P3317 HW from Lecture 16+17 and Recitation 9

Due Oct 30, 2018

Problem 1. Born-Openheimer potential for H_2^+

The H_2^+ ion consists of two protons, and one electron. Within the Born Oppenheimer approximation, we "integrate out" the electron to produce an effective potential felt by the protons. The Born-Oppenheimer potential is

$$V(R_1 - R_2) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|R_1 - R_2|} + \mathcal{E}(R_1 - R_2) \tag{1}$$

where the first term is the direct interaction between the protons, and the second term is the effective interaction from the electrons. In the case of H_2^+, this electronic contribution is the eigenvalue of a single electron problem,

$$\mathcal{E}\psi(r) = -\frac{\hbar^2}{2m_e}\nabla^2\psi(r) - \frac{e^2}{4\pi\epsilon_0}\left[\frac{1}{|R_1 - r|} + \frac{1}{|R_2 - r|}\right]\psi(r). \tag{2}$$

Adimensionalized, this equation reads

$$\mathcal{E}\psi(r) = -\frac{1}{2}\nabla^2\psi(r) - \left[\frac{1}{|R_1 - r|} + \frac{1}{|R_2 - r|}\right]\psi(r). \tag{3}$$

We will work with this adimensionalized form. Note, I have used the same symbols for dimensional and dimensionless quantities. This is very sloppy, but is pretty typical. I hate to encourage bad habits, but on the flip side, it is important to get used to interpreting these things.

1.1. How is the dimensionless energy related to the dimensionful energy? (Write the conversion factor in terms of the Rydberg energy E_R. Note: Wikipedia uses the symbol Ry instead of E_R.) How is the dimensionless length related to the dimensionful length? (Write the conversion factor in terms of the Bohr radius a_0.)

Solution 1.1 (2 points)**.** This is a conversion that we have done a lot in this class. We want to take

$$E_0 = \left(\frac{\hbar^2}{mr_0^2}\right) = \left(\frac{e^2}{4\pi\epsilon_0 r_0}\right). \tag{4}$$

Solving for r_0, we have

$$r_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2 m} = 5.20 \times 10^{-11}\text{m} = a_0. \tag{5}$$

and

$$E_0 = \frac{me^4}{16\pi^2\hbar^2\epsilon_0^2} = 27.2eV = 2E_R. \tag{6}$$

If you are interested in an analytic variational solution to Eq. (2) – you can look at Griffiths Chapter 7.3. It is kind of ugly though, because it is a 3D problem without spherical symmetry. A few years ago I had a homework problem that worked through it, but many students found it dissatisfying and mathematical. Instead we will numerically consider the 1D analog

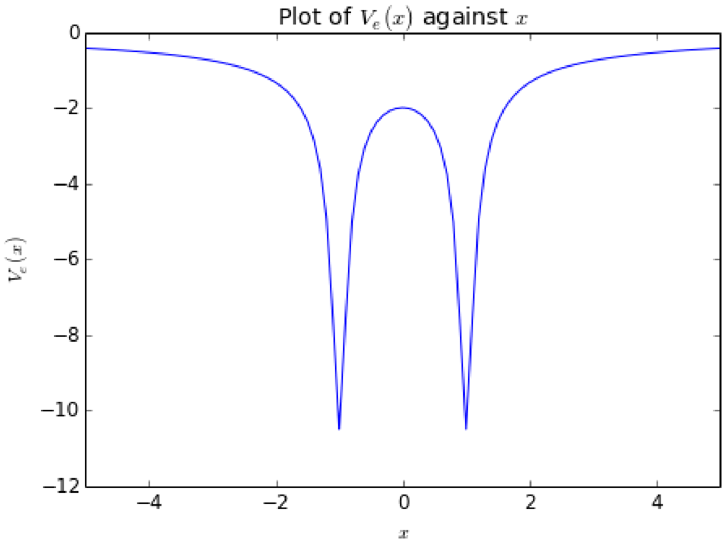
$$\mathcal{E}\psi(x) = -\frac{1}{2}\partial_x^2\psi(x) - \big[W(x - X_1) + W(x - X_2)\big]\psi(x), \tag{7}$$

where $W(x)$ is the Coulomb interaction between the nucleus and the electron. It turns out that the $1/x$ potential is not that well behaved in 1D, so we will use a truncated version

$$W(x) = \frac{1}{\sqrt{x^2 + \delta^2}}. \tag{8}$$

We will take δ to be a small number, so that this is similar to a $1/x$ potential. For your numerics take $\delta = 0.1$.

