

PHYS30201 Advanced Quantum Mechanics: Examples 2

8. Prove the following commutator relations. \hat{A} etc are arbitrary operators but $\hat{\mathbf{x}}$, $\hat{\mathbf{p}}$ and $\hat{\mathbf{L}}$ have their usual meanings. $V(x)$, $V(r)$ and $V(\mathbf{r})$ are arbitrary functions; the second depends only on the magnitude of the position vector \mathbf{r} whereas the third depends on all three components.

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

(b) $[\hat{L}_x, \hat{y}] = i\hbar\hat{z}$, $[\hat{L}_x, \hat{p}_y] = i\hbar\hat{p}_z$, $[\hat{L}_x, \sum_i \hat{p}_i^2] = 0$.

(c) $[\hat{p}_x, V(x)] = -i\hbar \frac{dV}{dx}$,

(d) $[\hat{p}_i, V(r)] = -i\hbar \hat{r}_i \frac{dV}{dr}$, $[\hat{\mathbf{p}}, V(\mathbf{r})] = -i\hbar \nabla V$ (where $\hat{r}_i = r_i/r$).

(e) $[\hat{L}_x, V(r)] = 0$

(Hint: You will only need to use the position representation where functions of x or r are involved. In that case it can be useful to provide an arbitrary wave function for derivative operators to act on. In the position representation we often write x for \hat{x} and \mathbf{r} for $\hat{\mathbf{x}}$, hence $V(x)$.)

9. Use Ehrenfest's theorem to show that for the one-dimensional harmonic oscillator in any state (not necessarily a stationary state),

$$m \frac{d^2 \langle \hat{x} \rangle}{dt^2} = -k \langle \hat{x} \rangle,$$

where k is the spring constant.

10. A particle of mass m is bound by a potential $V(\mathbf{r})$. Show that if the potential is spherically symmetric, $V = V(r)$, the expectation value of the angular momentum is conserved.

Now consider a non-spherically symmetric potential $V = V_0(r) + zV_1(r)$. Show that $\langle \hat{L}_z \rangle$ is still conserved, and that

$$\frac{d}{dt} \langle \hat{L}_x \rangle = -\langle \hat{y} V_1(r) \rangle \quad \text{and} \quad \frac{d}{dt} \langle \hat{L}_y \rangle = \langle \hat{x} V_1(r) \rangle$$

Show that the right-hand sides do indeed correspond to the components of the expectation value of the torque.

11. Fill in the details of the variational calculation for the $V(x) = \beta x^4$ potential discussed in the lectures, using as trial wavefunction $\Psi(x) = e^{-ax^2/2}$ to get an upper bound for the ground state energy of $3 \times 6^{1/3}/8 = 0.68$ in units of $(\hbar^4\beta/m^2)^{1/3}$.
12. A particle moves in a potential $V(x) = \beta x$ for $x > 0$ and $V(x) = \infty$ for $x < 0$. Sketch the potential and the rough form of the ground state solution. Use an appropriate state of the harmonic oscillator as a trial function (with x_0 as a variational parameter) to obtain an upper bound on E_0 . Try any other suitable trial function you can think of and see if it gives a better bound. (Hint: the exact answer is $2.338(\hbar^2\beta^2/2m)^{1/3}$. If you make the wrong choice of trial function, you might get an answer below this. Think carefully about what might have gone wrong, and why the variational principle is not violated.)

The solution to the differential equation $y''(z) - zy(z) + \mu y(z) = 0$ can be written in terms of Airy functions (these are special functions like Bessel functions whose roots can only be found numerically): $y = CAi(z - \mu) + DBi(z - \mu)$. You are strongly encouraged to use Mathematica (or a handbook of special functions) to explore these solutions, and to reproduce the exact result quoted above.

13. Consider the three-dimensional problem with potential $V(r) = -\beta e^{-\mu r}/r$. As is typically the case in 3D, for finite μ if the potential is too weak there will not be any bound-state solutions. Use a trial wavefunction $\Psi(r) = e^{-r/a}$ to find a value of β/μ , above which at least one bound state is guaranteed. What can we say in the $\mu \rightarrow 0$ limit?
14. Using products of $Z = 2$ hydrogenic single-particle wave functions, write down trial wave functions for the first two excited states of helium (the $1s^1 2s^1$ states of ortho- and parahelium). Which of the two could be used to generate a true upper bound on the energy level of the state?

Show the the electron-electron repulsion energy in the two states can be written $J + K$ for parahelium and $J - K$ for orthohelium, where

$$\begin{aligned}
 J &= \hbar c \alpha \int_0^\infty r_2 (R_{2,0}^{Z=2}(r_2))^2 \left(\int_0^{r_2} r_1^2 (R_{1,0}^{Z=2}(r_1))^2 dr_1 \right) dr_2 \\
 &+ \int_0^\infty r_2^2 (R_{2,0}^{Z=2}(r_2))^2 \left(\int_{r_2}^\infty r_1 (R_{1,0}^{Z=2}(r_1))^2 dr_1 \right) dr_2 \\
 K &= \hbar c \alpha \int_0^\infty r_2 R_{1,0}^{Z=2}(r_2) R_{2,0}^{Z=2}(r_2) \left(\int_0^{r_2} r_1^2 R_{1,0}^{Z=2}(r_1) R_{2,0}^{Z=2}(r_1) dr_1 \right) dr_2 \\
 &+ \int_0^\infty r_2^2 R_{1,0}^{Z=2}(r_2) R_{2,0}^{Z=2}(r_2) \left(\int_{r_2}^\infty r_1 R_{1,0}^{Z=2}(r_1) R_{2,0}^{Z=2}(r_1) dr_1 \right) dr_2
 \end{aligned}$$

and $R_{n,l}^{Z=2}(r)$ are the normalised radial wave functions as given in section A.3 of the notes. Given that the integrals contained in J and K are $34/(81a_0)$ and $32/(729a_0)$ respectively, estimate the first ionisation energy of each state. How might you refine your trial wave functions?