Quantum Mechanics III — Epiphany Term 2008

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Homework 4 – due 12 March 2008

Question 1. Consider a particle of mass M moving in the central potential $V(\mathbf{r}) = -V_0 e^{-|\mathbf{r}|/b}$, where V_0 and b are real positive constants. In spherical coordinates, write down the angular dependence of a Hamiltonian eigenfunction that is also eigenfunction of the $\hat{L}_z$ and of the $\hat{\mathbf{L}}^2$ operators. Also, give the differential equation that determines its radial dependence. Then, changing variable to $s = e^{-r/(2b)}$, find the explicit wave function for a bound state of zero total angular momentum, and the equation that fully determines the energies. Are there bound states for very small values of V_0?

Hint: Two solutions to the differential equations

$$\frac{d^2}{dz^2}f(z) + \frac{1}{z}\frac{d}{dz}f(z) + \left(1 - \frac{\beta^2}{z^2}\right) f(z)$$

are given by

$$f(z) = J_\beta(z) \quad \text{and} \quad f(z) = H_\beta(z)$$

for $\beta > 0$, with $J_\beta(z)$ the Bessel function of order β and $H_\beta(z)$ some other (independent) solution, which can be related to the Bessel function[1]. The Bessel function (for $\beta > 0$) has the property that $J_\beta(z) = (z/2)^\beta(1/\Gamma(1+\beta) + O(z^2))$ as $z \to 0$ ($\Gamma(z)$ is Euler's Gamma function, with $\Gamma(1+n) = n!$ for $n = 0, 1, 2, 3, \ldots$), and the other solution has the property $H_\beta(z) \propto z^{-\beta}$ as $z \to 0$. Don't hesitate to investigate properties of the Bessel functions and the Gamma function, for instance in Maple, Mathematica, on the web on Wikipedia, or in any good book about special functions.

Question 2. A particle of mass M moves in a potential

$$V(\mathbf{r}) = \frac{A}{|\mathbf{r}|^2} - \frac{B}{|\mathbf{r}|}$$

where A and B are real positive constants. Knowing that the hydrogen atom (case $A = 0$) has bound states energies

$$E = -\frac{MB^2}{2\hbar^2(N + \ell + 1)^2}\ , \quad N = 0, 1, 2, \ldots$$

in any state with total angular momentum ℓ, find the energies of the bound states in the potential V.

ANSWERS

1.

[1] We can take, for instance, $H_\beta(z) = J_{-\beta}(z)$ for $\beta \notin \mathbb{N}$, and $H_n(z) = \frac{\partial}{\partial\beta}(J_\beta(z) - (-1)^n J_{-\beta}(z))_{\beta=n}$ for $n \in \mathbb{N}$.

We want to solve simultaneously

$$\begin{aligned} \hat{L}_z\psi &= m\hbar\psi \\ \hat{\mathbf{L}}^2\psi &= \ell(\ell+1)\hbar^2\psi \\ \hat{H}\psi &= E\psi \end{aligned}$$

In spherical coordinates (r, θ, φ), with

$$\begin{aligned} x &= r\cos\theta\cos\varphi \\ y &= r\cos\theta\sin\varphi \\ z &= r\sin\theta \end{aligned}$$

these three equations can be solved by separation of variable. We write the wave function $\psi(r, \theta, \varphi)$ as

$$\psi(r, \theta, \varphi) = \frac{u(r)}{r} h(\varphi)\chi(\theta)$$

As seen in class, the product $h(\varphi)\chi(\theta)$ is a spherical harmonics:

$$h(\varphi)\chi(\theta) = Y_{\ell,m}(\theta,\varphi) = \begin{cases} (-1)^m \sqrt{\dfrac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}} (\sin\theta)^m \left(\dfrac{d}{d\cos\theta}\right)^m P_\ell(\cos\theta) e^{im\varphi} & m \geq 0 \\ \sqrt{\dfrac{(2\ell+1)(\ell+m)!}{4\pi(\ell-m)!}} (\sin\theta)^{-m} \left(\dfrac{d}{d\cos\theta}\right)^{-m} P_\ell(\cos\theta) e^{im\varphi} & m < 0 \end{cases}$$

where $P_\ell(x)$ are Legendre polynomials, and we must have $\ell = 0, 1, 2, 3, \ldots$ and $m = -\ell, -\ell + 1, \ldots, \ell - 1, \ell$. The radial equation becomes

$$-\frac{\hbar^2}{2M}\frac{d^2u}{dr^2} + \left(V(r) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2}\right) u = Eu$$

where $V(r) = -V_0 e^{-r/b}$.

