Quantum Mechanics MT 2019: Problem Sheet 1

Dirac notation

1.1 What physical phenomenon requires us to work with probability amplitudes rather than with probabilities?

1.2 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 $\langle b|$.

1.3 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

$$|\psi\rangle = a|A\rangle + b|B\rangle, \tag{1}$$

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) $b = \frac{1}{3} + i/\sqrt{2}$?

1.4 An electron can "tunnel" between potential wells that form a linear chain, so its state vector can be written as

$$|\psi\rangle = \sum_{n=-\infty}^{\infty} a_n|n\rangle, \tag{2}$$

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

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

(a) What is the probability of finding the electron in the n^{th} well?
(b) What is the probability of finding the electron in well 0 or anywhere to the right of it?

Operators

1.5 Let Q be the operator of an observable and let $|\psi\rangle$ be the state of our system.
(a) What are the physical interpretations of $\langle\psi|Q|\psi\rangle$ 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 Q? What is the operator $\sum_n q_n|q_n\rangle\langle q_n|$?

1.6 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?

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

1.8 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

1.9 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.

1.10 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.

1.11 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 $f(x)$.

1.12 Let A and B be two Hermitian operators. Prove that if $[A, B] = 0$ there exists a complete set of simultaneous eigenstates of the operators A and B, i.e.

$$A|u_j\rangle = a_j|u_j\rangle \ , \quad B|u_j\rangle = b_j|u_j\rangle, \tag{4}$$

and $\{|u_j\rangle\}$ form a basis of the LVS on which A and B act.

1.13 Prove that two observables are compatible if and only if the commutator between the associated Hermitian operators vanishes.

1.14 What does it mean to say that two operators commute? What is the significance of two observables having mutually commuting operators?

Given that the commutator $[P, Q] \neq 0$ for some observables P and Q, does it follow that for all $|\psi\rangle \neq 0$ we have $[P, Q]|\psi\rangle \neq 0$?

Quantum Mechanics MT 2019: Problem Sheet 2

Time dependence and the Schrödinger equation

2.1 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?

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

2.3 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 $|1\rangle$, $|2\rangle$, $\ldots$, $|n\rangle, \ldots$ 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?

2.4 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?

2.5 Let $\psi(x, t)$ be the correctly normalized wave function of a particle of mass m and potential energy $V(x)$. Write down the expressions for the expectation values of (a) $\hat{x}$; (b) $\hat{x}^2$; (c) $\hat{p}_x$; (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)?

2.6 Consider a quantum mechanical particle with Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}),$$

that is initially prepared in a state $|\psi(0)\rangle$. Using the TDSE show that the expectation value of an operator $\hat{Q}$ fulfils the following evolution equations

$$i\hbar\frac{d}{dt}\langle\psi(t)|\hat{Q}|\psi(t)\rangle = \langle\psi(t)|[\hat{Q}, H]|\psi(t)\rangle.$$

Consider the particular cases of the position and momentum operators and comment on the resulting equations

Wave Mechanics

2.7 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.

2.8 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 $W > \pi/2$.

2.9 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.

2.10 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

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

2.11 Given that the wavefunction is $\psi = A\mathrm{e}^{\mathrm{i}(kz-\omega t)} + B\mathrm{e}^{-\mathrm{i}(kz+\omega t)}$, 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.

2.12 Consider a free particle in one dimension with Hamiltonian

$$H = \frac{\hat{p}^2}{2m}. \tag{1}$$

Let the wave function of the particle at time $t = 0$ be a Gaussian wave packet

$$\psi(x,0) = \langle x|\psi(0)\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\frac{x^2}{4\sigma^2} + \frac{i}{\hbar}p_0 x}\ . \tag{2}$$

Show that in the momentum representation we have

$$\langle p|\psi(0)\rangle = \int dx\ \langle p|x\rangle\langle x|\psi(0)\rangle = \left[\frac{2\sigma^2}{\pi\hbar^2}\right]^{\frac{1}{4}} e^{-\frac{\sigma^2}{\hbar^2}(p-p_0)^2}. \tag{3}$$

Comment on the relation between the forms of the state in the position and momentum representations as a function of σ. By solving the TDSE show that the probability distribution function at time t can be written in the form

$$|\psi(x,t)|^2 = \frac{\sigma}{\sqrt{2\pi\hbar^2|b(t)|^2}} e^{-\frac{\sigma^2}{2\hbar^2|b(t)|^2}(x-p_0t/m)^2}\ , \tag{4}$$

and derive the form of the function $b(t)$. Explain what happens physically to the particle as time evolves.

