QM I _ Fall 2019
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Radial Schrödinger's equation

Examples :

Radial Schrödinger's equation

$$V(\vec{R}) = V(\hat{r}) \longrightarrow \text{Only depends on the distance}$$

$$\Rightarrow V(\vec{R}) = V(\hat{r}) \otimes \mathbb{1}_\theta \otimes \mathbb{1}_\varphi$$

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{r}) \longrightarrow P^2 = \hat{P}_r^{\,2} \otimes \mathbb{1} + \mathbb{1} \otimes \hat{P}_\Omega^{\,2}$$

$$P^2 = -\hbar^2 \nabla^2 \longrightarrow \text{Cartezian Coordinate is not good for this.}$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\hat{L}^2$$

Sch. eq

$$\frac{-\hbar^2}{2M}\left[\underbrace{\frac{1}{r}\frac{\partial^2}{\partial r^2} r}_{\hat{P}_r^{\,2}} - \underbrace{\frac{1}{\hbar^2 r^2}\hat{L}^2}_{\hat{P}_\Omega^{\,2}} + V(r)\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

Seperation of variables

$$\psi(\vec{r}) = R(r)\,\Omega(\theta,\varphi)$$

Should be eigenfunction of L^2. $\leftarrow Y_{\ell m}(\theta,\varphi)$

$$-\frac{\hbar^2}{2M}\cancel{Y_{\ell m}}\frac{\partial^2}{\partial r^2} rR(r) + \frac{\hbar^2\ell(\ell+1)\cancel{Y_{\ell m}(\theta,\varphi)}}{2Mr^2}\, rR(r) + \cancel{Y_{\ell m}}\, V(r)\, rR(r) = \cancel{Y_{\ell m}}\, E\, rR(r)$$

$$\Rightarrow -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2} U(r) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} U(r) + V(r)\, U(r) = E\, U(r)$$

$$U(r) = r\,R(r) \longrightarrow U_{E,\ell,m} \longrightarrow U_{E,\ell}$$

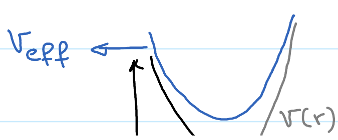
For bound states $E \to E_n$

$$\Rightarrow U_{n,\ell}(r)$$

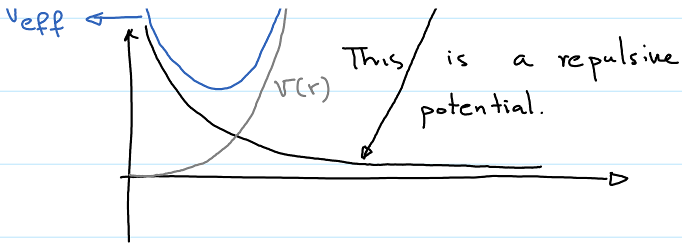
$$\boxed{-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2} U_{n\ell}(r) + \left(\frac{\ell(\ell+1)\hbar^2}{2Mr^2} + V(r)\right) U_{n\ell}(r) = E_n\, U_{n\ell}(r)}$$

Radial Sch eq

$$V_{eff} = V(r) + \underbrace{\frac{\ell(\ell+1)\hbar^2}{2Mr^2}}_{}$$



This is a repulsive



To have bound states, $V(r)$ should be attractive.

* This is effectively a 1-D potential problem.
But

$$r \geq 0$$

$$\Rightarrow \lim_{r \to 0} u_{n\ell}(r) = 0$$

(Similar to $r \to \infty$).

* The larger the ℓ, the harder it would be to bound the state. This is similar to the classical behavior If angular momentum is to large, the attractive potential needs to be strong enough to compensate.