1.2. Plot the function $V_e(x) = -W(x-X_1)-W(x-X_2)$ for x running from -5 to 5 with $X_1 = -3/2$ and $X_2 = 3/2$. Choose a scale for your axes so that the main features can be seen. Label your axes. *Do not submit a program which plots this, just submit this graph.*



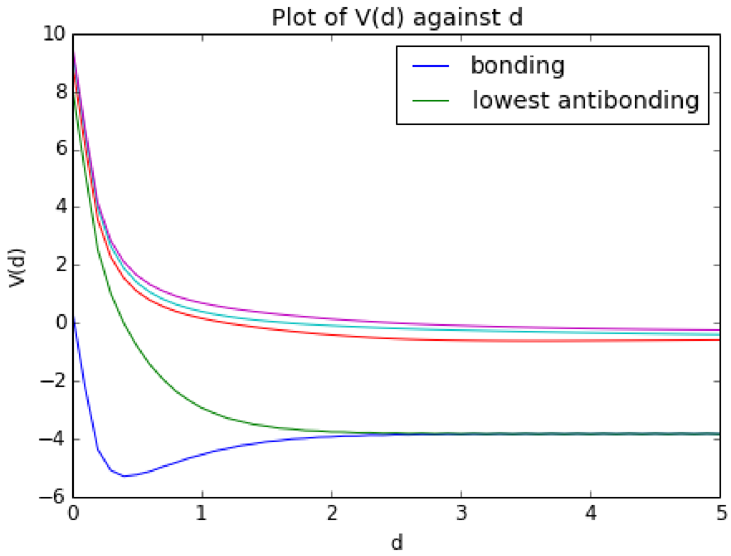
Solution 1.2 (5 points)**.**

1.3. Write a program which will numerically solve Eq. (7), finding the 5 eigenvalues closest to -8, for fixed $d = X_1 - X_2$. [These will be the 5 lowest eigenvalues.] Take $\delta = 0.1$, and a real space grid running from $x = -10$ to 10 with a grid spacing of 0.1. Place the two "protons" symmetrically, $X_1 = d/2$ and $X_2 = -d/2$.

To make `eigsh` return eigenvalues close to -8, make one of its arguments `sigma=-8`.

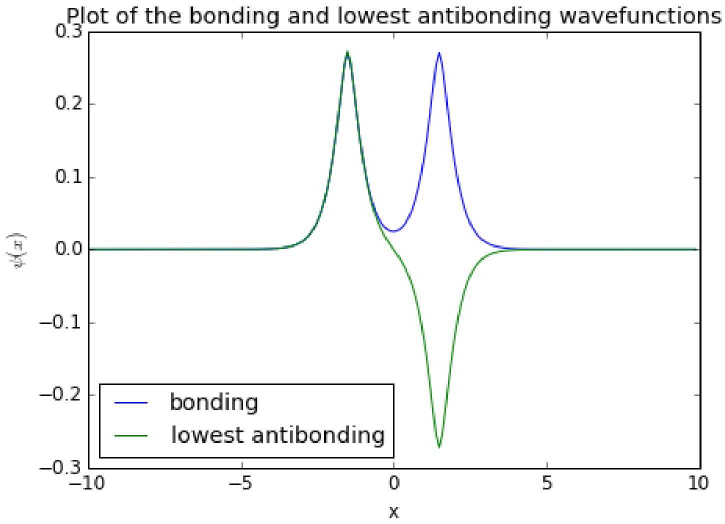
Tabulate the function $\mathcal{E}(d)$, for these 5 states, with d running from 0 to 5 in steps of 0.1. *Do not hand this in – this is just so that you can plot V.*

Make a properly labeled plot of the Born-Oppenheimer potential $V(d) = \mathcal{E}(d) + W(d)$ as a function of d for these 5 orbitals. [We add $W(d)$, as this is the direct interaction between the protons.] *Do not submit your program, just submit this graph with your homework.* Annotate your graph (either by hand or with the computer) to point out the potential coming from the bonding orbital and from the lowest antibonding orbital.



Solution 1.3 (5 points).

1.4. Plot the electronic wavefunction for the lowest bonding and antibonding orbitals when the nuclei are separated by a distance $d = 3$. Label your graph, and mark which is bonding, and which is antibonding. *Do not submit your program, just submit the graph.*



Solution 1.4 (5 points).

Problem 2. Semiclassical Molecule I want you to model the excitation spectrum of a neutral diatomic molecule. Generically there are three types of excitations:

electronic – an electron is promoted to a higher level

vibrational – the distance between the two atoms oscillates

rotational – the atoms rotate around one-another

Here you will estimate the energy scale of each of these excitations.

