Physics 312 – First Pledged Problem Set

1. The ground state of hydrogen is described by the wavefunction

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-r/a_0},$$

where a_0 is the Bohr radius.

(a) Compute the charge density

$$\rho(\mathbf{r}) = e\left|\psi(\mathbf{r})\right|^2.$$

and plot $4\pi r^2 \rho$ as a function of the dimensionless variable r/a_0. Does the plot peak at $r = a_0$?

We have

$$\begin{aligned} \rho(\mathbf{r}) &= e\left|\frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-r/a_0}\right|^2 \\ &= \frac{1}{\pi}\frac{e}{a_0^3} e^{-2r/a_0}. \end{aligned}$$

Thus

$$4\pi r^2 \rho(\mathbf{r}) = 4\frac{e}{a_0}\left(\frac{r}{a_0}\right)^2 e^{-2\frac{r}{a_0}}.$$

A plot of this function is below.
We see that the plot does peak at $r = a_0$.

(b) Compute the average value of r. Is it equal to a_0?

We have

$$\begin{aligned} \langle r\rangle &= \int \psi^\dagger(\mathbf{r})\, r\psi(\mathbf{r})\, d^3r \\ &= \int r\left|\psi(\mathbf{r})\right|^2 d^3r \\ &= \int_0^\infty r\frac{1}{\pi}\left(\frac{1}{a_0}\right)^3 e^{-2r/a_0} 4\pi r^2\, dr \\ &= 4a_0\int_0^\infty \beta^3 e^{-2\beta}\, d\beta, \end{aligned}$$

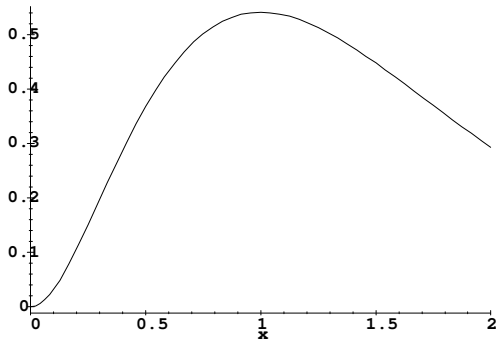

Figure 1:

where $\beta = r/a_0$. The remaining integral computed by hand, looked up, or done by computer, and is found to be equal to $3!/2^4 = 3/8$. Thus

$$\langle r \rangle = \frac{3}{2} a_0.$$

We see that $\langle r \rangle$ is *not* equal to a_0.

(c) Does the electron have a definite value of r? Does it have a definite speed? Does it have a definite angular momentum? Does it have a definite energy? If the answer to any of these questions is yes, give the value of the quantity.

The Hamiltonian that describes the electron is

$$\begin{aligned} H &= \frac{\mathbf{p}^2}{2m_e} + V(\mathbf{r}) \\ &= -\frac{\hbar^2}{2m_e}\boldsymbol{\nabla}^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}. \end{aligned}$$

We know from basic quantum mechanics that an eigenfunction of a system described by a Hamiltonian H will also be an eigenfunction of an operator $\mathcal{O}$ if and only if $\mathcal{O}$ commutes with H. One can check that r and $v = p/m$ do not commute with H, while $L^2 = L_x^2 + L_y^2 + L_z^2$ and H itself do commute with H. Therefore the electron has a definite energy and angular momentum, but not a definite radius or speed. The value of the angular momentum is $L = \sqrt{l(l+1)}\hbar = 0$ and the value of the energy is $E = -13.6$ eV.

(d) Compute the electric field due to this charge density everywhere in space. (Hint: use Gauss's theorem.) Add it to the field of the proton. Plot the total (radial) field as a function of r/a_0 for $r > a_0/2$ to check that it decreases exponentially.

