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$\boxed{\det e^{L} = e^{\mathrm{Tr} L}}$, $\underline{L = P^{-1} T P}$, $\mathrm{Tr} L = \mathrm{Tr}(P^{-1} T P)$

$= \mathrm{Tr}(P P^{-1} T)$

$= \mathrm{Tr}(T)$ — (1)

$e^{L} = e^{P^{-1}TP} = P^{-1} e^{T} P$

$\therefore \det e^{L} = \det(P^{-1} e^{T} P) = \det e^{T}$

$= e^{\lambda_1} e^{\lambda_2} \cdots e^{\lambda_n} = e^{\lambda_1 + \lambda_2 + \cdots + \lambda_n}$

$= e^{\mathrm{Tr} T}$

$= e^{\mathrm{Tr} L}$ (from (1))

$$T = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix}$$

Schrödinger equation (SE)

Non Dimensionalization $\quad -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$

or $\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}(V-E)\psi$ or $L^2 \frac{d^2\psi(x)}{dx^2} = \frac{2mL^2}{\hbar^2}(V-E)\psi$ — (1)

Redefine $x^* = x/L$, $E^* = \frac{2mL^2}{\hbar^2}(V-E)$, $\psi(x^*) = \psi(x)$

(1) $\times \Rightarrow \frac{d^2\psi(x)}{d(x/L)^2} = \frac{2mL^2}{\hbar^2}(V-E)\psi(x)$

$$\therefore \boxed{\frac{d^2\psi^*(x^*)}{dx^{*2}} = E^*\psi(x^*)}$$

$\phi = \frac{d\psi^*}{dx^*}$, $\frac{d\phi}{dx^*} = \frac{d^2\psi}{dx^{*2}} = f(\psi, x^*)$ with $\psi(x_0) = \psi_0$.

$= f(\psi, x^*, V, E)$.

(A) Infinite Well : $V(x=0) = V(x=L) = \infty$

$\psi(x=0) = \psi(x=L) = 0$.

SE : $\boxed{\frac{d^2\psi(x^*)}{dx^{*2}} + E^*\psi(x^*) = 0}$, $E^* = \frac{2mEL^2}{\hbar^2}$

(B) Harmonic Oscillator : $V(x) = \frac{1}{2} m\omega^2 x^2$ $\qquad l = \sqrt{\frac{\hbar}{m\omega}}$

$\psi(x = -\infty) = \psi(x = +\infty) = 0$

SE: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{m\omega^2 x^2}{2}\psi(x) = E\psi(x)$, $x^* = x/l = x\sqrt{\frac{m\omega}{\hbar}}$

$E^* = \frac{2E}{\hbar\omega}$

or $-\frac{\cancel{\hbar^2}}{2\cancel{m}}\frac{d^2\psi(x^*)}{dx^{*2}}\frac{\cancel{m}\omega}{\cancel{\hbar}} + \frac{\cancel{m}\omega^{\cancel{2}}}{2}x^{*2}\psi(x^*)\frac{\hbar}{\cancel{m\omega}} = E\psi(x^*)$

$\therefore \frac{d^2\psi(x^*)}{dx^{*2}} = \left(\frac{2E}{\hbar\omega} - x^{*2}\right)\psi(x^*) = (E^* - x^{*2})\psi(x^*)$

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$$\phi = \frac{d\psi(x^*)}{dx^*}, \quad \frac{d\phi}{dx^*} = (E^* - x^{*2})\psi(x^*)$$

odd parity $\psi(x^* = \frac{L}{\ell}) = 1 \xrightarrow{\text{seek}} \psi(x^* = 1) = 0$.

$\phi(x^* = \frac{L}{\ell}) = 0$.

