Quantum Mechanics

Second year physics course

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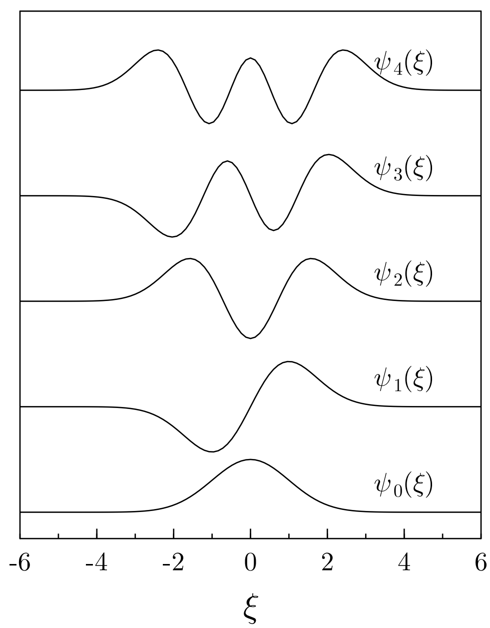

Questions*

MICHAELMAS 2015

*These problems are designed to develop skills in manipulating quantum-mechanical operators and solving problems. The first two sheets are designed for tutorials in Michaelmas term, with the third serving as work for the vacation. Most of the problems are taken or adapted from a previous problem sheet and therefore feature questions from *The Physics of Quantum Mechanics* by James Binney and David Skinner (OUP).

Quantum Mechanics: Problems

Problem sheet 1: (Michaelmas Term, Weeks 5–6)

■ *Matter waves*

1.1 Find the kinetic energy in eV (electron volts) of a neutron, an electron and an electromagnetic wave, each of wavelength 0.1 nm. (For the electron and the neutron, first try a non-relativistic formula for the kinetic energy, and then justify afterwards why it was reasonable to do that.)

1.2 For the electron and the neutron in the previous problem, estimate in each case the approximate wavelength below which the non-relativistic formula would fail to give a good answer (and make a reasonable choice for what 'good' means here).

1.3 A beam of neutrons with energy E runs horizontally into a crystal. The crystal transmits half the neutrons and deflects the other half vertically upwards. After climbing to height H these neutrons are deflected through 90° onto a horizontal path parallel to the originally transmitted beam. The two horizontal beams now move a distance L down the laboratory, one distance H above the other. After going distance L, the lower beam is deflected vertically upwards and is finally deflected into the path of the upper beam such that the two beams are co-spatial as they enter the detector. Given that particles in both the lower and upper beams are in states of well-defined momentum, show that the wavenumbers k, k' of the lower and upper beams are related by

$$k' \simeq k \left(1 - \frac{m_{\mathrm{n}} g H}{2E}\right).$$

In an actual experiment (R. Colella *et al.*, *Phys. Rev. Lett.*, **34**, 1472, 1975) $E = 0.042\,\mathrm{eV}$ and $LH \sim 10^{-3}\,\mathrm{m}^2$ (the actual geometry was slightly different). Determine the phase difference between the two beams at the detector. Sketch the intensity in the detector as a function of H.

■ *Wave mechanics*

1.4 Particles move in the potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases}.$$

Particles of mass m and energy $E > V_0$ are incident from $x = -\infty$. Show that the probability that a particle is reflected is

$$\left(\frac{k-K}{k+K}\right)^2,$$

where $k \equiv \sqrt{2mE}/\hbar$ and $K \equiv \sqrt{2m(E - V_0)}/\hbar$. Show directly from the time-independent Schrödinger equation that the probability of transmission is

$$\frac{4kK}{(k+K)^2}$$

and check that the flux of particles moving away from the origin is equal to the incident particle flux.

1.5 Show that the energies of bound, odd-parity stationary states of the square potential well

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ V_0 > 0 & \text{otherwise} \end{cases},$$

are governed by

$$\cot(ka) = -\sqrt{\frac{W^2}{(ka)^2} - 1} \quad \text{where} \quad W \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad \text{and} \quad k^2 = 2mE/\hbar^2.$$

Show that for a bound odd-parity state to exist, we require $W > \pi/2$.

1.6 A free particle of energy E approaches a square, one-dimensional potential well of depth V_0 and width $2a$. Show that the probability of being reflected by the well vanishes when $Ka = n\pi/2$, where n is an integer and $K = (2m(E + V_0)/\hbar^2)^{1/2}$. Explain this phenomenon in physical terms.

