

Summary.  
of Connection Rules.

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I.  $x < x_r$

$$\text{p}(x) = \sqrt{2m [E - v(x)]} \geq 0$$

$$S(x, x_r) \cancel{=} = \int_{x_r}^x p(x') dx' \geq 0, \uparrow$$

$$\Psi_I(x) = \frac{1}{\sqrt{p(x)}} \left[ C_r e^{\frac{i}{\hbar} S(x, x_r) + i\pi/4} + C_d e^{-\frac{i}{\hbar} S(x, x_r) - i\pi/4} \right]$$

II.  $x > x_r$

$$p(x) = i \sqrt{2m [v(x) - E]} = i |p(x)|$$

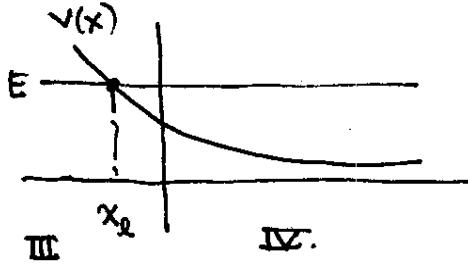
$$K(x, x_r) \cancel{=} = \int_{x_r}^x |p(x')| dx' \geq 0, \uparrow$$

$$\Psi_{II}(x) = \frac{1}{\sqrt{|p(x)|}} \left[ C_g e^{\frac{i}{\hbar} K(x, x_r)} + C_d e^{-\frac{i}{\hbar} K(x, x_r)} \right]$$

$$\begin{pmatrix} C_g \\ C_d \end{pmatrix} = \begin{pmatrix} i & -i \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} C_r \\ C_d \end{pmatrix}, \quad \begin{pmatrix} C_r \\ C_d \end{pmatrix} = \begin{pmatrix} -i/2 & 1 \\ i/2 & 1 \end{pmatrix} \begin{pmatrix} C_g \\ C_d \end{pmatrix}.$$

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$$\text{III. } \psi(x) = i\sqrt{2m[v(x)-E]} = i|\rho(x)|.$$

$$K(x, x_e) = \int_{x_e}^x |\rho(x')| dx' < 0, \uparrow$$

$$\Psi_{\text{III}}(x) = \frac{1}{\sqrt{|\rho(x)|}} (c_g e^{K(x, x_e)/\hbar} + c_d e^{-K(x, x_e)/\hbar})$$

$$\text{IV. } \rho(x) = \sqrt{2m[E - v(x)]} \geq 0.$$

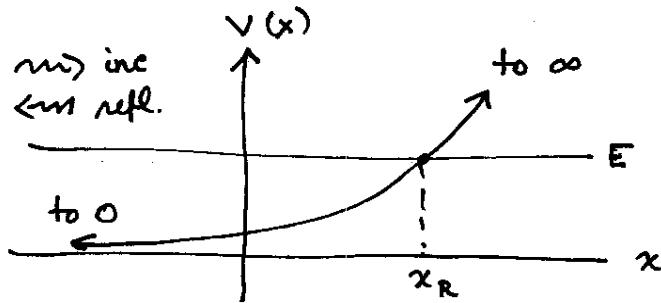
$$S(x, x_e) = \int_{x_e}^x \rho(x') dx' = \geq 0, \uparrow.$$

$$\Psi_{\text{IV}}(x) = \frac{1}{\sqrt{\rho(x)}} \left( \cancel{c_g} c_r e^{\frac{i}{\hbar} S(x, x_e) - i\pi/4} + c_d e^{-\frac{i}{\hbar} S(x, x_e) + i\pi/4} \right)$$

$$\begin{pmatrix} c_g \\ c_d \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -i & i \end{pmatrix} \begin{pmatrix} c_r \\ c_d \end{pmatrix}, \quad \begin{pmatrix} c_r \\ c_d \end{pmatrix} = \begin{pmatrix} 1 & i/2 \\ 1 & -i/2 \end{pmatrix} \begin{pmatrix} c_g \\ c_d \end{pmatrix}$$

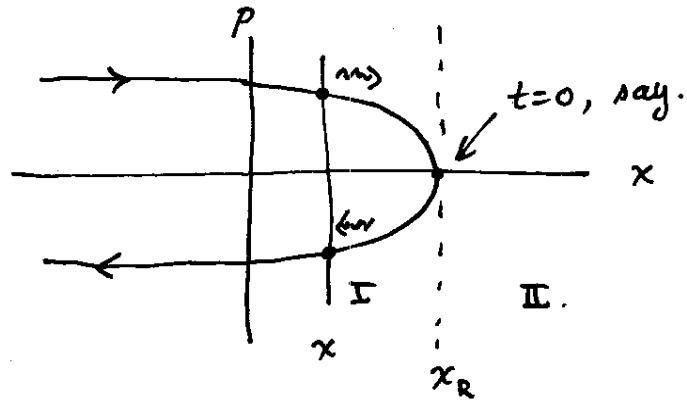
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Now do some problems. First:



A simple scattering problem. Will have incident, reflected waves, but no transmitted wave because can't get through  $\infty$  barrier.

