ where

$$M_0 = \alpha^{-3/2} \times \frac{9}{64}(3\pi)^{1/2} \times (\frac{\hbar c}{G})^{3/2} \times \frac{1}{m_p^2}, \tag{13}$$

and R becomes imaginary for M in excess of M_0. That is, the white dwarf cannot have a mass larger than M_0; if M is larger than M_0, the Pauli pressure is not strong enough to support the gas up against the gravitational collapse.

(d) Perform numerical calculation for Eq. (13) to show that M_0 is comparable to the solar mass (note that α is on the order of unity). I remark that more detailed analysis with determination of α leads to

$$M_0 \approx 1.4 \times \text{solar mass}. \tag{14}$$

This is the celebrated Chandrasekhar limit, and has been upheld by astronomical observations.