Problem set -4

11. Bound states and scattering states for an attractive square well.

This numerical exercise illustrates the relation between bound states and scattering resonances. Consider an attractive square well (depth -V$_0$) with width a=1. Use the notation from the class but we will set $m=1, \hbar=1$ and the attractive potential is in terms of $\lambda^2=2V_0$. Define $p^2=\lambda^2+k^2$. Let $u_k(r)=rR(r)$. Consider s-wave scattering, we can then write $u(r)=B\sin kr$ for r<1 and $u(r)=\sin(kr+\delta)$. We have derived the expression for the phase shift in the class.

(a) Show that

$$B^2=\frac{k^2}{k^2+\lambda^2\cos^2 p}$$

The B^2 measures the probability of finding the particle inside the potential well. Clearly the probability reaches a local maximum whenever cos p=0. This allows us to locate the resonances.

(b) From the solution of the bound state equation, find the value of λ (called λ_2) where the potential well can accommodate two bound states. For whatever λ_2 you choose, identify the binding energy of the second state. Now choose a value of λ which is slightly smaller than λ_2 until that you have only one bound state. Calculate the phase shift and B^2 for a range of k^2 from near zero till you pass the first resonance. This shows that as the potential becomes weaker the second bound state has been moved to become a resonance. Plot the phase shift near the resonance region, as well as B^2 and the s-wave cross section in the same region to see if the width from the cross section and from B^2 are very close to each other.

(c) For λ slightly greater than λ_2 so that the second resonance is barely bound. Calculate the scattering length a$_s$ and show that the position of the second bound state is given by E=$-\frac{1}{2a_s^2}$ (recall we use $m=1, \hbar=1$). Try another value of λ, and show that this relation is correct.

12. **Scattering from a hard sphere**.

In this exercise you will use partial wave expansion method to calculate the cross sections and differential cross sections. A hard sphere means that the potential is infinite for $r \le a$ and zero elsewhere.

(a) Low-energy limit. Calculate the phase shift for s-wave and show that the cross section is given by $4\pi a^2$-- four times the classical value.

(b) Calculate the phase shifts and plot the differential cross section for ka=5. Check how many partial waves you need to get reasonable convergence in the infinite sum. Note that classically the maximum angular momentum is 5. You can use Mathematica or any other programs to extract the values of spherical Bessel and Neuman functions.

(c) Go to the EM textbook and check out the expression for the diffraction of a disk of radius a by light and compare the diffraction pattern predicted there for the equivalent ka to the present one.

13. **Scattering by N scattering centers**--like by a crystal lattice.

Consider N static identical spherically symmetric scatters placed on a straight line such that the n-th scatterer is at the point (n-1)**a**. Choose **a** to be along the z-axis. Assume that the potential is weak and you can calculate the cross section using the Born approximation. Show that the differential cross section can be expressed as

$$\frac{d\sigma}{d\omega}(\theta,\phi) = \frac{d\sigma}{d\omega}(\theta,\phi)\,|_B\; F(q)^2$$

where the first term on the right is the Born cross section from a single scatterer and F(q) is called the structure factor. Find the structure factor as well. Sketch $F(q)^2$ vs scattering angle for N=4. (Note the similarity to radiation by antennas.)

14. **Normalization of continuum wave functions**.

Assume that the radial wave function R(r)=u(r)/r, the normalization for the bound state wave function is well understood. In this exercise we will walk through the procedure to normalize the continuum wavefunctions. In the asymptotic region, the continuum wave function can be written as

$$R_k(r) = u_k(r)/r \to \frac{A}{r}\sin(kr - \ell\pi/2 + \delta) \quad \text{as } r \to \infty \tag{1}$$

if we have a short range potential. If there is a Coulomb potential at large distance then you need to add a logarithmic term in the phase plus a Coulomb phase.

We say that the continuum wave function R_k is **normalized per unit momentum k** if

$$\int_0^\infty u_k(r)u_{k'}(r)dr = \delta(k-k') \tag{2}$$

Similarly we say that the continuum wave function R_E is normalized **per unit energy** if

$$\int_0^\infty u_E(r)u_{E'}(r)dr = \delta(E-E') \tag{3}$$

We want to derive what A should be if the wave functions are normalized to either scheme.

The expression (2) is equivalent to

$$\int_0^\infty u_k(r)dr \int_{k-\Delta}^{k+\Delta} u_{k'}(r)dk' = 1 \qquad (4)$$

We will use (4) to find out what A should be in (1).

Start with the Schrodinger equation for u_k and $u_{k'}$ and *do integration by parts* to construct expression like (4) except by setting the upper limit in r to a large number a. You can then use (1) for the u's at r=a. You will need the integral

$$\int_0^\infty \frac{\sin x}{x} dx = \frac{\pi}{2}$$

which you can prove by using contour integration. From this procedure prove that

$$A = \sqrt{\frac{2}{\pi}}$$

if the wave function is normalized in the k-scale and

$$A = \sqrt{\frac{2}{\pi k \hbar}}$$

if the wave function is normalized per unit energy as in equation (3).

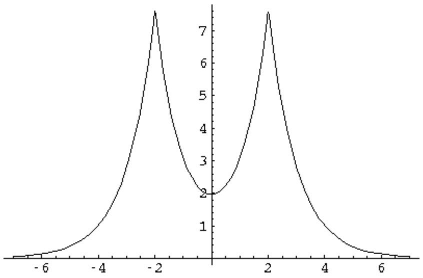
Note that different normalization will give you different expressions for the density of states. If the wave function is normalized per unit energy, then the density of states $\rho(E) = 1$. If the wave function is normalized per unit in k-space, then the density of state $\rho_k(E) = dn/dk = \frac{dn}{dE}\frac{dE}{dk} = \hbar k$.