We have from Gauss's law that

$$\int_{\partial S} \mathbf{E}(\mathbf{r}) \cdot d\mathbf{a} = \frac{1}{\epsilon_0} \int_S \rho(r)\, d^3 r,$$

for any closed surface S. Because the charge density is spherically symmetric, it follows that the electric field will be radial. Thus if we choose for S a sphere of radius r centered at the origin, we find that

$$E(r)\, 4\pi r^2 = \frac{1}{\epsilon_0} \int_0^r \rho(r')\, 4\pi r'^2\, dr',$$

so

$$E(r) = \frac{1}{\epsilon_0} \frac{1}{r^2} \int_0^r \rho(r')\, r'^2\, dr'.$$

$$= \frac{e}{\pi\epsilon_0}\int_0^r \left(\frac{r'}{a_0}\right)^2 e^{-2r'/a_0}\, d\left(\frac{r'}{a_0}\right)$$
$$= \frac{e}{\pi\epsilon_0}\int_0^R R'^2 e^{-2R'}\, dR',$$

where $R = r/a_0$ and $R' = r'/a_0$. The remaining integral can be done by *Maple* or the like, but is also easily done by hand. First we perform a change of variable:

$$\frac{e}{\pi\epsilon_0}\int_0^R R'^2 e^{-2R'}\, dR' = \frac{e}{8\pi\epsilon_0}\int_0^{2R} \beta^2 e^{-\beta}\, d\beta,$$

where β is simply equal to $2R'$. Now we perform two integrations by parts:

$$\begin{aligned}\int_0^{2R} \beta^2 e^{-\beta}\, d\beta &= -\beta^2 e^{-\beta}\big|_0^{2R} + \int_0^{2R} 2\beta e^{-\beta}\, d\beta \\ &= -(2R)^2 e^{-2R} - 2\beta e^{-\beta}\big|_0^{2R} + \int_0^{2R} 2e^{-\beta} \\ &= -4R^2 e^{-2R} - 4Re^{-2R} + 2 - 2e^{-2R} \\ &= 2 - \left(1 + 2R + 2R^2\right) e^{-2R}.\end{aligned}$$

Therefore we have

$$\begin{aligned}E(r) &= \frac{1}{r^2}\frac{e}{8\pi\epsilon_0}\left[2 - \left(1 + 2R + 2R^2\right) e^{-2R}\right] \\ &= \frac{1}{4\pi\epsilon_0}\frac{e}{a_0^2}\left[\frac{a_0^2}{r^2} - \left(1 + \frac{a_0}{r} + \frac{a_0^2}{2r^2}\right) e^{-2r/a_0}\right].\end{aligned}$$

The field due to the proton is just the Coulomb field

$$E(r) = -\frac{1}{4\pi\epsilon_0}\frac{e}{r^2},$$

so adding this to our previous result we find that the total field is

$$E_{\text{tot}}(r) = -\frac{1}{4\pi\epsilon_0}\frac{e}{a_0^2}\left(1 + \frac{a_0}{r} + \frac{a_0^2}{2r^2}\right) e^{-2r/a_0}.$$

A plot of this field is below.

(e) Compute the potential by integrating the field from r to infinity.

Using Maple or the like to do the integration, we find that

$$\begin{aligned}V(r) &= \int_r^\infty E_{\text{tot}}(r')\, dr' \\ &= -\frac{1}{4\pi\epsilon_0}\frac{e}{a_0}\left(\frac{1 + \frac{r}{a_0}}{2\frac{r}{a_0}}\right)\exp\left(-2r/a_0\right).\end{aligned}$$

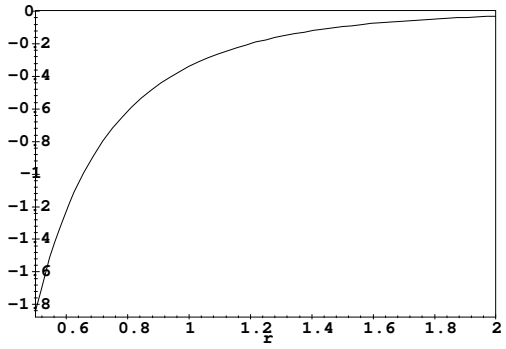

Figure 2:

2. Read the short section on impurity levels on page 368 of *Kittel and Kroemer* and look up the dielectric constants of Si and Ge, as well as the effective masses for the valence and conduction bands. Then:

(a) Compute the "effective Bohr radius" for donor and acceptor ground states. The easy way to do this is to scale the usual Bohr radius by the appropriate factors.