Quantum Mechanics MT 2019: Problem Sheet 3 (Christmas Break)

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 $E(p, x) \equiv p^2/2m + \frac{1}{2}m\omega^2x^2$ 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 $\langle x|2\rangle = \text{constant} \times (x^2/\ell^2 - 1)\mathrm{e}^{-x^2/4\ell^2}$, 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

$$\hat{x}_{jk} = \ell \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots & & & & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & & & & & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots & & & & \\ & & \sqrt{3} & \cdots & & & & & \\ \cdots & & \cdots & & \cdots & & \cdots & & \\ & & & \cdots & 0 & \sqrt{n-1} & \cdots & & \\ & & & & \sqrt{n-1} & 0 & \sqrt{n} & & \\ & & & & & \sqrt{n} & 0 & \sqrt{n+1} & \cdots \\ & & & & & & \sqrt{n+1} & 0 & \\ \cdots & & \cdots & & \cdots & & \cdots & & \cdots \end{pmatrix}$$

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 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 $\hat{B}$.

3.10 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.

3.11 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 $\langle Q\rangle \equiv \int_{-\infty}^{\infty} \psi^* \hat{Q}\psi \,\mathrm{d}x$.

3.12 (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 $0 \le x \le a$.

(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.

3.13 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).

Some off-syllabus stuff you may find interesting

3.14 **Numerical solutions of the Schrödinger equation** By following the discussion given in the lecture notes construct numerical solutions for the first 10 eigenstates $|\phi_n\rangle$ of the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \lambda\hat{x}^4.$$

for $\frac{\lambda\ell^4}{\hbar\omega} = 0.1$. You can download a MATHEMATICA file for doing this from the course webpage. Now use the eigenvectors to obtain an expression for the ground state of the harmonic oscillator Hamiltonian ($\lambda = 0$) in terms of the eigenstates of H

$$|0\rangle \approx \sum_{n=0}^{N} \langle\phi_n|0\rangle \ |\phi_n\rangle.$$

Now assume that we initially prepare our system in the state $|\Phi(0)\rangle = |0\rangle$ and then consider time evolution under the Hamiltonian H. We have

$$|\Phi(t)\rangle \approx \sum_{n=0}^{N} \langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}|\phi_n\rangle. \tag{1}$$

We now want to determine the probability density $|\langle x|\Phi(t)\rangle|^2$ to find the particle at position x at time t. To do this we express $|\Phi(t)\rangle$ in terms of harmonic oscillator wave functions $\psi_k(x)$

$$\begin{aligned}\langle x|\Phi(t)\rangle \ &\approx \ \sum_{n=0}^{N}\langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}\langle x|\phi_n\rangle = \sum_{n=0}^{N}\langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}\langle x|\sum_{k=0}^{\infty}|k\rangle\langle k|\phi_n\rangle \\ &\approx \ \sum_{k=0}^{N}\sum_{n=0}^{N}\langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}\langle k|\phi_n\rangle \ \psi_k(x). \end{aligned} \tag{2}$$

In the last step we have cut off the sum over k in the resolution of the identity, which is justified because $\langle k|\phi_n\rangle\langle\phi_n|0\rangle$ are negligible for large k. We have explicit expression for the harmonic oscillator wave functions and know $\langle k|\phi_n\rangle$ and E_n from our numerics. We therefore can plot $P(x,t) = |\langle x|\Phi(t)\rangle|^2$ for any given time. In order to keep our discussion very general we note that we essentially have two dimensionful quantities in our problem

- A time scale $1/\omega$.
- A length scale ℓ.

