J.D. Jackson

221A Lecture Notes for Sept 25, 27, 29, 2006
(substituting for Hitoshi Murayama)

Sept 25 start

WKB Semi-classical Approximation

Often it is true that the wavelength of the matter waves is short compared with the natural scale of changes of the potential, for example. In such circumstances, the solutions to the Schrodinger equation can be approximated by a method originated by Liouville, by Lord Rayleigh in a physics context, and called the W(entzel) K(ramers) B(rillouin) approximation, or sometimes the J(effreys)WKB method. It is analogous to the first-order wave (eikonal) correction to geometric optics.

Sound waves: density of medium (and so the speed of sound) changes slowly in one wavelength

Light: index of refraction changes slowly in one wavelength

Q-M: particle has a relatively well defined local kinetic energy and so wavelength ie

$$\bar{\lambda} = \frac{\hbar}{p} = \frac{\hbar}{\sqrt{2m(E-V(\vec{x}))}}$$

The method starts by analogy with $\psi(\vec{x}) = e^{i\vec{p}_{local}\cdot\vec{x}/\hbar}$ and writes the wave function in the form,

$$\psi(\vec{x},t) = e^{\frac{i}{\hbar}\bar{S}(\vec{x},t)}$$

where $\bar{S}$ is a complex function that is the quantum analog of Hamilton's principal function (See Goldstein, 2nd ed., Chapter 10). We substitute into the time-dependent Schrodinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

and find $$-\frac{\partial\bar{S}}{\partial t} = \frac{1}{2m}\left[(\vec{\nabla}\bar{S})^2 + \frac{\hbar}{i}\nabla^2\bar{S}\right] + V$$

In the limit of $\hbar \to 0$, or, said differently, in the limit that $\hbar|\nabla^2 \bar{S}| << |\vec{\nabla}\bar{S}|^2$, we get the lowest order approximation for S, called S_0, satisfying
$$\frac{\partial \bar{S}_0}{\partial t} + \frac{(\vec{\nabla}\bar{S}_0)^2}{2m} + V = 0$$

This equation is, in fact, the Hamilton-Jacobi equation of classical mechanics and $\bar{S}_0(\vec{x},t)$ is Hamilton's principal function. With $\bar{S}_0 = S_0 - Et$, we have $E = \frac{(\vec{\nabla}S_0)^2}{2m} + V$ and we can identify $\vec{p}(\vec{x},t) = \frac{\vec{\nabla}S_0}{m}$.

Hamilton's work in 1834 showed how optics and classical mechanics were related. Schrödinger recalled Hamilton's 1834 paper in his discovery of wave mechanics.

Let us now consider $\bar{S}(\vec{x},t) = S(\vec{x}) - Et$ and so study the equation,
$$(\vec{\nabla}S)^2 - i\hbar\nabla^2 S = 2m(E - V(\vec{x})) \equiv p^2(\vec{x})$$

In the spirit of a semi-classical approximation, we write an expansion of $S(\vec{x})$ in powers of $\hbar$:
$$S(\vec{x}) = S_0(\vec{x}) + \hbar S_1(\vec{x}) + \hbar^2 S_2(\vec{x}) + \cdots$$

Substitution gives
$$-i\hbar(\nabla^2 S_0 + \hbar\nabla^2 S_1 + \cdots) + (\vec{\nabla}S_0 + \hbar\vec{\nabla}S_1 + \cdots)^2 = p^2(x)$$

Coeff of $\hbar^0$: $(\vec{\nabla}S_0)^2 - p^2(x) = 0$

Coeff of $\hbar^1$: $2(\vec{\nabla}\bar{S}_0)\cdot(\vec{\nabla}S_1) - i\nabla^2 S_0 = 0$

Coeff of $\hbar^2$: $(\vec{\nabla}S_1)^2 + 2(\vec{\nabla}S_0)\cdot\vec{\nabla}S_2 - i\nabla^2 S_1 = 0$

and so on.

These equations can be solved, in principle at least, to whatever order one wishes to retain.

WKB Solutions in One-Dimension

In practice, the 1-d solution is most useful (also simplest!).

($\hbar^0$): $\frac{d}{dx}S_0(x) = \pm p(x)$, with solution $S_0(x) = \pm\int^x p(x')dx'$

Note that $p(x) = \sqrt{2m(E-V)}$ is real in classically allowed regions and imaginary in classically forbidden regions. Thus $e^{iS_0/\hbar}$ oscillates (decays or grows) in the classically allowed (forbidden) regions.

