Homework 3 for Physics 531

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Virial Theorem With $H = \frac{\vec{\mathbf{p}}^2}{2m} + V(\vec{\mathbf{x}})$, we can remove vanishing components of the commutator so that $[\vec{\mathbf{x}} \cdot \vec{\mathbf{p}}, H] = [\vec{\mathbf{x}}, \vec{\mathbf{p}} \cdot \vec{\mathbf{p}}]\frac{\vec{\mathbf{p}}}{2m} + \vec{\mathbf{x}}\big[\vec{\mathbf{p}}, V(\vec{\mathbf{x}})\big]$. Then,

$$[\vec{\mathbf{x}} \cdot \vec{\mathbf{p}}, H] = i\hbar \left[\sum_i \left(\delta_{ij} p_j + p_j \delta_{ij}\right) \frac{p_i}{2m} + \sum_i x_i \left(-\frac{\partial V(\vec{\mathbf{x}})}{\partial x_i}\right)\right] = i\hbar \left(\frac{\vec{\mathbf{p}}^2}{m} - \vec{\mathbf{x}} \cdot \nabla V\right) \tag{1}$$

By taking the expectation value of either side and applying the Heisenberg equation of motion as in (2.2.19) we obtain the necessary,

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \vec{\mathbf{x}} \cdot \vec{\mathbf{p}} \rangle = \frac{1}{i\hbar} \big\langle [\vec{\mathbf{x}} \cdot \vec{\mathbf{p}}, H] \big\rangle = \frac{\langle \vec{\mathbf{p}} \rangle^2}{m} - \langle \vec{\mathbf{x}} \cdot \nabla V \rangle \tag{2}$$

For $\Omega = \vec{\mathbf{x}} \cdot \vec{\mathbf{p}}$, the LHS of (2) vanishes when $\frac{\mathrm{d}\langle \Omega \rangle}{\mathrm{d}t} = 0$, that is when the expectation value of Ω with respect to some state does not vary with time. In other words, applying Ehrenfest's theorem to the operator $\Omega = \vec{\mathbf{x}} \cdot \vec{\mathbf{p}}$, this implies that $\frac{\mathrm{d}}{\mathrm{d}t} \langle \vec{\mathbf{x}} \cdot \vec{\mathbf{p}} \rangle = \left\langle \frac{\partial (\vec{\mathbf{x}} \cdot \vec{\mathbf{p}})}{\partial t} \right\rangle$

The upside-down harmonic oscillator The upside-down harmonic oscillator has Hamiltonian $H = \frac{p^2}{2m} - \frac{m\omega^2 x^2}{2}$. Given a candidate solution to Schrodinger's equation in the suggested form of $\psi(x,t) = A(t) \exp\big\{-B(t)x^2\big\}$, calculate that

$$\frac{\partial \psi(x,t)}{\partial t} = \exp\Big\{-Bx^2\Big\} \left[\frac{\mathrm{d}A}{\mathrm{d}t} - Ax^2 \frac{\mathrm{d}B}{\mathrm{d}t}\right] = \psi(x,t) \left[\frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}t} - x^2 \frac{\mathrm{d}B}{\mathrm{d}t}\right] \tag{3}$$

Solving the Schrodinger equation for one-dimensional potentials gives that

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \psi(x,t) \left[\frac{\hbar^2}{m} B(1 - 2Bx^2) + V(x)\right] \tag{4}$$

$$= \psi(x,t) \left[\frac{\hbar^2 B}{m} - x^2 \left(\frac{k}{2} + 2\frac{\hbar^2 B^2}{m}\right)\right] \tag{5}$$

The last line obtains by substituting the given inverse potential into (4). Dividing (3) and (5) throughout by $\psi(x,t)$ results in the condition,

$$\frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}t} - x^2 \frac{\mathrm{d}B}{\mathrm{d}t} = \frac{1}{i\hbar} \left[\frac{\hbar^2}{m} B - x^2 \left(\frac{k}{2} + 2\frac{\hbar^2}{m} B^2\right)\right] \tag{6}$$

The desired solution follows trivially by collecting like terms in x,

$$i\hbar \frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\hbar^2}{m} AB \tag{7}$$

$$i\hbar \frac{\mathrm{d}B}{\mathrm{d}t} = \frac{k}{2} + 2\frac{\hbar^2}{m} B^2 \tag{8}$$