Vanderpol oscillator: $\ddot{x} - \epsilon(1 - x^2)\dot{x} + x = 0 \Rightarrow \begin{array}{l} \dot{y} = x/\epsilon \\ \dot{x} = \epsilon(x - \frac{x^3}{3} - y) \end{array}$

$y'' + 5y' = 5x, \quad y(0) = 1, \; y(1) = 0.$ $\qquad u_\alpha' = v_\alpha$

$u_\alpha'' + 5u_\alpha' = 5x, \quad u_\alpha(0) = 1, \; u_\alpha'(0) = \alpha$ $\qquad v_\alpha' = -5v_\alpha + 5x$

Step

1. $y''(x) = f(y(x), y'(x), x), \; y(x_0) = a, \; y(x_N) = b.$ (BVP)

2. $\Rightarrow u_\alpha''(x) = f(u_\alpha(x), u_\alpha'(x), x), \; u_\alpha(x_0) = a, \; u_\alpha'(x_0) = \alpha$ (IVP). (RK4)

$g(\alpha) = u_\alpha(x_N) - y(x_N) = u_\alpha(x_N) - b) = 0$ [Find α]

3. Bisection / Newton-Raphson $\Rightarrow z_\alpha = \frac{du_\alpha(x)}{d\alpha}, \; z_\alpha(x_0) = \frac{da}{d\alpha} = 0, \; z_\alpha'(x_0) = \frac{d\alpha}{d\alpha} = 1$

4. $\alpha = \frac{\alpha_1 + \alpha_2}{2}$

$z_\alpha''(x) = \frac{\partial f}{\partial u_\alpha} z_\alpha(x) + \frac{\partial f}{\partial u_\alpha'} z_\alpha'(x)$ (IVP) (RK4)

$$\alpha_{j+1} = \alpha_j - \frac{u_{\alpha_j}(x_N - b)}{z_{\alpha_j}(x_N)} \Rightarrow y(x) = u_{\alpha_{j+1}}(x)$$

Bisection $\Rightarrow$ Step 1 + step 2 + step 4.

NR $\Rightarrow$ Step 1 + (Step 2 + step 3) + step 4.

Linear Shooting $f(y(x), y'(x), x) \to$ linear $\Rightarrow$ 1. $y''(x) + P(x)y'(x) + Q(x)y(x) = R(x)$ (inhomogeneous)

with $y(x_0) = a, \; y(x_N) = b.$ (BVP)

2. (a) $u''(x) + P(x)u'(x) + Q(x)u(x) = R(x), \quad u(x_0) = a, \; u'(x_0) = 0$ (IVP) (RK4)

(b) $v''(x) + P(x)v'(x) + Q(x)v(x) = 0 \qquad v(x_0) = 0, \; v'(x_0) = s, \; (s \neq 0)$

3. $$y(x) = u(x) + \frac{b - u(x_N)}{v(x_N)} v(x), \; (v(x_N) \neq 0)$$

[homogeneous $(R(x) = 0) \to$ Step 1 + 2(b) + 3 $= y(x) = \frac{b}{v(x_N)} v(x)$ as $u(x) = 0$]

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Schrödinger Equation Shooting from left

(BVP)

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x) \begin{cases} \lim\limits_{x\to\pm\infty} V(x)\to\infty, \ \psi(x)\to 0 \\ \& \lim\limits_{x\to\pm a} V(x)>>, \ \psi(x)\to 0 \end{cases}$$

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x), \quad \psi(-a)=0, \quad \psi'(-a)=S. \quad \text{(IVP)}$$

$$\psi_{j+1} = 2\left[\frac{m(\Delta x)^2}{\hbar^2}(V_j - E) + 1\right]\psi_j - \psi_{j-1}, \quad \psi_0 = 0, \ \psi_1 = S$$

Normalization $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = A$ so that $\psi_{N-1} = 0$. (right BC)

solve for given E. But how to know E?