Phase space picture:



Define flux of inc, refl. waves by

$$J = \operatorname{Re} [\psi^* \left( -i\frac{\hbar}{m} \frac{d}{dx} \psi \right)] \quad \psi = \psi_{\text{inc}} \text{ or } \psi_{\text{refl.}}$$

Then define

$$R = \text{reflection probability} = \left| \frac{J_{\text{refl}}}{J_{\text{inc}}} \right|.$$

Obvious in this case that  $R = 1$ . Now solve by WKB theory.

Boundary conditions are, no growing wave in region II, hence  $C_g = 0$ .

Take  $C_d = 1$ , arb. normalization. Then

$$\begin{pmatrix} C_g \\ C_d \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} C_r \\ C_e \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (\text{see p. 1}).$$

Thus in region I,

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$$\Psi_I(x) = \frac{1}{\sqrt{p(x)}} \left[ e^{\frac{i}{\hbar} S(x, x_r) + i\frac{\pi}{4}} + e^{-\frac{i}{\hbar} S(x, x_r) - i\frac{\pi}{4}} \right]$$

$$= \frac{2}{\sqrt{p(x)}} \cos \left[ \frac{S(x, x_r)}{\hbar} + \frac{\pi}{4} \right].$$

Wave fn is real. This is due to t-reversal invariance (more later).

Also nondegenerate. Write soln also this way:

$$\Psi_I(x) = \frac{e^{i\pi/4}}{\sqrt{p(x)}} \left[ e^{\frac{i}{\hbar} S(x, x_r)} + r e^{-\frac{i}{\hbar} S(x, x_r)} \right]$$

where  $r = e^{-i\pi/2} = -i = \text{reflection amplitude}$ .

From defin of R and T, find

$$R = |r|^2 = 1, \text{ as expected.}$$

Interpret this. Classical particles move along classical orbit, and as they do, accumulate phase

$$S(t) = \int_0^t p(t') \frac{dx(t')}{dt'} dt',$$

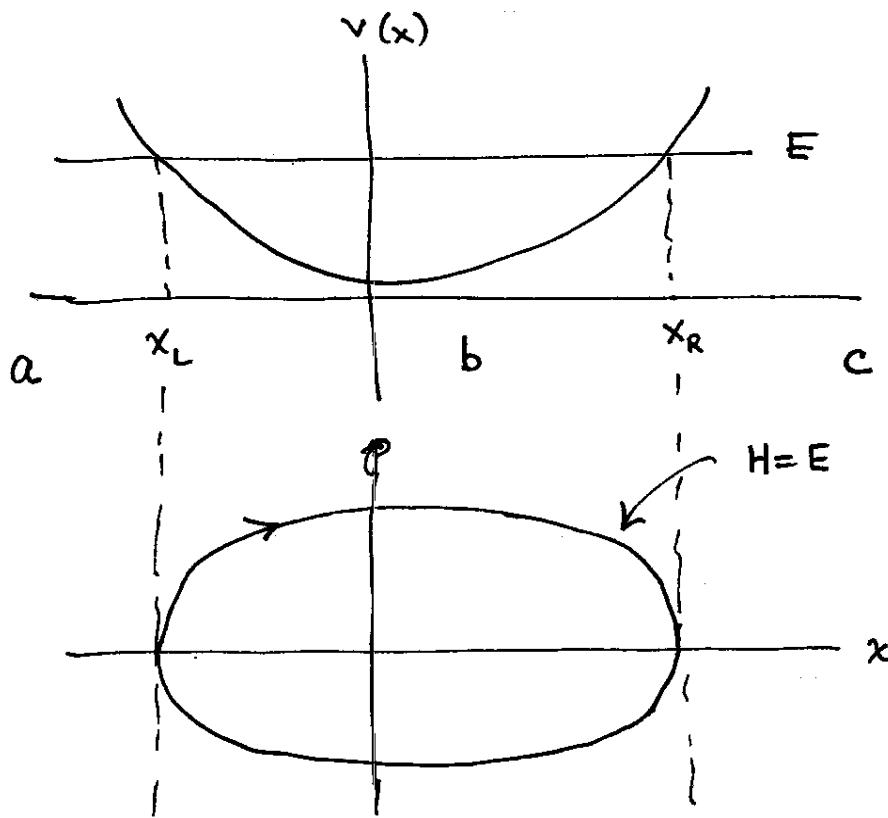
which is same as  $S(x)$  except that it's  $S$  as seen by the particle. It's a single valued function of time along the orbit, unlike  $S(x)$  ( $S$  viewed from a fixed  $x$  value) which is double valued. But two  $S$ 's are the same if  $t=0$  is the t.p.  $x_r$ . Then we think of particles carrying wave forward with themselves,

