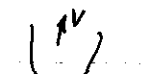
Physical Systems - last class! Spring 2007
29 May E/Z

Ch 16 - VARIATIONAL METHOD - WORKS BEST FOR low n.
WKB - BEST for high n.

GOAL - Try to find approximate ψ and E for tricky $V(r)$

gaussian for 

METHOD - Draw $V(r)$
- Guess form for $\psi(r) = f(\alpha)$ where α = unknown parameter
- Calculate $E(\alpha) = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$

where $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(r)$ as usual

- Minimize $E(\alpha)$: Solve $\frac{\partial E}{\partial \alpha} = 0$ for α_0

- Sub in: $E_0 = E(\alpha_0)$ is an UPPER BOUND on ground state

- $\psi(\alpha_0)$ may or may not be of the same form as the true $\psi(r)$

Ex (p. 440) For $V(x) = \lambda x^4$ (λ = some constant - not wavelength!)
Guess $\psi = e^{-\alpha x^2/2}$

$E(\alpha) = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \dfrac{\hbar^2\alpha}{4m} + \dfrac{3\lambda}{4\alpha^2}$ (after doing Gaussian integrals)

$\frac{\partial E}{\partial \alpha} =$

$\alpha_0 =$

$E_0 =$

Variational Method:

Ex: $V = \frac{1}{2} m\omega^2 x^2$. Guess $\psi = e^{-\alpha x^2/2}$

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \ldots$$

$$\frac{\partial E}{\partial \alpha} =$$

$\alpha_0 = \left(\frac{m\omega}{\hbar}\right)^{1/2} \to E_0 = \hbar\omega/2$: The approximation HAPPENS to give the exact E_0

because the true $\psi(r)$ = gaussian. (lucky!)

Ex. p. 441 : $V = \frac{-e^2}{r}$ (coulomb). Guess $\psi = e^{-\alpha r^2}$

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \ldots \qquad = \frac{3\hbar^2\alpha}{2m} - \sqrt{\frac{2}{\pi}}\, 2e^2 \sqrt{\alpha}$$

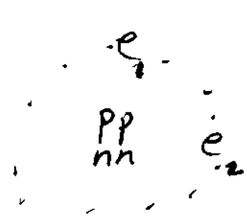
$$\frac{\partial E}{\partial \alpha} =$$

$$\alpha_0 =$$

$$E_0 =$$

Compare to true $E_0 = -\frac{me^4}{2\hbar^2}$ (eq. 13.1.19-20)

$Z = 2$



Variational Method... HELIUM Ground state (p. 442)

(16.1.11) $H = -\frac{\hbar^2}{2m}(\nabla_1^2 - \nabla_2^2) - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} - \frac{e^2}{r_{12}}$

electron 1 electron 2 mutual repulsion between electrons - neglect

(16.1.14) Guess $\psi = cZ^{3/2} e^{-Z(r_1+r_2)/a_0}$ Let Z = unknown parameter.

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \ldots = c'\left[4Z - Z^2 - \frac{5}{8}Z\right]$$

$$\frac{\partial E}{\partial Z} =$$

$$Z_0 =$$

$$E(Z_0) =$$

Moral: "even a poor approximation to ψ can give a good approximation to E_0".

16.2 APPROX METHOD #2: WKB METHOD

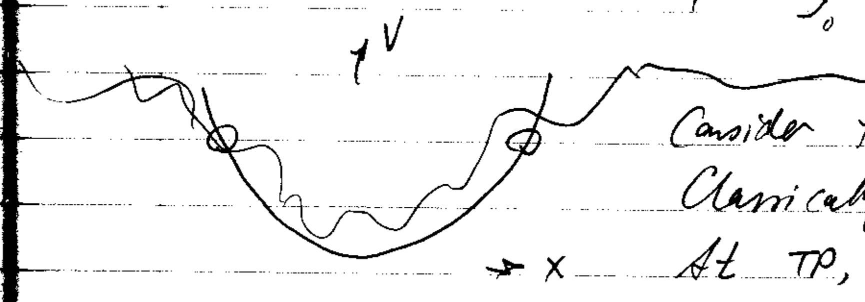
Wentzel-Kramers-Brillouin

PLANE-WAVE APPROXIMATION IN SLOWLY-VARYING $V(x)$
(adiabatic)