With the constants a and ω as defined, note that $a = \sqrt{\frac{\hbar}{m\omega}}$. Express (8) as

$$i\frac{\mathrm{d}B}{\mathrm{d}t} = \omega \left(\frac{m}{2\hbar}\omega + 2B^2 a^2\right) = \frac{\omega}{2a^2} + 2B^2 a^2 \omega \tag{9}$$

Integrate by parts to solve the separated equation as,

$$\int \frac{i}{\frac{\omega}{2a^2} + 2a^2\omega B^2}\,\mathrm{d}B(t) = \frac{2ia^2}{\omega}\int \frac{1}{1+4a^4B^2}\,\mathrm{d}B(t) \tag{10}$$

$$= \frac{i}{\omega}\int \frac{1}{1+(2a^2B)^2}\,\mathrm{d}(2a^2B)^2 \tag{11}$$

$$\int 1\,\mathrm{d}t = \frac{i\arctan\left(2a^2B(t)\right)}{\omega} + C \tag{12}$$

This results in,

$$B(t) = \frac{1}{2a^2}\tan\left(\frac{\omega}{i}(t+c)\right) \tag{13}$$

$$= \frac{1}{2a^2}\tan\left(-i\omega t + \phi\right) \tag{14}$$

$$= \frac{1}{2a^2}\frac{\sin 2\phi - i\sinh 2\omega t}{\cos 2\phi + \cosh 2\omega t} \tag{15}$$

where $\phi = -i\omega c$ and the last line follows by definition of the hyperbolic tangent and some substitution.[1] Note substituting back, we have $\phi = -c\sqrt{-\frac{k}{m}}$. Note the initial condition,

$$B(0) = -\frac{1}{x^2}\left(-\frac{x^2}{2d} - \ln\sqrt{2\pi}\,(A)\right) = \frac{1}{2}\left[\frac{1}{d} + \frac{1}{x^2}\ln\left(2\pi A^2\right)\right] \tag{16}$$

Using (14), we also have that

$$\phi = \arctan\left\{\frac{\hbar}{\sqrt{mk}}\left[\frac{1}{d} + \frac{1}{x^2}\ln\left(2\pi A^2\right)\right]\right\} \tag{17}$$

Physically, ϕ gives an initial phase shift contingent on the spring constant as well as the initial position x_0 and dispersion d of the generating wave packet. Using (14) calculate that

$$\left|\psi(x,t)\right| = \left|A(t)\right|\exp\left\{-\frac{x^2}{2a^2}\left[\tan\left(\phi - i\omega t\right) + \tan\left(\phi + i\omega t\right)\right]\right\} \tag{18}$$

$$= \left|A(t)\right|\exp\left\{-\frac{x^2}{2a^2}\left[\frac{2\sin\left(2\phi\right)}{\cos\left(2\phi\right) + \cosh\left(2\phi\right)}\right]\right\} \tag{19}$$

Note that for the suggested $A(t) = (2\pi)^{1/4}\left[b\cos(\phi - i\omega t)\right]^{-1/2}$ we have that $A\cdot B$ (ignoring constants factors) has the form,

$$AB \sim \frac{i\sinh\left(i\phi + t\omega\right)}{\cosh\left(i\phi + t\omega\right)^{3/2}\sin(2\phi)^{1/4}} \tag{20}$$

$$i\frac{\mathrm{d}A}{\mathrm{d}t} \sim \frac{i\omega\sinh\left(\frac{i\phi+t\omega}{2}\right)\cosh\left(\frac{i\phi+t\omega}{2}\right)}{\cosh^{3/2}(i\phi+t\omega)\sin^{1/4}(2\phi)} \tag{21}$$

$$= \frac{i\omega\sinh\left(i\phi + t\omega\right)}{2\cosh^{3/2}(i\phi+t\omega)\sin^{1/4}(2\phi)} \tag{22}$$

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[1] Alternatively, solve the differential equation by letting $y(t) = \frac{1}{sa^2}\frac{iv(t)}{\omega}$ the integral becomes $t + c = \int \frac{\mathrm{d}v(t)/\mathrm{d}t}{v(t)^2-\omega^2}$, which first leads to $-\frac{1}{\omega}\tanh^{-1}\left(\frac{v(t)}{\omega}\right) = t+c$. Solving $v(t) = -w\tanh\big(\omega(t+c)\big)$ leads us to the another expression for (14) as in $B(t) = -\frac{i\tanh\big(\omega(t+c)\big)}{2a^2}$ which corresponds to the alternative form stated in (15).