1.7 A particle of energy E approaches from $x < 0$ a barrier in which the potential energy is $V(x) = V_\delta \delta(x)$. Show that the probability of its passing the barrier is

$$P_{\text{tun}} = \frac{1}{1 + (K/2k)^2} \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad K = \frac{2mV_\delta}{\hbar^2}.$$

1.8 Given that the wavefunction is $\psi = Ae^{\mathrm{i}(kz-\omega t)} + Be^{-\mathrm{i}(kz+\omega t)}$, where A and B are constants, show that the probability current density is

$$\boldsymbol{J} = v\big(|A|^2 - |B|^2\big)\,\hat{\boldsymbol{z}},$$

where $v = \hbar k/m$. Interpret the result physically.

1.9 Let $\psi(x,t)$ be the correctly normalised wavefunction of a particle of mass m and potential energy $V(x)$. Write down expressions for the expectation values of (a) $\hat{x}$; (b) $\hat{x}^2$; (c) the momentum $\hat{p}_x$; (d) $\hat{p}_x^2$; (e) the energy.

What is the probability that the particle will be found in the interval (x_1, x_2)?

Quantum Mechanics: Problems

Problem sheet 2: (Michaelmas Term, Weeks 7–8)

■ *Dirac notation*

2.1 How is a wavefunction $\psi(x)$ written in Dirac's notation? What's the physical significance of the complex number $\psi(x)$ for given x?

2.2 Given that $|\psi\rangle = e^{i\pi/5}|a\rangle + e^{i\pi/4}|b\rangle$, express $\langle\psi|$ as a linear combination of $\langle a|$ and $\langle b|$.

2.3 An electron can be in one of two potential wells that are so close that it can 'tunnel' from one to the other. Its state vector can be written

$$|\psi\rangle = a|A\rangle + b|B\rangle,$$

where $|A\rangle$ is the state of being in the first well and $|B\rangle$ is the state of being in the second well and all kets are correctly normalised. What is the probability of finding the particle in the first well given that: (a) $a = i/2$; (b) $b = e^{i\pi}$; (c) $b = \frac{1}{3} + i/\sqrt{2}$?

2.4 Let $\hat{Q}$ be the operator of an observable and let $|\psi\rangle$ be the state of our system.

(a) What are the physical interpretations of $\langle\psi|\hat{Q}|\psi\rangle$ and $|\langle q_n|\psi\rangle|^2$, where $|q_n\rangle$ is the n^{th} eigenket of the observable Q and q_n is the corresponding eigenvalue?

(b) What is the operator $\sum_n |q_n\rangle\langle q_n|$, where the sum is over all eigenkets of $\hat{Q}$? What is the operator $\sum_n q_n|q_n\rangle\langle q_n|$?

(c) If $u_n(x)$ is the wavefunction of the state $|q_n\rangle$, write down an integral that evaluates to $\langle q_n|\psi\rangle$.

■ *Time dependence and the Schrödinger equation*

2.5 Write down the time-independent (TISE) and the time-dependent (TDSE) Schrödinger equations. Is it necessary for the wavefunction of a system to satisfy the TDSE? Under what circumstances does the wavefunction of a system satisfy the TISE?

2.6 Why is the TDSE first-order in time, rather than second-order like Newton's equations of motion?

2.7 A particle is confined in a potential well such that its allowed energies are $E_n = n^2\mathcal{E}$, where $n = 1, 2, \ldots$ is an integer and $\mathcal{E}$ a positive constant. The corresponding energy eigenstates are $|1\rangle$, $|2\rangle$, …, $|n\rangle$, … At $t = 0$ the particle is in the state

$$|\psi(0)\rangle = 0.2|1\rangle + 0.3|2\rangle + 0.4|3\rangle + 0.843|4\rangle.$$

(a) What is the probability, if the energy is measured at $t = 0$, of finding a number smaller than $6\mathcal{E}$?

(b) What is the mean value and what is the rms deviation of the energy of the particle in the state $|\psi(0)\rangle$?

(c) Calculate the state vector $|\psi\rangle$ at time t. Do the results found in (a) and (b) for time t remain valid for arbitrary time t?

(d) When the energy is measured it turns out to be $16\mathcal{E}$. After the measurement, what is the state of the system? What result is obtained if the energy is measured again?

2.8 A particle moves in the potential $V(\boldsymbol{x})$ and is known to have energy E_n. (a) Can it have well-defined momentum for some particular $V(\boldsymbol{x})$? (b) Can the particle simultaneously have well-defined energy and position?

■ *Hermitian operators*

2.9 Which of the following operators are Hermitian, given that $\hat{A}$ and $\hat{B}$ are Hermitian: $\hat{A}+\hat{B}$; $c\hat{A}$; $\hat{A}\hat{B}$; $\hat{A}\hat{B}+\hat{B}\hat{A}$.

Show that in one dimension, for functions which tend to zero as $|x| \to \infty$, the operator $\partial/\partial x$ is not Hermitian, but $-\mathrm{i}\hbar\partial/\partial x$ is. Is $\partial^2/\partial x^2$ Hermitian?