We use these scales to introduce dimensionless variables parametrizing the time and position by $x = z\ell$, $t = \tau/\omega$. The probability to observe our particle in the interval $[x, x+dx]$ is $P(x,t)dx = p(z,\tau)dz$, where

$$p(z,\tau) = |\langle z\ell|\Phi(\tau/\omega)\rangle|^2\ell.$$

The nice thing is that $p(z,\tau)$ no longer contains any dimensionful quantities

$$p(z,\tau) \ \approx \ \left|\frac{e^{-z^2/4}}{(2\pi)^{\frac{1}{4}}}\sum_{k=0}^{N}\sum_{n=0}^{N}\langle\phi_n|0\rangle \ \langle k|\phi_n\rangle \ e^{-i(E_n/\hbar\omega)\tau}\frac{H_k(z/\sqrt{2})}{\sqrt{k!2^k}}\right|^2. \tag{3}$$

Plot $p(x,\tau)$ as a function of z for some values of τ.

Quantum Mechanics HT 2020: Problem Sheet 4

Transformations

4.1 *Reflection symmetry around a point* $\mathbf{x}_0$

Let $P_{\mathbf{x_0}}$ be the operator that induces reflections around a point $\mathbf{x_0}$. Argue that

$$\begin{aligned} \hat{P}_{\mathbf{x_0}}|\mathbf{x_0}+\mathbf{x}\rangle &= |\mathbf{x_0}-\mathbf{x}\rangle \ , \\ \hat{P}_{\mathbf{x_0}}\hat{\mathbf{x}}\hat{P}_{\mathbf{x_0}} &= 2\mathbf{x_0}\mathbf{1}-\hat{\mathbf{x}} \ , \\ \hat{P}_{\mathbf{x_0}}\hat{\mathbf{p}}\hat{P}_{\mathbf{x_0}} &= -\hat{\mathbf{p}}, \end{aligned}$$

and that the transformed wave function fulfils

$$\psi'(\mathbf{x}) = \psi(2\mathbf{x_0}-\mathbf{x}).$$

4.2 For which potentials V is the Hamiltonian $H = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})$ translationally invariant?

4.3 Show that the orbital angular momentum operators $\hat{L}_a$ $(a = x, y, z)$ are Hermitian.

4.4 A spinless QM system is called *rotationally invariant* if its Hamiltonian commutes with the orbital angular momentum operators $[H, \hat{L}_a] = 0$, $a = x, y, z$. Rotational invariance expresses the fact the energy measurements remain unchanged under rotations of the system. If the Hamiltonian commutes only with $\hat{L}_z$ it is called invariant under rotations around the z-axis. Consider Hamiltonians of the form

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}).$$

Show that potentials that depend only on the distance $\|\mathbf{x}\|$ lead to rotationally symmetric Hamiltonians, while potentials that depend on x and y only through the combination $x^2 + y^2$ leads to Hamiltonians that invariant under rotations around the z-axis.

4.5 Show that

$$\lim_{N\to\infty}\left[1+\frac{x}{N}\right]^N = e^x.$$

Give arguments that an analogous formula holds for operators.

4.6 *Heisenberg equations of motion for the SHO*

Derive the Heisenberg equations of motion for the creation and annihilation operators in the simple harmonic oscillator and show that their solution is

$$a(t) = a(0)e^{-i\omega t} \ , \quad a^\dagger(t) = a^\dagger(0)e^{i\omega t} \ .$$

From these, obtain equations of motion for the position and momentum operators. Comment on the relation of your results to Ehrenfest's theorem.

Orbital angular momentum

4.7 (a) Show by explicit calculation using $\hat{L}_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k$ that $[\hat{L}_i, \hat{x}_j] = \mathrm{i}\hbar\epsilon_{ijk}\hat{x}_k$ and $[\hat{L}_i, \hat{p}_j] = \mathrm{i}\hbar\epsilon_{ijk}\hat{p}_k$.

(b) Evaluate $[\hat{L}_x, \hat{L}_y]$ by writing $\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$ and using the results from part (a) of this question.