* $$\psi_{n,\ell,m}(\vec{r}) = R_{n\ell}(r)\, Y_{\ell m}(\theta, \varphi)$$

Note that L_z does not appear in the eq which implies all m give the same energy:

$$n, \ell \to m = 2\ell + 1 \text{ degeneracy (at least)}$$

Example 1: Free particle

$$V(r)=0 \Rightarrow V_{eff} = \frac{\ell(\ell+1)\hbar^2}{2Mr^2}$$

$$\Rightarrow -\frac{\hbar^2}{2M}\frac{1}{r}\frac{d^2}{dr^2}(rR(r)) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2}R(r) = E$$

$$k=\sqrt{\frac{2ME}{\hbar^2}} \quad , \quad \rho = kr$$

$$\frac{d^2}{dr^2}(rR(r)) = 2\frac{dR(r)}{dr} + r\frac{d^2R(r)}{dr^2}$$

$$\frac{\cancel{k}}{\rho}\left[2\cancel{k}\frac{dR(\rho)}{d\rho} + \left(\frac{\rho}{\cancel{k}}\right)(\cancel{k^2})\frac{d^2R(\rho)}{d\rho^2}\right] - \frac{\ell(\ell+1)\hbar^2\cancel{k^2}}{\rho^2}R(\rho) = -\cancel{k^2}R(\rho)$$

$$\Rightarrow \frac{d^2R(\rho)}{d\rho^2} + \frac{2}{\rho}\frac{dR(\rho)}{d\rho} + \left[1 - \frac{\ell(\ell+1)\hbar^2}{\rho^2}\right]R(\rho) = 0$$

$\hookrightarrow$ Spherical Bessel eq.

$$R_\ell(\rho) = A_\ell J_\ell(\rho) + B_\ell n_\ell(\rho)$$

We also have $\lim_{\rho\to 0} R_\ell(\rho)$ should be finite $\leadsto$ $B_\ell = 0$. ($n_\ell(\rho)$ diverge at $\rho=0$)

$$\psi_{k,l,m}(\vec{r}) = j_l(kr)\, Y_{lm}(\theta,\varphi)$$

Ⓐ Which one was easier? Spherical or Cartesian Coordinates?

Ⓐ How are the solutions related?

Ⓐ What is the CSCO for the solutions in

* Spherical Coordinates?
* Cartesian " ?

Example 2: Potential Well

$$V(r) = \begin{cases} -V_0 & 0 \leq r \leq a \\ 0 & a < r \end{cases}$$

$\boxed{0 \leq r \leq a} \longrightarrow$

$$\frac{d^2 R(\tilde{\rho})}{d\tilde{\rho}^2} + \frac{2}{\tilde{\rho}} \frac{dR(\tilde{\rho})}{d\tilde{\rho}} + \left[1 - \frac{l(l+1)\hbar^2}{\tilde{\rho}^2}\right] R(\tilde{\rho}) = 0$$

$$\tilde{\rho} = qr \quad , \quad q = \sqrt{\frac{2m(V_0+E)}{\hbar^2}}$$

$$\hbar^2$$

$$\psi_{k,l,m}(\vec{r}) = j_\ell(qr)\, Y_{\ell m}(\theta, \varphi)$$

$\boxed{r > a}$ $E > 0$ $\rightsquigarrow$ Similar to free particle

+ B.C.

$-V_0 \leq E \leq 0 \Rightarrow k \to ik$

$$R_\ell(\rho) = C h_\ell^{(1)}(\rho) + D h_\ell^{(2)}(\rho)$$

$$\begin{cases} h_\ell^{(1)} = j_\ell(\rho) + i n_\ell(\rho), \\ h_\ell^{(2)} = j_\ell(\rho) - i n_\ell(\rho) \end{cases} \quad : r \to \infty \quad h_\ell^{(2)} \rightsquigarrow \infty$$

$$R_\ell(\rho) = h_\ell^{(1)}(\rho)$$

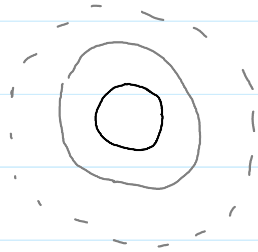
$$\psi_{k\ell m}(\vec{r}) = h_\ell^{(1)}(ikr)\, Y_{\ell m}(\theta, \varphi)$$

$\to$ B.C.

$$\Rightarrow k \cot(kr) = -q$$

Example 3: Isotropic Harmonic Potential

$$V(r) = \frac{1}{2} m \omega^2 r^2$$



Potential gets stronger as we get away from the center.