2.10 Given that $\hat{A}$ and $\hat{B}$ are Hermitian operators, show that $\mathrm{i}[\hat{A}, \hat{B}]$ is a Hermitian operator.

2.11 Given that for any two operators $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$, show that

$$(\hat{A}\hat{B}\hat{C}\hat{D})^\dagger = \hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger.$$

■ *Commutators*

2.12 Show that if there is a complete set of mutual eigenkets of the Hermitian operators $\hat{A}$ and $\hat{B}$, then $[\hat{A}, \hat{B}] = 0$. Explain the physical significance of this result.

2.13 Does it always follow that if a system is an eigenstate of $\hat{A}$ and $[\hat{A}, \hat{B}] = 0$ then the system will be in a eigenstate of $\hat{B}$? If not, give a counterexample.

2.14 Show that

(a) $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

(b) $[\hat{A}\hat{B}\hat{C}, \hat{D}] = \hat{A}\hat{B}[\hat{C}, \hat{D}] + \hat{A}[\hat{B}, \hat{D}]\hat{C} + [\hat{A}, \hat{D}]\hat{B}\hat{C}$. Explain the similarity with the rule for differentiating a product.

(c) $[\hat{x}^n, \hat{p}] = \mathrm{i}\hbar n\hat{x}^{n-1}$

(d) $[f(\hat{x}), \hat{p}] = \mathrm{i}\hbar\frac{\mathrm{d}f}{\mathrm{d}x}$ for any function $f(x)$.

Quantum Mechanics: Problems

Problem sheet 3: (Christmas vacation)

■ *The simple harmonic oscillator*

3.1 After choosing units in which everything, including $\hbar = 1$, the Hamiltonian of a harmonic oscillator may be written $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2)$, where $[\hat{x}, \hat{p}] = \mathrm{i}$. Show that if $|\psi\rangle$ is a ket that satisfies $H|\psi\rangle = E|\psi\rangle$, then

$$\frac{1}{2}(\hat{p}^2 + \hat{x}^2)(\hat{x} \mp \mathrm{i}\hat{p})|\psi\rangle = (E \pm 1)(\hat{x} \mp \mathrm{i}\hat{p})|\psi\rangle.$$

Explain how this algebra enables one to determine the energy eigenvalues of a harmonic oscillator.

3.2 Given that $\hat{a}|n\rangle = \alpha|n-1\rangle$ and $E_n = (n + \frac{1}{2})\hbar\omega$, where the annihilation operator of the harmonic oscillator is

$$\hat{a} \equiv \frac{m\omega\hat{x} + \mathrm{i}\hat{p}}{\sqrt{2m\hbar\omega}},$$

show that $\alpha = \sqrt{n}$. Hint: consider $|\hat{a}|n\rangle|^2$.

3.3 The pendulum of a grandfather clock has a period of 1 s and makes excursions of 3 cm either side of dead centre. Given that the bob weighs 0.2 kg, around what value of n would you expect its non-negligible quantum amplitudes to cluster?

3.4 Show that the minimum value of $E(p, x) \equiv p^2/2m + \frac{1}{2}m\omega^2 x^2$ with respect to the real numbers p, x when they are constrained to satisfy $xp = \frac{1}{2}\hbar$, is $\frac{1}{2}\hbar\omega$. Explain the physical significance of this result.

3.5 How many nodes are there in the wavefunction $\langle x|n\rangle$ of the nth excited state of a harmonic oscillator?

3.6 Show that for a harmonic oscillator that wavefunction of the second excited state is $\langle x|2\rangle$ = constant $\times$ $(x^2/\ell^2 - 1)\mathrm{e}^{-x^2/4\ell^2}$, where $\ell \equiv \sqrt{\hbar/2m\omega}$ and find the normalising constant.

3.7 Use

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) = \ell(\hat{a} + \hat{a}^\dagger)$$

to show for a harmonic oscillator that in the energy representation the operator $\hat{x}$ is

$$\hat{x}_{jk} = \ell \left(\begin{array}{ccccccccc}
0 & \sqrt{1} & 0 & 0 & \ldots & & & & \\
\sqrt{1} & 0 & \sqrt{2} & 0 & & & & & \\
0 & \sqrt{2} & 0 & \sqrt{3} & \ldots & & & & \\
 & & \sqrt{3} & \ldots & & & & & \\
\ldots & & \ldots & & \ldots & & \ldots & & \\
 & & & \ldots & 0 & \sqrt{n-1} & \ldots & & \\
 & & & & \sqrt{n-1} & 0 & \sqrt{n} & & \\
 & & & & & \sqrt{n} & 0 & \sqrt{n+1} & \ldots \\
 & & & & & & \sqrt{n+1} & 0 & \\
\ldots & & \ldots & & \ldots & & \ldots & & \ldots
\end{array} \right)$$

Calculate the same entries for the matrix $\hat{p}_{jk}$.