(c) Show that in the position representation we have

$$\langle\mathbf{x}|\hat{L}_i|\psi\rangle = \hat{\mathrm{L}}_i\psi(\mathbf{x}) \ ,$$

and obtain explicit expressions for the differential operators $\hat{\mathrm{L}}_i$. Show that for any differentiable function f

$$(\hat{\mathrm{L}}_x\hat{\mathrm{L}}_y - \hat{\mathrm{L}}_y\hat{\mathrm{L}}_x)f(x,y,z) = \mathrm{i}\hbar\hat{\mathrm{L}}_z f(x,y,z).$$

Since this holds for any f it can be written as an operator equation $[\hat{\mathrm{L}}_x, \hat{\mathrm{L}}_y] = \hat{\mathrm{L}}_x\hat{\mathrm{L}}_y - \hat{\mathrm{L}}_y\hat{\mathrm{L}}_x = \mathrm{i}\hbar\hat{\mathrm{L}}_z$, as you will have found in part (b). Deduce similar expressions for $[\hat{\mathrm{L}}_y, \hat{\mathrm{L}}_z]$ and $[\hat{\mathrm{L}}_z, \hat{\mathrm{L}}_x]$.

(d) Defining $\hat{\boldsymbol{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$, show that (Hint: remember $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$)

$$[\hat{L}_x, \hat{\boldsymbol{L}}^2] = [\hat{L}_y, \hat{\boldsymbol{L}}^2] = [\hat{L}_z, \hat{\boldsymbol{L}}^2] = 0.$$

(e) Show that in spherical polar co-ordinates the differential operators $\hat{\mathrm{L}}_i$ take the form

$$\hat{\mathrm{L}}_x \;=\; i\sin\phi\frac{\partial}{\partial\theta} + i\cot\theta\cos\phi\frac{\partial}{\partial\phi}\;, \quad \hat{\mathrm{L}}_y = -i\cos\phi\frac{\partial}{\partial\theta} + i\cot\theta\sin\phi\frac{\partial}{\partial\phi}\;, \quad \hat{\mathrm{L}}_z = -i\frac{\partial}{\partial\phi}\;.$$

4.8 (a) Verify that the three functions $\cos\theta$, $\sin\theta\,\mathrm{e}^{\mathrm{i}\phi}$ and $\sin\theta\,\mathrm{e}^{-\mathrm{i}\phi}$ are all eigenfunctions of $\hat{\boldsymbol{L}}^2$ and $\hat{\mathrm{L}}_z$.

(b) Find normalization constants N for each of the above functions so that

$$\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\;\sin\theta\,N^2\,|\psi(\theta,\phi)|^2 = 1.$$

(c) Once normalized, these functions are called spherical harmonics and given the symbol $Y_\ell^m(\theta,\phi)$. Hence deduce that your results are consistent with the functions:

$$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta; \qquad Y_1^1(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{\mathrm{i}\phi}; \qquad Y_1^{-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{-\mathrm{i}\phi}.$$

(Note, you can't use this method to get the signs of Y_1^0, Y_1^1 and Y_1^{-1}. The minus sign in Y_1^1 can be deduced by using a raising operator $\hat{L}_+$ on Y_1^0. This is not required.)

(d) Rewrite these functions in terms of Cartesian variables [$x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$]. Sketch $|Y_1^0|^2$, $|Y_1^1|^2$ and $|Y_1^{-1}|^2$. (They are angular functions, so keep r fixed and look only at the angle dependence. A cross section in the x–z plane will do. Why?)

4.9 The angular part of a system's wavefunction is

$$\langle\theta,\phi|\psi\rangle \propto (\sqrt{2}\cos\theta + \sin\theta\,\mathrm{e}^{-\mathrm{i}\phi} - \sin\theta\,\mathrm{e}^{\mathrm{i}\phi}).$$

What are the possible results of measurement of (a) $\hat{\boldsymbol{L}}^2$, and (b) $\hat{L}_z$, and their probabilities? What is the expectation value of $\hat{L}_z$?

4.10 A system's wavefunction is proportional to $\sin^2\theta\,\mathrm{e}^{2\mathrm{i}\phi}$. What are the possible results of measurements of (a) $\hat{L}_z$ and (b) $\hat{\boldsymbol{L}}^2$?

4.11 A system's wavefunction is proportional to $\sin^2\theta$. What are the possible results of measurements of (a) $\hat{L}_z$ and (b) $\hat{\boldsymbol{L}}^2$? Give the probabilities of each possible outcome.

4.12 A particle of mass m is described the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - e\mathcal{E}\hat{x}.$$

(a) What is the physical origin of the last term in $\hat{H}$?