The radial sch eq.:

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}\left(r R_{n\ell}(r)\right) + \left(\underbrace{\frac{\ell(\ell+1)\hbar^2}{2Mr^2} + V(r)}\right) r R_{n\ell}(r) = E_n r R_{n\ell}(r)$$

$$V_{eff}(r) = \frac{1}{2} m \omega^2 r^2 + \frac{\ell(\ell+1)\hbar^2}{2M r^2}$$

How do we solve this?

This is an important example.

We follow basically the exact steps for the Hydrogen atom.

① Asymptotic behavior.

a) $r \to 0$

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}\left(U_{n\ell}(r)\right) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} U_{n\ell}(r) = 0$$

$$U_{n\ell}(r) \sim r^{\ell+1}$$

b) $r \to \infty$

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}\left(U_{n\ell}(r)\right)+\frac{1}{2}M\omega^2 r^2 U_{n\ell}(r)=0$$

$$U_{n\ell}(r) \sim e^{-m\omega\, r^2/2\hbar}$$

② We make a guess

$$U_{n\ell}(r)=f(r)\, r^{\ell+1}\, e^{-\frac{M\omega r^2}{2\hbar}}$$

and rewrite the sch. eq for f(r).

$$-\frac{\hbar^2}{2M}\underbrace{\frac{d^2}{dr^2}\left(U_{n\ell}(r)\right)}+\left(\frac{\ell(\ell+1)\hbar^2}{2Mr^2}+V(r)\right)U_{n\ell}(r) = E_n U_{n\ell}(r)$$

a) $$\frac{d^2}{dr^2}\left[f(r)\, r^{\ell+1} e^{-\frac{M\omega r^2}{2\hbar}}\right]= r^{\ell+1} e^{-\frac{M\omega r^2}{2\hbar}}\frac{d^2 f(r)}{dr^2}$$

$$+\frac{df}{dr}\left[2(\ell+1)\, r^{\ell}\, e^{-\frac{M\omega r^2}{2\hbar}}-\frac{2M\omega r}{\hbar}\, r^{\ell+1}\, e^{-\frac{M\omega r^2}{2\hbar}}\right]$$

$$+f(r)\left[\ell(\ell+1)\, r^{\ell-1}\, e^{-\frac{M\omega r^2}{2\hbar}}+\left(\frac{M\omega r}{\hbar}\right)^2 r^{\ell+1}\, e^{-\frac{M\omega r^2}{2\hbar}}\right.$$

$$\left.+\left[(\ell+1)+(\ell+2)\right]\left(\frac{-M\omega r}{\hbar}\right) r^{\ell}\, e^{-\frac{M\omega r^2}{2\hbar}}\right]$$

$$= r^{\ell+1} e^{-\frac{M\omega r^2}{2\hbar}}\left[\frac{d^2 f}{dr^2}+\frac{df}{dr}\left(\frac{2(\ell+1)}{r}-2\frac{M\omega r}{\hbar}\right)+f\left(\frac{\ell(\ell+1)}{r^2}+\left(\frac{M\omega r}{\hbar}\right)^2-\frac{(2\ell+3)M\omega}{\hbar}\right)\right]$$

b) $\Rightarrow$ Putting it all back together and dividing by

$$-\frac{2M}{\hbar^2}\, r^{\ell+1}\, e^{-\frac{M\omega}{2\hbar}r^2}$$ gives:

$$\frac{d^2 f}{dr^2} + \frac{df}{dr}\left[\frac{2(l+1)}{r} - \frac{2M\omega r}{\hbar}\right] + \left[\frac{2ME}{\hbar^2} - (2l+3)\frac{M\omega}{\hbar}\right] f = 0$$

