Year 2 - Quantum Mechanics Revision Lecture

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Office Hours

- I will hold four office hours between now and the exam
  - These will be in my office, Blackett 506
- The times and dates are already listed on Blackboard and on the Level 3 notice board
  - Week 4: Tue 22 May 12.00, Thu 24 May 14.00
  - Week 5: Tue 29 May 12.00
  - Week 6: Thu 7 June, 14.00

Exam format

- This is the fourth year I have taught this course
  - The syllabus has also been unchanged for (at least) the previous five years
- The exam this year will be in the same format, style and level as for (at least) the last eight years
  - Two hours
  - 3/6 questions required
  - Do not assume anything either way about Qu 6...

2011 Exam Question 4, Part i

4. When considering radial motion in both classical and quantum mechanics, systems with a central potential $V(r)$ can be treated as having an *effective potential*

$$V_{\mathrm{Eff}}(r) = \frac{L^2}{2mr^2} + V(r),$$

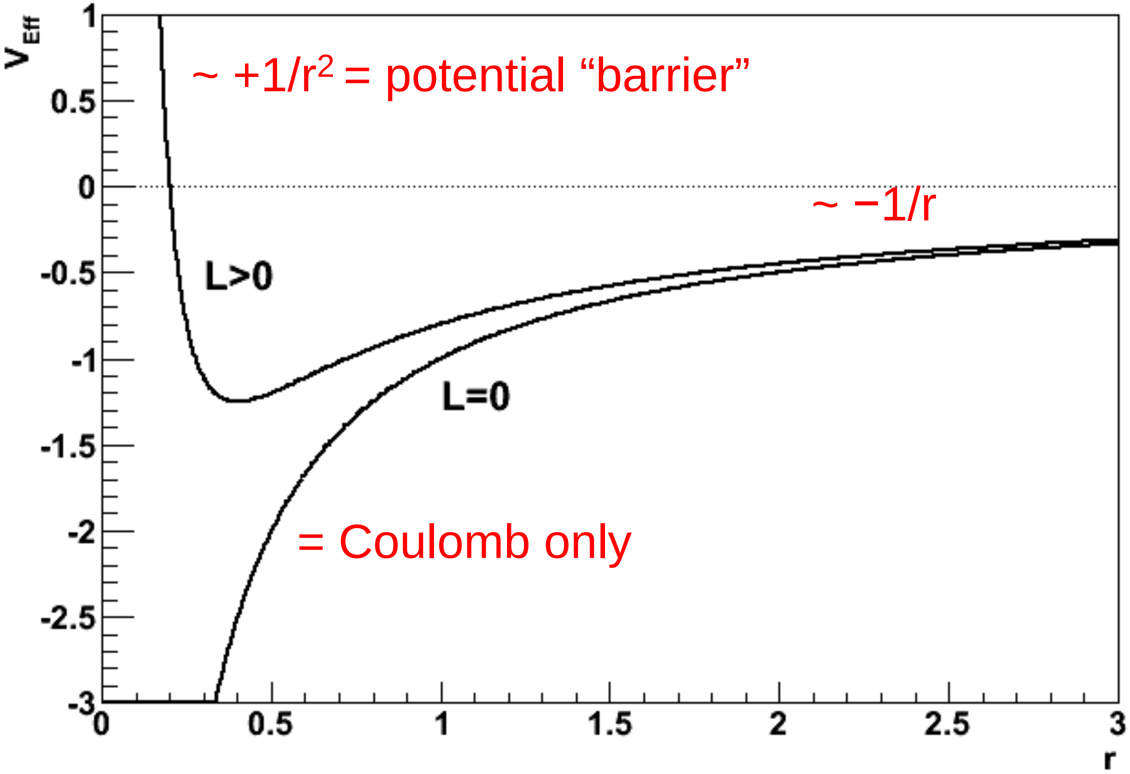
where L is the magnitude of the orbital angular momentum, which is constant for a central potential. Consider the case of an electron orbiting a proton in a hydrogen atom.