(b) Which of the observables represented by the operators $\hat{\boldsymbol{L}}^2$, $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ are constants of the motion assuming (i) $\mathcal{E} = 0$; (ii) $\mathcal{E} \neq 0$ (Hint: Use the results for $[\hat{L}_i, \hat{x}]$ from [4.6].)

4.13 Show that $\hat{L}_i$ commutes with $\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{p}}$.

Quantum Mechanics HT 2020: Problem Sheet 5

Spin and $S > 1$ Systems

5.1 Write down the expression for the commutator $[\sigma_i, \sigma_j]$ of two Pauli matrices. Show that the anticommutator of two Pauli matrices is

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}.$$

5.2 Let $\boldsymbol{n}$ be any unit vector and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ be the vector whose components are the Pauli matrices. Why is it physically necessary that $\boldsymbol{n} \cdot \boldsymbol{\sigma}$ satisfy $(\boldsymbol{n} \cdot \boldsymbol{\sigma})^2 = I$, where I is the 2×2 identity matrix? Let $\boldsymbol{m}$ be a unit vector such that $\boldsymbol{m} \cdot \boldsymbol{n} = 0$. Why do we require that the commutator $[\boldsymbol{m} \cdot \boldsymbol{\sigma}, \boldsymbol{n} \cdot \boldsymbol{\sigma}] = 2\mathrm{i}(\boldsymbol{m} \times \boldsymbol{n}) \cdot \boldsymbol{\sigma}$? Prove that these relations follow from the algebraic properties of the Pauli matrices. You should be able to show that $[\boldsymbol{m} \cdot \boldsymbol{\sigma}, \boldsymbol{n} \cdot \boldsymbol{\sigma}] = 2\mathrm{i}(\boldsymbol{m} \times \boldsymbol{n}) \cdot \boldsymbol{\sigma}$ for any two vectors $\boldsymbol{n}$ and $\boldsymbol{m}$.

5.3 Let $\boldsymbol{n}$ be the unit vector in the direction with polar coordinates (θ, ϕ). Write down the matrix $\boldsymbol{n} \cdot \boldsymbol{\sigma}$ and find its eigenvectors. Hence show that the state of a spin-half particle in which a measurement of the component of spin along $\boldsymbol{n}$ is certain to yield $\frac{1}{2}\hbar$ is

$$|+, \boldsymbol{n}\rangle = \sin(\theta/2)\, \mathrm{e}^{\mathrm{i}\phi/2}|-\rangle + \cos(\theta/2)\, \mathrm{e}^{-\mathrm{i}\phi/2}|+\rangle,$$

where $|\pm\rangle$ are the states in which $\pm\frac{1}{2}$ is obtained when s_z is measured. Obtain the corresponding expression for $|-, \boldsymbol{n}\rangle$. Explain physically why the amplitudes in the previous equation have modulus $2^{-1/2}$ when $\theta = \pi/2$ and why one of the amplitudes vanishes when $\theta = \pi$.

5.4 For a spin-half particle at rest, the operator $\boldsymbol{J}$ is equal to the spin operator $\boldsymbol{S}$. Use the properties of the Pauli spin matrices to show that in this case the rotation operator $U(\boldsymbol{\alpha}) \equiv \exp(-\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{J}/\hbar)$ is

$$U(\boldsymbol{\alpha}) = I \cos\left(\frac{\alpha}{2}\right) - \mathrm{i}\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma} \sin\left(\frac{\alpha}{2}\right),$$

where $\hat{\boldsymbol{\alpha}}$ is the unit vector parallel to $\boldsymbol{\alpha}$. Comment on the value this gives for $U(\boldsymbol{\alpha})$ when $\alpha = 2\pi$.

5.5 Explain why a spin-$\frac{1}{2}$ particle in a magnetic field $\boldsymbol{B}$ has a Hamiltonian given by

$$H = -\gamma \boldsymbol{S} \cdot \boldsymbol{B},$$

where γ is the gyromagnetic ratio which you should define. In a coordinate system such that $\boldsymbol{B}$ lies along the z-axis, a proton is found to be in a eigenstate $|+, x\rangle$ of $\hat{S}_x$ at $t = 0$. Find $\langle \hat{S}_x \rangle$ and $\langle \hat{S}_y \rangle$ for $t > 0$.

