Quantum Mechanics A
Fall 2010
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Problem Set 7

Problem 1

A particle of mass m is under the influence of a 1D harmonic oscillator (HO) potential with a Hamiltonian of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2. \tag{1}$$

Assume that the ground-state wave-function is a Gaussian of the form

$$\psi(x) = A\exp(-\alpha x^2) \tag{2}$$

a) Determine the pre-factor A such that the state $\psi(x)$ is normalized.

b) Calculate the expectation value of the HO Hamiltonian with the state given above as a function of the parameter α, i.e.,

$$E(\alpha) = \langle\psi|\hat{H}|\psi\rangle \tag{3}$$

c) Determine the parameter α by minimizing the expectation value $E(\alpha)$ with respect to α. What is the value α_0 at which the energy has a minimum?

d) Compare the energy and the wave-function obtained by using the optimum value α_0 found above, with the exact ground-state energy and wave-function for the HO.

e) Plot the energy expectation value $E(\alpha)$ as a function of α. In a different Figure, plot together the potential as a function of x and the wavefunction as a function of x. Use three different values for α, $\alpha = \alpha_0$, $\alpha = \alpha_0/2$ and $\alpha = 2\alpha_0$. The classical lowest energy state is the one in which the particle is at the minimum of the potential i.e., at $x = 0$, which corresponds to a state obtained as a limit of $\alpha \to \infty$. Explain why? What is the expectation value of the Hamiltonian in this limit?

Problem 2

A particle of mass m is under the influence of a 1D potential of the so-called Lennard-Jones form

$$V(x) = -4\epsilon\left(\left(\frac{\sigma}{x}\right)^6 - \left(\frac{\sigma}{x}\right)^{12}\right), \tag{4}$$

with a Hamiltonian of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{5}$$

a) Draw this potential and show that its minimum is at $x_0/\sigma = 2^{1/6}$.

b) Now assume that the amplitude of the zero-point motion of the particle in the ground state is small; this assumption allows you to expand the potential near the minimum $x = x_0$. Show that the leading term is of the form

$$V(x) = V(x_0) + \frac{1}{2}m\omega^2(x - x_0)^2 \tag{6}$$

namely, there is no linear term in $x - x_0$. What is the value of the parameter ω introduced above?

c) What is the ground state energy of the Hamiltonian using the harmonic approximation (given by Eq. 6) for the potential? What is the ground state wavefunction?

d) Calculate the expectation value

$$(\Delta x)^2 \equiv \langle\psi_0|(x - x_0)^2|\psi_0\rangle \tag{7}$$

in the ground state within the harmonic approximation (6).

e) Find a critical value λ_c for the dimensionless combination

$$\lambda = \frac{\hbar^2}{m\sigma^2\epsilon} \tag{8}$$

such that for $\lambda > \lambda_c$ there is no bound state.

f) What is the value of $\Delta x/\sigma$ as the value of λ becomes the critical λ_c. Do you think that the harmonic approximation could still be valid for $\lambda = \lambda_c$?

Problem 3

A 1D harmonic oscillator with the familiar Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2, \tag{9}$$

is prepared in an initial state with a wave-function of the following form

$$\phi(x) = Ax^2\exp(-\frac{m\omega}{2\hbar}x^2). \tag{10}$$

a) Find the normalization constant A.

b) Write the above initial state as a linear combination of the eigenstates of the harmonic oscillator.

c) Assume that the harmonic oscillator at $t = 0$ is in a state described by the above wave-function. Find the state of the system $|\psi(t)\rangle$ at a later time t.

d) Show that the expectation value of $\hat{x}$ is zero at all times. Find the expectation value of $\hat{x}^2$, i.e., $\langle\psi(t)|\hat{x}^2|\psi(t)\rangle$ as a function of time. Plot the quantity

$$\sigma(t) = \sqrt{\langle\psi(t)|\hat{x}^2|\psi(t)\rangle}. \tag{11}$$

as a function of t. Can you interpret your result?

Problem 4

a) Derive and solve the equations of motion for the Heisenberg operators $a(t)$ and $a^\dagger(t)$ for the harmonic oscillator.

b) Calculate the commutator $[a(t), a^\dagger(t')]$.

Problem 5

a) Show that

$$[\mathbf{r}, f(\mathbf{p})] = i\hbar\nabla_{\mathbf{p}} f(\mathbf{p}), \tag{12}$$

for any arbitrary function $f(\mathbf{p})$ of the momentum operator.

b) Using this result show that

$$e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{d}}\mathbf{r}e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{d}} = \mathbf{r} + \mathbf{d} \tag{13}$$

where $\mathbf{d}$ is c-vector.

c) Show that the wave-function of the state

$$|\Phi\rangle = e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{d}}|\Psi\rangle \tag{14}$$

is the same as the wave-function of the state $|\psi\rangle$, only shifted a distance $\mathbf{d}$.

d) Write out $\langle x|\Phi\rangle$ explicitly if $|\Psi\rangle$ is the ground state of the 1D harmonic oscillator.

e) Show that $|\Phi\rangle$ develops in the Schrödinger representation by

$$|\Phi(t)\rangle = e^{-\frac{i}{\hbar}\mathbf{p}(-t)\cdot\mathbf{d}}|\Psi(t)\rangle \tag{15}$$

where $\mathbf{p}(-t)$ is the momentum operator in the Heisenberg representation at time $-t$.