(i) Write down an expression for $V(r)$ for the Coulomb potential experienced by the electron. Qualitatively sketch the form of $V_{\mathrm{Eff}}(r)$ for the two cases of $L = 0$ and $L > 0$. Hence, explain under what condition would the particle be able to approach very close to the centre of the potential. [4 marks]

2011 Exam Answer 4, Part i

(i) The Coulomb potential for the hydrogen atom is

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$



2011 Exam Question 4, Part ii

(ii) Treating the atom as a classical system with $L > 0$, show that the radius of the circular orbit for a given L is

$$r_C = \frac{4\pi\epsilon_0 L^2}{me^2}.$$

[4 marks]

2011 Exam Answer 4, Part ii

(ii) The particle will orbit classically at the radius r_C where the forces balance. This is when

No radial force
$$\frac{dV_{\text{Eff}}}{dr} = 0 = -\frac{L^2}{mr_C^3} + \frac{e^2}{4\pi\epsilon_0 r_C^2}$$

Hence

$$\frac{L^2}{mr_C} = \frac{e^2}{4\pi\epsilon_0} \quad \text{so} \quad r_C = \frac{4\pi\epsilon_0 L^2}{me^2}$$

Alternative: Since for a circular orbit $L = mvr$, then setting the forces equal gives

so v = L/mr

$$\frac{e^2}{4\pi\epsilon_0 r_C^2} = \frac{mv^2}{r_C} = \frac{m}{r_C}\frac{L^2}{m^2 r_C^2} = \frac{L^2}{mr_C^3} \quad \text{so} \quad r_C = \frac{4\pi\epsilon_0 L^2}{me^2}$$

as before. [4 marks]

Coulomb = centrifugal

2011 Exam Question 4, Part iii

(iii) Neglecting spin terms, the quantum energy eigenstates in a central potential can be written

$$u_{n\,l\,m_l} = \frac{\chi_{n\,l}(r)}{r}\, Y_{l\,m_l}(\theta, \phi),$$

where $Y_{l\,m_l}$ are the normalised spherical harmonics. Show that the eigenstate is normalised if the radial function satisfies

$$\int |\chi_{n\,l}|^2\, dr = 1.$$

[2 marks]

QM knowledge

- All physical states must be normalised to get correct probabilities
  - 1D: $\int \psi(x)^* \psi(x)\, dx = 1$
  - 3D: $\int \psi(\mathbf{r})^* \psi(\mathbf{r})\, d^3r = 1$
- In 3D using spherical harmonics, the integral becomes
  - $\int \psi(r,\theta,\phi)^* \psi(r,\theta,\phi)\, r^2 dr \sin(\theta) d\theta\, d\phi = 1$

2011 Exam Answer 4, Part iii

(iii) To be normalised, the energy eigenstate must satisfy

$$\int |u|^2 \, d^3r = 1 = \int_0^\infty \frac{|\chi|^2}{r^2} r^2 \, dr \underbrace{\int |Y|^2 \, d\Omega}_{=1} = \int_0^\infty |\chi|^2 \, dr$$

since the spherical harmonics are normalised. [2 marks]

N.B. Element of solid angle $d\Omega = \sin(\theta) d\theta \, d\phi$

2011 Exam Question 4, Part iv

(iv) For a given l, the radial function solution with the lowest energy has $n = l + 1$ and is given by

$$\chi_{nl} = Ar^n e^{-r/na_0},$$

where $a_0 = 4\pi\epsilon_0\hbar^2/me^2$ is the Bohr radius and A is a normalisation constant. Show that

$$|A|^2 = \frac{1}{(2l+2)!}\left[\frac{2}{(l+1)a_0}\right]^{2l+3}.$$

[5 marks]

Standard integral:

$$\int_0^\infty r^m e^{-\alpha r}\,dr = \frac{m!}{\alpha^{m+1}}.$$

QM knowledge

- Properties of the hydrogen atom
  - Quantum numbers are constrained by $n > l$
  - Energy goes up with n

2011 Exam Answer 4, Part iv

(iv) From above

N.B. Squares

$$\int_0^\infty |\chi|^2\, dr = 1 = \int_0^\infty |A|^2 r^{2n} e^{-2r/na_0}\, dr$$

With $m = 2n$ and $\alpha = 2/na_0$ then

Notation in standard integral

$$\int_0^\infty |\chi|^2\, dr = 1 = |A|^2 \frac{m!}{\alpha^{m+1}} = |A|^2 (2n)! \left(\frac{na_0}{2}\right)^{2n+1}$$

Since $n = l + 1$, then this requires

$$|A|^2 = \frac{1}{2n!}\left(\frac{2}{na_0}\right)^{2n+1} = \frac{1}{(2l+2)!}\left[\frac{2}{(l+1)a_0}\right]^{2l+3}$$

[5 marks]

2011 Exam Question 4, Part v

(v) For a particle in the state given in part (iv), show that the expectation value of the particle radius is

$$\langle r \rangle = \frac{(2l+3)(l+1)}{2}\, a_0 .$$

[3 marks]