5.6 Write down the 3×3 matrix that represents S_x for a spin-one system in the basis in which S_z is diagonal (i.e., the basis states are $|0\rangle$ and $|\pm\rangle$ with $S_z|+\rangle = |+\rangle$, etc.)

A beam of spin-one particles emerges from an oven and enters a Stern–Gerlach filter that passes only particles with $J_z = \hbar$. On exiting this filter, the beam enters a second filter that passes only particles with $J_x = \hbar$, and then finally it encounters a filter that passes only particles with $J_z = -\hbar$. What fraction of the particles stagger right through?

5.7 A system that has spin angular momentum $\sqrt{6}\hbar$ is rotated through an angle ϕ around the z-axis. Write down the 5×5 matrix that describes a rotation by an angle ϕ around the z-axis.

5.8 * *Vector operators* (Optional, off-syllabus problem)

(a) Show that expectation values of the position operators in a state $|\psi\rangle$ transform like a classical vector under a rotation around an axis $\mathbf{n}$ by an angle α.
(b) Show that the commutation relations $[\hat{V}_j, \hat{J}_k] = i\hbar\epsilon_{jkl}\hat{V}_l$ are equivalent to

$$\hat{V}_j + \frac{d\alpha}{i\hbar}[\hat{V}_j, \mathbf{n} \cdot \hat{\mathbf{J}}] = \sum_k \left(R(\mathbf{n}d\alpha)\right)_{jk} \hat{V}_k \ ,$$

where $\mathbf{n}$ is a unit vector and $R(\mathbf{n}d\alpha)$ is the rotation matrix around the axis $\mathbf{n}$ by an angle $d\alpha$.

Composite systems

5.10 A system AB consists of two non-interacting parts A and B. The dynamical state of A is described by $|a\rangle$, and that of B by $|b\rangle$, so $|a\rangle$ satisfies the TDSE for A and similarly for $|b\rangle$. What is the ket describing the dynamical state of AB? In terms of the Hamiltonians $H_{\rm A}$ and $H_{\rm B}$ of the subsystems, write down the TDSE for the evolution of this ket and show that it is automatically satisfied. Do $H_{\rm A}$ and $H_{\rm B}$ commute? How is the TDSE changed when the subsystems are coupled by a small dynamical interaction $H_{\rm int}$? If A and B are harmonic oscillators, write down $H_{\rm A}$, $H_{\rm B}$. The oscillating particles are connected by a weak spring. Write down the appropriate form of the interaction Hamiltonian $H_{\rm int}$. Does $H_{\rm A}$ commute with $H_{\rm int}$? Explain the physical significance of your answer.

5.11 Explain what is implied by the statement that "the physical state of system A is correlated with the state of system B." Illustrate your answer by considering the momenta of cars on (i) London's circular motorway (the M25) at rush-hour, and (ii) the road over the Nullarbor Plain in southern Australia in the dead of night.

5.12 Consider a system of two particles of mass m that each move in one dimension along a given rod. Let $|1;x\rangle$ be the state of the first particle when it's at x and $|2;y\rangle$ be the state of the second particle when it's at y. A complete set of states of the pair of particles is $\{|xy\rangle\} = \{|1;x\rangle|2;y\rangle\}$. Write down the Hamiltonian of this system given that the particles attract one another with a force that's equal to C times their separation.

Suppose that the particles experience an additional potential $V(x,y) = \frac{1}{2}C(x+y)^2$. Show that the dynamics of the two particles is now identical with that of a single particle that moves in two dimensions in a particular potential $\Phi(x,y)$, and give the form of Φ.

5.13 In the lectures we considered measurements by Alice and Bob on an entangled pair of spins prepared in a singlet state. Bob measures the component of spin along an axis that is inclined by angle θ to that used by Alice. Given the expression

$$|-,\boldsymbol{b}\rangle = \cos(\theta/2)\,\mathrm{e}^{\mathrm{i}\phi/2}|-\rangle - \sin(\theta/2)\,\mathrm{e}^{-\mathrm{i}\phi/2}|+\rangle,$$

for the state of a spin-half particle in which it has spin $-\frac{1}{2}$ along the direction $\boldsymbol{b}$ with polar angles (θ,ϕ), with $|\pm\rangle$ the states in which there is spin $\pm\frac{1}{2}$ along the z-axis, calculate the amplitude that Bob finds the positron's spin to be $-\frac{1}{2}$ given that Alice has found $+\frac{1}{2}$ for the electron's spin. Hence show that the corresponding probability is $\cos^2(\theta/2)$.