($\hbar^1$):
$$i\frac{d^2S_0(x)}{dx^2} = 2\frac{dS_0}{dx}\frac{dS_1}{dx} *$$

$$\frac{dS_1}{dx} = \frac{i}{2}\frac{dp(x)/dx}{p(x)} = i\frac{d}{dx}\ln\sqrt{p(x)}$$

$$\therefore\ iS_1(x) = \ln\frac{1}{\sqrt{p(x)}} + \text{constant}.$$

Correct to first order in $\hbar$ inclusive, we have

$$i\frac{S(x)}{\hbar} = \pm\frac{i}{\hbar}\int^x p(x')dx' + \ln\left(\frac{1}{\sqrt{p(x)}}\right)$$

The WKB solution, to this order, is therefore

$$\psi_{WKB}(\vec{x}) = \frac{A}{\sqrt{k(x)}}\exp\left(\pm i\int^x k(x')dx'\right)$$

where $k(x) = \sqrt{\frac{2m}{\hbar^2}(E-V(x))}$ is the local wave number.

The oscillatory wave function is just a straightforward manifestation of deBroglie waves with a potential. The factor out front is understandable, too. Since $|\psi|^2 \propto$ probability density, we have $P(x)dx \propto \frac{1}{k(x)}dx \propto \frac{1}{v(x)}dx$. With $dx = v\,dt$, we see that $P(x)$ is proportional to the time the particle spends in the neighborhood of x. This is just the classical probability.

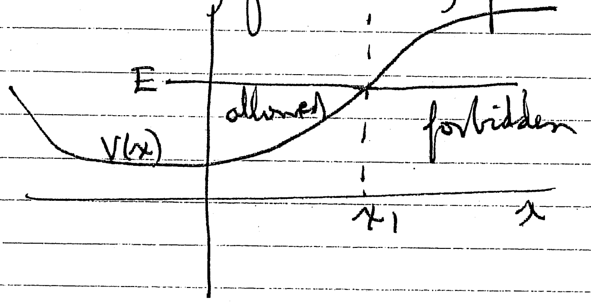
The above solution is appropriate in the classically allowed regions. For the classically forbidden regions we have

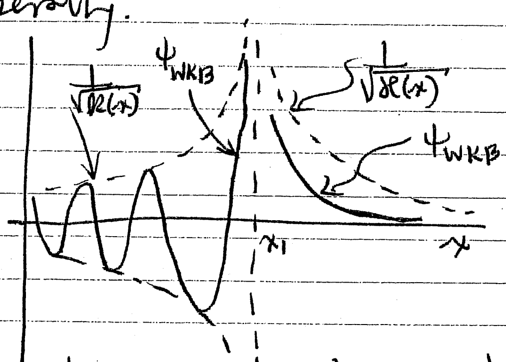
$$\psi(x) = \frac{A'}{\sqrt{\varkappa(x)}} \exp\left(\pm \int^{x} \varkappa(x')\,dx'\right)$$

where $\varkappa(x) = \sqrt{\frac{2m}{\hbar^2}(V(x)-E)}$.

Failure of WKB at classical turning points

The WKB solutions in the classically allowed and forbidden regions are physically understandable. But near the classical turning points they fail miserably.





At $x=x_1$, the WKB solutions diverge as $\frac{1}{\sqrt{k(x)}}$ or $\frac{1}{\sqrt{\varkappa(x)}}$. This unphysical (classical) behavior prevents us from implementing the continuity of the wave function as a function of x.

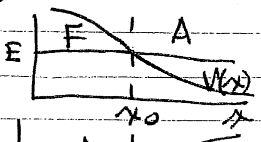
Connection formulas

By addressing the solution of the Schrodinger equation in the neighborhood of a classical turning point, we deduce the following "connection formulas":