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making the phase  $S(t)/\hbar$  as they go, with  $S = \int p dx$ . 9/20/07

But extra rule applies in t.p. crossing: particle's phase suffers a  $-\pi/2$  phase shift (hence the factor  $r$ ). With this interpretation, phase of both WKB waves is accounted for.

Now do case of oscillator (not nec. H.O.).



Let regions be a, b, c ( $a, c = \text{class. forb.}, b = \text{class. allow.}$ ).

If particles accumulate phase  ~~$\int p dx$~~   $\frac{1}{\hbar} \int p dx$  as they move around orbit, but lose  $\pi/2$  at each turning point, then the total accumulated phase around the orbit is

$$\frac{1}{\hbar} \oint p dx - \pi.$$

Notice,  $\oint p dx = \text{phase space area of orbit.}$

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If you want returning wave to be in phase with original wave (to get a single-valued wave function), then must have

$$\frac{1}{\hbar} \oint p dx - \pi = 2n\pi, \quad n=0,1,2,\dots$$

This means,

$$\text{area of orbit} = \oint p dx = (n + \frac{1}{2}) 2\pi\hbar = (n + \frac{1}{2}) \hbar$$

$\hbar = 2\pi\hbar$ . This is the easy way to understand the Bohr-Sommerfeld quantization rule. The classical orbit that satisfy this condition (for integer  $n$ ) are said to be allowed or quantized. Their energies are the energy eigenvalues  $E_n$  (approximately).

Now a more rigorous derivation. Write down the <sup>WKB</sup> wave fun in regions a, b, c.

$$\Psi_a(x) = \frac{1}{\sqrt{|p(x)|}} \left[ a_g e^{K(x, x_L)/\hbar} + a_d e^{-K(x, x_L)/\hbar} \right]$$

$$\Psi_b(x) = \frac{1}{\sqrt{|p(x)|}} \left[ b_r e^{\frac{i}{\hbar} S(x, x_L) - i\frac{\pi}{4}} + b_l e^{-\frac{i}{\hbar} S(x, x_L) + i\pi/4} \right]$$

$$= \frac{1}{\sqrt{|p(x)|}} \left[ b'_r e^{\frac{i}{\hbar} S(x, x_R) + i\pi/4} + b'_l e^{-\frac{i}{\hbar} S(x, x_R) - i\pi/4} \right]$$

$$\Psi_c(x) = \frac{1}{\sqrt{|p(x)|}} \left[ c_g e^{K(x, x_R)/\hbar} + c_d e^{-K(x, x_R)} \right]$$

There are two expressions for  $\Psi_b(x)$  (hence two pairs of

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coefficients,  $(b_r, b_e)$  and  $(b'_r, b'_e)$ ), since we have represented  $\psi$  in the class. allowed region in two ways, from the two turning points (see summary or Notes 5.) But these two expressions must be equal.

To find all coefficients, work from the left. In region a, must have  $a_d = 0$  (since  $e^{-k/x}$  blows up as  $x \rightarrow -\infty$ ).

Take  $a_g = 1$ . Then from p.2,

$$\begin{pmatrix} b_r \\ b_e \end{pmatrix} = \begin{pmatrix} 1 & i/2 \\ 1 & -i/2 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

To get  $b'_r$ , set  $b_r = 1$ , equate right-going waves:

$$e^{\frac{i}{\hbar} S(x, x_L) - i\pi/4} = b'_r e^{\frac{i}{\hbar} S(x, x_R) + i\pi/4}.$$

$$\text{Now, } S(x, x_L) = \int_{x_L}^x p dx = \left( \int_{x_L}^{x_R} + \int_{x_R}^x \right) p dx = S(x_R, x_L) + S(x, x_R).$$

$$\text{But } S(x_R, x_L) = \int_{x_L}^{x_R} p dx = \frac{1}{2} \oint p dx = \frac{1}{2} \text{ area of orbit.}$$

$$\text{Write area} = \oint p dx = \Phi \hbar, \quad \text{defining dim'less number } \Phi.$$

