Mathematical Tripos Part IB Quantum Mechanics

Michaelmas Term 2024 Prof. Frank Verstraete

Example Sheet 2

1. A particle of mass m is confined to a one-dimensional box $0 \le x \le a$ (the potential U(x) is zero inside the box, and infinite outside). Show that the energy eigenvalues are $E_n = \hbar^2 \pi^2 n^2 / 2ma^2$ for $n = 1, 2, \ldots$, and determine corresponding normalised energy eigenstates $\chi_n(x)$. Show that the expectation value and the uncertainty for a measurement of \hat{x} in the state χ_n are given by

$$\langle \hat{x} \rangle_n = \frac{a}{2}$$
 and $(\Delta x)_n^2 = \frac{a^2}{12} \left(1 - \frac{6}{\pi^2 n^2} \right)$.

Does the limit $n \to \infty$ agree with what you would expect for a classical particle in this potential?

2. Write down the time-independent Schrödinger equation for the wavefunction of a particle moving in a potential $U(x) = -U\delta(x)$, where U is a positive constant and $\delta(x)$ is the Dirac delta function. Integrate the equation over the interval $-\epsilon < x < \epsilon$, for a positive constant ϵ , and hence deduce that there is a discontinuity at x = 0 in the derivative of $\chi(x)$:

$$\lim_{\epsilon \to 0} \left[\chi'(\epsilon) - \chi'(-\epsilon) \right] = -\frac{2mU}{\hbar^2} \chi(0) \; .$$

By using this condition to relate appropriate solutions for x > 0 and x < 0, find the unique bound and normalisable eigenstate of the Hamiltonian, and determine its energy eigenvalue E(with E < 0).

3. Consider a square well potential with U(x) = -U for |x| < a and U(x) = 0 otherwise (U is a positive constant). Show that there are no bound states (normalisable energy eigenfunctions) which satisfy $\chi(-x) = -\chi(x)$ (i.e. which have odd parity) if $a^2U < (\pi\hbar)^2/8m$.

4. Sketch the potential

$$U(x) = -\frac{\hbar^2}{m} \mathrm{sech}^2 x \; .$$

Show that the time-independent Schrödinger equation for a particle in this potential can be written

$$\hat{A}^{\dagger}\hat{A}\chi = (\mathcal{E}+1)\chi$$

where $\mathcal{E} = 2mE/\hbar^2$ and

$$\hat{A} = \frac{\mathrm{d}}{\mathrm{d}x} + \tanh x , \quad \hat{A}^{\dagger} = -\frac{\mathrm{d}}{\mathrm{d}x} + \tanh x .$$

Show, by integrating by parts, that for any normalised wavefunction χ ,

$$\int_{-\infty}^{\infty} \chi^* \hat{A}^{\dagger} \hat{A} \chi \, \mathrm{d}x = \int_{-\infty}^{\infty} (\hat{A} \chi)^* (\hat{A} \chi) \, \mathrm{d}x$$

and deduce that the eigenvalues of $\hat{A}^{\dagger}\hat{A}$ are non-negative. Hence show that the ground state (with lowest energy) has $\mathcal{E} \geq -1$. Show that a wavefunction $\chi_0(x)$ is an energy eigenstate with $\mathcal{E} = -1$ iff

$$\frac{\mathrm{d}\chi_0}{\mathrm{d}x} + \tanh x \,\chi_0 = 0 \; .$$

Find and sketch $\chi_0(x)$.

5. Write down the Hamiltonian H for a harmonic oscillator of mass m and frequency ω . Express $\langle H \rangle$ in terms of $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, Δx and Δp , all defined for some normalised state ψ . Use the Uncertainty Relation to deduce that $E \geq \frac{1}{2}\hbar\omega$ for any energy eigenvalue E.

6. The energy levels of the harmonic oscillator are $E_n = (n + \frac{1}{2})\hbar\omega$ for n = 0, 1, 2, ... and the corresponding stationary state wavefunctions are

$$\chi_n(x) = h_n(y)e^{-y^2/2}$$
 where $y = (m\omega/\hbar)^{1/2}x$

and h_n is a polynomial of degree *n* with $h_n(-y) = (-1)^n h_n(y)$. Using *only* the orthogonality relations

$$(\chi_m, \chi_n) = \delta_{mn} \,,$$

determine χ_2 and χ_3 up to an overall constant in each case.

Give an expression for the quantum state of the oscillator $\psi(x,t)$ if the initial state is $\psi(x,0) = \sum_{n=0}^{\infty} c_n \chi_n(x)$, where c_n are complex constants. Deduce that

$$|\psi(x, 2p\pi/\omega)|^2 = |\psi(-x, (2q+1)\pi/\omega)|^2$$

for any integers $p, q \ge 0$. Comment on this result, considering the particular case in which $\psi(x, 0)$ is sharply peaked around position x = a.

7. A particle of mass m is in a one-dimensional infinite square well (a potential box) with U = 0 for 0 < x < a and $U = \infty$ otherwise. The normalised wavefunction for the particle at time t = 0 is

$$\psi(x,0) = Cx(a-x) \; .$$

(i) Determine the real constant C.

(ii) By expanding $\psi(x, 0)$ as a linear combination of energy eigenfunctions (found in Example 1 above), obtain an expression for $\psi(x, t)$, the wavefunction at time t.

(iii) A measurement of the energy is made at time t > 0. Show that the probability that this yields the result $E_n = \hbar^2 \pi^2 n^2 / 2ma^2$ is $960/\pi^6 n^6$ if n is odd, and zero if n is even. Why should the result for n even be expected? Which value of the energy is most likely, and why is its probability so close to unity?

8. Consider the Schrödinger Equation in one dimension with potential U(x). Show that for a stationary state, the probability current J is independent of x.

Now suppose that an energy eigenstate $\chi(x)$ corresponds to scattering by the potential and that $U(x) \to 0$ as $x \to \pm \infty$. Given the asymptotic behaviour

$$\chi(x) \sim e^{ikx} + Be^{-ikx}$$
 $(x \to -\infty)$ and $\chi(x) \sim Ce^{ikx}$ $(x \to +\infty)$

show that $|B|^2 + |C|^2 = 1$. How should this be interpreted?

9. A particle is incident on a potential barrier of width a and height U. Assuming that U = 2E, where $E = \hbar^2 k^2 / 2m$ is the kinetic energy of the incident particle, find the transmission probability.

[Work through the algebra, which simplifies in this case, rather than quoting the general result.]

10. Consider the time-independent Schrödinger Equation with potential $U(x) = -U\delta(x)$. Show that there is a scattering solution with energy eigenvalue $E = \hbar^2 k^2/2m$ for any real k > 0 and find the transmission and reflection coefficients $A_{tr}(k)$ and $A_{ref}(k)$ (that correspond to the transmission and reflection coefficients defined in the notes as T and R respectively). [*Recall from Example* **2** that the energy eigenfunction χ is continuous, but satisfies $\chi'(0+) - \chi'(0-) = -(2mU/\hbar^2)\chi(0)$.]

Is the solution above still an eigenfunction of the Hamiltonian if k is allowed to take complex values? Show that $A_{tr}(k)$ and $A_{ref}(k)$ are singular at $k = i\kappa$ for a certain real, positive value of

 κ . By first re-scaling the scattering solution, find a bound state (normalisable) solution in the potential. What is the energy of this bound state?

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