

$$E = \frac{1}{2} L \dot{r}^2(t) + \frac{1}{2} C v^2(t)$$

$$\hat{E} \Psi(v, t) = \frac{1}{2} L \hat{p}^2 \Psi(v, t) + \frac{1}{2} C v^2 \Psi(v, t)$$

WKB unlikely on final

$$i \hbar \frac{\partial}{\partial t} \Psi(v, t) = - \frac{\hbar \omega_0^2}{2C^2} \frac{\partial^2}{\partial v^2} \Psi(v, t) + \frac{1}{2} C v^2 \Psi(v, t)$$

How to make quantum world

- guess \hat{H}
- work with analog problem to get form of \hat{H}
- work from classical Lagrangian (see notes)

⇒ can verify using Ehrenfest.

Janis: We're moving into 8.06.

Q: How do we know that it works?

New systems - predictive capabilities.

WKB - Jeffries, Wentzel, Kramers, Br.M (...?)

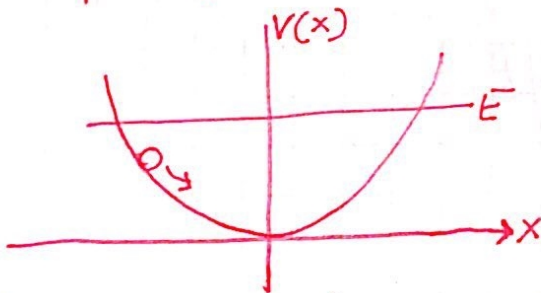
Think about the classical problem:

$$E = \frac{p^2(x)}{2m} + V(x(t))$$

$$\frac{d}{dt} x(t) = \frac{p(t)}{m} \quad \frac{d}{dt} p(t) = - \frac{d}{dx} V(x(t))$$

$$\Rightarrow p = \pm \sqrt{2m(E - V(x))} \rightarrow \hbar k(x)$$

$\Psi \sim e^{ik(x)x}$ ← doesn't work very well.
 $\sim e^{i \int^x k(x') dx'}$ flux conserving



WKB transformation

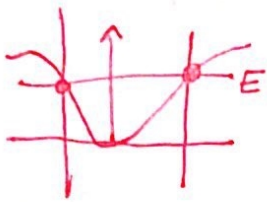
$$E = \hbar^2 \gamma^2 - \hbar^{1/2} \gamma \frac{d^2}{dy^2} \hbar^{1/2} \gamma + V(y)$$

⇒ non-linear differential eq'n.

1) Normalized version of the problem

$$E \Psi(y) = - \frac{d^2}{dy^2} \Psi(y) + V(y) \Psi(y)$$

$$\Psi(y) = \begin{cases} \frac{\sin \phi(y)}{\sqrt{\gamma(y)}} & \gamma(y) = \frac{d}{dy} \phi(y) & \phi(y) = \int^y \gamma(y') dy \\ \frac{\cos \phi(y)}{\sqrt{\gamma(y)}} & e^{\pm i \phi(y)} & \end{cases}$$



The new nonlinear eq'n is actually really hard to solve

However, you can get an approximate sol'n:

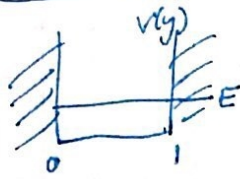
$$E \approx y^2(y) + V(y) \quad \eta(y) \approx \pm \sqrt{E - V(y)}$$

Near turning pts, WKB approximation not as accurate

$$\Psi(y) = \frac{\sin \phi(y)}{\eta^{1/2}} = \frac{\sin\left(\int \sqrt{E - V(y)} dy\right)}{[E - V(y)]^{1/4}}$$

Areas used: establishing boundary conditions for scattering. Normalization of WKB sol'n

2) Application: establishing E



$$E \Psi(y) = -\frac{d^2}{dy^2} \Psi(y) + V(y) \Psi(y)$$

$$\Psi(y) = \sin(ky) \Rightarrow k = n\pi$$

$$E = n^2 \pi^2$$

$$\Psi(y) = \frac{\sin \phi}{\sqrt{\eta}} \quad \eta = \frac{d\phi}{dy}$$

proposal make $0 = y_{\min}$, $l = y_{\max} \Rightarrow \int_{y_{\min}}^{y_{\max}} \eta(y) dy = \phi(y_{\max}) - \phi(y_{\min}) = n\pi$