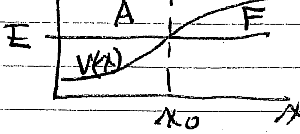
$$\frac{1}{2}\frac{1}{\sqrt{\varkappa(x)}}\, e^{-\xi'} \longrightarrow \frac{1}{\sqrt{k(x)}} \cos\left(\xi - \frac{\pi}{4}\right)$$

$$\frac{1}{\sqrt{\varkappa(x)}}\, e^{+\xi'} \longleftarrow \frac{1}{\sqrt{k(x)}} \cos\left(\xi + \frac{\pi}{4}\right) = -\frac{1}{\sqrt{k(x)}} \sin\left(\xi - \frac{\pi}{4}\right)$$

where $\xi = \int_{x_0}^{x} k(x')\,dx'$, $\xi' = \int_{x}^{x_0} \varkappa(x')\,dx'$ for



and $\xi = \int_{x}^{x_0} k(x')\,dx'$, $\xi' = \int_{x_0}^{x} \varkappa(x')\,dx'$ for

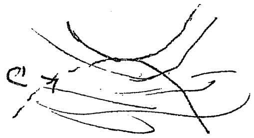


Sept 25
end

i Sept 27 Start 09.24.06

Method of Steepest Descent

In mathematical physics we are often faced with integrals of the form
$$I = \int_C dz\, e^{\lambda f(z)} g(z)$$
where λ is a positive parameter, often large, and $f(z)$ ~~is~~ and $g(z)$ are analytic. The method of steepest descent exploits the properties of analytic functions to distort the path C so that the dominant contribution to the integral comes from a relatively short part of the new contour. We look for a point (or set of points) where $f(z)$ is a ~~maximum~~ extremum or stationary ie $f'(z_0) = 0$. In the neighborhood of z_0 we make a Taylor Series expansion:



$$f(z) = f(z_0) + \cancelto{0}{f'(z_0)(z-z_0)} + \tfrac{1}{2} f''(z_0)(z-z_0)^2 + \cdots$$

Then we choose $z - z_0 = \rho e^{i\varphi}$, where ρ is real and φ is constant (in the neighborhood of z_0) and pick φ so that $\lambda f''(z_0) e^{2i\varphi}$ is <u>real</u> and <u>negative</u>.

Then $f(z) \simeq f(z_0) - \frac{1}{2}|f''(z_0)|\rho^2$

and
$$I \simeq \int_{-\infty}^{\infty} d\rho\, e^{i\varphi} g(z_0)\, e^{\lambda f(z_0)}\, e^{-\frac{\lambda}{2}|f''(z_0)|\rho^2}$$

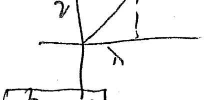
Note, if λ is complex, choose $\lambda f''(z_0) e^{2i\varphi}$ real & negative.

[If desired one can expand $g(z_0)$ around $z = z_0$.] But take care.]

$$\boxed{I \simeq g(z_0)\, e^{i\varphi}\, e^{\lambda f(z_0)} \frac{\sqrt{2\pi}}{\sqrt{\lambda |f''(z_0)|}}}$$

<u>Useful integral:</u>
$$\int_{-\infty}^{\infty} dt\, e^{-\mu t^2} = \frac{\sqrt{\pi}}{\sqrt{|\mu|}}\, e^{-i\frac{\alpha}{2}}$$

where $\mu = \lambda + i\nu$ with $\lambda > 0$ and $\mu = |\mu| e^{i\alpha}$

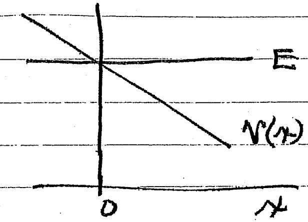


$-\frac{\pi}{2} < \alpha < \frac{\pi}{2}$; $|\mu| = \sqrt{\lambda^2 + \nu^2}$

Derivation of the Connection formulas:

We consider a solvable problem in the neighborhood of a classical turning point.

Linear potential



$$p^2(x) = 2m(E-V(x)) = 2mCx$$

$$\left(\frac{p^2}{2m} - Cx\right)\psi(x) = 0$$

Solve in momentum space ie put $x = i\hbar\frac{d}{dp}$. Define $q = p/(2m\hbar C)^{\frac{1}{3}}$. Then the momentum-space Schrodinger equation is

$$\left(\frac{d}{dq} + iq^2\right)\varphi(q) = 0$$

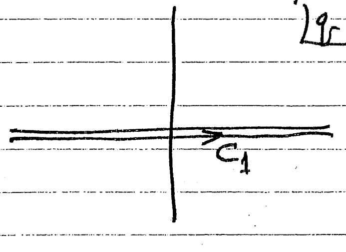
begin here!

with the solution, $\varphi(q) = e^{-iq^3/3}$

Defining $y = (2mC\hbar)^{\frac{1}{3}}x/\hbar$, the (unnormalized) coordinate-space wave function is $\psi(y) = \int dq\, e^{i(qy - q^3/3)}$

There are two linearly independent solutions. These will be chosen by treating q as a complex variable and choosing different contours of integration to define the different solutions.

