

# MA4A7 Quantum Mechanics: Basic Principles and Probabilistic Methods

## PROBLEM SHEET 1

Volker Betz

February, 2010.

### 1. Orders of magnitude: harmonic oscillator

We rescaled the Schrödinger equation for the harmonic oscillator, given by

$$i\partial_t\psi(x,t) = \left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{\kappa x^2}{2}\right)\psi(x,t),$$

to the standard form

$$i\partial_{\tilde{t}}\tilde{\psi}(\tilde{x},\tilde{t}) = \left(-\frac{1}{2}\partial_{\tilde{x}}^2 + \frac{\tilde{x}^2}{2}\right)\tilde{\psi}(\tilde{x},\tilde{t}).$$

For this we used the transformation  $\tilde{t} = \omega t$  with  $\omega = \sqrt{\kappa/m}$ ,  $\tilde{x} = \sqrt{m\omega/\hbar}x$ , and  $\tilde{\psi}(\tilde{x},\tilde{t}) = \psi(x,t)$ . Determine what a time and length interval of length one means in the rescaled variables, in the case of an electron in a quadratic force field. Use

$$m = \text{electron mass} = 0.91 \times 10^{-30} \text{ kg}, \quad \hbar = 1.05 \times 10^{-34} \text{ J} \times \text{sec}, \quad \kappa = 1.$$

### 2. The hydrogen atom

The Hamiltonian for the hydrogen atom in atomic units is

$$H = -\frac{1}{2}\Delta - \frac{1}{|x|} \quad \text{in } L^2(\mathbb{R}^3).$$

- Check that  $\psi(x) = e^{-\alpha|x|}/\sqrt{\pi}$  is an eigenfunction to  $H$  for some  $\alpha$  (which  $\alpha$ ? and what is the eigenvalue?). It is indeed the eigenfunction with lowest energy, called the ground state. We will learn how to prove this later in the lecture.
- Calculate the position and momentum uncertainty, and their product, for the hydrogen ground state. For the latter, use that the Fourier transform of  $\psi(x)$  is given by

$$\hat{\psi}(p) = \frac{8\pi\alpha}{(\alpha^2 + |p|^2)^2}.$$

For the integrals, use polar coordinates:

$$\int_{\mathbb{R}^3} f(|x|)dx = \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin(\theta)r^2 f(r).$$

For the radial integrals, integration by parts is useful.

- Calculate the expected distance from the nucleus,  $\langle\psi, |x|\psi\rangle$ , and the expected speed  $\frac{1}{(2\pi)^3}\langle\hat{\psi}, |p|\hat{\psi}\rangle$ .
- Convert these results back into physical units. One unit of length in atomic units is equal to  $\hbar^2/(me^2) \approx 0.5 \times 10^{-10}$  metres, and one unit of velocity is equal to  $e^2/\hbar \approx 2200$ km/s. Is the electron fast or slow compared to macroscopic speeds, the speed of sound, or the speed of light?

### 3. Symmetric operators

Let  $H$  be a symmetric operator on a complex Hilbert space.

- Show that all eigenvalues of  $H$  are real.
- Show that eigenvectors  $\psi_1, \psi_2$  to different eigenvalues  $E_1, E_2$  are orthogonal.
- Let  $\psi_1, \psi_2$  be two normalized eigenvectors to eigenvalues  $E_1, E_2$ . Define the superposition  $\psi_{1,2} = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$ . First guess and then compute the mean  $\langle H \rangle_{\psi_{1,2}}$  and the uncertainty  $(\Delta H)_{\psi_{1,2}}$ .

### 4. Ehrenfest equations via operators

- Prove first that for two linear operators  $A, B$ , we have  $[A^2, B] = A[A, B] + [A, B]A$ .
- For  $H = \frac{1}{2m}\sum_{j=1}^n P_j^2 + V$ , compute  $[H, X_j]$  and  $[H, P_j]$ , where  $X_j$  and  $P_j$  are position and momentum operators in the coordinate  $j$ , respectively.

c) Use this to prove the Ehrenfest equations.

5. **An alternative proof for the existence of  $e^{-itH}$ .**

Here is an alternative proof for the existence of solutions to the time-dependent Schrödinger equation. We assume that  $H$  is a self-adjoint, possibly unbounded, operator.

a) For  $\lambda > 0$ , define

$$H_\lambda := \frac{1}{2}\lambda^2 ((H + i\lambda)^{-1} + (H - i\lambda)^{-1}).$$

Using statements from the lecture, show that  $H_\lambda$  is well-defined and bounded for all  $\lambda > 0$

b) Show that for every  $\psi \in D(H^2)$ ,  $\|(H_\lambda - H)\psi\| \rightarrow 0$  as  $\lambda \rightarrow \infty$ .

c) Since  $H_\lambda$  is bounded,  $e^{itH_\lambda}$  exists. Prove that  $(e^{itH_\lambda})_\lambda$  is a Cauchy sequence for  $\lambda \rightarrow \infty$ , e.g. take  $\lambda_n = 1/n$ . To do this, check that

$$e^{iH_{\lambda'}} - e^{iH_\lambda} = \int_0^1 \partial_s (e^{isH_{\lambda'}} e^{i(1-s)H_\lambda}) ds.$$

Show that  $H_\lambda$  is self-adjoint, which implies  $\|e^{iH_\lambda}\| = 1$ . Then compute the derivative under the integral, and use this to estimate the difference above, for  $\psi \in D(H^2)$ . Since  $D(H^2)$  is dense, the proof is finished.