JWKB

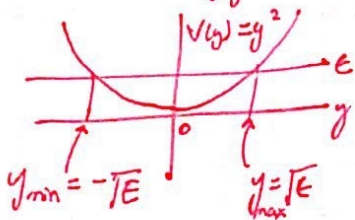
$$\eta = \sqrt{E - V(y)} \rightarrow \sqrt{E}$$

$$\int_0^l \sqrt{E} dE = n\pi \quad \sqrt{E} = n\pi \Rightarrow E_n = n^2 \pi^2$$

numbering for square well

3) Try the Simple Harmonic Oscillator

$$E \Psi = -\frac{d^2}{dy^2} \Psi + y^2 \Psi$$



$$\int_{y_{\min}}^{y_{\max}} \eta(y) dy = \int_{-\sqrt{E}}^{\sqrt{E}} \sqrt{E - y^2} dy = \frac{\pi}{2} E$$

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

For SHO, ground state at $n=0$

SHO numbering

$$E_n = 2n+2 \text{ JWKB}$$

$$E_n = 2n+1 \text{ exact}$$

Reverse phase Constraint

$$\int_{y_{min}}^{y_{max}} \psi(y) dy = (n+1)\pi - \frac{\pi}{4} - \frac{\pi}{4}$$

SHO

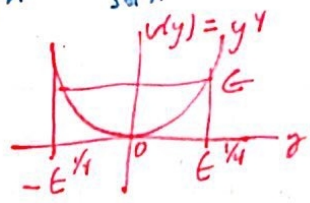
if left boundary in sol'n
if right boundary in sol'n

$$\int_{-\sqrt{E}}^{\sqrt{E}} \sqrt{E - y^2} dy = \frac{\pi}{2} E = (n+1)\pi - \frac{\pi}{2}$$

$$E_n = 2n+1$$

$$E\psi = -\frac{d^2}{dy^2} \psi + y^2 \psi$$

$$JWKB: \psi(y) = \sqrt{E - y^2}$$



$$\int_{-E^{1/4}}^{E^{1/4}} \sqrt{E - y^4} dy = (n + \frac{1}{2})\pi = \frac{2E^{3/4} \Gamma(\frac{5}{2}) \Gamma(\frac{3}{2})}{\Gamma(\frac{7}{4})}$$

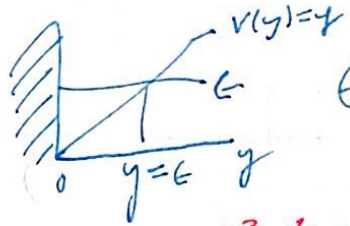
$$E_n = \left[\frac{\pi(n + \frac{1}{2}) \Gamma(\frac{7}{4})}{2 \Gamma(\frac{5}{4}) \Gamma(\frac{3}{2})} \right]^{4/3}$$

approximations

n	exact	JWKB
0	1.0604	0.8671
1	3.7517	3.7511
2	7.4557	7.4140
3	11.645	11.612
4	16.262	16.234

gets better as n gets larger

In his research, two-level system something high-order → he was able to use JWKB to get an exact answer.



$$E_n = \left[\frac{3}{2} (n + \frac{3}{4}) \pi \right]^{2/3}$$

n	exact	WKB
0	2.3381	2.3203
1	4.0879	4.0818
2	5.5206	5.5172
3	6.7867	6.7845

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

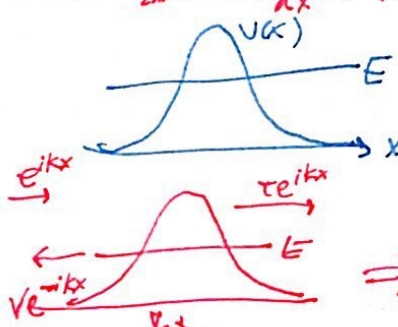
$$k(x) = \pm \sqrt{\frac{2m(E - V(x))}{\hbar^2}}$$

$$\psi(x) = \frac{\sin(kx)}{\sqrt{k(x)}}$$

$$E = -\frac{\hbar^2}{2m} k^2 V_0(x) \frac{d^2}{dx^2} k(x) + V(x) + \frac{\hbar^2}{2m} k^2(x)$$