We want real solutions.



We define 1st solution in terms of contour C_1 (the obvious one):

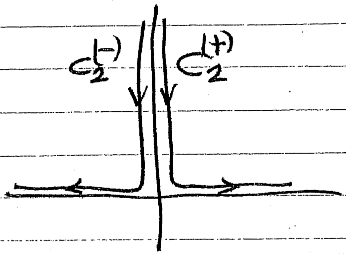
$$\psi_1(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dq\, e^{i(qy - q^3/3)}$$

$$= \frac{1}{\pi}\int_0^{\infty} \cos\left[\frac{q^3}{3} - yq\right] dq$$

This is ~~proportional~~ equal to the function $Ai(-y)$ — See Abramowitz & Stegun, p. 447, Eq. (10.4.32) — and is called an Airy function.

$$\psi_1(y) = Ai(-y)$$

For the second, linearly independent function we choose the contour C_2 (actually two contours)



$$\psi_2'(y) = \frac{i}{2\pi}\int_{C_2^{(-)}} + \frac{i}{2\pi}\int_{C_2^{(+)}}$$

On the vertical arm we take $q = i\tau$, $dq = i\,d\tau$

$$i(qy - q^3/3) = i\left(i\tau y - i^3\frac{\tau^3}{3}\right) = -\left(\tau y + \frac{\tau^3}{3}\right)$$

$$\therefore \psi_2(y) = \frac{1}{\pi}\int_0^\infty e^{-\left(\tau y + \frac{\tau^3}{3}\right)} d\tau + \underbrace{\frac{i}{2\pi}\int_0^{-\infty} dq\, e^{i(qy - q^3/3)}}_{\text{Put } q \to -q} + \frac{i}{2\pi}\int_0^\infty dq\, e^{i(qy - q^3/3)}$$

$$\psi_2(y) = \frac{1}{\pi}\int_0^\infty dq\left[e^{-\frac{q^3}{3} - qy} + \sin\left(\frac{q^3}{3} - qy\right)\right]$$

This function is equal to $Bi(-y)$, the second Airy function.

Connection formula for $\psi_1(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dq\, e^{i(qy - q^3/3)}$

Case 1 $y<0$ (forbidden region)

Put $y = -|y|$ Then $f(q) = -i(q|y| + q^3/3)$ $(\lambda = 1)$

$$f'(q) = -i(|y| + q^2)$$

$$f''(q) = -2iq$$

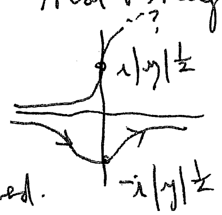
$f' = 0$ for $|y| + q^2 = 0$ i.e. $q_0 = \pm i\sqrt{|y|}$, where $f''(q_0) = \pm 2|y|^{\frac{1}{2}}$

and $f(q_0) = -i\left(\pm i|y|^{3/2} - \frac{1}{3}(\pm i)|y|^{3/2}\right) = \pm\frac{2}{3}|y|^{3/2}$

Now look at $q - q_0 = \rho e^{i\varphi}$ and $\pm 2|y|^{\frac{1}{2}} e^{2i\varphi}$ real & negative

For the upper sign we need $2\varphi = \pi$ or $\varphi = \frac{\pi}{2}$

lower $\varphi = 0$



Upper path is excluded. Only lower path is allowed.