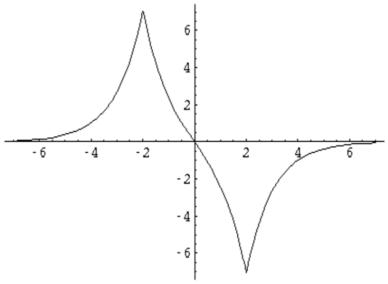
Note that according to Fermi Golden rule (later) the transition rate is proportional to $|< 0 | T | f_T >|^2 \ \rho_T(E)$ where f is the final state continuum wave function, 0 stands for the initial state and T is some transition operator. Clearly this exercise shows that the transition rate does not depend on how you normalize the continuum wave function.

15. In this exercise we learn how to **Construct approximate electronic wave functions of the $\mathbf{H_2^+}$ molecule.**

To understand the structure of atoms, you need to start with the hydrogen atom. To understand diatomic molecules, we start with $\mathbf{H_2^+}$. In this exercise we will go over the procedure of getting the molecular orbitals and molecular potential energies qualitatively and derive the quantum numbers. The two protons are assumed to be fixed in space with separation R, and we want to know what are the eigenstates of the electron as R is varied.

(a) Recall Prob. 6 you worked out the wave function of an electron in an attractive delta potential and the case of two delta potentials separated by R. In the later case, the first solution of the wavefunction is symmetric and the second solution is antisymmetric. We will use **gerade (g)** and **ungerade (u)** to describe each, respectively. Clearly at large distance R, the two wavefunctions can be written approximately as f(x-R/2) +f(x+R/2) and the second solution as f(x-R/2)-f(x+R/2), the gerade and ungerade states. The gerade state is lower in energy and has larger density in the region between the two centers. They should look like

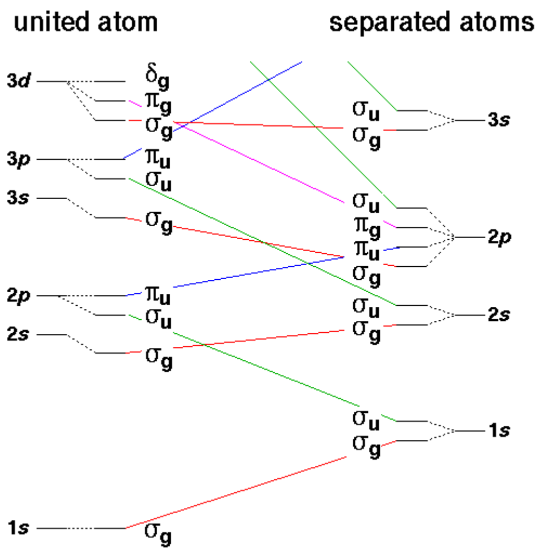




(b) We will use this concept to construct the "correlation diagram" of $\mathbf{H_2^+}$**.** The electron can associate with one or the other protons. We will use the internuclear axis as the quantization axis and use σ for m=0, π for |m|=1 and δ for |m|=2. For large R, the two 1sσ orbital from each center can form gerade and ungerade combinations. Thus write the two states as σ_g 1s and σ_u 1s, respectively. **Sketch the wavefunctions for these two states in a plane containing the internuclear axis**, indicate regions of + and - of the total wavefunction.

(c) Next you can construct the similar combination from 2s, and clearly you can get σ_g 2s and σ_u 2s, and again you know the gerade state is lower than the ungerade state. The next that you can do is to start from 2p. You can start with $2p_0$ from which you can obtain σ_g 2p and σ_u 2p. From $2p_1$ and $2p_{-1}$ first you can construct $2p_x$ and $2p_y$ for each atom. Of course they are degenerate with $2p_0$ or $2p_z$ since we use z as the quantization axis. Now try to combine $2p_x$ from each center to form π_g 2p and π_u 2p states. **Sketch the wavefunction of these four states.** Based on the relative magnitude of the density between the two centers justify that the relative energies should be $\sigma_g < \pi_u < \pi_g < \sigma_u$ for orbitals constructed from 2p. Note that the π_g 2p and π_u 2p are doubly degenerate since they can be constructed from either $2p_x$ or from $2p_y$.

(d) Now consider the other limit when the two protons are on top of each other ($R \rightarrow 0$), you would have hydrogen-like system, and you can label the states by hydrogenic quantum numbers. Assume that 2s is slightly below 2p. If you shift one of the proton slightly, you add an electric field and it will splits $2p_z$ and $2p_x$ (or $2p_y$). Which one will have lower energies? Follow this procedure, you can order the energy levels of $\mathbf{H_2^+}$ when the two protons are near each other (the united atom limit). In part (c) you have worked out the relative energies of H_2^+ in the separated atom limit. Now you need to connect the two regions, keeping in mind that the good quantum numbers are good for the whole curve. By doing so, you get the correlation diagram of $\mathbf{H_2^+}$**.**



More precise calculation will give you the real curves, but you see how the curves can be labelled. You can use united atom labels such as 2p σ_u from the united-atom limit or σ_g 2p from the separated atom limit.

Here is the actual potential curves for H_2^+.