At zero angular momentum, we have $\ell = 0$. Then,

$$Y_{0,0}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$$

With the change of variable $s = e^{-r/(2b)}$, we have $V(s) = -V_0 s^2$ and

$$\frac{d}{dr} = -\frac{s}{2b}\frac{d}{ds}\ , \qquad \frac{d^2}{dr^2} = \frac{1}{4b^2}\left(s^2\frac{d^2}{ds^2} + s\frac{d}{ds}\right)$$

so that at $\ell = 0$ we get, dividing by s^2,

$$-\frac{\hbar^2}{8Mb^2}\left(\frac{d^2u}{ds^2} + \frac{1}{s}\frac{du}{ds}\right) - \frac{Eu}{s^2} - V_0 u = 0$$

If we want bound states, we must have $E = -|E| < 0$. Re-scaling the s variable to $s' = \frac{\sqrt{8Mb^2V_0}}{\hbar}s$, this becomes the equation that gives Bessel functions (of real order and arguments), with $\beta^2 = 8Mb^2|E|/\hbar^2$. A general solution is

$$u(s) = AJ_{\sqrt{8Mb^2|E|}/\hbar}\left(\frac{\sqrt{8Mb^2V_0}}{\hbar}s\right) + BH_{\sqrt{8Mb^2|E|}/\hbar}\left(\frac{\sqrt{8Mb^2V_0}}{\hbar}s\right)$$

In a bound state, the wave function vanishes (decays exponentially) as $r \to \infty$, where the potential is 0. The point $r \to \infty$ is the point $s = 0$, so that we must take a solution that vanishes as $s \to 0$. From the form of the Bessel function as the argument goes to zero, we are lead to $B = 0$,

$$u(s) = AJ_{\sqrt{8Mb^2|E|}/\hbar}\left(\frac{\sqrt{8Mb^2V_0}}{\hbar}s\right)$$

This vanishes proportionally to $s^{\sqrt{8Mb^2|E|}/\hbar} = e^{-r\sqrt{2M|E|}/\hbar}$ as $r \to \infty$. Also, in order for the probability $r^2 \sin\theta|\psi(r,\theta,\varphi)|^2 drd\theta d\varphi = \sin\theta|u(r)|^2 drd\theta d\varphi/(4\pi)$ to be well-defined at $r = 0$ (in particular, to be the same if we approach the point $r = 0$ from any θ direction), we must have $u(r) \to 0$ as $r \to 0$. That is, $u(s) = 0$ at $s = 1$, which leads to

$$J_{\sqrt{8Mb^2|E|}/\hbar}\left(\frac{\sqrt{8Mb^2V_0}}{\hbar}\right) = 0$$

This is the equation that determines the possible energies.

We expect bound states to be present certainly for V_0 large enough. For small values of V_0, we can see if there are bound states by taking the leading term of the expansion of the Bessel function at small arguments:

$$J_{\sqrt{8Mb^2|E|}/\hbar}\left(\frac{\sqrt{8Mb^2V_0}}{\hbar}\right) \approx \left(\frac{\sqrt{8Mb^2V_0}}{2\hbar}\right)^{\sqrt{8Mb^2|E|}/\hbar} \frac{1}{\Gamma\left(1+\sqrt{8Mb^2|E|}/\hbar\right)}$$

The Gamma function is finite for any positive argument, so that this is never zero for any positive value of $|E|$.

2.

The radial equation for this potential, with total angular momentum ℓ, is

$$-\frac{\hbar^2}{2M}\frac{d^2u}{dr^2} + \left(\frac{A}{r^2} - \frac{B}{r} + \frac{\ell(\ell+1)\hbar^2}{2Mr^2}\right)u = Eu \tag{1}$$

The left-hand side can be written by putting the A-term and centrifugal term together:

$$-\frac{\hbar^2}{2M}\frac{d^2u}{dr^2} + \left(-\frac{B}{r} + \frac{\ell(\ell+1)\hbar^2 + 2MA}{2Mr^2}\right)u$$

We know that at $A = 0$, solutions to equation (1) with negative energies (because we want a bound state, and the potential is 0 at infinity) and with appropriate boundary conditions have energies

$$E = -\frac{MB^2}{2\hbar^2(N+\ell+1)^2}\ , \quad N = 0, 1, 2, \ldots$$

For $A \neq 0$, we have exactly the same equation, but with the centrifugal term in $1/r^2$ modified, as if we had a different angular momentum ℓ'. The new value is such that

$$\ell'(\ell'+1)\hbar^2 = \ell(\ell+1)\hbar^2 + 2MA$$

which gives

$$\ell' = \frac{1}{2}\left(-1 \pm \sqrt{\frac{8MA}{\hbar^2} + (1+2\ell)^2}\right)$$

and the energies of bound states are

$$E = -\frac{MB^2}{2\hbar^2(N+\ell'+1)^2}\ , \quad N = 0, 1, 2, \ldots$$