Then $\psi_1(y) \simeq \frac{\sqrt{2\pi}}{2\pi\sqrt{2}|y|^{\frac{1}{4}}}\, e^{-\frac{2}{3}|y|^{3/2}} = \frac{1}{2\sqrt{\pi}|y|^{\frac{1}{4}}}\, e^{-\frac{2}{3}|y|^{\frac{3}{2}}}$

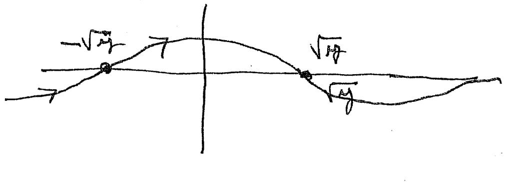
Case 2 $y > 0$ (allowed region)

$$f(q) = i(yq - q^3/3),\quad f'(q) = i(y - q^2),\quad f''(q) = -i2q$$

$f' = 0$ for $q_0 = \pm\sqrt{y}$. $f(q_0) = \pm i\frac{2}{3}y^{3/2}$; $f''(q_0) = \mp 2iy^{\frac{1}{2}}$

With $q - q_0 = \rho e^{i\varphi}$, we require $\mp i e^{2i\varphi}$ = real & negative.

$\therefore\ e^{2i\varphi \mp i\frac{\pi}{2}} = -1$ For upper sign, $\varphi = -\frac{\pi}{4}$; lower sign, $\varphi = +\frac{\pi}{4}$.



We have two contributions.

$$\psi_1(y) \simeq \frac{1\sqrt{2\pi}}{2\pi\sqrt{2}\,y^{\frac{1}{4}}}\left(e^{i\frac{\pi}{2}} e^{-i\frac{2}{3}y^{\frac{3}{2}}} + \text{c.c.}\right)$$

$$\therefore\ \psi_1(y) \simeq \frac{1}{\sqrt{\pi}\,y^{\frac{1}{4}}}\cos\left(\frac{2}{3}y^{3/2} - \frac{\pi}{4}\right)$$

iii

Left as exercise to show $y^{3/2}$ etc.

Relation to WKB functions

Classically forbidden solution is $\psi(x) \propto \frac{1}{\sqrt{\varkappa(x)}} \exp\left(\pm \int_x^0 \varkappa(x')dx' \right)$ for $x<0$

With linear potential we have $V(x) - E = C'(-x)$

so $\varkappa(x') = \sqrt{-\frac{k^2(x')}{\hbar^2}} = \sqrt{\frac{2mC'}{\hbar^2}(-x')}$

Define $\xi' = \int_x^0 \varkappa(x')dx' = \sqrt{\frac{2mC'}{\hbar^2}} \int_0^{|x|} (x')^{\frac{1}{2}} dx' = \frac{2}{3}\sqrt{\frac{2mC'}{\hbar^2}} |x|^{3/2}$

But $y = \left(\frac{2mC'}{\hbar^2}\right)^{\frac{1}{3}} x \quad \therefore \xi' = \frac{2}{3}|y|^{\frac{3}{2}}$ and $\frac{1}{|y|^{\frac{1}{4}}} \propto \frac{1}{\sqrt{\varkappa(x)}}$

Thus our result for "large" y of $\psi_1(y)$ is proportional and joins smoothly with the WKB solution in terms of the integral $\xi'(x)$.

Similarly the classically allowed region has a corresponding matching with $\xi(x) = \int_0^x k(x')dx' \qquad k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V(x))}$.

With

$$y<0 \qquad \psi_1 \simeq \frac{1}{2\sqrt{\pi}|y|^{\frac{1}{4}}} e^{-\frac{2}{3}|y|^{\frac{3}{2}}}$$

$$y>0 \qquad \psi_1 \simeq \frac{1}{\sqrt{\pi}\, y^{\frac{1}{4}}} \cos\left(\frac{2}{3}y^{\frac{3}{2}} - \frac{\pi}{4}\right)$$

we obtain the first connection formula:

$$\frac{1}{2\sqrt{\varkappa(x)}} e^{-\xi'} \longrightarrow \frac{1}{\sqrt{k(x)}} \cos\left(\xi - \pi/4\right)$$

as stated earlier.