From Table 13.1 on page 357 of *Kittel and Kroemer* we obtain the following values:

Element	**Effective Mass of Holes**	**Effective Mass of Electrons**	**Dielectric Constant**
Si	0.58 m_e	1.06 m_e	11.7
Ge	0.35 m_e	0.56 m_e	15.8

The Bohr radius for hydrogen is given (in MKS units) by

$$a_{0,\text{hydrogen}} = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2},$$

which is equal to 0.0529 nm. As a rough approximation, we can treat the acceptor and donor atoms as hydrogen-like atoms by replacing m_e by the effective electron mass (m_{eff}) and ϵ_0 by $\kappa\epsilon_0$, where κ is the dielectric constant of the material. Thus we have

$$a_0 = \frac{4\pi\kappa\epsilon_0\hbar^2}{m_{eff}e^2} = \frac{\kappa}{(m_{eff}/m_e)}a_{0,\text{hydrogen}}.$$

Substituting, we find the following values for the effective Bohr radii:

Element	a_0 **for Holes**	a_0 **for Electrons**
Si	20.2 a_0	11.0 a_0
Ge	45.1 a_0	28.2 a_0

(b) Compute the ionization energies and compare with Table 13.2.

The ionization energy of the hydrogen atom is given by

$$E_{ion,\text{hydrogen}} = \frac{m_e e^4}{2\left(4\pi\epsilon_0\right)^2\hbar^2},$$

which is equal to 13.6 eV. Performing the same approximations as before we find that

$$E_{ion} = \frac{m_{eff}e^4}{2\left(4\pi\kappa\epsilon_0\right)^2\hbar^2} = \frac{(m_{eff}/m_e)}{\kappa^2}E_{ion,\text{hydrogen}}.$$

Thus we find the following table:

more accurate than that.

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3. Compute the bias voltage of a germanium p-n junction at 77 K, at room temperature, and at 500 K. Comment on the effect of increased temperature on the performance of such a junction.

We have from page 17 of *Melissinos* that

$$V_{bi} = \frac{k_B T}{e} \ln\left(\frac{N_D N_A}{n_i^2}\right),$$

and we have from page 8 that

$$n_i = N_s e^{\frac{-E_g}{2k_B T}}.$$

Combining these two relations we have that

$$\begin{aligned} V_{bi} &= \frac{k_B T}{e} \ln\left(\frac{N_D N_A}{N_s^2 e^{-E_g/k_B T}}\right) \\ &= \frac{E_g}{e} + \frac{k_B T}{e} \ln\left(\frac{N_D N_A}{N_s^2}\right). \end{aligned}$$

The exact values of N_A and N_D will depend on the doping, but for representative values we can use the ones given in Figures 1.8(b) and 1.8(c) on page 15 of *Melissinos*. These are $N_A = 10^{16}$ cm^{-3} and $N_D = 10^{15}$ cm^{-3}. On page 9 of *Melissinos*, we learn that for germanium $n_i \approx 10^{13}$ cm^{-3} and $E_g = 0.7$ eV at room temperature (300 K). From there data we determine that $N_s \approx 8\ 10^{18}$ cm^{-3}. Plugging these values into the expression for the bias voltage we find that $V_{bi} = 0.596$ V, 0.295 V, and 0.025 V at 77 K, room temperature (300 K), and 500 K, respectively.

Since the bias voltage decreases with temperature, the performance of the junction becomes worse as the temperature decreases.