Then:

$$\frac{1}{\hbar} S(x, x_L) = \frac{1}{2} \Phi + \frac{1}{\hbar} S(x, x_R).$$

$$\text{So... } e^{\frac{i}{\hbar} S(x, x_R) + \frac{1}{2} \Phi e^{-i\pi/4}} = b'_r e^{\frac{i}{\hbar} S(x, x_R) + i\pi/4},$$

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or,

$$b_r' = e^{\frac{i}{2}\Phi - \frac{i\pi}{2}} = -i e^{i\Phi/2}$$

$$\text{Sim. find, } b_e' = +i e^{-i\Phi/2}.$$

Then from summary, get

$$\begin{pmatrix} c_g \\ c_d \end{pmatrix} = \begin{pmatrix} i & -i \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} b_r' \\ b_e' \end{pmatrix} = \begin{pmatrix} 2 \cos \Phi/2 \\ \sin \Phi/2 \end{pmatrix}.$$

Bdry condns require,  $c_g = 0, \cos \Phi/2 = 0, \Rightarrow$ 

$$\Phi = (n + 1/2) 2\pi$$

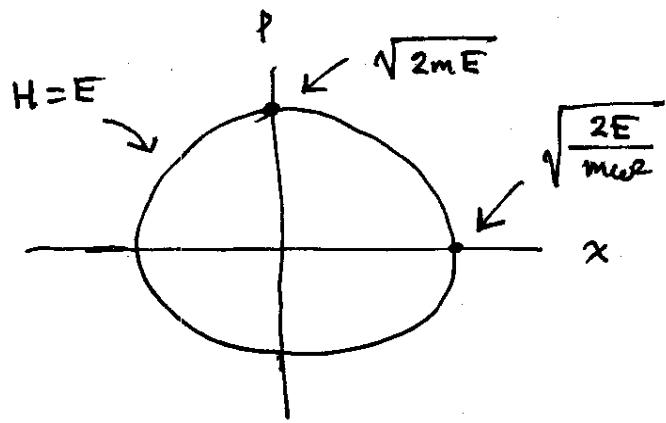
$$\Rightarrow \boxed{\text{area} = (n + 1/2) 2\pi \hbar = \oint p dx} \quad \text{Bohr-Sommerfeld rule.}$$

Also get,  $c_d = (-1)^n$ , and can now write  $\psi$  in region b,

$$\boxed{\psi = \frac{2}{\sqrt{p(x)}} \cos \left[ \frac{S(x, x_L)}{\hbar} - \frac{\pi}{4} \right]}$$

Example, H.O.  $H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$ .

Most of work in using B-S rule is classical. Plot HO orbits in phase space,

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$$\text{Area of ellipse} = \pi ab = \pi \sqrt{2mE} \sqrt{\frac{2E}{m\omega^2}} = \frac{2\pi E}{\omega} = (n + \frac{1}{2}) 2\pi \hbar,$$

hence

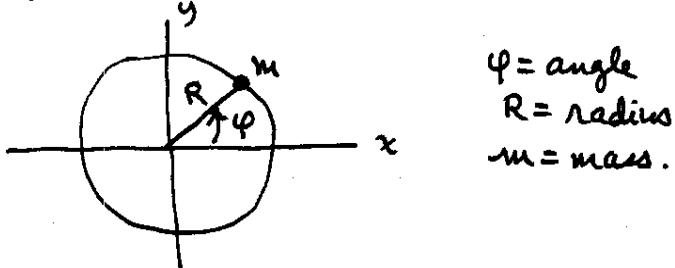
$$E_n = (n + \frac{1}{2}) \hbar \omega$$

the exact answer.

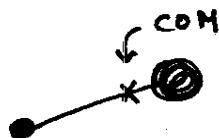
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Another example of Bohr-Sommerfeld rule: Rigid rotor. One model is free particle confined to a circle:



Another model is a rigid rotor in a plane, a model of a diatomic molecule, that rotates about its center of mass.