Second solution By the same methods we can show that

Classically forbidden $(y<0)$ $\quad \psi_2(y) \simeq \frac{1}{\sqrt{\pi}} \frac{e^{2/3|y|^{3/2}}}{|y|^{1/4}}$

Classically allowed $(y>0)$ $\quad \psi_2(y) \simeq \frac{1}{\sqrt{\pi}} \frac{1}{y^{1/4}} \cos\left(\overset{\frac{2}{3}y^{\frac{3}{2}}}{\xi} + \pi/4\right) = \frac{-1}{\sqrt{\pi}\, y^{\frac{1}{4}}} \sin\left(\frac{2}{3}y^{\frac{3}{2}} - \frac{\pi}{4}\right)$

The second connection formula is

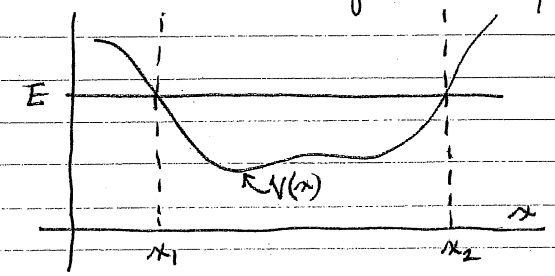
$$\frac{1}{\sqrt{\varkappa(x)}} e^{+\xi'} \longleftarrow \frac{-1}{\sqrt{k(x)}} \sin\left(\xi - \pi/4\right)$$

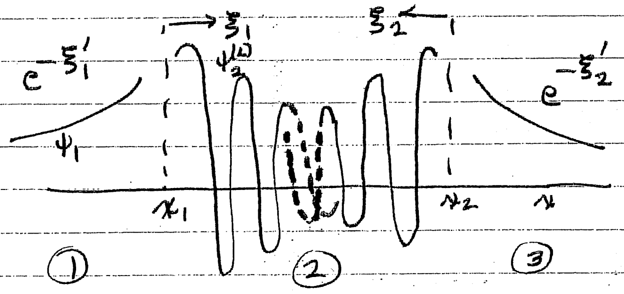
Sept 27 end

Sept 29 Starts

WKB Quantization Rule for Bound States

Consider a potential of the form shown in the sketch.





We have $k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V(x))}$ in CA region and define

$$\xi_1 = \int_{x_1}^{x} k(x')dx'$$

$$\xi_2 = \int_{x}^{x_2} k(x')dx'$$

In CF regions to the left and right we have $\kappa(x) = \sqrt{\frac{2m}{\hbar^2}(V(x) - E)}$

and define $\xi_1' = \int_{x}^{x_1} \kappa(x')dx'$

$$\xi_2' = \int_{x_2}^{x} \kappa(x')dx'$$

On the left

Then the solution that is asymptotically

$$\psi_1 = \frac{A}{2\sqrt{\kappa(x)}} e^{-\xi_1'}$$

connects across $x = x_1$ to $\psi_2^{(L)} = \frac{A}{\sqrt{k(x)}} \cos\left(\xi_1 - \frac{\pi}{4}\right)$

On the Right

The solution $\psi_3 \rightarrow \frac{A'}{2\sqrt{\kappa(x)}} e^{-\xi_2'}$ connects with $\psi_2^{(R)} = \frac{A'}{\sqrt{k(x)}} \cos\left(\xi_2 - \frac{\pi}{4}\right)$

In the CA region, the two solutions $\psi_2^{(L)}$ and $\psi_2^{(R)}$ will not, in general, be the same. Only for certain energy eigenvalues will they connect together to form a proper eigenfunction (single valued & unique).

Requirements

(a) $|A'| = |A|$

(b) $\cos\left(\xi_1 - \frac{\pi}{4}\right) = \pm \cos\left(\xi_2 - \frac{\pi}{4}\right) = \pm \cos\left(\frac{\pi}{4} - \xi_2 - \xi_1 + \xi_1\right)$

$$= \pm \cos\left[\xi_1 - \frac{\pi}{4} - \left(\frac{\pi}{2} + \xi_1 + \xi_2\right)\right]$$

$\therefore \xi_1 + \xi_2 - \frac{\pi}{2} = n\pi \quad , n = 0, 1, 2, \ldots$ (negative n are excluded because $\xi_1 + \xi_2 \geq 0$)

The quantization rule is thus $\xi_1 + \xi_2 = \left(n + \frac{1}{2}\right)\pi$

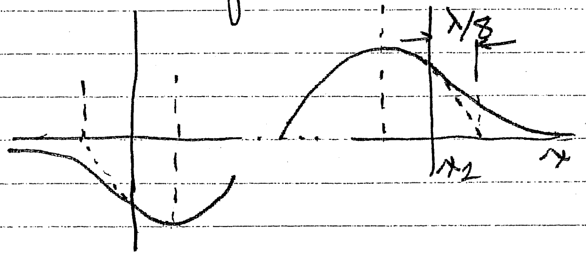
or

$$\int_{x_1}^{x_2} k(x')\,dx' = (n+\tfrac{1}{2})\pi$$

If we multiply by $2\hbar$, we can write it as $\oint p\,dq = (n+\frac{1}{2})(\overset{h}{\overset{\downarrow}{2\pi\hbar}})$

This differs from the Sommerfeld-Wilson quantization rule of the old quantum theory ~~by~~ only by having $(n+\frac{1}{2})$ instead of n.

