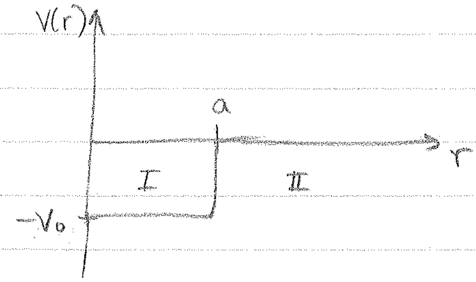
Bound States of the Spherical Potential Well

Schrödinger equation:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2}\left(E - V(r)\right)\right] R(r) = 0$$

Potential:



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

Bound states occur for energies: $-V_0 < E < 0$.

Define $\frac{2m}{\hbar^2}\left(E - V(r)\right) = \begin{cases} \frac{2m}{\hbar^2}(E + V_0) = q^2 & \text{inside} \\ \frac{2m}{\hbar^2} E \quad = -\kappa^2 & \text{outside} \end{cases}$ in this case $E = -|E|$

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2} + \begin{pmatrix} q^2 \\ -\kappa^2 \end{pmatrix}\right] R(r) = 0.$$

Inside the well, require solution be regular at origin:

$R_I(r) = A\, j_\ell(qr)$ in region I: $r < a$

Outside the well, want solutions that decrease exponentially:

$R_{II}(r) = B\, h_\ell^{(1)}(i\kappa r)$ in region II: $r > a$

[$h_\ell^{(2)}(-i\kappa r)$ works, too]

Continuity at boundary: $R_I(a) = R_{II}(a) \Rightarrow A\, j_\ell(qa) = B\, h_\ell^{(1)}(i\kappa a)$ [*]

Smoothness at boundary: $R_I'(a) = R_{II}'(a) \Rightarrow A \frac{\partial}{\partial r} j_\ell(qa) = B \frac{\partial}{\partial r} h_\ell^{(1)}(i\kappa a)$ [**]

Divide [**] by [*] for an eigen condition: $q \frac{\partial}{\partial r} \ln j_\ell(r)\Big|_{r=qa} = i\kappa \frac{\partial}{\partial r} \ln h_\ell^{(1)}(r)\Big|_{r=i\kappa a}$

For $\ell = 0$, the condition from log derivatives is:

$$q \frac{\partial}{\partial r} \ln \frac{\sin r}{r}\Bigg|_{r=qa} = i\kappa \frac{\partial}{\partial r} \ln \frac{-i e^{ir}}{r}\Bigg|_{r=i\kappa a}$$

$$q\left(\cot r - \frac{1}{r}\right)_{r=qa} = i\kappa\left(i - \frac{1}{r}\right)_{r=i\kappa a}$$

$$q \cot qa - \frac{\cancel{q}}{\cancel{q}a} = -\kappa - \frac{i\kappa}{i\kappa a}$$

cancel

$\zeta = \sqrt{\frac{2ma^2V_0}{\hbar^2}}$

$$\cot qa = \frac{-\kappa}{q} \quad \text{or} \quad \text{Write} \quad \kappa = \frac{1}{a}\sqrt{-(qa)^2 + \zeta^2}$$

$$-\cot qa = \frac{\sqrt{-(qa)^2 + \zeta^2}}{qa} \quad \text{(same as for 1D potential well)}$$

This is a transcendental equation: plot both sides and find intersections numerically for q

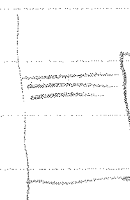
LIMIT: Deep potential well

$q = \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$

Take $qa \gg \ell$ high energy (close to zero as opposed to close to V_0) low angular momentum, ℓ.

$$q\frac{\partial}{\partial r} \ln j_\ell(qa) = i\kappa \frac{\partial}{\partial r} \ln h_\ell^{(1)}(i q_{II} a)$$

Use asymptotic formula



looking at these states.

$$j_\ell(qa) \simeq \frac{1}{qa} \sin\left(qa - \frac{\ell\pi}{2}\right)$$

$$q\frac{\partial}{\partial r}\left(\frac{1}{r}\sin\left(r - \frac{\ell\pi}{2}\right)\Bigg|_{r=qa}\right) = i\kappa \frac{\partial}{\partial r} \ln h_\ell^{(1)}(i\kappa a)$$

$$q\left(-\frac{1}{qa} + \frac{1}{qa}\cot\left(qa - \frac{\ell\pi}{2}\right)\right) =$$

$$-\frac{1}{a} + \frac{1}{a}\cot\left(qa - \frac{\ell\pi}{2}\right) = i\kappa \frac{\partial}{\partial r} \ln h_\ell^{(1)}(i\kappa a)$$

Notice RHS doesn't depend on V_0, since $\kappa = \sqrt{\frac{2m}{\hbar^2}|E|}$.