2.1. What is the typical bond length in a diatomic molecule (such as CO, or H_2)? Feel free to look this up in a textbook or on the web. You could also figure it out with dimensional analysis. We just need an order of magnitude.

Solution 2.1 (2 points)**.** Dimensional analysis suggests it should be of order the Bohr radius (0.5 Angstroms). In fact, the bond lengths of H_2 and CO are $0.74\,\text{Å}$ and $1.128\,\text{Å}$ respectively.

2.2. One can roughly model the electronic states by considering the electrons to be trapped in a square box of size given by your solution to 2.1. If so, what is the energy scale of electronic excitations (in eV)?

Solution 2.2 (2 points)**.** Using $L = 1\,\text{Å}$, the ground state energy for a particle trapped in a cube of sides L is

$$3 \times \frac{\hbar^2\pi^2}{2mL^2} = 3 \times \frac{(6.62606957 \times 10^{-34})^2 \times \frac{1}{4\pi^2} \times \pi^2}{2 \times 9.10938291 \times 10^{-31} \times (10^{-10})^2}\,\text{J} = 1.8 \times 10^{-17}\,\text{J} \sim 100\,\text{eV} \tag{9}$$

This is a bit on the big side. The electronic wavefunction is a bit more spread out than this, and a few eV is more realistic.

One can estimate the vibrational energy by approximating the Born-Openheimer potential as a harmonic oscillator $V(r) \sim \frac{1}{2}k(r - r_0)^2$, where r_0 is the equilibrium size of the molecule, and r is the separation between the nucleii. We will use dimensional analysis to estimate the constant k.

2.3. What units does k have?

Solution 2.3 (1 point)**.** The spring constant has units of Energy/length^2, or mass/time^2 or force/length.

2.4. The Born Oppenheimer potential comes from the solution of an electronic problem in the presence of the nuclei. List the dimensional quantities that it seems reasonable for k to depend on. Can you construct a unique k from these? If you have too many dimensional quantities, check to see if any of them are similar in size. Since we are looking for a numerical answer, these all are equivalent for us. If you still have too many, critically evaluate them and discard ones which are less likely to play a role in this physics. If you have too few dimensional quantities, look at Eq. (2). This is the equation for the Born-Oppenheimer potential, so they should all be there. Maybe you missed a fundamental constant like $\hbar$?

Use these numbers to estimate k (in physical units).

Solution 2.4 (2 points)**.** There are a number of arguments here. The simplest is that the only relevant energy scale is the Rydberg energy E_R, and the only relevant length scale is the Bohr radius, and hence one expects

$$k \sim \frac{E_R}{a_0^2} \sim \frac{10\text{eV}}{0.2\text{Å}^2} \sim 50\frac{\text{eV}}{\text{Å}^2}. \tag{10}$$

A slightly longer argument is to note that

- We expect Planck constant $\hbar$ to be involved.
- Since the actual interactions are electrostatic, we also expect $\frac{e^2}{4\pi\epsilon_0}$ to be involved.
- Part of the interactions is the electrostatic attraction of the nuclei to the electron cloud. Since the size of the electron cloud is important in this case, we expect the electron mass m_e to be involved.
- As m_p appears in the kinetic terms of the nuclei, it might affect the separation of the nuclei and hence the potential seen by the electron, and hence the size of the electron cloud, but it is clear from this long chain of argument that the effects are very indirect. Since it has the same dimensions as m_e, it seems more reasonable to consider m_e in place of m_p.

Let us now construct a unique k out of $\hbar$, $\frac{e^2}{4\pi\epsilon_0}$ and m_e. Keeping in mind that

$$[\hbar] = \frac{ML^2}{T}, \quad \left[\frac{e^2}{4\pi\epsilon_0}\right] = \frac{ML^3}{T^2}, \quad [m_e] = M \tag{11}$$

We find that

$$k \sim m_e^3 \left(\frac{e^2}{4\pi\epsilon_0}\right)^4 \hbar^{-6} - 1557\,\frac{\text{J}}{\text{m}^2} \sim 100\frac{\text{eV}}{\text{Å}^2}. \tag{12}$$

2.5. The energy of these vibrations should be $\hbar\omega = \hbar\sqrt{k/m}$, where m should be a the nuclear mass. Estimate the energy of vibrational excitations (in eV).

