Mathematical Tripos Part IB | **Michaelmas Term 2023**

Quantum Mechanics | **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

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

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 $\chi(x)$:

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

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 $a^2 U < (\pi\hbar)^2/8m$.

4. Sketch the potential

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

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 $\mathcal{E} \ge -1$. 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 $n = 0, 1, 2, \ldots$ and the corresponding stationary state wavefunctions are

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

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, $q \geq 0$. 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

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

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 $E = \hbar^2k^2/2m$ 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 $E = \hbar^2k^2/2m$ for any real $k > 0$ and find the transmission and reflection coefficients $A_{\rm tr}(k)$ and $A_{\rm ref}(k)$(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 $A_{\rm tr}(k)$ and $A_{\rm ref}(k)$ 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?

Comments to: fv285@cam.ac.uk