Homework 2

Due Feb. 15, beginning of class

This exercise is an example of multichannel scattering. We will take the simplest example of a two-channel problem. The radial Schrödinger equation is given by (in atomic units)

$$\left(-\frac{1}{2\mu}\mathbf{I}\frac{d^2}{dR^2}+\mathbf{V}\right)\mathbf{F}=E\mathbf{F}$$

with

$$\mathbf{V}=\begin{pmatrix} \frac{a+b}{(1+c)R} & \mathcal{E}\frac{R}{2}d \\ \mathcal{E}\frac{R}{2}d & \frac{a-b}{(1-c)R}-\omega \end{pmatrix}.$$

The various terms in this expression are defined as

$$\begin{aligned} a &= (1+R)e^{-2R} \\ b &= \left(1-\frac{2R^2}{3}\right)e^{-R} \\ c &= \left(1+R+\frac{R^2}{3}\right)e^{-R} \\ d &= \frac{1}{2}(1-\tanh(R-6.5)). \end{aligned}$$

In addition, we will assume $\mu = 918$ a.u. and $\omega = 0.06$ a.u., and we will consider both $\mathcal{E}$=0.001 and 0.005 a.u.

If we imagine these are Born-Oppenheimer potentials, then this Schrödinger equation models the process of predissociation (see the discussion on p. 555-556 of Bransden and Joachain). We will see later this semester that it also models the behavior of a molecule in an intense laser field via the Floquet representation. For now, though, we will treat it as a scattering problem. We will ignore angular momentum in this example and concentrate on the multichannel aspects.

(a) Plot the diabatic potentials. Calculate the energies of any bound states for these potentials (i.e. ignore the coupling).

(b) Calculate and plot the adiabatic potentials for each value of $\mathcal{E}$, showing clearly the avoided crossing that emerges. Discuss the effect of changing $\mathcal{E}$ between the two sets of potentials. Compare the energy gap you find with the simple estimate predicted by the two-channel linear model we discussed in class. Calculate the energies of any bound states for these potentials, ignoring any non-adiabatic coupling.

(c) Calculate and plot all possible cross sections for total energies in the range –0.06 a.u. to 0.06 a.u. for each $\mathcal{E}$.

(d) Discuss your cross sections physically as a function of energy and of $\mathcal{E}$. Make sure to comment on any resonances you find and on the threshold behaviors you observe.

(e) For the resonances, find their positions and widths. Do these resonances correlate to any of the bound states you found in (a) or (b)? Identify each as a *shape* or *Feshbach* resonance. Justify your label.

(f) Pick one of the resonances you found and plot the radial wave functions for three energies: two resonance widths below the resonance and two above, and right at the resonance energy. Discuss these wave functions physically, relating their behavior to the resonance.