Solution 2.5 (2 points)**.** The argument that I like best is that the

$$\hbar\omega = \sqrt{\frac{m_e}{m}}\hbar\sqrt{\frac{k}{m_e}}, \tag{13}$$

but that $\hbar\sqrt{k/m_e}$ must be a typical electronic energy scale. The mass ratio $\sqrt{m/m_e} \sim 50$, so the vibrational energy should be about 50 times smaller than the electronic excitation energy. Using our previous estimate, this would be of order eV.
Alternatively, we can directly use our $k = 100eV/\AA^2$, and find

$$\hbar\omega = \hbar\sqrt{\frac{k}{m_p}} = 0.6\,\text{eV}. \tag{14}$$

2.6. For the rotational energy scales, we can use the classical expression, $E = L^2/2I$. Quantum mechanically, what are the allowed values of L?

Solution 2.6 (1 point)**.** Quantum-mechanically, $L^2 = \hbar^2\ell(\ell+1)$, where ℓ is a nonnegative integer.

2.7. From the geometry of the diatomic molecule, estimate the moment of inertia I.

Solution 2.7 (2 points)**.** Treating it as a dumb-bell shaped molecule,

$$I = 2 \times m_p \times \left(\frac{L}{2}\right)^2 = 8.4 \times 10^{-48}\,\mathrm{kgm}^2 \tag{15}$$

2.8. Estimate the energy (in eV) of the rotational excitations.

Solution 2.8 (2 points)**.** The argument that I like best is that

$$E_{\mathrm{rot}} = \frac{L^2}{2I} \sim \frac{\hbar^2}{ma_0^2} \sim \frac{m_e}{m}\frac{\hbar^2}{m_e a_0^2} \tag{16}$$

the last quantity is the electronic energy, and hence $E_{\mathrm{rot}} \sim 0.05\mathrm{eV}$.
Alternatively, I plug in $L = \hbar$, and I from Eq. (15) to get

$$\frac{L^2}{2I} = \frac{\hbar^2}{I} = 0.008\,\mathrm{eV} \tag{17}$$

One shouldn't sweat these factors of 5 in this sort of estimation.

Problem 3. Paschen-Back effect The electronic and nuclear spins of Rubidium-87 are coupled by the "hyperfine interaction." This is basically the dipole-dipole coupling between these spins. Of course, the typical magnetic moment of a nucleus is very very small, so the coupling is quite weak. Nonetheless, one can detect this splitting by "Magnetic Resonance" – the same technology which is used in the "Magnetic Resonance Imaging" used for medical diagnosis.

The model used for the Hyperfine splitting is

$$H = -g_e\mu_e\hat{S}_zB - g_{\mathrm{Rb}}\mu_N\hat{I}_zB + A_{hf}\hat{\mathbf{S}}\cdot\hat{\mathbf{I}} \tag{18}$$

where B is a magnetic field in the $\hat{z}$ direction. Numerically $\mu_e = 10^{-23}\mathrm{J/T}$, and $\mu_N = 5\times10^{-27}\mathrm{J/T}$, $g_e \approx 2/\hbar$, $g_{\mathrm{Rb}} \approx 3/\hbar$, and $A_{hf} = \hbar \times 1.5\mathrm{GHz}/\hbar^2$. The nuclear spin is 3/2. and the electronic spin is 1/2. The operator $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ corresponds to the electronic spin, and $\hat{\mathbf{I}} = (\hat{I}_x, \hat{I}_y, \hat{I}_z)$ corresponds to the nuclear spin.

We want to understand the behavior of the energy levels as a function of the magnetic field.

3.1. Give two independent dimensionless numbers that can be made from $\mu_e, \mu_N, B, A_{hf}, \hbar$? [Hint there are only two such numbers, and as usual they are not unique.]

Solution 3.1 (3 points)**.** The simplest thing is to see that there are three energies in the Hamiltonian: $\mu_e\hbar B$, $\mu_N\hbar B$, $A_{hf}\hbar^2$. Their ratios will be dimensionless, for example:

$$\begin{aligned} \Pi_1 &= \mu_b/\mu_e && (19) \\ \Pi_2 &= \frac{\mu_e B}{\hbar A_{hf}}. && (20) \end{aligned}$$

As always, any products or ratios of these also work.

3.2. Given that the ratio μ_b/μ_e is so small, it is reasonable to drop it from the problem, and consider the simplified model

$$H = -g_e\mu_e S_z B + A_{hf} S \cdot I. \tag{21}$$

Convert this equation to dimensionless units. Measure angular momenta in units of $\hbar$, energy in units of $A_{hf}\hbar^2$ and B in units of $A_{hf}\hbar/g_e\mu_e$. **Use this dimensionless expression for the rest of the problem. I do not want to see you write A_{hf} or g or $\hbar$ for the rest of this problem.** [Except for your graph at the end.]