These are equal up to a factor of ω, which follows by multiplying (21) through by $\hbar$ and incorporating the factor of $\frac{1}{2a^2} \cdot \frac{1}{\sqrt{a}}$ into (20). Putting these together, our wave equation is given by

$$\psi(x,t) = \lim_{t\to\infty} \psi(x,t) \left(\frac{1}{(2\pi)^{1/4}}\right) \frac{1}{\sqrt{a\cos(\phi - i\omega t)\sqrt{\sin(2\phi)}}} \exp\left\{-\frac{x^2}{2a^2}\tan(\phi - i\omega t)\right\} \tag{23}$$

To find the late time behavior, first consider the limit $\lim_{t\to\infty} B(t)$,

$$\lim_{t\to\infty} B(t) = \frac{1}{2a^2} \lim_{t\to\infty} \frac{\sin 2\phi - i\sinh 2\omega t}{\cos 2\phi + \cosh 2\omega t} \tag{24}$$

$$= -\frac{i}{2a^2} \lim_{t\to\infty} \frac{\tanh 2\omega t}{1 + \frac{\cos 2\phi}{\cosh 2\omega t}} \tag{25}$$

$$\approx -\frac{i\omega}{2} + i\omega \exp\{-2\omega t\}\cos 2\phi + \omega\exp\{-2\omega t\}\sin 2\phi + \mathcal{O}\left(\frac{1}{\exp\{4\omega t\}}\right) \tag{26}$$

Substituting (with some of the simplification through Mathematica), the desired result obtains, that is

$$\psi(x,t) \approx \sqrt{\frac{1}{b}\sqrt{\frac{2}{\pi}}} \exp\left\{\frac{ix^2}{2a^2} - \frac{x^2}{b^2}\exp\{-2\omega t\} - \frac{\omega t + i\phi}{2}\right\} \tag{27}$$

To get the limiting expectation value, $\langle x^2\rangle$ consider that $\left|\psi(x,t)\right|^2$ is real and therefore must have probability proportional to the real component of the exponential function. Thus we must evaluate $\langle x^2\rangle \approx \exp\left\{-2\,\mathrm{Re}\left\{B(t)\right\}\right\}$. Returning to (26), only one term below fourth exponential order is real, and so we have

$$|\psi|^2 \approx \exp\left\{-2x^2\left(\omega\exp\{-2\omega t\}\sin 2\phi\right)\right\} \tag{28}$$

Completing this as a Gaussian, we have that

$$\left\langle x^2\right\rangle = \frac{\exp\{2\omega t\}}{4\omega\sin 2\phi} \tag{29}$$

The function disperses over time. This appears to correspond to the classical limit, modulo the expectation value. Compute first that,

$$\frac{\partial\psi(x,t)}{\partial x} = -2ABx\exp\left\{-Bx^2\right\} = -2xB(t)\psi(x,t) \tag{30}$$

This leads to

$$\left[-i\hbar\frac{\partial}{\partial x} - \frac{x}{a^2}\right]\psi = \left(2i\hbar B - \frac{1}{a^2}\right)x\psi \tag{31}$$

Noting that $p = -i\hbar\frac{\partial}{\partial x}$, compute the expectation value of the spread

$$\left\langle\left[p - \frac{x}{a^2}\right]^2\right\rangle = \left\langle x^2\right\rangle\left|2i\hbar B - \frac{1}{a^2}\right|^2 \tag{32}$$

$$= \frac{\exp\{2\omega t\}}{4\omega\sin 2\phi}\left|2i\hbar B - \frac{1}{a^2}\right|^2 \tag{33}$$

$$= \frac{a^2\exp\{2\omega t\}}{4\sin 2\phi}\left(\frac{4}{a^4\exp\{4\omega t\}}\right) \tag{34}$$

$$= \frac{\omega\exp\{-2\omega t\}}{\sin 2\phi} \tag{35}$$

If not for $x^2 \gg a^2$, it would be incorrect to use $\langle x^2 \rangle = \frac{\exp\{2\omega t\}}{4\omega \sin 2\phi}$ as in (29) since the coefficient on the highest-order term that is included would not vanish. In this limit, however, we have $\left\langle \left[p - \frac{x}{a^2}\right]^2 \right\rangle \to \langle p^2 \rangle$, and clearly the limiting terms commute. Note that $x^2 \gg a^2$ is equivalent to $x^2 \ll \omega^2$ and so when the "frequency" becomes very high, the commutator approaches zero.