1. Bisection $\to E = \frac{E_{min} + E_{max}}{2}$ (Estimate E_{min} & E_{max})
2. shooting from left $\psi_{j+1}^{(E)} = 2\left[\frac{m(\Delta x)^2}{\hbar^2}(V_j - E)+1\right]\psi_j^{(E)} - \psi_{j-1}^{(E)}, \quad \psi_0^{(E)} = 0, \psi_1^{(E)} = S.$
3. node counting $n' = n$ & goto ① till $|E_{max} - E_{min}| \leq \epsilon$

Multiple shooting

Left shoot

$$\vec{\psi}_{j+1}^{(E)} = 2\left[\frac{m(\Delta x)^2}{\hbar^2}(V_j - E) + 1\right]\vec{\psi}_j^{(E)} - \vec{\psi}_{j-1}^{(E)}$$

$$\vec{\psi}_0^{(E)} = 0, \quad \vec{\psi}_1^{(E)} = S$$

Right shoot

$$\overleftarrow{\psi}_{j-1}^{(E)} = 2\left[\frac{m(\Delta x)^2}{\hbar^2}(V_j - E) + 1\right]\overleftarrow{\psi}_j^{(E)} - \overleftarrow{\psi}_{j+1}^{(E)}$$

$$\overleftarrow{\psi}_{N-1}^{(E)} = 0, \quad \overleftarrow{\psi}_{N-2}^{(E)} = S'$$

continuity $\Rightarrow \vec{\psi}^{(E)} = \overleftarrow{\psi}^{(E)}$, Differentiability $g(E) = \psi_{m+1}^{(E)} + \psi_{m-1}^{(E)} - 2\psi_m^{(E)} = 0$

Numerov's Integrator

$$-\frac{\hbar^2}{2m}\frac{Y_{j+1}^{(E)} - 2Y_j^{(E)} + Y_{j-1}^{(E)}}{(\Delta x)^2} + (V_j - E)\psi_j^{(E)} = 0, \quad \text{with}$$

$$Y_j^{(E)} = \left[1 - \frac{m}{6\hbar^2}(\Delta x)^2(V_j - E)\right]\psi_j^{(E)}.$$

Cooley's Energy Correction

$$E^{(K+1)} = E^{(K)} + \frac{\psi_m^{(E_0)*}}{\sum_{j=0}^{N-1}|\psi_j^{(E_0)}|^2}\left[-\frac{\hbar^2}{2m}\frac{Y_{m+1}^{(E_0)} - 2Y_m^{(E_0)} + Y_{m-1}^{(E_0)}}{(\Delta x)^2} + (V_m - E_0)\psi_m^{(E_0)}\right]$$

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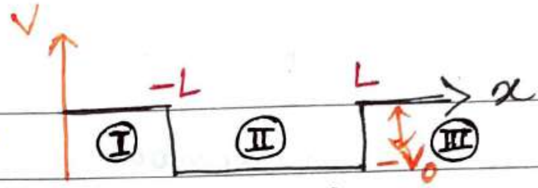

Finite Potential Well

$x < -L,\ V(x) = 0$

Region ① : TISE $\quad -\frac{\hbar^2}{2m}\psi''(x) = E\psi(x) \Rightarrow \psi''(x) = k^2\psi(x) \quad k = \frac{\sqrt{-2mE}}{\hbar}$

$\psi(x) = Ae^{-kx} + Be^{kx} = Be^{kx}$ as $x \to -\infty,\ A = 0.$

Region ② $\quad -L < x < L,\ V(x) = -V_0$

TISE $\quad -\frac{\hbar^2}{2m}\psi''(x) - V_0\psi(x) = E\psi(x) \Rightarrow \psi''(x) = -q^2\psi(x),\ q = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

$\psi(x) = C'e^{-iqx} + D'e^{iqx} = C\sin(qx) + D\cos(qx)$

Region ③ $\quad x > L,\ V(x) = 0,\ \psi(x) = Fe^{-kx}$

(Even parity) $\quad \psi^+(x) = Be^{kx},\ \underbrace{D\cos(qx),\ Be^{-kx}}_{(x=L)}$

(Odd parity) $\quad \psi^-(x) = -Be^{kx},\ C\sin(qx),\ Be^{-kx}$

$\frac{\psi'(x)}{\psi(x)} = \frac{d}{dx}\ln\psi(x) =$ continuous; $\quad \left.\frac{\psi^{+}(x)'}{\psi^+(x)}\right|_{x=L} \Rightarrow \frac{-Dq\sin(qL)}{D\cos(qL)} = \frac{-Bke^{-kL}}{Be^{-kL}}$