Solution 3.2 (2 points)**.** If we put bars on our dimensionless quantities,

$$\begin{aligned} \bar{S} &= \frac{S}{\hbar} && (22) \\ \bar{I} &= \frac{I}{\hbar} && (23) \\ \bar{H} &= \frac{H}{A_{hf}\hbar^2} && (24) \\ \bar{B} &= B\frac{g_e\mu_e}{\hbar A_{hf}}. && (25) \end{aligned}$$

We then have

$$\bar{H} = -\bar{B}\bar{S}_z + \bar{S} \cdot \bar{I}. \tag{26}$$

In the remainder we will leave off the bars.

For the following two subproblems it will be helpful to use the fact that for a spin-1/2 S the states obey: (note in our dimensionless units, all of these hbars are equal to unity)

$$\begin{aligned} S_z|S = 1/2, m_s = 1/2\rangle &= (\hbar/2)|S = 1/2, m_s = 1/2\rangle && (27) \\ S_z|S = 1/2, m_s = -1/2\rangle &= (-\hbar/2)|S = 1/2, m_s = -1/2\rangle && (28) \\ S_+|S = 1/2, m_s = 1/2\rangle &= 0 && (29) \\ S_+|S = 1/2, m_s = -1/2\rangle &= \hbar|S = 1/2, m_s = 1/2\rangle && (30) \\ S_-|S = 1/2, m_s = 1/2\rangle &= \hbar|S = 1/2, m_s = -1/2\rangle && (31) \\ S_-|S = 1/2, m_s = -1/2\rangle &= 0. && (32) \end{aligned}$$

[If you take PHYS 4443 you will derive these.] Similarly, for a spin-3/2 I the states obey:

$$
\begin{aligned}
I_z|I=3/2, m_I=3/2\rangle &= (3\hbar/2)|I=3/2, m_I=3/2\rangle && (33)\\
I_z|I=3/2, m_I=1/2\rangle &= (\hbar/2)|I=3/2, m_I=1/2\rangle && (34)\\
I_z|I=3/2, m_I=-1/2\rangle &= (-\hbar/2)|I=3/2, m_I=-1/2\rangle && (35)\\
I_z|I=3/2, m_I=-3/2\rangle &= (-3\hbar/2)|I=3/2, m_I=-3/2\rangle && (36)\\
I_+|I=3/2, m_I=3/2\rangle &= 0 && (37)\\
I_+|I=3/2, m_I=1/2\rangle &= \sqrt{3}\hbar|I=3/2, m_I=3/2\rangle && (38)\\
I_+|I=3/2, m_I=-1/2\rangle &= \sqrt{7/2}\hbar|I=3/2, m_I=1/2\rangle && (39)\\
I_+|I=3/2, m_I=-3/2\rangle &= \sqrt{3}\hbar|I=3/2, m_I=-1/2\rangle && (40)\\
I_-|I=3/2, m_I=3/2\rangle &= \sqrt{3}\hbar|I=3/2, m_I=1/2\rangle && (41)\\
I_-|I=3/2, m_I=1/2\rangle &= \sqrt{7/2}\hbar|I=3/2, m_I=-1/2\rangle && (42)\\
I_-|I=3/2, m_I=-1/2\rangle &= \sqrt{3}\hbar|I=3/2, m_I=-3/2\rangle && (43)\\
I_-|I=3/2, m_I=-3/2\rangle &= 0. && (44)
\end{aligned}
$$

[Again, you will derive this in PHYS 4443.] In recitation you had a chance to play with a computer algebra system which knows about these operators.

If we specify both the electronic and nuclear spin quantum numbers, we will write something like

$$|m_s=1/2, m_I=1/2\rangle = |S=1/2, m_s=1/2\rangle \otimes ||I=3/2, m_I=1/2\rangle. \qquad (45)$$

The S operators only act on the S quantum numbers, and similarly with I. For example

$$S_-|m_s=1/2, m_I=1/2\rangle = \hbar|m_s=-1/2, m_I=1/2\rangle \qquad (46)$$

or

$$I_+|m_s=1/2, m_I=1/2\rangle = \sqrt{3}\hbar|m_s=1/2, m_I=3/2\rangle. \qquad (47)$$

Finally, you will find the following identity useful:

$$
\begin{aligned}
S\cdot I &= S_zI_z + S_xI_x + S_yI_y && (48)\\
&= S_zI_z + \frac{1}{2}\left(S_+I_- + S_-I_+\right) && (49)
\end{aligned}
$$

3.3. There is a unique eigenstate of this Hamiltonian with $m_f = m_s + m_I = 2$, it is $|m_s = 1/2, m_I = 3/2\rangle$. Calculate its energy as a function of B. This linear behavior is similar to what happens if you just have a single level of a spin-1/2 electron – it is known as the Zeeman effect.