Classical mech. first.

$$L = \text{Lagrangian} = K.E. = \frac{1}{2} m R^2 \dot{\varphi}^2$$

$$P_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = m R^2 \dot{\varphi} = I \dot{\varphi} \quad \text{where } I = m R^2 = \text{moment of inertia.}$$

Physically  $P_\varphi$  is z-component of angular mom ( $L_z$ ) but just write  $P_\varphi$  for it to avoid confusion with  $L$  (Lagrangian).

$$H = \text{Hamiltonian} = H(\varphi, P_\varphi) = \frac{P_\varphi^2}{2I}.$$

Quantize this by DeMo's rule,  $P_\varphi \rightarrow -i\hbar \frac{d}{d\varphi}$ . Then Sch. eqn is

$$-\frac{\hbar^2}{2I} \frac{d^2 \psi}{d\varphi^2} = E \psi,$$

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where  $\psi(\varphi)$  is the wave fn.  $\psi$  must be periodic

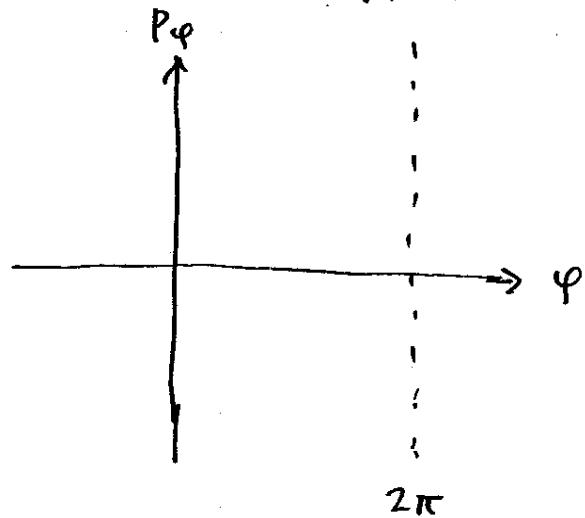
$\psi(\varphi + 2\pi) = \psi(\varphi)$ , so solns are

$$\psi_m(\varphi) = e^{im\varphi}, \quad m=0, \pm 1, \pm 2, \dots$$

$$E_m = \frac{\hbar^2 m^2}{2I}.$$

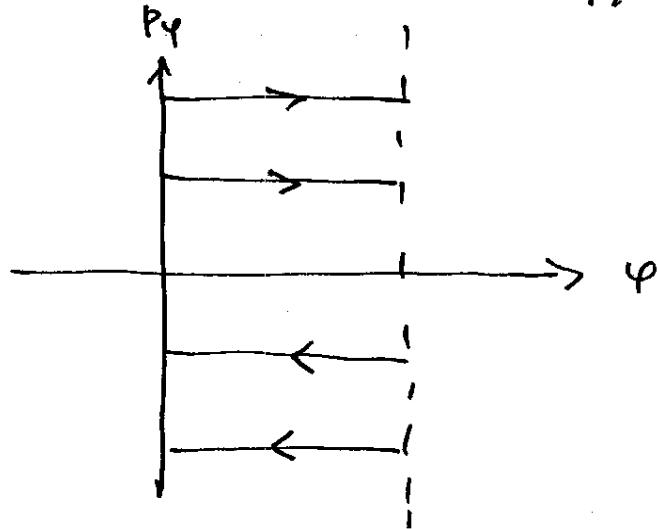
These are also eigenfns of  $P_\varphi$  with eigenvalue  $mi\hbar$ .

Now do it by Bohr-Sommerfeld. Classical phase space is strip  $0 \leq \varphi < 2\pi$  in  $\varphi - P_\varphi$  plane:



or if you glue line  $\varphi=0$  and  $\varphi=2\pi$ , you get a cylinder.

Classical orbits are  $H=E=\text{const}$  or  $P_\varphi=\text{const}$ .



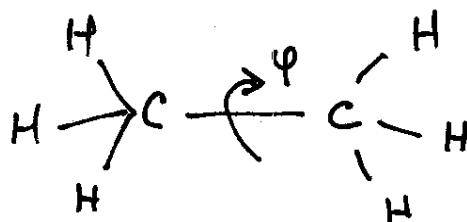
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According to B-S, the quantized orbits have area  $\oint p_\varphi d\varphi$  9/20/07  
 $= m \cdot 2\pi\hbar$ , where  $m = \text{integers}$ , not  $m + \frac{1}{2}$  because there are no turning points. The geom. meaning of  $\oint p_\varphi d\varphi$  is that it is the area betw. the orbit and the  $\varphi$ -axis. And,  $p_\varphi = \text{const}$  along the orbit, so,

$$\oint p_\varphi d\varphi = 2\pi p_\varphi = m \cdot 2\pi\hbar,$$

or  $p_\varphi = m\hbar$ ,  $E = \frac{n^2\hbar^2}{2I}$ . Again, exact answer.

Case of ethane molecule  $\text{CH}_3\text{CH}_3$  was discussed in class.



Here there is a potential  $V(\varphi)$  that has 3-fold periodicity in  $0 \leq \varphi < 2\pi$ .

