# Midterm Exam (221B), due Mar 22, 5pm

1. Use Thomas–Fermi model of atoms to answer the following questions.
   (a) Solve the differential equation numerically for neutral atoms and obtain a plot of Thomas–Fermi function $\chi(x)$ for $x < 20$.
   (b) Based on this result, argue why higher $l$ orbitals have higher energies with a given principal quantum number $n$.
   (c) Calculate the total binding energy of an atom.
   (d) Show that the "radius" of atoms depends only weakly on $Z$, consistent with the empirical fact. The radius is naively infinite in this model because the charge density extends smoothly to infinity. Define the radius $R$ instead to contain $Z-1$ electrons

$$Z - 1 = \int_0^R 4\pi r^2 dr \rho(r). \tag{1}$$

   Plot $R$ in Å as a function of $Z$.

2. Consider a nucleus as a sphere with a uniform charge density.
   (a) Calculate the Rutherford scattering cross section of an electron by a nucleus together with the form factor using the first Born approximation.
   (b) Comparing it to the data in J. B. Bellicard et al, *Phys. Rev. Lett.*, **19**, 527 (1967), estimate the size of Calcium nuclei, using the location of dips in the cross sections.
   (c) Comparing it to the data in J. B. Bellicard et al, *Phys. Rev. Lett.*, **19**, 242 (1967), estimate the size of lead nuclei, using the location of dips in the cross sections.
   (d) Discuss $A$ dependence of the size of nuclei.
   Note Even though the electrons used in these experiments are relativistic, it is still true that the form factor is the Fourier transform of the charge density to the extent that we ignore the nuclear recoil. Be careful, however, to use the electron momentum and energy with the relativistic formula $E = cp$, and regard the form factor a function of momentum trasnfer $q^2 = 2p^2(1 - \cos\theta)$.

3. Interatomic potential in a diatomic molecule can be well approximated by Morse potential,

$$V(r) = V_0(e^{-2(r-r_0)/b} - 2e^{-(r-r_0)/b}), \tag{2}$$

where $r$ is the distance between two nuclei. It turns out that energy levels can be obtained exactly for the bound states with this potential. Consider only the radial motion (vibration) of the molecule, and ignore rotation. In other words, the Schrödinger equation is

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r)\right)\psi(r) = E\psi(r). \tag{3}$$

Answer the following questions.

(a) Plot the inter-proton potential by Heitler–London (see lecture notes) and show that Morse potential with $b = 0.92a_0$, $r_0 = 1.64254a_0$, and $V_0 = 0.116\frac{e^2}{a_0}$ approximates it well.

(b) Rewrite the Schrödinger equation using the variable $\xi = K_0 b e^{-(r-r_0)/b}$. Use $K_0 = \sqrt{2\mu V_0}/\hbar$, $\kappa = \sqrt{-2mE}/\hbar$.

(c) At large $\xi$, show that $\psi(\xi) \sim e^{-c\xi}$. Determine the constant $c$.

(d) Define $\psi(\xi) = w(\xi)e^{-c\xi}$ and write down the equation for $w(\xi)$.

(e) Solve for $w(\xi)$ in power series: $w(\xi) = \xi^\alpha(1 + c_1\xi + c_2\xi^2 + \cdots + c_n\xi^n + \cdots)$. Determine $\alpha$, and obtain the recursion relation between $c_n$ and $c_{n-1}$.

(f) Unless power series expansion in $w(\xi)$ stops at finite $n$, $w(\xi) \sim e^{2c\xi}$ and does not give a normalizable $\psi(\xi)$. Therefore, at some $n$, $c_n$ must vanish. Show that the energy eigenvalues are therefore given by

$$E_n = -\frac{\hbar^2}{2\mu b^2}\left(K_0 b - n + \frac{1}{2}\right)^2. \tag{4}$$

Note Actually, $\xi$ extends only up to $K_0 b e^{r_0/b}$, but in practice it is quite large. Also for larger $\xi$, or equivalently small $r$, the Morse potential is no longer a good approximation but the potential behaves as $e^2/r$ and diverges. Therefore, requiring exponentially damping wave function for large $\xi$ is a good approximate method to solve the problem.

(g) Show that for $n \ll K_0 b$ the energy eigenvalues can be approximated by those of a harmonic oscillator $n\hbar\omega$. Determine $\omega$.

(h) Compare the first excitation energies for rotation, vibration, and electronic excitation, and verify that they are widely separated to justify Born–Oppenheimer approximation.