QM knowledge

- The expectation value for operator Q is
  - $\langle Q \rangle = \int \psi(\mathbf{r})^* \, Q \, \psi(\mathbf{r}) \, d^3r$

2011 Exam Answer 4, Part v

Y terms not written as they normalise to 1 again

Exactly as before but with one more power of r

(v) The expectation value of r is given by

$$\langle r \rangle = \int u^* \hat{r} u \, d^3 r = \int |u|^2 r \, d^3 r = \int_0^\infty r |\chi|^2 \, dr = \int_0^\infty |A|^2 r^{2n+1} e^{-2r/na_0} \, dr$$

$$= |A|^2 (2n+1)! \left(\frac{na_0}{2} \right)^{2n+2} = (2n+1) \left(\frac{na_0}{2} \right) = \frac{(2l+3)(l+1)}{2} a_0$$

[3 marks]

Now need to substitute in value of $|A|^2$ found in part iv

2011 Exam Question 4, Part vi

(vi) Explain what is meant by the correspondence principle and show that in the correspondence limit, the expectation value of the radius agrees with the classical value r_C. [2 marks]

QM knowledge

- The correspondence principle says classical mechanics must be a limit of quantum mechanics
  - Several ways to state the correspondence limit
  - Size >> λ, $\hbar$ -> 0, quantum numbers -> ∞, Ehrenfest…

2011 Exam Answer 4, Part vi

(vi) The correspondence principle states that the classical limit should correspond to the limit of large quantum numbers. Specifically, for large l, then

$$\langle r \rangle \approx \frac{l \times 2l}{2} a_0 = l^2 a_0$$

Approximation to (l+1)(2l+3)

The quantum angular momentum is this limit is

$$L^2 = l(l+1)\hbar^2 \approx l^2 \hbar^2$$

so $l^2 \approx L^2/\hbar^2$

so

$$\langle r \rangle \approx \frac{L^2 a_0}{\hbar^2} = \frac{L^2}{\hbar^2} \frac{4\pi\epsilon_0 \hbar^2}{me^2} = \frac{4\pi\epsilon_0 L^2}{me^2} = r_C$$

[2 marks]

2011 Exam Question 4 Report

Question 4

This question was attempted by a very small number of candidates. Almost all did it well and got quite high marks, although one did very poorly.

Part (i) seemed straightforward, with most sketches being reasonable and the correct condition, namely $L = 0$, being stated. Similarly, being a simple classical calculation, part (ii) was mainly correctly done. Part (iii) was done well, with almost all candidates knowing the correct volume element in spherical polars. The calculations in part (iv) and (v) were done without problems by most candidates. However, many of the answers to part (vi) did not clearly state what is meant by the correspondence principle and did not specify which limit was needed. In addition, the approximations used in this limit were often not applied consistently.

2011 Exam Question 6, Part i

(i) The component operators for the spin angular momentum of a spin 1/2 particle satisfy $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$, and cyclic permutations. What does this imply for an attempt to measure the three spin components simultaneously? [3 marks]

QM knowledge

- Compatible variable pairs share all eigenstates
  - Their operators commute
- Non-compatible variable pairs cannot generally both be in eigenstates
  - Hence cannot have definite measurement outcomes
- If measure one of the two variables
  - Wavefunction collapses to its eigenstate
- If then measure the other variable
  - Wavefunction collapses to different eigenstate
  - First measurement eigenstate is lost

2011 Exam Question 6, Part ii

(ii) A general form for a two-component spin state is

$$\chi = \begin{pmatrix} \cos(\theta/2)e^{i\alpha} \\ \sin(\theta/2)e^{i\beta} \end{pmatrix}.$$

where θ, α and β are parameters.

(a) Show that this state is normalised. [1 mark]

(b) Show that the expectation value of the spin x component is given by

$$\langle S_x \rangle = \frac{\hbar}{2} \sin\theta \cos\phi,$$

where $\phi = \beta - \alpha$. [6 marks]

(c) The other two expectation values of the spin components are given by

$$\langle S_y \rangle = \frac{\hbar}{2} \sin\theta \sin\phi, \qquad \langle S_z \rangle = \frac{\hbar}{2} \cos\theta.$$

(Do not prove this.) Comment on the fact that the expectation values only depend on the combination $\beta - \alpha$ and not on these two values individually. [1 mark]

The spin component operators are $\hat{S}_i = \hbar\sigma_i/2$, where the Pauli spin matrices are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