Quantum Mechanics HT 2019: Problem Sheet 6

The Hydrogen Atom

[6.1] Some things about hydrogen's gross structure that it's important to know (ignore spin throughout, and you may set the reduced mass to be equal to the electron mass):

(a) What quantum numbers characterise stationary states of hydrogen?

(b) What combinations of values of these numbers are permitted?

(c) Give the formula for the energy of a stationary state in terms of the Rydberg $\mathcal{R}$. What is the value of $\mathcal{R}$ in eV?

(d) How many stationary states are there in the first excited level and in the second excited level?

(e) What is the wavefunction of the ground state?

(f) Write down an expression for the mass of the reduced particle.

(g) We can apply hydrogenic formulae to any two charged particles that are electrostatically bound. How does the ground-state energy then scale with (i) the mass of the reduced particle, and (ii) the charge Ze on the nucleus? (iii) How does the radial scale of the system scale with Z?

[6.2] An electron is in the ground state of a hydrogen-like atom with nuclear charge $+Ze$. For simplicity neglect the difference between the reduced mass and the electron mass.

(a) What is its average distance from the nucleus?

(b) At what distance from the nucleus is it most likely to be found?

(c) Show that the expectation value of the potential energy of the electron is the same as that given by the Bohr model, namely $-Ze^2/4\pi\epsilon_0 r_0$ where $r_0 = a_0/Z$.

(d) Show that the expectation value of the kinetic energy is equal to the value given by the Bohr model, namely $Ze^2/8\pi\epsilon_0 r_0$.

(e) Hence verify that the expectation value of the total energy agrees with the Bohr model.

[6.3] Show that the speed of a classical electron in the lowest Bohr orbit is $v = \alpha c$, where $\alpha = e^2/4\pi\epsilon_0\hbar c$ is the fine-structure constant. What is the corresponding speed for a hydrogen-like Fe ion (atomic number $Z = 26$)? Given these results, what fractional errors must we expect in the energies of states that we derive from non-relativistic quantum mechanics.

[6.4] Show that the electric field experienced by an electron in the ground state of hydrogen is of order $5 \times 10^{11}\,\mathrm{V\,m^{-1}}$. Why is it impossible to generate comparable macroscopic fields using charged electrodes. Lasers are available that can generate beam fluxes as big as $10^{22}\,\mathrm{W\,m^{-2}}$. Show that the electric field in such a beam is of comparable magnitude.

[6.5] Positronium consists of an electron e^- and a positron e^+ (both spin-half and of equal mass) in orbit around one another. What are its energy levels? By what factor is a positronium atom bigger than a hydrogen atom?

[6.6] Muonium consists of an electron e^- and a positive muon μ^+ (both spin-half particles but $m_\mu = 206.7 m_\mathrm{e}$) in orbit around one another. What are its energy levels? By what factor is muonium atom bigger than a hydrogen atom?

[6.7] The emission spectrum of the He^+ ion contains the Pickering series of spectral lines that is analogous to the Lyman, Balmer and Paschen series in the spectrum of hydrogen

Balmer $i = 1, 2, \ldots$	0.456806	0.616682	0.690685	0.730884
Pickering $i = 2, 4, \ldots$	0.456987	0.616933	0.690967	0.731183

The table gives the frequencies (in $10^{15}\,\mathrm{Hz}$) of the first four lines of the Balmer series and the first four even-numbered lines of the Pickering series. The frequencies of these lines in the Pickering series are almost coincident with the frequencies of lines of the Balmer series. Explain this finding. Provide a quantitative explanation of the small offset between these nearly coincident lines in terms of the reduced mass of the electron in the two systems. (In 1896 E.C. Pickering identified the odd-numbered lines in his series in the spectrum of the star ζ Puppis. Helium had yet to be discovered and he believed that the lines were being produced by hydrogen. Naturally he confused the even-numbered lines of his series with ordinary Balmer lines.)