In order that limit $V_0 \to \infty$ be finite in LHS, $\cot\left(qa - \frac{l\pi}{2}\right)$ must drop faster than q rises.

$\cot(x)$ hits 0 at $x = \left(n + \frac{1}{2}\right)\pi \quad n = 0, 1, \ldots$

So $qa - \frac{l\pi}{2} = \frac{\pi}{2}$

$$\underbrace{\sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}}_{\text{expand}} \times a - \frac{l\pi}{2} = \left(n + \frac{1}{2}\right)\pi, \quad n = 0, 1, \ldots$$

$$\sqrt{\frac{2m}{\hbar^2}}\left(1 - \frac{|E|}{2V_0} + O(|E|^2)\right) a - \frac{l\pi}{2} = \left(n + \frac{1}{2}\right)\pi$$

Solving for $|E|$:

$$\boxed{\frac{|E|}{2V_0} = 1 - \sqrt{\frac{\hbar^2}{2mV_0 a^2}}\left(n + l + \frac{1}{2}\right)\pi}$$

Formula good for large n (giving large q_I)

For general ℓ, the condition for bound state is:

$$q \frac{j_\ell'(q_I a)}{j_\ell(q_I a)} = i\kappa \frac{h_\ell^{(1)\prime}(i q_{II} a)}{h_\ell^{(1)}(i q_{II} a)}$$

Use: $j_\ell'(qa) = j_{\ell-1}(qa) - \frac{\ell+1}{qa} j_\ell(qa)$

$h_\ell^{(1)\prime}(\kappa a) = h_{\ell-1}^{(1)}(\kappa a) - \frac{\ell+1}{i\kappa a} h_\ell^{(1)}(qa)$ (recurrence relations)

$$q \frac{j_{\ell-1}(qa)}{j_\ell(qa)} - \cancel{\frac{\ell+1}{a}} = i\kappa \frac{h_{\ell-1}^{(1)}(i\kappa a)}{h_\ell^{(1)}(i\kappa a)} - \cancel{\frac{(\ell+1)}{a}}$$

$$q \frac{j_{\ell-1}(qa)}{j_\ell(qa)} = i\kappa \frac{h_{\ell-1}^{(1)}(i\kappa a)}{h_\ell^{(1)}(i\kappa a)}$$

Exercise: What is the condition for the appearance of a bound state at zero energy ($E=0$) for any ℓ? Careful: $h_\ell^{(1)}(0)$ is singular.

Solution: $\kappa = \sqrt{\frac{2m}{\hbar^2}E} \xrightarrow{E\to 0} 0$, but $h_\ell^{(1)}(i\kappa a) \to$ diverges as $\kappa \to 0$, so we have to be careful about RHS:

Small x behavior: $h_\ell^{(1)}(x) \sim \frac{-i(2\ell-1)!}{2^\ell \ell!} \frac{1}{x^{\ell+1}} + \dots = -i(2\ell-1)!! \frac{1}{x^{\ell+1}}$

$$\text{RHS} \longrightarrow i\kappa \frac{-i(2(\ell-1)-1)!!}{-i(2\ell-1)!!} \frac{(i\kappa a)^{\ell+1}}{(i\kappa a)^{\ell}} \xrightarrow{\kappa=0} 0 \quad \text{(fine)}$$

Hence $q \frac{j_{\ell-1}(qa)}{j_\ell(qa)} = 0$ with $q \xrightarrow{E=0} \sqrt{\frac{2mV_0}{\hbar^2}} = \frac{\zeta}{a}$

or $\boxed{j_{\ell-1}(\zeta) = 0}$ is the condition for the appearance of a zero-energy bound state.