33-756 Homework 4

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1. Delta Functions in d Dimensions

Consider a d-dimensional system with delta function potential. What are the symmetries of this system? Is there a particular dimension for which the symmetry is enhanced?

In any dimension, there is a reflection symmetry about any coordinate, as long as the reflection is centered around the delta function. Since this potential is spherically symmetric, there is also an $SO(d)$ symmetry for a d-dimensional potential. In $d = 2$, there is an additional symmetry of scale invariance. In d dimensions, the action is

$$S = \int \mathrm{d}t\, \frac{1}{2} m\dot{x}^2 - A\delta^{(d)}(x)$$

If we scale both time and space,

$$(x', t') = (\gamma x, \lambda t)$$

we want to find what value of d makes the action invariant. $\mathrm{d}t' = \lambda\, \mathrm{d}t$ and $\dot{x}' = \frac{\mathrm{d}}{\mathrm{d}t'} x' = \frac{\gamma}{\lambda}\dot{x}$, so

$$\begin{aligned} S' &= \int \lambda\, \mathrm{d}t \left(\frac{1}{2} m \frac{\gamma^2}{\lambda^2} \dot{x}^2 - A\delta^{(d)}(\gamma x) \right) \\ &= \int \mathrm{d}t\, \frac{1}{2} m \frac{\gamma^2}{\lambda} \dot{x}^2 - \frac{\lambda}{\gamma^d} \delta^{(d)}(x) \end{aligned}$$

For this to be invariant, we require $\frac{\gamma^2}{\lambda} = 1$ and $\frac{\lambda}{\gamma^d} = 1$, so $d = 2$.

2. Inverse Square Potential

Consider the problem of a particle moving in a spherical potential

$$V(r) = \frac{A\hbar^2}{2Mr^2}.$$

Write out the Schrödinger equation for this system utilizing the spherical symmetry. Next, rewrite the equation in terms of the dimensionless variable $\rho = kr$ where $k = \sqrt{2ME/\hbar^2}$. The solution to this differential equation is a special function. Show that there are no bound state solutions to the equation which are physically sensible. Finally, explain how you could have guessed this using physical reasoning using the results of the previous homework. As a side note, classically there is a theorem by Bertrand that states the only potentials with closed bound orbits are r^2 and $1/r$.

Because of the spherical symmetry of the potential, we can expand the wave function as

$$\sum_{lm} Y_{lm}(\theta,\varphi)R(r)$$

so we can write the Schrödinger equation in terms of the angular momentum operator and act it on the spherical harmonics:

$$\left[-\frac{\hbar^2}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\hbar^2(l(l+1)+A)}{2M}\frac{1}{r^2}\right]R(r)=ER(r)$$

Next, by the chain rule, we can reduce the radial differential to

$$\frac{\hbar^2}{2M}\left[-\frac{1}{r}\frac{\partial^2}{\partial r^2}r+(l(l+1)+A)\frac{1}{r^2}\right]R(r)=ER(r)$$

We then make the following substitution:

$$\rho = kr \qquad \frac{\partial^2}{\partial\rho^2}=\left(\frac{\partial r}{\partial\rho}\right)^2\frac{\partial^2}{\partial r^2}=\frac{1}{k^2}\frac{\partial^2}{\partial r^2}$$

$$\left[-E\frac{1}{\rho}\frac{\partial^2}{\partial\rho^2}\rho+E(l(l+1)+A)\frac{1}{\rho^2}\right]R=ER$$

Substituting $R(r)=\frac{U(\rho)}{\sqrt{\rho}}$, we get

$$\frac{U-4\rho(U'+\rho U'')}{4\rho^{5/2}}+\frac{(l(l+1)+A)}{\rho^{5/2}}U-\frac{\rho^2}{\rho^{5/2}}U=0$$

or

$$0=\rho^2U''(\rho)+\rho U'(\rho)+\left[\rho^2-\underbrace{\left\{l(l+1)+A+\frac{1}{4}\right\}}_{\alpha^2}\right]U(\rho)$$

