Applied Physics 195 / Physics 195 — Assignment #1

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Date: September 9th, 2015
Due: **12:45pm + 10 min grace period**, September 18th, 2015; slide your work under through the door at Maxwell-Dworkin Room 131.

Problem 1 (50 pt): Tight binding calculation with $N = 2$ solid

We revisit the tight-binding calculation of the 2-atom system—hydrogen molecule ion with covalent one-electron bond—of Lecture #1, given the importance of the method which we will later extend to N-atom solids. Protons 1 and 2 are separated by distance d. Let $|1\rangle$ be the ground state of an electron with energy ϵ_0 due to its Coulomb interaction with Proton 1 alone (potential energy: V_1). $|2\rangle$ is the electron ground state with energy ϵ_0 due to interaction with Proton 2 alone (potential energy V_2). $|1\rangle$ and $|2\rangle$ then satisfy:

$$\left[p^2/(2m) + V_1\right]|1\rangle = \epsilon_0|1\rangle; \quad (1)$$

$$\left[p^2/(2m) + V_2\right]|2\rangle = \epsilon_0|2\rangle. \quad (2)$$

The energy eigenstates $|\psi\rangle$ and eigenvalues E of the electron with both protons then satisfy

$$H|\psi\rangle = E|\psi\rangle, \quad (3)$$

where $H = p^2/(2m) + V_1 + V_2$. In 2-state approximation, $|1\rangle$ and $|2\rangle$ serve as approximate orthonormal basis.

(a) Express H as a matrix in the basis of $|1\rangle$ and $|2\rangle$. You may use $\delta \equiv -\langle 1|V_1|2\rangle$ (can you argue δ is positive?)

(b) Find the lower and higher eigen energies, $E = E_L$ and $E = E_H$, and corresponding eigenstates $|\psi\rangle = |\psi_L\rangle$ and $|\psi\rangle = |\psi_H\rangle$ as linear combinations of $|1\rangle$ and $|2\rangle$. How do E_L and E_H compare in magnitude to ϵ_0? From $|\psi_L\rangle$, can you see electron delocalization? As d decreases, how does E_L behave? Do you expect attraction or repulsion?

(c) To understand the role of the non-vanishing off-diagonal elements of H (which are related to δ), describe, quantitatively, the time evolution of the electron state, which is prepared to be $|2\rangle$ at $t = 0$.

Problem 2 (50 pt): Van der Waals attraction

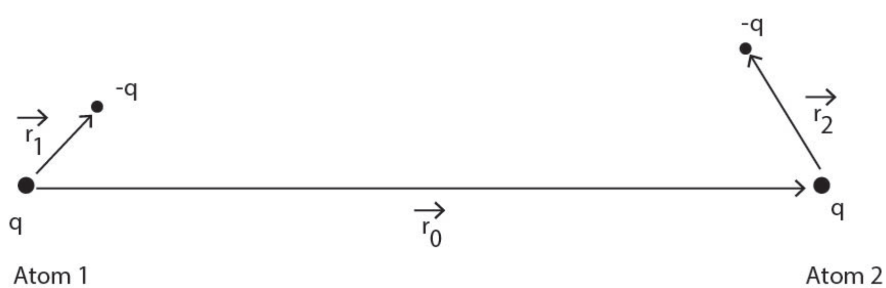

Figure 1:

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:

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

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

$$H_2 = \frac{p_2^2}{2m} - \frac{q^2}{4\pi\epsilon_0}\frac{1}{r_2}. \tag{5}$$

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

$$H_d \equiv \frac{q^2}{4\pi\epsilon_0}\left[\frac{1}{r_0} - \frac{1}{|\vec{r}_0 - \vec{r}_1|} - \frac{1}{|\vec{r}_0 + \vec{r}_2|} + \frac{1}{|\vec{r}_0 - \vec{r}_1 + \vec{r}_2|}\right] \tag{6}$$

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

$$H_d \approx \frac{q^2}{4\pi\epsilon_0}\frac{\vec{r}_1\cdot\vec{r}_2 - 3(\vec{r}_1\cdot\hat{r}_0)(\vec{r}_2\cdot\hat{r}_0)}{r_0^3} \tag{7}$$

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 (50pt): 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

$$\mu = k_BT \ln\left[\exp\left(\frac{\epsilon_F}{k_BT}\right) - 1\right]. \tag{8}$$

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

$$\epsilon = [(pc)^2 + (m_e c^2)^2]^{1/2} = [(\hbar ck)^2 + (m_e c^2)^2]^{1/2} \tag{9}$$

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

$$U = 2 \times \frac{V}{(2\pi)^3} \int_0^{k_F} \epsilon(k) d^3\vec{k} \tag{10}$$

while k_F is connected to N via

$$N = 2 \times \frac{V}{(2\pi)^3} \int_0^{k_F} d^3\vec{k}. \tag{11}$$

We define a unit-less quantity a_F as

$$a_F \equiv \frac{\hbar k_F}{m_e c} \tag{12}$$

and we consider the strongly relativistic case of $a_F \gg 1$. Show that with $a_F \gg 1$, U of Eq. (10) can be approximated as

$$U \approx \frac{V m_e^4 c^5}{4\pi^2 \hbar^3} (a_F^4 + a_F^2). \tag{13}$$

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

$$P \approx \frac{m_e^4 c^5}{12\pi^2 \hbar^3} (a_F^4 - a_F^2). \tag{14}$$

(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

$$4\pi R^2 P = \alpha \frac{GM^2}{R^2} \tag{15}$$

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. (14) into Eq. (15), 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

$$M_0 = \alpha^{-3/2} \times \frac{9}{64} (3\pi)^{1/2} \times (\frac{\hbar c}{G})^{3/2} \times \frac{1}{m_p^2}, \tag{16}$$

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. (16) 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

$$M_0 \approx 1.4 \times \text{solar mass}. \tag{17}$$

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