PHY 303, I-Semester 2023/24, Assignment 5

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Due-date: 22 Oct 2023

(1) Wave function discontinuities [8 pts tot]: Consider the normalised wavefunction

$$\Psi(x) = \begin{cases} \frac{1}{\sqrt{L}} & \text{for } -\frac{L}{2} \leq x \leq \frac{L}{2} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

for $L > 0$, describing a particle with free Hamiltonian $\hat{H} = \hat{p}^2/(2m)$.

(a) Show formally that the function has two discontinuities, then find the corresponding momentum space wavefunction $\Psi(p)$ and draw both probability densities, for position and for momentum measurements [5pts].

(b) Show that the expectation value of the kinetic (=total) energy in the state is infinite regardless of L, and discuss the implications of this for discontinuities in wavefunctions [3pts].

(2) Bound states on two delta-function potentials [10pts tot]: Consider a double delta-function potential

$$V(x) = -\alpha[\delta(x-a) + \delta(x+a)]. \tag{2}$$

(a) Show that a wavefunction solving the TISE for the potential above must satisfy the condition

$$\lim_{\epsilon\to 0}\left[\phi(a+\epsilon)' - \phi(a-\epsilon)'\right] = -\frac{2m}{\hbar^2}\alpha\phi(a). \tag{3}$$

and a similar one involving location $x = -a$ [2pts].

(b) With that, show that the Ansatz

$$\phi(x) = \begin{cases} Ae^{-\kappa x} & \text{for } x \leq -a, \\ B(e^{\kappa x} \pm e^{-\kappa x}) & \text{for } -a < x \leq a, \\ Ae^{\kappa x} & \text{for } x > a, \end{cases} \tag{4}$$

can solve the TISE. Why can we choose this Ansatz?. Find the parameter κ required for this separately for $\pm$ and the equation linking it and the energy E. Solve that equation, numerically if need be [6pts].

(c) Discuss all solutions to this equation graphically. How many bound states are there? Is there always a bound state? [2 pts]

(3) Measurements: [**12 pts**] Consider a Hilbertspace with three basis vectors $|\, a\,\rangle$, $|\, b\,\rangle$, $|\, c\,\rangle$, and three operators:

$$\hat{O}_1 = \kappa\,(|\, a\,\rangle\langle\, a\,| - |\, c\,\rangle\langle\, c\,|)\,, \tag{5}$$
$$\hat{O}_2 = \frac{\kappa}{\sqrt{2}}\,(|\, a\,\rangle\langle\, b\,| + |\, b\,\rangle\langle\, a\,| + |\, b\,\rangle\langle\, c\,| + |\, c\,\rangle\langle\, b\,|)\,, \tag{6}$$
$$\hat{O}_3 = \frac{\kappa}{\sqrt{2}}\,(-i|\, a\,\rangle\langle\, b\,| + i|\, b\,\rangle\langle\, a\,| + -i|\, b\,\rangle\langle\, c\,| + i|\, c\,\rangle\langle\, b\,|)\,. \tag{7}$$
$$\tag{8}$$

(a) Find the matrix representation of these operators in the basis $\{|\, a\,\rangle, |\, b\,\rangle, |\, c\,\rangle\}$, all eigenvectors and eigenvalues for each and all commutators among those three operators.

(b) From that derive an uncertainty relation between the three observables described by $\hat{O}_j$. Also discuss uncertainties between $\hat{O}_2$ and $\hat{O}_\perp \equiv \hat{O}_1^2 + \hat{O}_3^2$.

(c) Suppose the system is initially in the state $|\, \Psi\,\rangle = (|\, a\,\rangle - |\, b\,\rangle + i|\, c\,\rangle)/\sqrt{3}$. From this discuss the following sequence:

  (i) What is the probability to find $o_2 = 0, \pm\kappa$ upon measuring $\hat{O}_2$?

  (ii) Suppose we measured $o_2 = \kappa$, what is the probability to measure $o_2 = \kappa$ if the measurement is repeated immediately after the first?

  (iii) Immediately following that, we measure $\hat{O}_1$ and suppose we find $o_1 = \kappa$. Immediately after this step, we measure $\hat{O}_2$ again, which answers can we find, and with which probabilty?

(d) What changes if you swap the final measurement of $\hat{O}_1$ in the list above with a measurement of $\hat{O}_\perp$? Discuss all similarities and differences, and relate whatever you find to the uncertainty relations you have derived earlier.

(4) Box inside a box: [**10pts**] Consider the infinite square well potential, with an additional step potential inside:

$$\bar{V}(x) = \begin{cases} \infty & x \leq 0, \\ 0 & 0 < x \leq \frac{a}{2} - \frac{L}{2}, \\ V_0 > 0 & \frac{a}{2} - \frac{L}{2} < x \leq \frac{a}{2} + \frac{L}{2} \\ 0 & \frac{a}{2} + \frac{L}{2} < x \leq a \\ \infty & x > a. \end{cases} \tag{9}$$

Let us assume that $V_0 < \frac{\hbar^2\pi^2}{2ma^2}$. Let us denote the usual infinite square well potential without that step (as in lecture notes Eq. (2.10)) by $V(x)$, and define two Hamiltonians $\hat{\bar{H}} = \hat{T} + \bar{V}(x)$ and $\hat{H} = \hat{T} + V(x)$, where $\hat{T}$ is the kinetic energy operator of a particle of mass m in one dimension.

(a) Make a drawing of this potential. Argue why all eigenstates $\bar{\phi}_n(x)$ of the present Hamiltonian $\hat{\hat{H}}$ can be expressed in terms of eigenstates $\phi_n(x)$ of the usual Hamiltonian $\hat{H}$. Then find an argument, why it might be justified, for the above low value of V_0, to attempt to express the new lowest energy eigenstates of $\hat{\hat{H}}$ only using the M lowest energy eigenstates of $\hat{H}$, for small M, let's say $M = 3$.

(b) Write the present Hamiltonian $\hat{\hat{H}}$ explicitly in matrix form, using only the $M = 3$ lowest energy eigenstates of $\hat{H}$ as a basis (i.e. Eq. (2.18) of lecture notes, for $n = 1, 2, 3$). Explicitly find a matrix in terms of parameters, solving any integrations that might be required.

(c) Using that matrix representation, find the new eigenstates and eigenenergies, make a drawing of the former, and compare the latter explicitly with the eigenenergies of $\hat{H}$.

(d) Now adapt the code which was provided for Assignment 3 Q4, to numerically solve the TISE, to numerically find eigenstates and energies of $\hat{\hat{H}}$ under conditions as discussed above, and thus verify your calculations. Choose parameters for which at least some of the lowest three new eigenstates visibly differ from the old ones, and discuss physical reasons for the differences (or absence thereof).