6. **Dynamics via spectral decomposition**

Let  $H$  be any self-adjoint operator. Assume that  $(E_n)_{n \in \mathbb{N}}$  are eigenvalues of  $H$  with corresponding eigenfunctions  $\psi_n$ . For coefficients  $\alpha_n \in \mathbb{C}$  with  $\sum_{n \geq 1} |\alpha_n|^2 < \infty$ , define  $\phi = \sum_{n=1}^{\infty} \alpha_n \psi_n$ .

a) Show that  $\phi \in D(H)$  if and only if  $\sum_{n=1}^{\infty} |E_n \alpha_n|^2 < \infty$ .

b) Under the assumption that  $\sum_{n=1}^{\infty} |E_n^2 \alpha_n|^2 < \infty$ , show that the unique solution to the equation  $i\partial_t \psi = H\psi$ ,  $\psi(0) = \phi$  is given by

$$\psi(t) = \sum_{n=1}^{\infty} \alpha_n e^{-iE_n t} \psi_n.$$

7. **Energy of the harmonic oscillator**

Consider the harmonic oscillator with Hamiltonian  $H = -\frac{1}{2}\partial_x^2 + \frac{x^2}{2}$ . From the time evolution of the observables it follows that

$$\begin{aligned} \langle X(t) \rangle_{\psi_0} &\equiv \langle \psi(\cdot, t), X\psi(\cdot, t) \rangle \equiv \langle \psi_0, X(t)\psi_0 \rangle = \sin(t)\langle P \rangle_{\psi_0} + \cos(t)\langle X \rangle_{\psi_0}, \\ \langle X(t) \rangle_{\psi_0} &= \cos(t)\langle P \rangle_{\psi_0} - \sin(t)\langle X \rangle_{\psi_0}, \end{aligned}$$

for any initial state  $\psi_0$ . So the classical energy  $(p^2 + x^2)/2$  of the expected values is given by

$$E_{\text{class}} = \frac{1}{2}(\langle P \rangle_{\psi_0}^2 + \langle X \rangle_{\psi_0}^2).$$

Show that  $E_{\text{class}}$  is strictly smaller than the quantum energy  $\langle H \rangle_{\psi_0}$ , for any given initial state  $\psi_0$ . Find the initial state that minimizes the difference.

*Hint:* Use the uncertainty principle.

8. **Eigenfunctions and eigenvalues of the two-dimensional harmonic oscillator**

Let  $H = -\frac{1}{2}\Delta + V(x, y)$  be a Schrödinger operator in  $L^2(\mathbb{R}^2)$ .

a) Assume that the potential  $V(x, y)$  is a sum of two independent potentials:  $V(x, y) = V_1(x) + V_2(y)$ . Define  $H_1 = -\frac{1}{2}\partial_x^2 + V_1(x)$ ,  $H_2 = -\frac{1}{2}\partial_y^2 + V_2(y)$ . Assume that we know eigenfunctions  $\psi_1(x)$  and  $\psi_2(y)$  of  $H_1$  and  $H_2$ , with eigenvalues  $E_1$  and  $E_2$ , respectively. Find an eigenfunction of  $H$  and the corresponding eigenvalue. (Hint: try products)

b) Find all the eigenvalues and eigenfunctions of the two-dimensional harmonic oscillator  $H = -\frac{1}{2}\Delta + |x|^2$ ,  $x \in \mathbb{R}^2$ . For this, first find all the eigenfunctions that can be constructed as in a). Using the facts that the eigenspaces of the one-dimensional harmonic oscillator span  $L^2(\mathbb{R})$  (you don't need to prove this), show that the spaces you have found span  $L^2(\mathbb{R}^2)$ . (Hint: use that any  $L^2$  function can be approximated by a finite weighted sum of indicator functions of squares in  $\mathbb{R}^2$ , up to an error of order  $\varepsilon/2$ . Then approximate each indicator function up to a sufficiently small error.)

c) Determine the dimension of each eigenspace of the two-dimensional harmonic oscillator. Try to guess (or calculate, if you want) the eigenvalues and the dimension of each eigenspace for the  $n$ -dimensional harmonic oscillator.