$\left.\frac{\psi^-(x)'}{\psi^-(x)}\right|_{x=L} = \frac{Cq\cos(qL)}{C\sin(qL)} = \frac{-Bke^{-kL}}{Be^{-kL}}$

$$\boxed{\begin{aligned} \therefore\ & q\tan(qL) = k \\ \therefore\ & q\cot(qL) = -k \end{aligned}}$$

Transcendental solution

Nondimensional variable: $\quad z = qL = \frac{\sqrt{2m(E+V_0)}}{\hbar},\ z_0 = \frac{L\sqrt{2mV_0}}{\hbar}$

$k^2 + q^2 = \frac{-2mE}{\hbar^2} + \frac{2mE + V_0}{\hbar^2} = \frac{2mV_0}{\hbar^2} = \frac{z_0^2}{L^2}.$

$\therefore k^2L^2 + q^2L^2 = z_0^2$ or $k^2L^2 + z^2 = z_0^2$ or $\frac{k^2L^2}{q^2L^2} = \frac{z_0^2 - z^2}{z^2} = \frac{z_0^2}{z^2} - 1$

$\therefore \frac{k}{q} = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}. \quad \therefore q\tan(qL) = k \Rightarrow$

$$\boxed{\begin{aligned} \tan z &= \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \\ \cot z &= -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \end{aligned}}$$

$\cancel{z = \frac{\sqrt{2mE}}{\hbar} + \frac{z_0}{L}}$

$\therefore \cancel{E = \frac{\hbar^2}{2m}\left[z - \frac{z_0}{L}\right]^2}$

$\frac{z^2\hbar^2}{2m} = E + V_0$

$E = \frac{z^2\hbar^2}{2m} - V_0$

Hydrogen atom

$-\frac{\hbar^2}{2\mu}\frac{d^2U(r)}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{r}\right]U(r) = EU(r)$

or $\quad \frac{d^2U(r)}{dr^2} + \left[\frac{2E\mu}{\hbar^2} + \frac{2\mu e^2}{r\hbar^2} - \frac{l(l+1)}{r^2}\right]U(r) = 0 \qquad$ a.u. $e = 1 = \hbar = 1$, $\mu = 1$

$\therefore \frac{d^2U(r)}{dr^2} = -\left[2E + \frac{2}{r} - \frac{l(l+1)}{r^2}\right]U(r)$

So $V(r) = +\frac{dU(r)}{dr},\quad \frac{dV(r)}{dr} = -\left[2E + \frac{2}{r} - \frac{l(l+1)}{r^2}\right]U(r)$

$\hbar = \mu = 1 = e = 1$

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Isotropic anharmonic oscillator $V(r) = \frac{1}{2}Kr^2 + \frac{1}{3}br^3$.

TISE $-\frac{\hbar^2}{2\mu}\frac{d^2U(r)}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} + \frac{1}{2}Kr^2 + \frac{1}{3}br^3\right]U(r) = EU(r)$

or. $\frac{d^2U(r)}{dr^2} + \left[2E - \frac{l(l+1)}{r^2} - Kr^2 - \frac{2}{3}br^3\right]U(r)$

$\therefore V(r) = +\frac{dU}{dr}$, $\frac{dV(r)}{dr} = \left(\frac{l(l+1)}{r^2} + Kr^2 + \frac{2}{3}br^3 - 2E\right)U(r)$

Yukawa $V(r) = -\frac{e^2}{r}e^{-r/a} = -\frac{e^{-r/a}}{r}$, $e = 1$.

$V(r) = \frac{dU}{dr}$, $\frac{dV(r)}{dr} = \left[\frac{l(l+1)}{r^2} - \frac{2}{r}e^{-r/a} - 2E\right]U(r)$

Isotropic Morse $V(r) = D\left(e^{-2\alpha r'} - e^{-\alpha r'}\right)$, $r' = \frac{r - r_0}{r_0}$

$V(r) = \frac{dU}{dr}$, $\frac{dV(r)}{dr} = \left[\frac{l(l+1)}{r^2} + 2D\left(e^{-2\alpha r'} - e^{-\alpha r'}\right) - 2E\right]U(r)$