Noting the commutative relations,

$$\left[H, x_H(0)\right] = -i\hbar \frac{p_H(0)}{m} \tag{36}$$

$$\left[H, x_H(0)\right] = i\hbar m\omega^2 x_H(0) \tag{37}$$

apply the Baker-Hausdorff lemma to the equation $x_H(t) = \exp\left\{\frac{iHt}{\hbar}\right\} x_P(0) \exp\left\{-\frac{iHt}{\hbar}\right\}$, where the exponentials are naturally unitary. In fact we obtain,

$$x_H(t) = \exp\left\{\frac{iHt}{\hbar}\right\} x_P(0) \exp\left\{-\frac{iHt}{\hbar}\right\} \tag{38}$$

$$= x_H(0) + \frac{it}{\hbar}\left[H, x_H(0)\right] + \frac{i^2 t^2}{2\hbar^2}\left[H, \left[H, x_H(0)\right]\right] + \dots \tag{39}$$

Due to (36) and (37), we know the nested commutators simply alternate between $x_H(0)$ and $p_H(0)$. More precisely, for terms i^{2n} we have a coefficient $x_H(0)$ and for terms i^{2n+1} we have coefficient $\frac{p_H(0)}{m}$ for integers n. These separately constitute the series representation of $\cos(\cdot)$ and $\sin(\cdot)$ respectively and applying $\omega \to i\omega$

$$x_H(t) = x_H(0) \cos i\omega t + \left(\frac{p_H(0)}{m\omega}\right) \sin i\omega t \tag{40}$$

$$= x_H(0) \cosh(\omega t) + \left(\frac{p_H(0)}{m\omega}\right) \sinh \omega t \tag{41}$$

In series representation in the limit $t \to \infty$

$$x_H(t) \approx \exp\{\omega t\} \left[\frac{1}{2}\left(x_H(0) + \frac{p_H(0)}{m\omega}\right)\right] \tag{42}$$

In the limit, the particle oscillates around a fixed, time-independent amplitude as would be in the classical situation.

Spin Precession Compute generally that,

$$\frac{\mathrm{d}S_i}{\mathrm{d}t} = \frac{1}{i\hbar}[S_i, H] \tag{43}$$

$$= \frac{1}{i\hbar}\left[U^\dagger S_i^S U, H\right] \tag{44}$$

$$= \frac{\omega}{i\hbar} U^\dagger [S_i, S_z] U \tag{45}$$

or, in other words, treating the commutator as a Heisenberg operator and bringing forward the $|S_z\rangle$ eigenvalue ω. Naturally, $\frac{\mathrm{d}S_z}{\mathrm{d}t} = 0$ and also,

$$\frac{\mathrm{d}S_x}{\mathrm{d}t} = -\omega U^\dagger S_y U \tag{46}$$

$$\frac{\mathrm{d}S_y}{\mathrm{d}t} = \omega U^\dagger S_x U \tag{47}$$

The time-evolution operator as in Sakurai (2.1.43) and class is

$$\mathcal{U}(t) = \exp\left\{-\frac{iHt}{\hbar}\right\} \tag{48}$$

$$= \begin{pmatrix} \exp\left\{\frac{-i\omega}{2}\right\} & 0 \\ 0 & \exp\left\{\frac{i\omega}{2}\right\} \end{pmatrix} \tag{49}$$

These lead to the final spin operators,

$$S_x(t) = \frac{\hbar}{2}\begin{pmatrix} 0 & \exp\{i\omega t\} \\ \exp\{-i\omega t\} & \\ 0 & \end{pmatrix} \tag{50}$$

$$S_y(t) = \frac{i\hbar}{2}\begin{pmatrix} 0 & -\exp\{i\omega t\} \\ \exp\{-i\omega t\} & \\ 0 & \end{pmatrix} \tag{51}$$

$$S_z(t) = S_z(0) \tag{52}$$

corresponding to the Pauli matrices.[2]

[2] Specifically, the operators are integrated versions of the differentials previously given. For example, we have that

$$\begin{aligned} U^\dagger S_x U^\dagger &= \frac{\hbar}{2}\begin{pmatrix} \exp\left\{\frac{i\omega}{2}\right\} & 0 \\ 0 & \exp\left\{\frac{-i\omega}{2}\right\} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \exp\left\{\frac{-i\omega}{2}\right\} & 0 \\ 0 & \exp\left\{\frac{i\omega}{2}\right\} \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} 0 & \exp\{i\omega t\} \\ \exp\{-i\omega t\} & 0 \end{pmatrix} \\ U^\dagger S_y U^\dagger &= \frac{i\hbar}{2}\begin{pmatrix} 0 & -\exp\{i\omega t\} \\ \exp\{-i\omega t\} & 0 \end{pmatrix} \end{aligned}$$

The integration into the final operators provided is straightforward.