Phys 251A Problem Set 9
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1. Consider a particle on a ring of radius R with kinetic energy

$$H_0 = -\frac{1}{2mR^2}\partial_\phi^2$$

where ϕ is the azimuthal angle and the wavefunction $\psi(\phi) = \psi(\phi + 2\pi)$ is periodic.

(a) Calculate the energy eigenvalues and eigenfunctions of H_0.

The eigenfunctions are $|n\rangle = e^{in\phi}/\sqrt{2\pi}$ and the associated eigenvalues are $E_n = \frac{n^2}{2mR^2}$ for $n \in \mathbb{Z}$.

(b) Let us put the particle, which has charge q, in an electric field pointing in the x direction of strength ε, which leads to the full Hamiltonian

$$H = H_0 - q\varepsilon R\cos\phi.$$

Calculate the new ground state wavefunction to first order in ε.

We note that

$$\cos\phi\,|n\rangle = \frac{1}{2}(e^{i\phi} + e^{-i\phi})\,|n\rangle = \frac{1}{2}(|n+1\rangle + |n-1\rangle) \tag{1}$$

where we used the form of the eigenfunctions in the previous part. The first order correction to the ground state$|0\rangle$ is then

$$|0^{(1)}\rangle = \sum_{n\neq 0}\frac{\langle n|\,(-q\varepsilon R\cos\phi)\,|0\rangle}{E_0^{(0)} - E_n^{(0)}}\,|n\rangle = q\varepsilon R\left(\frac{1/2}{E_1^{(0)} - E_0^{(0)}}\,|1\rangle + \frac{1/2}{E_{-1}^{(0)} - E_0^{(0)}}\,|{-1}\rangle\right) = mR^3q\varepsilon(|1\rangle{+}|{-1}\rangle)$$

For the next part it is convenient to write the perturbed state in a slightly different way

$$|0^{(1)}\rangle = 2mR^3q\varepsilon\cos\phi\,|0\rangle \tag{2}$$

using again (1).

(c) Use the new ground state wavefunction to calculate the induced electric dipole moment in the x direction

$$p_x = \frac{\langle\psi|\,qx\,|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle\psi|\,qR\cos\phi\,|\psi\rangle}{\langle\psi|\psi\rangle}$$

to first order in ε. Then use this to calculate the polarizability of the system

$$\alpha = \left.\frac{dp_x}{d\varepsilon}\right|_{\varepsilon=0}$$

We note that the normalization $\langle\psi|\psi\rangle = (\langle\psi^{(0)}|{+}\langle\psi^1|)(|\psi^{(0)}\rangle{+}|\psi^1\rangle) = 1{+}O(\varepsilon^2)$ because $\langle\psi^{(0)}|\psi^{(1)}\rangle = 0$. So we can focus on the numerator to leading order in ε. Using

$$p_x = qR(\langle 0|\cos\phi\,|0^{(1)}\rangle + \langle 0^{(1)}|\cos\phi\,|0\rangle) = 4mq^2R^4\varepsilon\,\langle 0|\cos^2\phi\,|0\rangle = 2mq^2R^4\varepsilon$$

where we used

$$\langle 0| \cos^2\phi \, |0\rangle = \int \frac{d\phi}{2\pi} \cos^2\phi = \frac{1}{2}.$$

The polarizability is then

$$\alpha = 2mq^2R^4$$

2. *Upper and lower bounds on ground state energy.* You may find the following integrals useful.

$$\int_{-\infty}^{\infty} dx x^2 e^{-\frac{x^2}{d^2}} = d^3\frac{\sqrt{\pi}}{2}, \qquad \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{d^2}} = d\sqrt{\pi}$$

(a) Consider a Harmonic oscillator Hamiltonian

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2x^2$$

Bound the ground state energy from above with the variational principle (copied below) using a Gaussian trial state of variable width

$$E_0 \leq \frac{\langle\psi_d| H |\psi_d\rangle}{\langle\psi_d|\psi_d\rangle}, \qquad \psi_d(x) = e^{-\frac{x^2}{2d^2}}$$

Since d is arbitrary, optimize your bound by minimizing it over d. You will have an easier time if you use that $\langle x\rangle = \langle p\rangle = 0$.

We begin by computing the expectation values of x^2 and p^2 in the Gaussian wavepacket

$$\langle x^2\rangle = \frac{\int x^2 e^{-x^2/d^2}dx}{\int e^{-x^2/d^2}dx} = \frac{\frac{d}{dd^{-2}}\int e^{-x^2/d^2}dx}{\int e^{-x^2/d^2}dx} = \frac{\frac{d}{dd^{-2}}\sqrt{\pi/d^{-2}}}{\sqrt{\pi/d^{-2}}} = \frac{1}{2}d^2$$

and

$$\langle p^2\rangle = \frac{\langle p\psi|p\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int\left|-i\hbar\partial_x e^{-x^2/(2d^2)}\right|^2 dx}{\int e^{-x^2/d^2}dx} = \frac{\hbar^2}{d^4}\frac{\int x^2 e^{-x^2/d^2}dx}{\int e^{-x^2/d^2}}dx = \frac{\hbar^2}{d^4}\langle x\rangle^2 = \frac{\hbar^2}{2}d^{-2}$$