QM knowledge

- For a spin state vector χ
  - Hermitian conjugate: $\chi^+ = (\chi^*)^T = (\chi^T)^*$
  - Normalisation: $\chi^+\chi = 1$
  - Expectation value: $\langle Q \rangle = \chi^+ Q \chi$
- For any QM state, the overall phase is always unobservable
  - Must cancel out in calculation of any observable

2011 Exam Answer 6, Part ii

(ii) (a) The normalisation is given by Note –i as C.C.

$$\chi^\dagger\chi = [\cos(\theta/2)e^{-i\alpha} \quad \sin(\theta/2)e^{-i\beta}]\begin{bmatrix}\cos(\theta/2)e^{i\alpha}\\ \sin(\theta/2)e^{i\beta}\end{bmatrix} = \cos^2(\theta/2) + \sin^2(\theta/2) = 1$$

and hence the state is indeed normalised. [1 mark]

(b) Evaluating the x component expectation value gives

$$\begin{aligned}\langle S_x\rangle &= \chi^\dagger \hat{S}_x\chi = \frac{\hbar}{2}[\cos(\theta/2)e^{-i\alpha} \quad \sin(\theta/2)e^{-i\beta}]\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\cos(\theta/2)e^{i\alpha}\\ \sin(\theta/2)e^{i\beta}\end{bmatrix}\\ &= \frac{\hbar}{2}[\cos(\theta/2)e^{-i\alpha} \quad \sin(\theta/2)e^{-i\beta}]\begin{bmatrix}\sin(\theta/2)e^{i\beta}\\ \cos(\theta/2)e^{i\alpha}\end{bmatrix}\\ &= \frac{\hbar}{2}\cos(\theta/2)\sin(\theta/2)\left[e^{i(\beta-\alpha)} + e^{-i(\beta-\alpha)}\right] = \frac{\hbar}{2}\sin\theta\cos\phi\end{aligned}$$

[6 marks]

2011 Exam Answer 6, Part ii (cont)

(c) The state can be rewritten as

$$\chi = e^{i\alpha}\begin{pmatrix}\cos(\theta/2)\\ \sin(\theta/2)e^{i(\beta-\alpha)}\end{pmatrix} = e^{i\alpha}\begin{pmatrix}\cos(\theta/2)\\ \sin(\theta/2)e^{i\phi}\end{pmatrix}$$

or as

Overall phases

$$\chi = e^{i\beta}\begin{pmatrix}\cos(\theta/2)e^{i(\alpha-\beta)}\\ \sin(\theta/2)\end{pmatrix} = e^{i\beta}\begin{pmatrix}\cos(\theta/2)e^{-i\phi}\\ \sin(\theta/2)\end{pmatrix}$$

Hence, the absolute value of α (or equivalently β) corresponds to an overall phase, while the difference ϕ corresponds to a relative phase between the two terms. The overall phase of any state is not physically observable. Hence, any arbitrary value could be added to both α and β without changing any measurable property of the system. Hence, the expectation values, which are observable, can only depend on the difference $\phi = \beta - \alpha$.

[1 mark]

2011 Exam Question 6, Part iii

(iii) A general form of the Heisenberg uncertainty relation is

$$\Delta Q^2 \Delta R^2 \geq \left\langle \frac{i}{2}[\hat{Q}, \hat{R}] \right\rangle^2 ,$$

where ΔQ and ΔR are the RMS uncertainties in measurements of dynamical variables Q and R, such that $\Delta Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2$, and similarly for R. Consider the case of $\hat{Q} = \hat{S}_x$ and $\hat{R} = \hat{S}_y$.

(a) Evaluate the right-hand side of the above relation for the general state χ. What range of values can it take? [2 marks]

(b) Evaluate the left-hand side of the above relation for the general state χ and hence prove the relation is always satisfied. [5 marks]

(c) Show that when the equality holds for the relation, at least one of the expectation values $\langle S_x \rangle$ and $\langle S_y \rangle$ must be zero. [2 marks]

[Total 20 marks]

Each of the Pauli spin matrices satisfies:

$$\sigma_i^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I.$$

QM knowledge

- Observable operators must be Hermitian
  - For products of two Hermitian operators, {Q,R} and i[Q,R] are always Hermitian combinations
- The RMS uncertainty appears in the HUP and is given by
  - $\Delta Q^2 = (\Delta Q)^2 = \langle Q^2 \rangle - \langle Q \rangle^2$
- A minimum uncertainty state satisfies the equality of the HUP relation

