PHY 303, I-Semester 2023/24, Assignment 4

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Due-date: 8. Oct 2023

(1) Anharmonic oscillator [8pts]:

(a) The Hamiltonian for an oscillator of mass m with an anharmonic potential is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \kappa x^4, \tag{1}$$

for $\kappa > 0$. Write this Hamiltonian in terms of the same ladder operators that we defined for the harmonic oscillator [4 pts].

(b) Suppose the state of the particle in the anharmonic oscillator Eq. (1) is described by the wavefunction

$$\Psi(x) = \frac{1}{(\pi\sigma^2)^{1/4}} e^{-\frac{x^2}{2\sigma^2}}, \tag{2}$$

where $\sigma = \sqrt{\hbar/(m\omega)}$. Evaluate the expectation value of energy $\langle \hat{H} \rangle$ in state (2) for Hamiltonian (1) using two different methods: (i) Writing the corresponding integration over x and finding the result of the integral. (ii) Using your result of (a), writing $\Psi(x)$ and all functions appearing in an integral abstractly in terms of harmonic oscillator eigenstates $\phi_n(x)$ [from Eq. (2.65) of the lecture, but you do not need these details] [4pts].

(2) Correspondence principle [10pts]:

(a) Make your own exact figure for the drawing in example 15 in mathematica. In particular find x_{ctp} in term of the oscillator energy, then choose an energy E corresponding to a high lying harmonic oscillator state (say e.g. $n_0 = 20$) and plot $\rho(x)$ on top of $|\phi_{n_0}(x)|^2$ [5 pts].

(b) Now take the average of the probability density over a few states in the vicinity of E (say $n \pm 2$) thus calculatig $\bar{\rho}(x) = \sum_{n;|n-n_0|\leq 2} |\phi_n(x)|^2$ and compare again. Discuss what you find. Where does it agree, where does it not agree? How does agreement change when n_0 is varied? [5 pts].

(3) Harmonic oscillator [12 pts]

(a) Find the expectation values and uncertainties of $\hat{x}$ and $\hat{p}$ in each of the eigenstates of the Harmonic oscillator, and discuss the product of both uncertainties. [6pts]

(b) From that show the virial theorem $\langle \hat{T} \rangle = \langle \hat{V} \rangle$ relating the expectation values of kinetic and potential energies. [3pts]

(c) Now find the expectation value of the position in the superposition state $\Psi(x) = (\phi_0(x) + \phi_1(x))/\sqrt{2}$ at all times $t > 0$. [3pts] With which frequency does it oscillate?

(4) Quantum dynamics: [**10pts**] The code `Assignment4_program_draft_v1.nb` is set up to solve the TDSE. You only have to define a potential $V(x)$ and an initial state $\Psi(x, t = 0)$ at the indicated places.

Design your own question from here. I want you to: **(a)** make thorough contact with at least one concept of quantum dynamics encountered in the lecture so far. You can reproduce an example, assignment or tutorial question, analytical result, anything from the selection of week 3-5 problems. The only constraint is to look at genuine dynamics, i.e. something significant should vary in time, do not just look at a stationary state (even though you might want to do that for testing and warm up). **(b)**: Then extend that concept towards the unknown (by adding multiple copies of some feature in the potential, combining two features etc.). For both make many plots, verify whichever analytical results you may know, and extensively analyse your findings.

Please be careful about the following list of pitfalls

- We set $\hbar = m = 1$ to avoid any large unitful numbers. Thus mainly use numbers "of order one (0.1-10)" for definitions of potentials, initial states, spatial ranges and times.
- Numerics does not like infinities, hence if you want to use $V(x) \to \infty$, just make it larger than everything else (e.g. 100).
- Numerics also does not like discontinuities, rather use $(\tanh(x/\xi) + 1)/2$ with finite and visible ξ than $\theta(x)$ (Heaviside step function).
- The calculation will take longer, if you do brutal things to your wavefunction, or you go towards very "classical states" (very small quantum wavelength relative to $L_{\max}$). Best avoid these cases. If the solution has not been calculated after a few minutes, best change parameters. The more brutal dynamics you do, the more points you need (Increase `MinPoints`, `MaxPoints`).
- One way to see if anything goes wrong from the start, is set t_{fin} to a very low value.
- avoid wavefunctions hitting the edge of your domain $-L_{\max}$ or $L_{\max}$. If that happens the calculation ceases to make sense. To avoid it, enlarge $L_{\max}$, add a potential or decrease t_{fin}.
- Any numerical solution can be wrong. To make sure it is converged in terms of discretisation, check it does not change when you increase the number of points (`MinPoints`, `MaxPoints`) or increase the tolerances (`AccuracyGoal`, `PrecisionGoal`). Other good checks are whether energy $\langle \hat{H} \rangle$ or normalisation of the wavefunction stay conserved.

After the assignment, let us know about any additional pitfalls you encountered that were not listed here.

(5) Schrödinger's equation in momentum space [moved to/part of assignment 4]: [6 pts, from earlier Assignment 3 sheet] Suppose a particle of mass m can move in one dimension under the influence of the potential $V(x)$. In Eq. (2.93) of the lecture, we introduced the momentum space representation $\tilde{\phi}(k)$ of the wavefunction.

(a) Find also a momentum space representation of the TISE which a momentum space wavefunction has to fulfill.[1] *Hint: Your calculation should lead you towards the definition of the Fourier transformed potential:*

$$\tilde{V}(p-p') = \frac{1}{\sqrt{2\pi\hbar}} \int dx V(x) e^{-i\frac{(p-p')}{\hbar}x} \tag{3}$$

which should appear in your final equation. [3pts]

(b) Discuss the physical meaning of each term. Discuss what happens to the momentum probability distribution for the case $V(x) = 0$, or $V(x) \neq 0$. You may want to consider the change of the momentum space wavefunction during an infinitesimal time element dt [3pts].

[1] The TISE 1(.62) that we have considered so far is said to be in the "position space representation". Its momentum space variant should only have $i\hbar\frac{\partial}{\partial t}\tilde{\phi}(k,t) = \cdots$ as the left hand side.