The added $\frac{1}{2}$ is on account of the wave nature of quantum particles and the penetration into the classically forbidden region. There



is penetration equivalent to $\lambda/8$ (or $\frac{\pi}{4}$) at each end of the classically allowed region.

This phenomenon occurs in classical wave problems, eg. the lowering of the resonant frequency of a cavity because of finite conductivity and penetration by a skin depth into the metal.

WKB Estimate of Average Kinetic Energy in n^{th} state

With probability proportional to $\frac{\cos^2(\xi-\pi/4)}{k(x)} \simeq \frac{1}{2}\frac{1}{k(x)}$ on average

we write
$$\left\langle \frac{p^2}{2m}\right\rangle_n = \frac{\int_{x_1}^{x_2} \frac{\hbar^2}{2m}\frac{k^2(x)\,dx}{k(x)}}{\int_{x_1}^{x_2}\frac{dx}{k(x)}} = \frac{\hbar^2}{2m}\frac{\int_{x_1}^{x_2} k(x)\,dx}{\int_{x_1}^{x_2}\frac{dx}{k(x)}} = \frac{\pi(n+\frac{1}{2})\frac{\hbar^2}{2m}}{\int_{x_1}^{x_2}\frac{dx}{k(x)}}$$

What about the denominator? Consider the quantization condition and take the derivative of both sides with respect to E: Since $k = \sqrt{\frac{2m}{\hbar^2}(E-V(x))}$

$$\frac{d}{dE}\int_{x_1}^{x_2} k(x)\,dx = \frac{1}{2}\frac{2m}{\hbar^2}\int_{x_1}^{x_2}\frac{dx}{k(x)} + \cancelto{0}{\frac{dx_2}{dE}k(x_2)} - \cancelto{0}{\frac{dx_1}{dE}k(x_1)} = \pi\frac{dn}{dE}$$

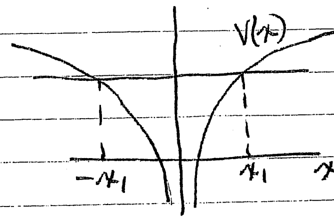
Thus
$$\frac{1}{\int_{x_1}^{x_2}\frac{dx}{k(x)}} = \frac{m}{\hbar^2 \pi}\frac{dE}{dn}$$

We find
$$\left\langle \frac{p^2}{2m}\right\rangle_n = \frac{1}{2}(n+\tfrac{1}{2})\frac{dE}{dn}$$

Strictly speaking, $E = E_{WKB}$.

Example of Eigenvalue problem

Bound states in a logarithmic potential



$$V(x) = V_0 \ln\left(\frac{|x|}{a}\right)$$

$$k(x) = \sqrt{\frac{2m}{\hbar^2}\left(E - V_0 \ln\frac{|x|}{a}\right)}$$

Turning point is $E = V_0 \ln\frac{x_1}{a}$ or $x_1 = a e^{E/V_0}$

$$k(x) = \sqrt{\frac{2mV_0}{\hbar^2}}\sqrt{\ln\frac{x_1}{a} - \ln\frac{|x|}{a}} = \sqrt{\frac{2mV_0}{\hbar^2}}\sqrt{\ln\frac{x_1}{|x|}}$$

The quantization rule is

$$(n+\tfrac{1}{2})\pi = \int_{-x_1}^{x_1} k(x)\,dx = 2\int_0^{x_1} k(x)\,dx = 2\sqrt{\frac{2mV_0}{\hbar^2}}\,x_1\int_0^1 \sqrt{\ln\left(\frac{1}{y}\right)}\,dy$$