③

$$f(r) = \sum_{i=0}^{\infty} a_i r^i \longrightarrow \text{Polynomial expansion}$$

$$\Rightarrow \sum_i i(i-1)\, a_i\, r^{i-2} + 2(l+1)\, i a_i r^{i-2} - \frac{2M\omega}{\hbar} i a_i r^i + \left[\frac{2ME}{\hbar^2} - (2l+3)\frac{M\omega}{\hbar}\right] a_i r^i = 0$$

$$\Rightarrow \sum_{i=0}^{\infty} i\left((i-1) + 2(l+1)\right) a_i r^{i-2} + \left(\frac{-2M\omega}{\hbar} i + \frac{2ME}{\hbar^2} - (2l+3)\frac{M\omega}{\hbar}\right) a_i r^i = 0$$

$$\Rightarrow \sum_i i(i+2l+1)\, a_i r^{i-2} + \left(\frac{2ME}{\hbar^2} - (2i+2l+3)\frac{M\omega}{\hbar}\right) a_i r^i = 0$$

$i=0$: $\quad i(i+2l+1)\, a_i\, r^{-2} = 0$ ✓

$i=1$ $\quad i(i+2l+1)\, a_1 r^{-1} = (2l+2)\, a_1 = 0 \Rightarrow a_1 = 0$

$i \geq 2$ $\quad (i+2)(i+2l+3)\, a_{i+2} = \left[-\frac{2ME}{\hbar^2} + (2i+2l+3)\frac{M\omega}{\hbar}\right] a_i$

→ All the odd terms vanish.

→ For the even terms

$$a_{i+2} = \frac{(2i+2l+3)M\hbar\omega - 2ME}{\hbar^2 (i+2)(i+2l+3)}\, a_i$$

$$\underbrace{\qquad\qquad\qquad}_{\xi_2}$$

$$\rightarrow f(r) = \sum_{i=0}^{\infty} a_{2i} \, r^{2i}$$

$$\lim_{r \to \infty} R_{n\ell}(r) = \infty \quad !!$$

How can we stop this from diverging?

$$a_i = 0 \quad \forall i \geq 2N$$

e.g. $a_0 \neq 0$, $a_2 = 0$

$$\Rightarrow \xi_0 = 0 \Rightarrow \left. \frac{(2i+2\ell+3)M\hbar\omega - 2ME}{\hbar^2 (i+2)(i+2\ell+3)} \right|_{i=0} = 0$$

$$\Rightarrow (2\ell+3)M\hbar\omega - 2ME = 0$$

$$E = \left(\frac{2\ell+3}{2}\right)\hbar\omega$$

$\rightarrow$ For the general case of ξ_{2N} we have:

$\boxed{i = 2N}$

$$\xi_{2N} = 0 \Rightarrow \left(2N+\ell+3/2\right)\hbar\omega = E$$

$n \rightarrow$ The energy quantum number.

$$E_n = \left(n + 3/2\right)\hbar\omega \quad , n = 0, 1, 2, \ldots$$

* Since $n = 2N + \ell$, for

Odd $n \rightarrow \ell$ is always odd

even $n \rightarrow \ell$ is " even.

e.g. $n=0 \rightarrow N=0, \ell=0$ $\quad g_0 = 1$

$n=1 \rightarrow N=0, \ell=1, m=\pm1, 0$ $\quad g_1 = 3$

$n=2 \rightarrow (N=1, \ell=0)$ or $(N=0, \ell=2)$ $\quad g_2 = 6$

$n=3 \rightarrow (N=1, \overset{3}{\ell}=1)$ or $(N=\overset{7}{0}, \ell=3)$ $\quad g_3 = 10$

$$g_n = \sum_{\substack{\text{allowed} \\ \ell}} (2\ell+1)$$

Odd n

$$\sum_{\ell=1,3\ldots}^{n} (2\ell+1)$$

1	3	5	...		n
n	$n-2$		...	3	1

$(n+1)\left(\frac{n+1}{2}\right)$

$$\rightarrow = 2(n+1)\left(\frac{n+1}{2}\right) + \frac{n+1}{2}$$

$$= \frac{n+1}{2}(n+1+1)$$

$$= \frac{1}{2}(n+1)(n+2)$$

Similarly for even $n \rightarrow g_n = \frac{1}{2}(n+1)(n+2)$