[Hint: Just act on this state with H, and use the given rules.]

Solution 3.3 (2 points)**.** Using the identity in Eq. (49), we note that

$$S \cdot I|m_s = 1/2, m_I = 3/2\rangle \quad = \quad S_z I_z I|m_s = 1/2, m_I = 3/2\rangle, \tag{50}$$

since both S_+ and I_+ give zero when they act on this state. Thus (in our dimensionless variables)

$$S \cdot I|m_s = 1/2, m_I = 3/2\rangle \quad = \quad \frac{3}{4} I|m_s = 1/2, m_I = 3/2\rangle. \tag{51}$$

Additionally,

$$S_z I|m_s = 1/2, m_I = 3/2\rangle \quad = \quad \frac{1}{2} I|m_s = 1/2, m_I = 3/2\rangle. \tag{52}$$

Hence

$$HI|m_s = 1/2, m_I = 3/2\rangle \quad = \quad \left[-\frac{1}{2}B + \frac{3}{4}\right] I|m_s = 1/2, m_I = 3/2\rangle. \tag{53}$$

Thus this is an energy eigenstate with energy

$$E = \frac{3}{4} - \frac{1}{2}B. \tag{54}$$

3.4. Find the eigenstates and eigenvalues of this Hamiltonian which have $m_f = 1$. These are linear combinations of

$$|A\rangle \quad = \quad |m_s = 1/2, m_I = 1/2\rangle \tag{55}$$

$$|B\rangle \quad = \quad |m_s = -1/2, m_I = 3/2\rangle \tag{56}$$

That is write $\psi = \alpha|A\rangle + \beta|B\rangle$, and write down a matrix eigenvalue equation for the vector

$$\vec{\psi} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \tag{57}$$

You will need to find the eigenvalues of that 2×2 matrix.

Plot energy vs magnetic field Be sure to label the axes so we know what units you are using. Choose your scale so that the important features can be seen.

This is the Paschen-Bach effect, sometimes called the nonlinear Zeeman effect.

Solution 3.4 (9 points – 4 for the Hamiltonian matrix, 1 for eigenvalues, 4 for graph)**.** We first note that

$$I \cdot S|A\rangle = \left(S_zI_z + \frac{1}{2}S_+I_- + \frac{1}{2}S_-I_+\right)|A\rangle. \tag{58}$$

These terms are

$$S_zI_z|A\rangle = \frac{1}{4}|A\rangle \tag{59}$$

$$S_+I_-|A\rangle = 0 \tag{60}$$

$$S_-I_+|A\rangle = \sqrt{3}|B\rangle. \tag{61}$$

Similarly

$$S_zI_z|B\rangle = -\frac{3}{4}|B\rangle \tag{62}$$

$$S_+I_-|B\rangle = \sqrt{3}|A\rangle \tag{63}$$

$$S_-I_+|B\rangle = 0. \tag{64}$$

Next we note that

$$S_z|A\rangle = \frac{1}{2}|A\rangle \tag{65}$$

$$S_z|B\rangle = -\frac{1}{2}|B\rangle. \tag{66}$$

Putting this together we have

$$H|A\rangle = \left(\frac{1}{4} - \frac{B}{2}\right)|A\rangle + \sqrt{3}/2|B\rangle \tag{67}$$

$$H|B\rangle = \left(-\frac{3}{4} + \frac{B}{2}\right)|B\rangle + \sqrt{3}/2|A\rangle. \tag{68}$$

Solution 3.4. Following the question, we now write $|\psi\rangle = \alpha|A\rangle + \beta|B\rangle$, in which case

$$\begin{aligned} H|\psi\rangle &= \left[\alpha\left(\frac{1}{4} - \frac{B}{2}\right) + \beta\frac{\sqrt{3}}{2}\right]|A\rangle && (69) \\ &\quad + \left[\alpha\frac{\sqrt{3}}{2} + \beta\left(-\frac{3}{4} + \frac{B}{2}\right)\right]|A\rangle. && (70) \end{aligned}$$

