May 2015 Preliminary Exam, Quantum Mechanics Problem 2

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Problem:

A point particle of mass m and electric charge q moves in a 3D harmonic oscillator potential with frequency ω and a uniform electric field of strength E pointing in the z-direction. The Hamiltonian is

$$H = \frac{\vec{p}^2}{2m} + \frac{m\omega^2\vec{r}^2}{2} - qEz \tag{1}$$

(a) What are the eigenenergies of this Hamiltonian?

(b) Find an expression for the ground state wave-function.

Assume now that the system is described by the above Hamiltonian only for $t < 0$, and that at $t = 0$ the electric field is suddenly turned off. For $t < 0$, the system is in its ground state.

(c) What is the probability that the system will end up in the new ground state right after the electric field is turned off?

(d) What is the expectation value of hte electric dipole moment $\vec{d} = q\vec{r}$ at some given time $t > 0$?

Solution:

(a) The electric field add a linear term to the harmonic oscillator Hamiltonian, which will result in a modified harmonic oscillator about some new z coordinate, with an additional overall energy shift. This can be seen by completing the square in the z component of H:

$$\frac{m\omega^2 z^2}{2} - qEz = \frac{m\omega^2}{2}\left(z^2 - \frac{2qE}{m\omega^2}z + \frac{q^2E^2}{m^2\omega^4}\right) - \frac{m\omega^2}{2}\frac{q^2E^2}{m^2\omega^4} = \frac{m\omega^2}{2}\left(z - \frac{qE}{m\omega^2}\right)^2 - \frac{q^2E^2}{2m\omega^2} \tag{2}$$

$$\implies H = \frac{\vec{p}^2}{2m} + \frac{m\omega^2\vec{r'}^2}{2} \tag{3}$$

where $\vec{r'}^2 = x^2 + y^2 + (z - \frac{qE}{m\omega^2})$. We now have the usual eigenenergies in terms of n_x, n_y, and $n_{z'}$:

$$E_{n_x,n_y,n_{z'}} = \left(n_x + n_y + n_{z'} + \frac{3}{2}\right)\hbar\omega - \frac{q^2E^2}{2m\omega^2} \tag{4}$$

(b) The ground state wave function for the 1D harmonic oscillator is the following:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{5}$$

This can either be memorized, or you can remember that the lowering operator has to kill this wave function and solve the first-order equation. The Hamiltonian is separable, so the 3D harmonic oscillator has the following ground state wave function:

$$\psi_0(\vec{r}) = \psi_0(x)\psi_0(y)\psi_0(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} exp\left(-\frac{m\omega}{2\hbar}\vec{r}^2\right) \tag{6}$$

The electric field caused a shift in the origin of our new harmonic oscillator, which can just be plugged into this equation, as follows:

$$\psi_0(\vec{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} exp\left(-\frac{m\omega}{2\hbar}\left(x^2 + y^2 + \left(z - \frac{qE}{m\omega^2}\right)^2\right)\right) \tag{7}$$

(c) Once the electric field is turned off, the Hamiltonian returns to the classic harmonic oscillator centered at the origin. To find the probability the system is in the classic ground state, consider the coefficient $|\langle 000|_E |000\rangle_0|^2$, which links the two states:

$$\langle 000|_E |000\rangle_0 = \int d^3\vec{r} \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} exp\left(-\frac{m\omega}{2\hbar}\left(2x^2 + 2y^2 + z^2 + \left(z - \frac{qE}{m\omega^2}\right)^2\right)\right) \tag{8}$$

The x and y direction are unchanged, so they must still be normalized. Therefore, we only need to consider changes to the z integral, which we can do by shifting the integration variable to $u = z - \frac{qE}{2m\omega^2}$:

$$\begin{aligned}
\langle 000|_E |000\rangle_0 &= \int du \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} exp\left(-\frac{m\omega}{2\hbar}\left(\left(u + \frac{qE}{2m\omega^2}\right)^2 + \left(u - \frac{qE}{2m\omega^2}\right)^2\right)\right) \\
&= \int du \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} exp\left(-\frac{m\omega}{2\hbar}\left(\left(u^2 + \frac{qE}{m\omega^2}u + \left(\frac{qE}{2m\omega^2}\right)^2\right) + \left(u^2 - \frac{qE}{m\omega^2}u + \left(\frac{qE}{2m\omega^2}\right)^2\right)\right)\right) \\
&= \int du \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} exp\left(-\frac{m\omega}{2\hbar}\left(2u^2 + \frac{q^2E^2}{2m^2\omega^4}\right)\right) \\
&= exp\left(-\frac{q^2E^2}{4\hbar m\omega^3}\right) \int du \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} exp\left(-\frac{m\omega}{2\hbar}\left(2u^2\right)\right) = exp\left(-\frac{q^2E^2}{4\hbar m\omega^3}\right)
\end{aligned} \tag{9}$$

$$\implies |\langle 000|_E |000\rangle_0|^2 = exp\left(-\frac{q^2E^2}{2\hbar m\omega^3}\right) \tag{10}$$

(d) Evaluate the average dipole moment as follows:

$$\left\langle \vec{d} \right\rangle = q\,\langle \vec{r} \rangle = q\,\langle 000|_E\, \vec{r}\, |000\rangle_E \tag{11}$$

The average position will be just the center of the shifted harmonic oscillator. The new Hamiltonian just reformulates the old wave function in a new basis of stationary states at t=0. Therefore,

$$\left\langle \vec{d} \right\rangle = q(0, 0, \frac{qE}{m\omega^2}) = \frac{q^2E}{m\omega^2}\hat{z} \tag{12}$$

However, the dipole moment doesn't stay here past this initial time because, although the states are stationary, they evolve at different rates because they have all different energies. Tyler Cochran proposed to me that this dipole moment might evolve classically, oscillating back and forth with amplitude as calculated above. This can be proven using both Virial theorems, taking the second derivative of the expectation value of the position, giving a single derivative of the expectation value of momentum, which is the negative expectation value of the gradient of the potential. The potential is quadratic in the position, so the gradient is linear in positions, giving a second order differential equation for position, solved with sines and cosines. I will update with the detailed calculation soon (hopefully). Sorry for the inconvenience until then.