This is the Bessel equation, and solutions for R are the spherical Bessel functions

$$R(r)=\sqrt{\frac{\pi}{2kr}}J_\alpha(kr)\equiv j_{\alpha-\frac{1}{2}}(kr)$$

However, for bound states, $E<0$, and $E=\frac{\hbar^2k^2}{2M}$ so then $k^2<0$ or k is imaginary. The Bessel equation can be solved for imaginary arguments, but then the solutions are the modified Bessel functions, which all diverge at $r\to\infty$, so any bound states would not be normalizable (are not physically sensible). In the previous homework, we found that the Runge-Lenz vector is conserved for conservative central forces, but this vector will not commute with a $\frac{1}{r^2}$ potential (we barely got it to work with a $\frac{1}{r}$ potential).

3. Perturbed Particle in a Box

Consider a particle in a box of length L. Suppose we place a delta function $V(x)=AL\delta(x)$ potential at the center of the box. Under what conditions (on A) do you expect to be able to treat this potential as a perturbation? Calculate the first-order energy shift to the nth level of the system as well as the shift in the wave function.

If $A << 1$ we can expand our eigenstates around the unperturbed Hamiltonian and find the low-order corrections for this system. In class, we learned that

$$E_n^{(1)} = \left\langle \psi_n^{(0)} \middle| AL\delta(x) \middle| \psi_n^{(0)} \right\rangle$$

In this case, the unperturbed wave functions for a particle in a box come in two different forms:

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{L}} \begin{cases} \sin\left(\frac{n\pi}{L}x\right) & n \text{ even} \\ \cos\left(\frac{n\pi}{L}x\right) & n \text{ odd} \end{cases}$$

Evaluating the expectation value of the potential, we find that for even n, there is no first-order perturbation to the energy:

$$E_n^{(1)} = \frac{2AL}{L} \int \delta(x) \sin^2\left(\frac{n\pi}{L}x\right) \sim \sin^2(0) = 0$$

However, for odd n, we get

$$E_n^{(1)} = 2A \int \delta(x) \cos^2\left(\frac{n\pi}{L}x\right) = 2A$$

We can then calculate the first-order shift in the wave function:

$$\left|\psi_n^{(1)}\right\rangle = \sum_{k \neq n} \frac{\left\langle \psi_k^{(0)} \middle| AL\delta(x) \middle| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} \left|\psi_k^{(0)}\right\rangle$$

In the numerator, if there is a single sine function in the integral, the whole thing will be zero, meaning that for n or k even, there is no first-order shift. However, if both are odd, then the numerator becomes:

$$\left\langle \psi_k^{(0)} \middle| AL\delta(x) \middle| \psi_n^{(0)} \right\rangle = 2A \int \delta(x) \cos\left(\frac{n\pi}{L}x\right) \cos\left(\frac{k\pi}{L}x\right) = 2A$$

In the denominator, we just have the unperturbed energies for a particle in a box, so the first-order correction to the wave function is

$$\left|\psi_n^{(1)}\right\rangle = \sum_{k \neq n} \frac{2A}{\frac{n^2\pi^2\hbar^2}{2mL^2} - \frac{k^2\pi^2\hbar^2}{2mL^2}} \left|\psi_k^{(0)}\right\rangle = \sum_{k \neq n} \frac{4AmL^2}{(n^2 - k^2)\pi^2\hbar^2} \left|\psi_k^{(0)}\right\rangle \qquad n, k \text{ odd}$$

4. Second-Order Energy Shift

Using the algorithm discussed in class, derive an expansion for the second-order energy shift in perturbation theory.