3.8 At $t = 0$ the state of a harmonic oscillator of mass m and frequency ω is

$$|\psi\rangle = \frac{1}{2}|N-1\rangle + \frac{1}{\sqrt{2}}|N\rangle + \frac{1}{2}|N+1\rangle.$$

Calculate the expectation value of x as a function of time and interpret your result physically in as much detail as you can.

■ *More problems on basic quantum mechanics*

3.9 An electron can 'tunnel' between potential wells that form a chain, so its state vector can be written

$$|\psi\rangle = \sum_{n=-\infty}^{\infty} a_n|n\rangle,$$

where $|n\rangle$ is the state of being in the nth well, where n increases from left to right. Let

$$a_n = \frac{1}{\sqrt{2}}\left(\frac{-\mathrm{i}}{3}\right)^{|n|/2} \mathrm{e}^{\mathrm{i}n\pi}.$$

(a) What is the probability of finding the electron in the nth well?

(b) What is the probability of finding the electron in well 0 or anywhere to the right of it?

3.10 A three-state system has a complete orthonormal set of states $|1\rangle, |2\rangle, |3\rangle$. With respect to this basis the operators $\hat{H}$ and $\hat{B}$ have matrices

$$\hat{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \hat{B} = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

where ω and b are real constants.

(a) Are $\hat{H}$ and $\hat{B}$ Hermitian?

(b) Write down the eigenvalues of $\hat{H}$ and find the eigenvalues of $\hat{B}$. Solve for the eigenvectors of both $\hat{H}$ and $\hat{B}$. Explain why neither matrix uniquely specifies its eigenvectors.

(c) Show that $\hat{H}$ and $\hat{B}$ commute. Give a basis of eigenvectors common to $\hat{H}$ and $\hat{B}$.

3.11 A system has a time-independent Hamiltonian that has spectrum $\{E_n\}$. Prove that the probability P_k that a measurement of energy will yield the value E_k is is time-independent. Hint: you can do this either from Ehrenfest's theorem, or by differentiating $\langle E_k, t|\psi\rangle$ w.r.t. t and using the TDSE.

3.12 Let $\psi(x)$ be a properly normalised wavefunction and $\hat{Q}$ an operator on wavefunctions. Let $\{q_r\}$ be the spectrum of $\hat{Q}$ and $\{u_r(x)\}$ be the corresponding correctly normalised eigenfunctions. Write down an expression for the probability that a measurement of Q will yield the value q_r. Show that $\sum_r P(q_r|\psi) = 1$. Show further that the expectation of Q is $\langle Q\rangle \equiv \int_{-\infty}^{\infty} \psi^* \hat{Q}\psi \,\mathrm{d}x$.

3.13 (a) Find the allowed energy values E_n and the associated normalized eigenfunctions $\phi_n(x)$ for a particle of mass m confined by infinitely high potential barriers to the region $0 \leq x \leq a$.

(b) For a particle with energy $E_n = \hbar^2 n^2 \pi^2 / 2ma^2$ calculate $\langle x \rangle$.

(c) Without working out any integrals, show that

$$\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \frac{a^2}{4}.$$

Hence find $\langle (x - \langle x \rangle)^2 \rangle$ using the result that $\int_0^a x^2 \sin^2(n\pi x/a)\,\mathrm{d}x = a^3(1/6 - 1/4n^2\pi^2)$.

(d) A classical analogue of this problem is that of a particle bouncing back and forth between two perfectly elastic walls, with uniform velocity between bounces. Calculate the classical average values $\langle x \rangle_\mathrm{C}$ and $\langle (x - \langle x \rangle)^2 \rangle_\mathrm{C}$, and show that for high values of n the quantum and classical results tend to each other.

3.14 A **Fermi oscillator** has Hamiltonian $\hat{H} = \hat{f}^\dagger \hat{f}$, where $\hat{f}$ is an operator that satisfies

$$\hat{f}^2 = 0, \quad \hat{f}\hat{f}^\dagger + \hat{f}^\dagger \hat{f} = 1.$$

Show that $\hat{H}^2 = \hat{H}$, and thus find the eigenvalues of $\hat{H}$. If the ket $|0\rangle$ satisfies $\hat{H}|0\rangle = 0$ with $\langle 0|0\rangle = 1$, what are the kets (a) $|a\rangle \equiv \hat{f}|0\rangle$, and (b) $|b\rangle \equiv \hat{f}^\dagger|0\rangle$?

In quantum field theory the vacuum is pictured as an assembly of oscillators, one for each possible value of the momentum of each particle type. A boson is an excitation of a harmonic oscillator, while a fermion in an excitation of a Fermi oscillator. Explain the connection between the spectrum of $\hat{f}^\dagger \hat{f}$ and the Pauli exclusion principle (which states that zero or one fermion may occupy a particular quantum state).