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

3.15 **A time-dependent scattering problem**

Consider the a particle in a potential of the form ($V_0 > 0$)

$$V(x) = \begin{cases} 0 & \text{if } |x| > a\ , \\ V_0 & \text{if } |x| < a\ . \end{cases} \tag{4}$$

(a) Show that the energy eigenstates with $E > V_0$ are given by

$$\psi_k(x) = \begin{cases} De^{ikx} + re^{-ikx} & \text{if } x < -a \\ Ae^{-iKx} + Be^{iKx} & \text{if } |x| < a \ , \\ te^{ikx} + Ce^{-ikx} & \text{if } x > a \ . \end{cases} \tag{5}$$

where $E = \frac{\hbar^2 k^2}{2m} = V_0 + \frac{\hbar^2 K^2}{2m}$ and

$$\begin{aligned} t &= \frac{2Kke^{-2ika}}{-i(k^2+K^2)\sin(2Ka) + 2kK\cos(2Ka)} \ , \\ r &= \frac{-Ie^{-2ika}(k^2-K^2)\sin(2Ka)}{-i(k^2+K^2)\sin(2Ka) + 2kK\cos(2Ka)} \ , \\ A &= \frac{e^{-iKa}}{2K}\left[e^{-ika}(K-k) + re^{ika}(K+k)\right] , \\ B &= \frac{e^{iKa}}{2K}\left[e^{-ika}(K+k) + re^{ika}(K-k)\right] . \end{aligned} \tag{6}$$

(b) At time $t = 0$ we prepare the system in a superposition of the energy eigenstates with $E > V_0$

$$\phi(x) = \frac{1}{N}\int_{\sqrt{2mV_0/\hbar^2}}^{\infty} dk \ e^{-\alpha(k-k_0)^2 - ikx_0} \ \psi_k(x) \ , \tag{7}$$

where

$$\alpha > 0 \ , \qquad k_0 > \sqrt{2mV_0/\hbar^2} \ , \quad x_0 < 0 \ , \tag{8}$$

and the normalization factor N ensures that our initial wave function is normalized to one

$$\int_{-\infty}^{\infty} dx \ |\phi(x)|^2 = 1. \tag{9}$$

Argue that the time evolved wave-function is given by

$$\phi(x,t) = \frac{1}{N}\int_{\sqrt{2mV_0/\hbar^2}}^{\infty} dk \ e^{-\alpha(k-k_0)^2 - ikx_0} e^{-\frac{i\hbar k^2}{2m}t} \ \psi_k(x) \ . \tag{10}$$

Use the MATHEMATICA program provided on the course web-page (or write your own MATLAB file) to plot the probability density $|\phi(x,t)|^2$ to find the particle at position x at time t (it is useful to transform to dimensionless variables first as is done in the lecture notes). Interpret the evolution in terms of a scattering process.