Physics 551 Homework 1

Due Friday 12 September 2014

1 Hamiltonian need not be defined on all of Hilbert space

Consider the Simple Harmonic Oscillator. The eigenstates of the Hamiltonian are labeled $|n\rangle$ and have energy

$$H\,|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle\ ,$$

for $n = 0, 1, \ldots$.

Consider the infintie series of (improperly normalized) states

$$|S_n\rangle = \sum_{m=0}^{n}\frac{1}{m+1}\,|m\rangle\ , \qquad \|S_n\|^2 \equiv \langle S_n|\,|S_n\rangle\ .$$

Also define the distance between two members of this state as usual,

$$D^2_{S_n,S_m} \equiv \Big(\,\langle S_n| - \langle S_m|\,\Big)\Big(\,|S_n\rangle - |S_m\rangle\,\Big)\,.$$

Show that the series *converges*,[1]

$$\lim_{n\to\infty}\mathrm{Sup}_{m>n}D_{S_n,S_m} = 0\,.$$

Therefore completeness requires that the state $S_\infty \equiv \lim_{n\to\infty} S_n$ exists. Find its squared norm $\langle S_\infty|\,|S_\infty\rangle$. (There is a closed-form expression!)

Next, find an expression for the expectation value of the energy in the state S_n,

$$E_{S_n} \equiv \langle S_n|\,H\,|S_n\rangle\ .$$

Show that, while each E_{S_n} exists and is finite, that $\lim_{n\to\infty} E_{S_n}$ diverges. (Here and throughout this course, if you don't want to make a rigorous proof, you are allowed to appeal to well known mathematical results, provided they really are well known.)

Therefore there is a state S_∞ which is present in the Hilbert space, but the Hamiltonian is not well defined on this state.

2 Energies in the WKB approximation

Consider a particle moving in 1 dimension under the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + ax^4$$

[1] Sup means "Supremum," meaning the smallest number which is at least as large as any member of a set.

which is an *an*harmonic oscillator.

First, argue on dimensional grounds that the ground state energy is a pure number times the dimensionful combination $\hbar^{4/3}a^{1/3}m^{-2/3}$.

Next, use the WKB approximation to estimate the energies of the ground and excited states. To do this, use the result that the WKB estimate of the phase accumulated in crossing the classically allowed region is $(n+1/2)\pi$. Here the classically allowed region is x such that $ax^4 < E$; and the phase accumulated is the WKB estimate $\int \sqrt{2m(E-V)}dx/\hbar$. **Hint**: you may need the integral

$$\int_{-1}^{1} \sqrt{1-x^4}\, dx = \frac{\pi^{1/2}\Gamma(5/4)}{\Gamma(7/4)} \simeq 1.748038369528\ldots .$$

Compare your results to the exact energies,

n	energy
0	$0.668\ (\hbar^4 a/m^2)^{1/3}$
1	$2.394\ (\hbar^4 a/m^2)^{1/3}$
2	$4.697\ (\hbar^4 a/m^2)^{1/3}$
3	$7.336\ (\hbar^4 a/m^2)^{1/3}$
4	$10.244\ (\hbar^4 a/m^2)^{1/3}$
5	$13.379\ (\hbar^4 a/m^2)^{1/3}$
6	$16.712\ (\hbar^4 a/m^2)^{1/3}$

3 Diatomic vibrational states

Atoms attract at large distance and repel at short distance. The Leonard-Jones potential

$$V(r) = -\frac{A}{r^6} + \frac{B}{r^{12}}$$

is a good model for the potential. The O_2 oxygen molecule has a bond length (inter-atomic spacing) of $r_0 = 120.75$ picometers and a binding energy of $V_0 = 5.115$ eV (electron volt). Assuming the bond length and binding energy are determined by the *classical* minimum of $V(r)$, express A and B in terms of V_0 and r_0.

An ^{16}O atom weighs 16 Atomic Mass Units (AMU). Use the WKB approximation to estimate the number of angular-momentum 0, bound (vibrational) states of the oxygen molecule. You may have to do one integral numerically or via Mathematica, and you will have to look up what an eV and an AMU are in real units.

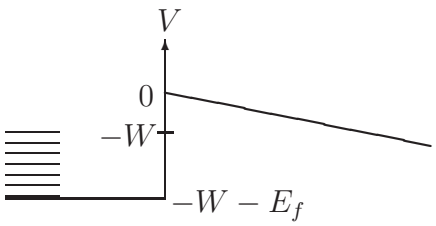
For extra credit, find the largest angular momentum ℓ for which a bound molecular state exists. This may be a little tricky and might require some numerics.

4 Tunneling from a metal

Inside a metal, conduction electrons are in a (nearly) flat potential. They have a range of kinetic energies, from 0 up to a maximum called the Fermi energy E_f.

At the boundary of the metal the potential rises by $E_f + W$, where W is the "work function" of the metal, equal to the energy which must be supplied to an electron to escape the metal. Taking the boundary to be at $x = 0$, the potential is then $-E_f - W$ for $x < 0$ and 0 for $x > 0$.

Now apply an electric field, so that, besides the step-function, there is also a linear component to the potential $V = -eE\,x$ outside the metal. (Here E is the electric field strength outside the metal; naturally there is no E field inside the metal, so the potential is flat inside.) Therefore, at some distance $d = W/eE$ from the metal's surface, an electron with energy E_f again becomes classically allowed.



Consider the wave function of an electron of energy $\varepsilon \leq E_f$, moving in the x direction inside the metal and impinging on the boundary. Calculate the wave function, in the WKB approximation, inside the metal, in the classically forbidden region, and in the classically allowed region outside the metal. (The wave function should be an almost perfect standing wave inside the metal, strictly shrinking in the forbidden region, and strictly a traveling wave moving away from the metal outside – that is, there is no incoming wave from outside the metal.)

Find the probability current leading away from the metal, as a function of the probability density inside the metal, ε, $W + E_f - \varepsilon$, and eE. How does the rate of escape vary with electron energy and with E-field, and can you explain this qualitatively?

[In this problem you should try to find the exponential factors, do not worry about factors of order 2 from doing careful matching. In any case the potential is more complicated within a few atomic lengths of the surface, which will correct your result by some large – but not exponential – factor.]