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4. Short questions.

(a) Using just the lattice parameter, compute the Fermi energy for aluminum and compare with the value given, for instance, in *Tipler*. (Hint: how many valance electrons per atom are there in Al?) If there is a discrepancy, it indicates that the effective mass of electrons in Al is different from the free electron mass.

Aluminum has a face-centered cubic lattice structure, and so it has four atoms per unit cell. The density and atomic weight (as found in the *CRC Handbook of Chemistry and Physics*) are 2.70 g/cm^3 and 26.98 g/mol, respectively. We learn from a periodic table that aluminum has three valence electron per atom. Therefore the volume occupied by one atom is (26.98 g/mol)(1 mol/6.022 10^{23} atoms)/(2.70 g/cm^3) = 1.66 10^{-23} cm^3/atom. Since there are four atoms per unit cell, the volume of the unit cell is four time this, or 6.64 10^{-23}

cm^3, and the lattice parameter is given by 4.05 10^{-8} cm. Since there are three valence electrons per atom, the number density of valence electrons is simply n_e = 3/(1.66 10^{-23} cm^3) = 18.1 10^{22} electrons/cm^3. From equation 1.4 on page 6 of *Melissinos* we see that

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n_e\right)^{2/3}.$$

Plugging in the appropriate quantities, we find that E_F = 7.38 10^{-21} J = 0.046 eV.

In Table 39-1 on page 1295 of *Tipler* (volume 2), the Fermi energy of aluminum is given as 11.7 eV. Therefore the effective mass of an electron in aluminum must be considerably different from that of a free electron.

(b) Using the measured resistivities, given by *Tipler* on page 722, compare the resistance (or, if you wish, the conductance) of an Al wire to that of a Cu wire having the same length and cross section.

From page 722 of *Tipler* we have $\rho_{\mathbf{Al}} = 2.8 \times 10^{-8}\ \Omega/\mathbf{m}$ and $\rho_{\mathbf{Cu}} = 1.7 \times 10^{-8}\ \Omega/\mathbf{m}$. On page 721 of *Tipler*, we learn that

$$R = \rho\frac{L}{A},$$

so if both wires have the same length and cross section then

$$\begin{aligned}\frac{R_{\mathbf{Al}}}{R_{\mathbf{Cu}}} &= \frac{\rho_{\mathbf{Al}}}{\rho_{\mathbf{Cu}}} \\ &= 1.65\end{aligned}$$

(c) Compare the resistance (or, if you wish, the conductance) of an Al wire to that of a Cu wire having the same length and weight.

Since the wires have the same weight we have $d_{\mathbf{Al}}A_{\mathbf{Al}}L = d_{\mathbf{Cu}}A_{\mathbf{Cu}}L$, or $A_{\mathbf{Al}}/A_{\mathbf{Cu}} = d_{\mathbf{Cu}}/d_{\mathbf{Al}}$, where d represents the density of the material. Therefore,

$$\begin{aligned}\frac{R_{\mathbf{Al}}}{R_{\mathbf{Cu}}} &= \frac{\rho_{\mathbf{Al}}}{\rho_{\mathbf{Cu}}}\frac{A_{\mathbf{Cu}}}{A_{\mathbf{Al}}} \\ &= \frac{\rho_{\mathbf{Al}}}{\rho_{\mathbf{Cu}}}\frac{d_{\mathbf{Al}}}{d_{\mathbf{Cu}}}.\end{aligned}$$

From Table 11-1 on page 333 of *Tipler* we see that $d_{\mathbf{Al}}/d_{\mathbf{Cu}} = 0.030$, so we have finally that $R_{\mathbf{Al}}/R_{\mathbf{Cu}} = 0.50$.

(d) You should have found from (b) and (c) that, at least by some criteria, Al is a better conductor than Cu. It is also much cheaper. Why then is Cu used for most electrical wiring?