Put $y = e^{-t^2}$ $\quad 0<t<\infty$

$$\sqrt{\ln\left(\tfrac{1}{y}\right)} = t$$

$$dy = -2te^{-t^2}dt$$

$$\therefore \int_0^1 \sqrt{\ln\left(\tfrac{1}{y}\right)}\,dy = 2\int_0^\infty t^2 e^{-t^2}dt$$

$$= -\frac{d}{d\lambda}\int_{-\infty}^{\infty} e^{-\lambda t^2}dt = -\frac{d}{d\lambda}\sqrt{\frac{\pi}{\lambda}} = \frac{\sqrt{\pi}}{2}$$

$$(n+\tfrac{1}{2})\pi = \cancel{2}\sqrt{\frac{2mV_0a^2}{\hbar^2}}\,e^{E/V_0}\,\frac{\sqrt{\pi}}{\cancel{2}}$$

$$\therefore E = V_0 \ln\left[(n+\tfrac{1}{2})\frac{\sqrt{\pi}\,\hbar}{\sqrt{2mV_0a^2}}\right]$$

[If we had s-wave states in a spherically symmetric potential, we must replace $n+\frac{1}{2} \to 2n+\frac{3}{2}$ in this formula.]

Average kinetic energy $\quad \left\langle \frac{p^2}{2m}\right\rangle_n = \frac{1}{2}(n+\tfrac{1}{2})\frac{dE}{dn}$

We have $\frac{dE}{dn} = \frac{V_0}{n+\frac{1}{2}}$. Hence $\left\langle\frac{p^2}{2m}\right\rangle_n = \frac{V_0}{2}$, independent of n.

The same result follows from the virial theorem:

$$\left\langle\frac{p^2}{2m}\right\rangle = \frac{1}{2}\left\langle x\frac{dV}{dx}\right\rangle = \frac{V_0}{2}.$$

Section 2.5 in Sakurai

Free-particle propagator

At $t = t_0$ a free particle is described by $\psi(\vec{x}, t_0)$.

At other times $\psi(\vec{x},t) = e^{-iH(t-t_0)/\hbar}\,\psi(\vec{x},t_0)$, $H = p^2/2m$.

We wish to express $\psi(\vec{x},t)$ in terms of a "propagator" from $(\vec{x}',t_0) \rightarrow (\vec{x},t)$, written as $K(\vec{x},\vec{x}',t,t_0)$

such that
$$\psi(\vec{x},t) = \int d^3x'\, K(\vec{x},\vec{x}',t,t_0)\,\psi(\vec{x}',t_0)$$

The form of H suggests using momentum space to find K

Write
$$\psi(\vec{x},t_0) = \frac{1}{(2\pi)^{3/2}}\int d^3k\, A(\vec{k})\, e^{i\vec{k}\cdot\vec{x}} \qquad (\vec{k} = \vec{p}/\hbar).$$

We need
$$e^{-iH(t-t_0)/\hbar}\, e^{i\vec{k}\cdot\vec{x}} = e^{i\vec{k}\cdot\vec{x}}\, e^{-i\hbar k^2(t-t_0)/2m}$$

Then
$$\psi(\vec{x},t) = \frac{1}{(2\pi)^{3/2}}\int d^3k\, A(\vec{k})\, e^{i\vec{k}\cdot\vec{x}}\, e^{-i\hbar k^2(t-t_0)/2m}$$

But
$$A(\vec{k}) = \frac{1}{(2\pi)^{3/2}}\int d^3x'\, e^{-i\vec{k}\cdot\vec{x}'}\,\psi(\vec{x}',t_0)$$

Hence
$$\psi(\vec{x},t) = \frac{1}{(2\pi)^3}\int d^3x'\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\, e^{-i\hbar k^2(t-t_0)/2m}\,\psi(\vec{x}',t_0)$$

The k-integral is called the free-particle propagator:
$$K(\vec{x},\vec{x}',t,t_0) = \frac{1}{(2\pi)^3}\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\, e^{-i\hbar k^2(t-t_0)/2m}$$

Note that $K = K(\vec{x}-\vec{x}', t-t_0)$

The integral can be done and gives explicitly (by completing square in exponent):
$$K(\vec{x}-\vec{x}', t-t_0) = \left(\frac{m}{2\pi i\hbar\tau}\right)^{3/2} \exp\left(\frac{imr^2}{2\hbar\tau}\right)$$

end Sept 29 where $\vec{r} = \vec{x}-\vec{x}'$, $\tau = t - t_0$.

Relation to heat conduction Kernel: $i\tau \rightarrow \tau_H$.