$$\int_{x_{min}}^{x_{max}} k(x) dx = (n+1)\pi - \frac{\pi}{4} - \frac{\pi}{4}$$

SHO numbering
left boundary
right boundary



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

$$\psi(x) = \frac{e^{\pm \alpha(x)}}{\sqrt{\alpha(x)}, \frac{\sinh \theta(x)}{\sqrt{\alpha(x)}, \frac{\cosh \theta(x)}{\sqrt{\alpha(x)}}$$

$$E = -\frac{\hbar^2}{2m} \alpha^{1/2} \frac{d^2 \alpha^{-1/2}}{dx^2} + V(x)$$

$$\approx -\frac{\hbar^2}{2m} \alpha^2$$

$$\Rightarrow T = |t|^2 \sim e^{-2G}$$

$$G = \int_{x_{min}}^{x_{max}} \alpha(x) dx$$

→ JWKB approx.

$$\alpha(x) = \pm \sqrt{\frac{2m(V(x) - E)}{\hbar^2}}$$

$V(x) = V_0 - eEx$ $0 < x < \frac{V_0}{eE}$ tunneling through triangle barrier ⇒ MOSFET & ... capacitor? ☆

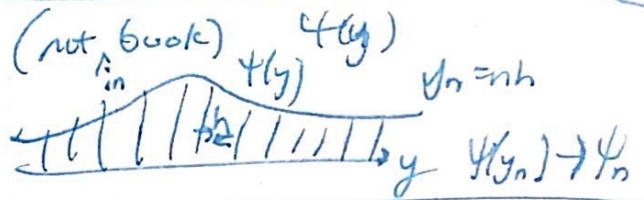
$$G = \int_0^{\frac{V_0}{eE}} \sqrt{\frac{2m(V_0 - eEx - E)}{\hbar^2}} dx$$

$$= \frac{2}{3} \sqrt{\frac{2m(V_0 - E)^3}{eE \hbar}}$$

WKB helps figure out how much exponential decay
 $T = e^{-2G}$

see other page for more notes

Numerical - Finite difference method



$$\epsilon \psi(y) = -\frac{d^2}{dy^2} \psi(y) + V(y)\psi(y)$$

$$\epsilon \psi(y_n) = -\left(\frac{d^2\psi}{dy^2}\right)_n + V(y_n)\psi(y_n)$$

$$\epsilon \psi_n = -\left(\frac{d^2\psi}{dy^2}\right)_n + V_n \psi_n$$

$$\epsilon \psi_n = \frac{-\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2} + V_n \psi_n + O(h^2)$$

$$\frac{h^2}{12} \left(\frac{d^4\psi}{dy^4}\right)_n$$

$$\psi(y_{n+1}) = \psi(y_n) + h\left(\frac{d\psi}{dy}\right)_n + \frac{h^2}{2}\left(\frac{d^2\psi}{dy^2}\right)_n + \dots$$

$$\psi(y_{n-1}) = \psi(y_n) - h\left(\frac{d\psi}{dy}\right)_n + \frac{h^2}{2}\left(\frac{d^2\psi}{dy^2}\right)_n + \dots$$

$$\psi(y_{n+1}) + \psi(y_{n-1}) = 2\psi(y_n) + \frac{2h^2}{2}\left(\frac{d^2\psi}{dy^2}\right)_n + \frac{2h^4}{4!}\left(\frac{d^4\psi}{dy^4}\right)_n + \dots$$

$$\left(\frac{d^2\psi}{dy^2}\right)_n = \frac{\psi(y_{n+1}) - 2\psi(y_n) + \psi(y_{n-1}))}{h^2} - \frac{h^2}{12}\left(\frac{d^4\psi}{dy^4}\right)_n + \dots$$

$$\left(\frac{d^2\psi}{dy^2}\right)_n \approx \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2}$$

$$\left(\frac{d^4\psi}{dy^4}\right)_n = \left(\frac{d}{dy^2}\left(\frac{d^2\psi}{dy^2}\right)\right)_n \approx \frac{\left(\frac{d^2\psi}{dy^2}\right)_{n+1} - 2\left(\frac{d^2\psi}{dy^2}\right)_n + \left(\frac{d^2\psi}{dy^2}\right)_{n-1}}{h^2}$$

$$\epsilon \psi_{n+1} + 10\psi_n + \psi_{n-1} = \frac{-\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2} + \frac{1}{12}(V_{n+1}\psi_{n+1} + 10V_n\psi_n + V_{n-1}\psi_{n-1})$$

Numerical Scheme