One reason copper is used rather than aluminum is that aluminum oxide does not conduct electricity, while copper oxide does. Like most metals, aluminum and copper quickly develop a thin layer of metal oxide when exposed to air. This means that if you strip two ends of an aluminum wire and twist them together, current will not want to flow across the splice. If the same procedure is repeated with copper, however, one finds that current readily flows across the splice. Thus, despite the fact that aluminum is cheaper, in most applications it is more convenient to use copper instead.

Another reason is that aluminum tends to expand more when heated, which significantly reduces the lifetime of splices.

(e) Why is the filament of an incandescent light bulb made of tungsten, rather than steel or copper?

From pages B-14, B-40, and E-88 of the *CRC Handbook of Chemistry and Physics, 66th Edition*, we learn that the melting points of copper, tungsten, and steel are $1083\ ^\circ$C, $3410\ ^\circ$C, and $1500\ ^\circ$C, respectively. We also learn from page 278 of *Bloomfield* that tungsten sublimes very slowly at temperatures below its melting point. Thus tungsten filaments can be run much hotter than filaments made of copper and steel before the filament melts or the rate of sublimation becomes intolerable. Because it can be run hotter, the tungsten filament also produces a richer, whiter light that is more similar to the light of the sun. For this reason, tungsten filaments are used in incandescent light bulbs instead of copper or steel.

(f) Why has silicon become the standard semiconductor material for most purposes? What are possible alternative materials?

One reason for the prevalence of silicon in semiconductor devices is that silicon is a readily available material. Sand (i.e. quartz) is simply silicon dioxide. Another reason is that when people first started to work with semiconductors they chose to work with silicon, and over the years manufacturers have developed tricks to make semiconductor components smaller, faster, etc. that are specific to silicon. It would cost a great deal of money to modify these techniques for use with other elements, so manufacturers continue to work with the traditional silicon.

Alternative materials that are used include germanium and gallium arsenide.

(g) Why is silicon not suitable for a light emitting diode? What materials are used for this purpose?

A material such as gallium arsenide is much more suitable than silicon for LEDs because GaAs is *direct gap* semiconductor, while Si is an *indirect gap* semiconductor. In both materials the states near the top of the valence band have zero momentum, but in GaAs the states at the bottom of the conduction band also have zero momentum, while in Si they have nonzero momentum. This is because the wavefunction changes sign in going from one Si atom to the next on the edge of the cubic cell. (See the picture of the energy bands of Si on

page 308 of the *Physicist's Desk Reference*.) This means that the momentum of an electron in GaAs changes very little when it emits or absorbs a photon, and thus light emission can occur directly in this material. In Si, however, photon emission is an indirect process that cannot occur unless the conduction band electron has a secondary process by which it can dispose of its momentum. (The terms *direct gap* and *indirect gap* refer to whether or not the bottom of the conduction band lines up directly above the top of the valence band in a plot versus momentum.)

Gallium arsenide has a bandgap of 1.4 eV, which corresponds to a red photon. Thus GaAs is used to make red LEDs. A wider bandgap, resulting in the emission of yellow or green light, is obtained by replacing some of the gallium atoms with aluminum, or by replacing some of the arsenic atoms with phosphorus.

(h) In a p-n junction at zero external bias, what is the sign of the net electrical charge on the p side? On the n side?

The net electric charge is negative on the p side and positive on the n side. This is because when the two pieces of semiconductor first make contact, there is a higher concentration of positive carriers on one side of the junction and a higher concentration of negative carriers on the other. Thus there is a diffusive current and positive carriers flow from the p side to the n side and negative carriers flow from the n side to the p side. Once the electrons cross into the p side of the junction they annihilate with a hole and similarly for the holes that cross into the n side. The new charge distribution produces an electric via Gauss's law, and the direction of the electric field is such that it *opposes* the diffusion current. The current continues to flow until the system reaches equilibrium, where the current due to diffusion is exactly the opposite of that due to the electric field.