2011 Exam Answer 6, Part iii

(iii) (a) The right-hand side of the relation is

From part i　　　From part ii

$$\left\langle \frac{i}{2}[\hat{S}_x, \hat{S}_y] \right\rangle^2 = \left\langle \frac{i}{2} i\hbar \hat{S}_z \right\rangle^2 = \left(-\frac{\hbar^2}{4} \cos\theta \right)^2 = \frac{\hbar^4}{16} \cos^2\theta$$

This can take values between 0 and $\hbar^4/16 = (\hbar/2)^4$. [2 marks]

(b) For any of the spin components

σ^2 = I given in question

$$\langle \hat{S}_i^2 \rangle = \frac{\hbar^2}{4} \langle \sigma_i^2 \rangle = \frac{\hbar^2}{4} \langle I \rangle = \frac{\hbar^2}{4}$$

$<I>=\chi^+ I\chi=\chi^+\chi=1$

Hence, the RMS uncertainties on the left-hand side are

$$\Delta S_x^2 = \langle \hat{S}_x^2 \rangle - \langle \hat{S}_x \rangle^2 = \frac{\hbar^2}{4} \left[1 - \sin^2\theta \cos^2\phi \right]$$

$$\Delta S_y^2 = \langle \hat{S}_y^2 \rangle - \langle \hat{S}_y \rangle^2 = \frac{\hbar^2}{4} \left[1 - \sin^2\theta \sin^2\phi \right]$$

From part ii

2011 Exam Answer 6, Part iii (cont)

The left-hand side is therefore

$$
\begin{aligned}
\Delta S_x^2 \Delta S_y^2 &= \frac{\hbar^4}{16}\left[1 - \sin^2\theta\cos^2\phi\right]\left[1 - \sin^2\theta\sin^2\phi\right] \\
&= \frac{\hbar^4}{16}\left[1 - \sin^2\theta\cos^2\phi - \sin^2\theta\sin^2\phi + \sin^4\theta\cos^2\phi\sin^2\phi\right] \\
&= \frac{\hbar^4}{16}\left[1 - \sin^2\theta + \sin^4\theta\cos^2\phi\sin^2\phi\right] \\
&= \frac{\hbar^4}{16}\left[\cos^2\theta + \sin^4\theta\cos^2\phi\sin^2\phi\right] \\
&= \left\langle \frac{i}{2}[\hat{S}_x, \hat{S}_y] \right\rangle^2 + \frac{\hbar^4}{16} \sin^4\theta\cos^2\phi\sin^2\phi
\end{aligned}
$$

RHS from above

All squares so must be ≥0

Since the second term above cannot be negative, then the uncertainty relation is always satisfied. [5 marks]

(c) For the equality to hold, the second term above must be zero. This can occur when any of the following hold

$$\sin\theta = 0, \qquad \cos\phi = 0, \qquad \sin\phi = 0$$

For the first case, then both $\langle S_x \rangle$ and $\langle S_y \rangle$ are zero. For the second case, $\langle S_x \rangle$ is zero, while for the third case, then $\langle S_y \rangle$ is zero. [2 marks]

2011 Exam Question 6 Report

Question 6

This question done by somewhat less than half of the candidates. Most of it was not previously seen material and some candidates found it difficult.

Most candidates knew that the non-zero commutator in part (i) meant the values of the spin components could not be known simultaneously, although few were able to explain this was due to not having the same eigenstates and so the collapse during measurements forces the wavefunction out of the eigenstate of the previously measured quantity. The normalisation calculation in part (ii)(a) and expectation value calculation in part (ii)(b) were mainly done correctly. However, very few candidates could answer part (ii)(c); the crucial fact that the overall phase of any state is unobservable was rarely stated. For part (iii)(a), a majority of candidates did not realise the commutator was already given in part (i) and spent time calculating it from scratch. Many also did not notice that $\langle \hat{S}_z \rangle$ was given in part (ii)(c) and again unnecessarily spent time calculating it explicitly. There were many arithmetic slips in this part. Most candidates got the correct expression for the LHS in part (iii)(b) in terms of trig functions, although many did not use the given relation $\sigma_i^2 = I$ and so yet again did a lot of unnecessary calculation. However, few were able to rearrange the LHS expression in terms of the RHS and so prove the uncertainty relation held. Many claimed it held even when previous mistakes meant what they had written down did not satisfy the relation, and hence they lost more marks. Also, due to arithmetical errors, many ended up comparing quantities with different dimensions, specifically different powers of $\hbar$, which should have indicated there was a mistake. Few candidates were able to do part (iii)(c) correctly; usually at least one of the three trig function conditions for equality was missed.

GOOD LUCK!