We equation this with

$$E|\psi\rangle = E\alpha|A\rangle + E\beta|B\rangle. \tag{71}$$

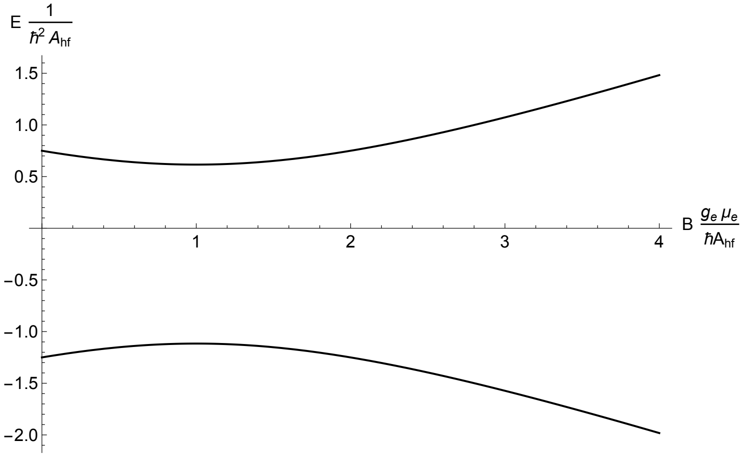
Equating the coefficients yields

$$E\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \frac{1}{4} - \frac{B}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{3}{4} + \frac{B}{2} \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \tag{72}$$

This is an eigenvalue problem, where the eigenvalues are

$$E = \frac{-1 \pm 2\sqrt{4 - 2B + B^2}}{4}. \tag{73}$$

We can then plot these energies, finding



Problem 4. Calculus of Variation

Some of you said that your analytical mechanics course did not formally define the math behind "Calculus of Variation". This problem works you through the formal definition. In a typical classical mechanics class one spends several weeks on this, so this is going to be a bit abbreviated.

Let $y(x)$ be an arbitrary function. We can define a functional $F[y]$ as an object which takes the function y and spits out a number. For example,

$$F[y] = \frac{1}{2}\int \frac{dx_1\,dx_2}{|x_1 - x_2|}y(x_1)y(x_2). \tag{74}$$

The variational derivative is defined by

$$\frac{\delta F[y]}{\delta y(x)} = \lim_{\eta\to 0} \frac{F[y+\eta s_x] - F[y]}{\eta}, \tag{75}$$

where $s_x(t) = \delta(t-x)$ is a Dirac delta function. So in this example

$$F[y+\eta s_x] = \frac{1}{2}\int \frac{dx_1\,dx_2}{|x_1 - x_2|}\left(y(x_1) + \eta\delta(x_1 - x)\right)\left(y(x_2) + \eta\delta(x_2 - x)\right). \tag{76}$$

4.1. Write $(F[y+\eta s_x] - F[y])/\eta$ as an integral over x_1 and x_2. Simplify the expression, but don't do the integrals. You should find two terms, one which is proportional to η, and one that is independent of η.

Solution 4.1 (2 points)**.** Multiplying out Eq. (76), we have

$$F[y+\eta s_x] = \frac{1}{2}\int \frac{dx_1\,dx_2}{|x_1 - x_2|}\left(y(x_1)y(x_2) + \eta\delta(x_1 - x)y(x_2) + \eta y(x_1)\delta(x_2 - x) + \eta^2\delta(x_1 - x)\delta(x_2 - x)\right) \tag{77}$$

Thus

$$\begin{aligned} \frac{F[y+\eta s_x] - F[y, s_x]}{\eta} &= \frac{1}{2}\int \frac{dx_1\,dx_2}{|x_1 - x_2|}\left(\delta(x_1 - x)y(x_2) + y(x_1)\delta(x_2 - x)\right) && (78) \\ &+ \frac{\eta}{2}\int \frac{dx_1\,dx_2}{|x_1 - x_2|}\delta(x_1 - x)\delta(x_2 - x) && (79) \end{aligned}$$

4.2. Since we will be taking the limit $\eta \to 0$, neglect the term proportional to η. Calculate the integrals for the other term, and hence evaluate

$$\frac{\delta F[y]}{\delta y(x)} = \lim_{\eta\to 0} \frac{F[y+\eta s_x] - F[y]}{\eta}. \tag{80}$$

Solution 4.2 (2 points)**.**

$$\begin{aligned} \frac{\delta F[y]}{\delta y(x)} &= \frac{1}{2}\int \frac{dx_1\,dx_2}{|x_1 - x_2|}\left(\delta(x_1 - x)y(x_2) + y(x_1)\delta(x_2 - x)\right) && (81) \\ &= \frac{1}{2}\int \frac{dx_2}{|x - x_2|}y(x_2) + \frac{1}{2}\int \frac{dx_1}{|x_1 - x|}y(x_1) && (82) \\ &= \int \frac{ds}{|x - s|}y(s). && (83) \end{aligned}$$

4.3. Consider a more generic symmetric Kernel,

$$G[y] = \frac{1}{2}\int dt_1\,dt_2\,K(t_1,t_2)y(t_1)y(t_2), \tag{84}$$

where $K(t_1,t_2) = K(t_2,t_1)$ is simply a function of two variables. Using any technique at your disposal, calculate

$$\frac{\delta G[y]}{\delta y(t)}. \tag{85}$$

Note: I changed the name of the dummy variables, but the logic should still be clear.