In perturbation theory, we had set up the expansion

$$\begin{aligned} &(H_0 + \lambda H_I)\left(|\psi_n\rangle + \lambda C_n^{[1]} |\psi_n\rangle + \lambda^2 C_n^{[2]} |\psi_n\rangle + \cdots\right) \\ &\qquad = \left(E_n^{[0]} + \lambda E_n^{[1]} + \lambda^2 E_n^{[2]} + \cdots\right)\left(|\psi_n\rangle + \lambda C_n^{[1]} |\psi_n\rangle + \lambda^2 C_n^{[2]} |\psi_n\rangle + \cdots\right) \end{aligned}$$

For shorthand, I will write $C_n^{[i]} |\psi_n\rangle \equiv \left|\psi_n^{[i]}\right\rangle$ with $C_n^{[0]} = 1$:

$$\begin{aligned} &(H_0 + \lambda H_I)\left(\left|\psi_n^{[0]}\right\rangle + \lambda \left|\psi_n^{[1]}\right\rangle + \lambda^2 \left|\psi_n^{[2]}\right\rangle + \cdots\right) \\ &\qquad = (E_n^{[0]} + \lambda E_n^{[1]} + \lambda^2 E_n^{[2]} + \cdots)\left(\left|\psi_n^{[0]}\right\rangle + \lambda \left|\psi_n^{[1]}\right\rangle + \lambda^2 \left|\psi_n^{[2]}\right\rangle + \cdots\right) \end{aligned}$$

From the first-order derivation, we already know what $\left|\psi_n^{[1]}\right\rangle$ and $E_n^{[1]}$ are, but now we want to find $E_n^{[2]}$. This value has a prefactor of λ^2 so we can multiply through and match powers of λ^2:

$$H_0\left|\psi_n^{[2]}\right\rangle + H_I\left|\psi_n^{[1]}\right\rangle = E_n^{[0]}\left|\psi_n^{[2]}\right\rangle + E_n^{[1]}\left|\psi_n^{[1]}\right\rangle + E_n^{[2]}\left|\psi_n^{[0]}\right\rangle$$

Next, we will project onto the unperturbed wave function:

$$\begin{aligned}
\left\langle\psi_n^{[0]}\middle| H_0 \middle|\psi_n^{[2]}\right\rangle + \left\langle\psi_n^{[0]}\middle| H_I \middle|\psi_n^{[1]}\right\rangle &= E_n^{[0]}\left\langle\psi_n^{[0]}\middle|\psi_n^{[2]}\right\rangle + E_n^{[1]}\left\langle\psi_n^{[0]}\middle|\psi_n^{[1]}\right\rangle + E_n^{[2]}\cancelto{1}{\left\langle\psi_n^{[0]}\middle|\psi_n^{[0]}\right\rangle} \\
\cancel{E_n^{[0]}\left\langle\psi_n^{[0]}\middle|\psi_n^{[2]}\right\rangle} + \left\langle\psi_n^{[0]}\middle| H_I \middle|\psi_n^{[1]}\right\rangle &= \cancel{E_n^{[0]}\left\langle\psi_n^{[0]}\middle|\psi_n^{[2]}\right\rangle} + E_n^{[1]}\left\langle\psi_n^{[0]}\middle|\psi_n^{[1]}\right\rangle + E_n^{[2]} \\
\left\langle\psi_n^{[0]}\middle| H_I \middle|\psi_n^{[1]}\right\rangle &= E_n^{[1]}\cancelto{0}{\left\langle\psi_n^{[0]}\middle|\psi_n^{[1]}\right\rangle} + E_n^{[2]} \\
\left\langle\psi_n^{[0]}\middle| H_I \middle|\psi_n^{[1]}\right\rangle &= E_n^{[2]}
\end{aligned}$$

From the first-order results, we know that

$$\left|\psi_n^{[1]}\right\rangle = \sum_{k\neq n} \frac{\left\langle\psi_k^{[0]}\middle| H_I \middle|\psi_n^{[0]}\right\rangle}{E_n^{[0]} - E_k^{[0]}}\left|\psi_k^{[0]}\right\rangle$$

so

$$E_n^{[2]} = \sum_{k\neq n} \frac{\left\langle\psi_k^{[0]}\middle| H_I \middle|\psi_n^{[0]}\right\rangle}{E_n^{[0]} - E_k^{[0]}}\left\langle\psi_n^{[0]}\middle| H_I \middle|\psi_k^{[0]}\right\rangle = \sum_{k\neq n} \frac{\left|\left\langle\psi_k^{[0]}\middle| H_I \middle|\psi_n^{[0]}\right\rangle\right|^2}{E_n^{[0]} - E_k^{[0]}}$$