Size of $V(x)$ variation << wavelength λ: $\left|\frac{d\lambda}{dx}\right| << 1$ (16.2.4)

$p = \hbar k = \frac{2\pi\hbar}{\lambda}$. $V(x)$ variation causes λ & p to vary, inducing a phase shift in V:

$\psi(x) = \psi(0) e^{\pm i\varphi/\hbar}$ where
$$\varphi = \int_0^x p(x)\,dx$$



Consider turning points.
Classically, $p = \sqrt{2m(E-V)}$
At TP, $V=0$, $p=0$
QM: $p \to 0$ means $\lambda \to \infty$

Near TP, wave spreads out - APPROX FAILS.

Away from TP, where $V(x)$ changes more slowly try the WKB method:

In constant V, $\psi(x) = \psi(0)\, e^{\pm ipx/\hbar}$ ← plane wave where $p = \sqrt{2m(E-V)}$
↑ amplitude

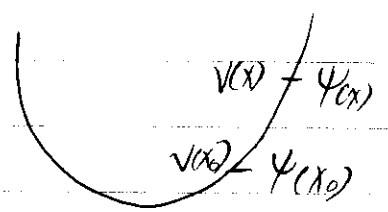
In slowly-varying V, calculate phase shift to planewave

(16.2.7) are $\varphi = \int_0^x p(x)\,dx = \varphi_0 + \hbar\varphi_1 + \ldots$ where

(16.2.9) $\varphi_0 = \pm\int p(x)\,dx$ and $\varphi_1 = i \ln\sqrt{p} + \text{const}$

Finally, WKB $\psi(x) = \psi(x_0)\sqrt{\frac{p(x_0)}{p(x)}}\, e^{\pm \frac{i}{\hbar}\int_{x_0}^{x} p(x)\,dx}$

Semiclassical argument:



Probability$(x) \sim \psi^2(x) \sim \frac{1}{v}$

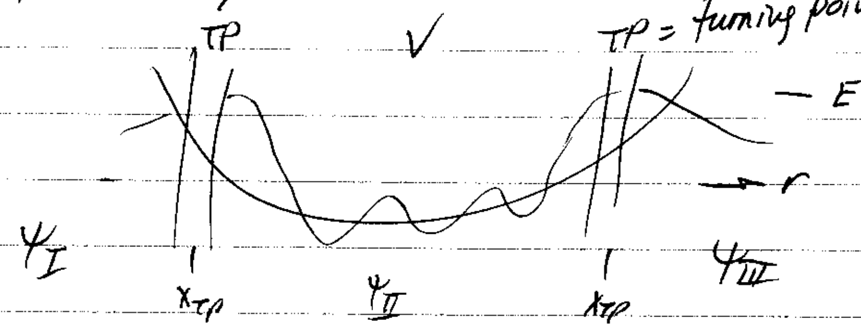
$$\frac{\psi^2(x)}{\psi^2(x_0)} = \frac{p(x_0)}{p(x)}$$

Accumulated phase shift between TP.

(16.2.33) quantization condition =

Approximating bound states : $\Sigma\varphi = \int_{x_1}^{x_2} p(x)\,dx = (n+\frac{1}{2})\pi\hbar$

TP = turning point transition region



Get ~~plane wave~~ damped exp. solutions for ψ_I & ψ_{III} (16.2.28)

Match across TP to oscillating solution in ψ_{II}

Solve for two unknown parameters (BC)

Approximate E from $x_{tp} = \frac{E}{k} y$ (scaling argument) where y is determined from quantization condition. WORKS BEST FOR HIGH n.