Solution 4.3 (2 points)**.** The only difference here compared to the last problem is that we need to replace $1/|x_1 - x_2|$ with $K(x_1, x_2)$. Thus without any extra work,

$$\frac{\delta G[y]}{\delta y(t)} = \int ds\ K(t,s)y(s). \tag{86}$$

4.4. Consider a Kernel of the form:

$$K(t_1, t_2) = -m\delta''(t_1 - t_2) - m\omega^2\delta(t_1 - t_2) \tag{87}$$

where $\delta(t)$ is the Dirac delta function, and

$$\delta''(t) = \frac{\partial^2}{\partial t^2}\delta(t). \tag{88}$$

By integrating by parts in the variables t_1 and t_2, show that

$$G[y] = \int dt \left(\frac{1}{2}m(y'(t))^2 - \frac{1}{2}m\omega^2(y(t))^2\right) \tag{89}$$

Solution 4.4 (2 points)**.** It is easiest to break the expression into two pieces:

$$\begin{aligned}
G[y] &= G_1[y] + G_2[y] &(90)\\
G_1[y] &= \frac{-m}{2}\int dt_1\, dt_2\, \delta''(t_1 - t_2)y(t_1)y(t_2) &(91)\\
&= \frac{m}{2}\int dt_1\, dt_2\, \frac{\partial^2\delta(t_1 - t_2)}{\partial t_1 \partial t_2}y(t_1)y(t_2) &(92)\\
G_2[y] &= \frac{-m\omega^2}{2}\int dt_1\, dt_2\, \delta(t_1 - t_2)y(t_1)y(t_2). &(93)
\end{aligned}$$

We integrate by parts on G_1, first with respect to t_1,

$$G_1[y] = \frac{-m}{2}\int dt_1\, dt_2\, \frac{\partial\delta(t_1 - t_2)}{\partial t_2})y'(t_1)y(t_2), \tag{94}$$

then with respect to t_2

$$G_1[y] = \frac{m}{2}\int dt_1\, dt_2\, \delta(t_1 - t_2)y'(t_1)y'(t_2), \tag{95}$$

We then use the delta-function on one of the integrals, and rename the variables to get

$$G_1[y] = \frac{m}{2}\int dt\ \left(y'(t)\right)^2. \tag{96}$$

For G_2, we just do one of the integrals, and rename the variables to get

$$G_2[y] = \frac{-m\omega^2}{2}\int dt\ (y(t_1))^2. \tag{97}$$

Adding these up gives the desired expression.

4.5. By taking the result from problem 4.3, and substituting in Eq. (87), show that

$$\frac{\delta G[y]}{\delta y(t)} = -my''(t) - m\omega^2 y(t), \tag{98}$$

and hence Newton's equations for the simple harmonic oscillator can be written as

$$\frac{\delta G[y]}{\delta y(t)} = 0 \tag{99}$$

[Note, most classical mechanics courses use slightly different notation for this.]

Solution 4.5 (2 points)**.** We begin with

$$\frac{\delta G[y]}{\delta y(t)} = \int ds\ K(t,s) y(s). \tag{100}$$

We then substitute in the expression of the kernel,

$$\begin{aligned} \frac{\delta G[y]}{\delta y(t)} &= \int ds\ \left[-m\delta''(s-t) - m\omega^2\delta(s-t)\right] y(s) && (101) \\ &= \int ds\ \left[-m\frac{\partial^2\delta(s-t)}{\partial s^2} - m\omega^2\delta(s-t)\right] y(s). && (102) \end{aligned}$$

We integrate by parts twice to get

$$\frac{\delta G[y]}{\delta y(t)} = \int ds\ \left[-m\delta(s-t)y''(s) - m\omega^2\delta(s-t)y(s)\right]. \tag{103}$$

We then do the s integral to find,

$$\frac{\delta G[y]}{\delta y(t)} = -my''(t) - m\omega^2 y(t), \tag{104}$$

which is the desired expression.

Problem 5. Feedback

5.1. How long did this homework take?

5.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair