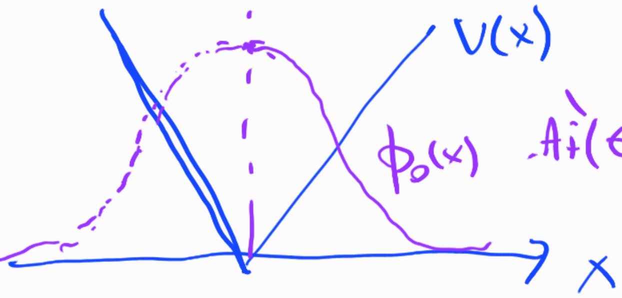
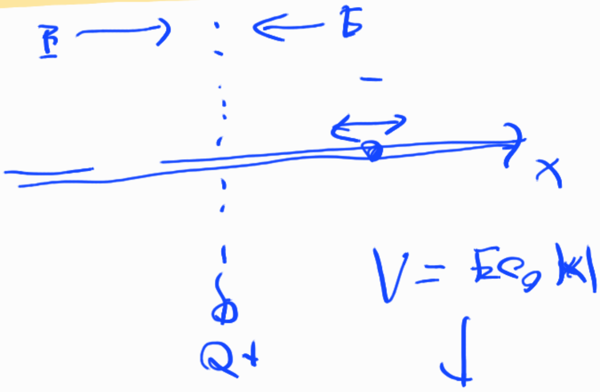
QM II – cv3 | Variační metoda a WKB



$Ai(\epsilon_0) = 0$

$Ai(\epsilon_1) = 0$



$V = E e_0 |x|$

$\downarrow$

$V = |q|$

PŘESNÉ

- $\psi_0(q) \simeq e^{-\alpha q^2}$

$$E[\psi] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = f(\alpha)$$

- první excit. stav: zákl. stav $\mathcal{H} = \mathcal{H}_S \oplus \mathcal{H}_L$

$$\psi_1(q) = q\, e^{-\alpha q^2}$$

$$E[\psi_1] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{2}{\sqrt{2\pi}}\frac{1}{\sqrt{\alpha}} + 3\alpha$$

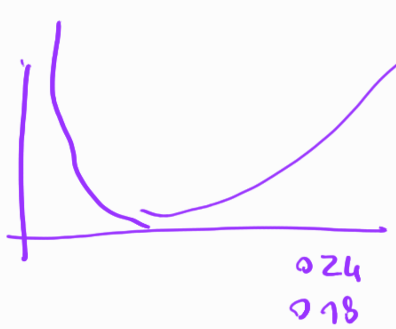
min $E'(\alpha) = 3 - \frac{1}{\sqrt{2\pi}}\alpha^{-\frac{3}{2}} = 0$

$$\alpha_0 = \left(3\sqrt{2\pi}\right)^{-2/3}$$

$E_1 \approx E[\alpha_0] = 2.3448$ ... Přesné: 2.338

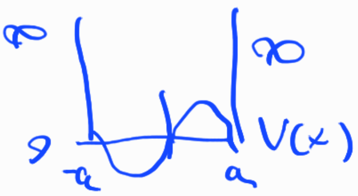
ΔE 0.006

- základní stav $\psi_\alpha(x) = \frac{1}{x^2+\alpha^2}$



$E[\alpha] = \frac{1}{2}\frac{1}{\alpha^2} + \frac{2}{\pi}\alpha$ ... $\alpha = \sqrt[3]{\frac{\pi}{2}}$ ... $E_0 = 1.11006$

ÚLOHA 2 Částice v kruhové potenciálové jámě



$a = 1$ $\quad \epsilon = \frac{\hbar^2}{2m}\frac{1}{a^2}$

$\hat{H} = -\Delta$ ...

... vlnové fce ≈ 0 mě jámy

ψ ... L^2(disku poloměru 1) } třída fcí
$\psi(r=1) = 0$

$\langle\psi|H|\psi\rangle$

① $\psi(x,y) = \sin\left(\frac{r}{\pi}\right)$

② $\psi(x,y) = \cos\left(\frac{2r}{\pi}\right) \to E[\psi]$

$= \int \psi^* \Delta\psi \, d^2r$

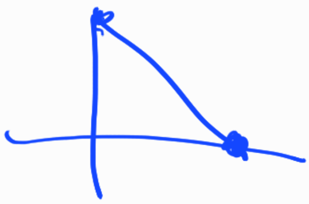
$= \int \nabla\psi \cdot \nabla\psi \, dr$

$f(r) \quad \nabla f = f'(r)\vec{e}_r$

$r\,d\varphi\,dr$

$[f'(r)]^2 \cdot r$

$\sin^2 \cdot r\,dr$
$\cos^2 \cdot r\,dr$

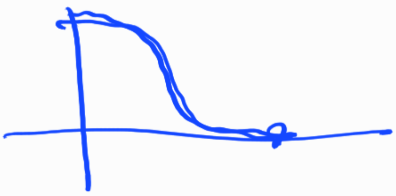


$m = 0$

③ $\psi(x,y) = (1-r)$

$e^{im\varphi} = 1$

$(1-r)^2$



= polynom v $(1-r)$

Excit. stavy: $\psi = a\phi_1 + b\phi_2$ $\begin{vmatrix} \langle\phi_1|H|\phi_1\rangle & \langle\phi_1|H|\phi_2\rangle \\ \langle\phi_2|H|\phi_1\rangle & \langle\phi_2|H|\phi_2\rangle \end{vmatrix}$

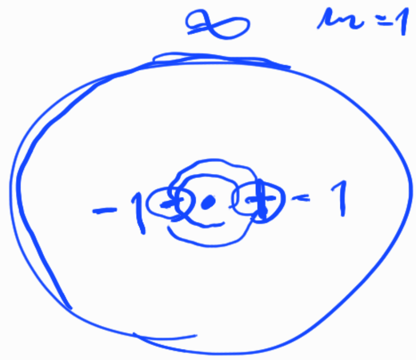
Hylleraas–Undheim vl. č. E_0, E_1 ← aprox. zákl. a 1. ex. stav

• symetrie: rotační symetrie
$\hat{L} = i\hbar\partial_\varphi \quad [\hat{H}, \hat{L}] = 0 \quad \ldots e^{im\varphi}$

$\{\hat{H}, \hat{L}\}$ -- $\psi(r,\varphi) = f(r)e^{im\varphi}$

různé hodnoty $m \to \mathcal{H} = \mathcal{H}_{m=0} \oplus \mathcal{H}_{m=1} \oplus \mathcal{H}_{m=2} \oplus$

$E^{|m|}_{n=0,1,2,\ldots}$



Exit. stav $m = \pm 1$ -- $E^{|m|}_{n=0}$

$\psi(r,\varphi) = f(r)\, e^{im\varphi}$

- $f(r)|_{r=1} = 0$ -- $f(0) = 0$

$f(r) = r(1-r)$ -- $p\{r(1-r)\}$

Přesné řešení: $-\Delta\psi(x,y) = E\psi(x,y)$ v obl. Ω

$\psi(r=1) = 0$

$\hookrightarrow \psi(r,\varphi) = f(r)e^{im\varphi}$ $m \in \mathbb{Z}$

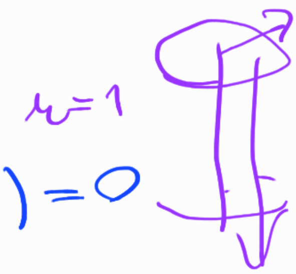
Laplace v polárních souř.:

$$\frac{\partial^2}{\partial r^2}\psi + \frac{1}{r}\frac{\partial}{\partial r}\psi + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\psi + E\psi = 0 \qquad \left(\frac{\partial^2}{\partial\varphi^2} \to -m^2\right)$$

$\psi(x) = f(kr)e^{im\varphi}$ -- $E = k^2$ $z = kr$

$$f''(z) + \frac{1}{z}f'(z) + \left[1 - \frac{m^2}{z^2}\right]f = 0$$

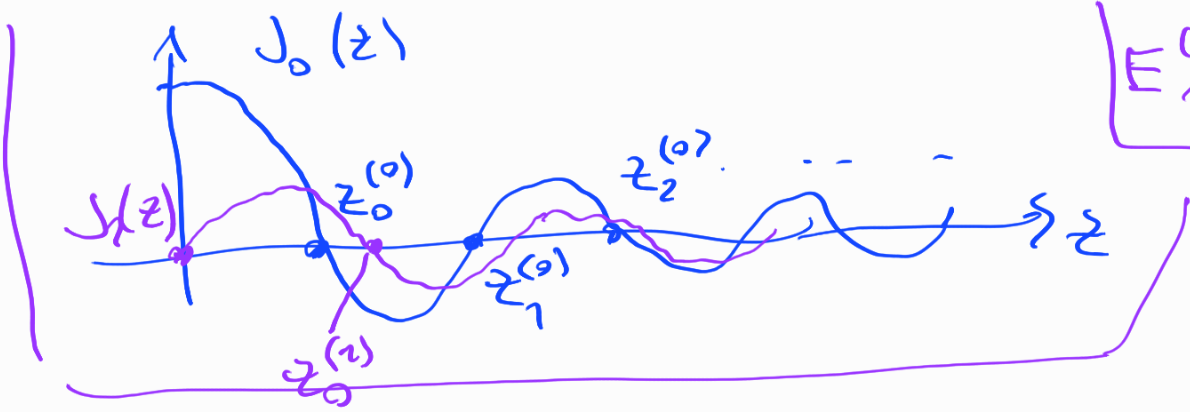
Besselova rovnice $J_m(z)$



$\Rightarrow \psi(x,y) = J_m(kr)e^{im\varphi}$ $J_m(kr) = 0$

kořeny Bessel. fcí $J_m(z^{(m)}_n) = 0$

$n = \ldots$ $r = 1 \Rightarrow k = \frac{1}{z^{(m)}_n}$



$$E_n^{(m)} = k^2 = \frac{1}{\left(z_n^{(m)}\right)^2}$$

1) Odvození (WKB) asymptot Airyho funkcí

↑ Duhy

Def: $Ai''(x) = x\,Ai(x)$

$$\rightarrow \quad Ai = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{t^3}{3} + xt\right)dt = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\left(\frac{t^3}{3} + xt\right)}dt$$

$$e^{if(t)}$$

$$\rightarrow \quad f'(t) = 0 = t^2 + x$$

Metoda stacionární fáze

$$\rightarrow \quad t_0 = \sqrt{-x}$$

$$f''(t) = 2t_0$$

$$f(t) \simeq t_0\Big(x + \frac{1}{3}\underbrace{(-x)}_{t_0^2}\Big] + t_0\,(t-t_0)^2 = \frac{2}{3}x t_0 + t_0(t-t_0)^2$$

Taylor — 0. ř., 1. ř. = 0, 2. ř.

1) $x > 0 \quad t_0 = \pm i\sqrt{|x|}$. $\quad (+) \; (-)$

$$Ai(x) \simeq \frac{1}{2\pi} e^{i i\sqrt{x}\,\frac{2}{3}x}\int_{-\infty}^{\infty} e^{(-\sqrt{x})(t - i\sqrt{x})^2}dt = \frac{1}{2\sqrt{\pi\sqrt{x}}}e^{-\frac{2}{3}x^{3/2}}$$

Gauss

$$\boxed{Ai(x) \underset{x>0}{\simeq} \frac{1}{2\sqrt{\pi\sqrt{x}}}e^{-\frac{2}{3}x^{3/2}}} \qquad x \to \infty$$

(2) $x < 0$ .. $f_0 = \sqrt{x}$

$$Ai(x) = \frac{1}{\sqrt{i\pi\sqrt{x}}} e^{\frac{2i}{3} x^{3/2}} + \; - \; -$$

$\cos\left(\frac{2}{3}x^{3/2} + \frac{\pi}{4}\right)$