. We therefore have

$$E \leq \langle H\rangle = \frac{1}{2m}\langle p^2\rangle + \frac{1}{2}m\omega^2\langle x^2\rangle = \frac{\hbar^2}{4md^2} + \frac{1}{4}m\omega^2d^2.$$

The above bound is valid for all d. We can optimize the bound by minimizing the right hand side with respect to d. To do so we calculate the minimum of the function $f(\lambda) = \frac{\hbar^2}{4m\lambda} + \frac{1}{4}m\omega^2\lambda$. Differentiating f and setting the derivative to zero yields $d = \sqrt{\lambda} = \sqrt{\hbar/m\omega}$. The bound above then yields

$$E \leq \frac{1}{4}\hbar\omega + \frac{1}{4}\hbar\omega = \frac{1}{2}\hbar\omega$$

(b) We will now lower bound the ground state energy. Using the Heisenberg uncertainty principle, show that the ground state energy is lower bounded as

$$E_0 \geq \frac{\hbar^2}{8m\langle x^2\rangle} + \frac{1}{2}m\omega^2\langle x^2\rangle$$

where $\langle x^2\rangle$ is the expectation value in the ground state of x^2. By computing the minimum of the function $f(\lambda) = \frac{\hbar^2}{8m\lambda} + \frac{1}{2}m\omega^2\lambda$, show that

$$E_0 \geq \frac{1}{2}\hbar\omega$$

and that this lower bound matches the upper bound of the previous part, pinning the ground state energy to the value $\frac{1}{2}\hbar\omega$.

We use the Heisenberg uncertainty relation of the ground state wavefunction together with $\langle x\rangle = \langle p\rangle$, by symmetry, to lower bound

$$\langle(\Delta p)^2\rangle = \langle p^2\rangle \geq \frac{\hbar^2}{4\langle(\Delta x)^2\rangle} = \frac{\hbar^2}{4\langle x^2\rangle}$$

Taking the expectation value in the actual ground state, we then have

$$E_0 = \frac{1}{2m}\langle p^2\rangle + \frac{1}{2}m\omega^2\langle x^2\rangle \geq \frac{\hbar^2}{8m\langle x^2\rangle} + \frac{1}{2}m\omega^2\langle x^2\rangle.$$

Note that on the right hand side we should still interpret $\langle x^2\rangle$ as the expectation value in the g round state, which we (nominally) do not know. We can, however, know that the right hand side is greater than or equal to the minimum of $f(\lambda) = \frac{\hbar^2}{4m\lambda} + \frac{1}{4}m\omega^2\lambda$, since the right hand side above can be interpreted as $f(2\langle x^2\rangle)$ (we are making a slightly different definition of f here for convenience in order to use what we did in the previous part. We found in the previous part that $f(\lambda)$ has a minimum value of $\hbar\omega/2$. We therefore conclude

$$E_0 \geq \hbar\omega/2$$

Combined with the previous part, we have that E_0 is upper and lower bounded by $\hbar\omega/2$ so that it must be equal to $\hbar\omega/2$ (which matches the exact solution).

(c) Now consider

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + \lambda|x|$$

where λ has units of energy per unit length. Upper bound the ground state energy of H using a gaussian trial state, as you did in part (a), and optimize the value of d.

The expectation value of the first term is the same as in part (a):

$$\langle\frac{p^2}{2m}\rangle = \frac{\hbar^2}{4md^2}.$$

For the second term we evaluate the integral directly, using the symmetry under $x \to -x$ to restrict to $x > 0$ and multiply by two:

$$\frac{\int_{-\infty}^{\infty}|x|e^{-x^2/d^2}dx}{\int_{-\infty}^{\infty}e^{-x^2/d^2}dx} = \frac{1}{d\sqrt{\pi}}\int_0^\infty 2xe^{-x^2/d^2} = \frac{d}{\sqrt{\pi}}\int_0^\infty 2ue^{-u^2} = \frac{d}{\sqrt{\pi}}(e^{-u^2})\big|_\infty^0 = \frac{d}{\sqrt{\pi}}$$

We therefore have

$$E_0 \leq \langle H\rangle = \frac{\hbar^2}{4md^2} + \frac{d\lambda}{\sqrt{\pi}}.$$

Minimizing with respect to d we have

$$\frac{\hbar^2}{2md^3} = \frac{\lambda}{\sqrt{\pi}} \quad \Longrightarrow \quad d = \left(\frac{\sqrt{\pi}\hbar^2}{2m\lambda}\right)^{1/3}$$

or

$$E = \frac{1}{2}\left(\frac{\hbar^2}{2md^2}\right) + \frac{\lambda d}{\sqrt{\pi}} = \frac{1}{2}\left(\frac{\hbar^2\lambda^2}{2\pi m}\right)^{1/3} + \left(\frac{\hbar^2\lambda^2}{2\pi m}\right)^{1/3} = \frac{3}{2}\left(\frac{\hbar^2\lambda^2}{2\pi m}\right)^{1/3}$$