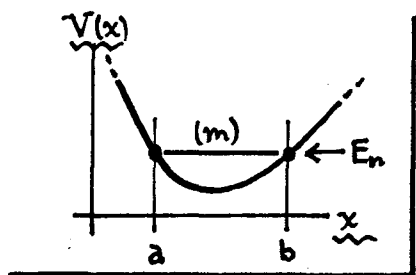


Other Applications of the WKB Method to QM

We have now solved two prototype QM problems by using the WKB approximation, viz.

① Bound states of a 1D potential well.

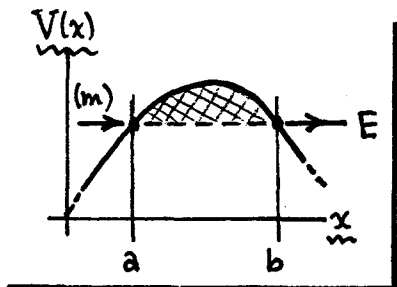


WKB (Bohr-Sommerfeld) Energy Quantization:

$$\int_a^b \sqrt{2m[E_n - V(x)]} dx = (n + \frac{1}{2})\pi\hbar, \quad n = 0, 1, 2, \dots \quad (1)$$

(approxⁿ good for: $k_{av}(b-a) \gg 1$; limit of ψ_{WKB} validity).

② Tunneling thru a 1D potential barrier.



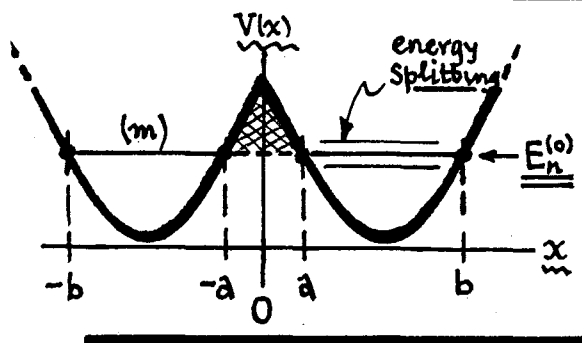
WKB barrier transmission coefficient:

$$T = \exp \left\{ -\frac{2}{\hbar} \int_a^b \sqrt{2m[V(x) - E]} dx \right\}. \quad (2)$$

(approxⁿ good for: $K_{av}(b-a) \gg 1$; limit of ψ_{WKB} validity).

Combinations of these problems (i.e. $V(x) = \cup + \wedge + \cup + \dots$) provide a rich variety of QM models. We shall now survey a few such models.

1) First we look at a double (or multiple) well.



The well of type ① above is reflected thru the origin to form a symmetric "double well" as sketched.

The wells are coupled-- in the sense that the energy levels E_n of the RH well depend in part on the presence of the LH well. Specifically, coupling is

provided by QM tunneling back & forth thru the potential barrier between $-a$ & a .

This tunneling has a novel effect on the well energies: each energy $E_n^{(0)}$ is split.

Details are left to an assigned problem. Results go as follows...

1. Let $E_n^{(0)}$ be the n^{th} energy level of either well alone, calculated from...

$$\rightarrow \int_a^b \sqrt{2m[E_n^{(0)} - V(x)]} dx = (n + \frac{1}{2})\pi \hbar, \text{ for one well.} \quad (3a)$$

2. Let $\omega_n^{(0)}$ be the oscillation frequency for the particle in one well...

$$\left\{ \begin{array}{l} \text{natural} \\ \text{oscillation} \\ \text{period} \end{array} \right\} \frac{2\pi}{\omega_n^{(0)}} = 2 \int_a^b \frac{dx}{p_n^{(0)}(x)/m}, \quad \text{w/ } p_n^{(0)}(x) = \sqrt{2m[E_n^{(0)} - V(x)]}. \quad (3b)$$

For m rattling about in one well, this is the time elapsed between successive presentations to the barrier.

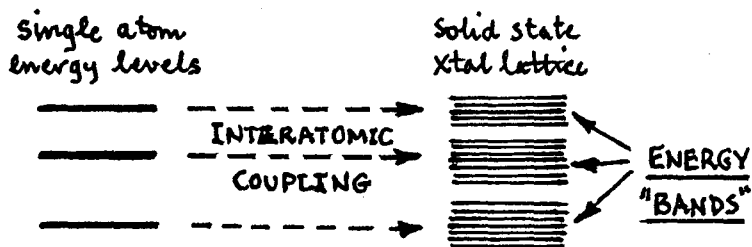
3. The energy level $E_n^{(0)}$ in Eq. (3a) is split as follows...

$$E_n^{(0)} \xrightarrow[\text{tunnel}]{\text{QM}} E_n = E_n^{(0)} \pm \Delta E_n, \text{ i.e. } E_n^{(0)} \rightarrow \begin{array}{l} E_n^{(0)} + \Delta E_n \\ E_n^{(0)} - \Delta E_n \end{array}$$

$$\text{w/ } \Delta E_n = \left(\frac{\hbar \omega_n^{(0)}}{2\pi} \right) \exp \left\{ (-) \int_{-a}^{+a} \sqrt{(2m/\hbar^2)[V(x) - E_n^{(0)}]} dx \right\}. \quad (3c)$$

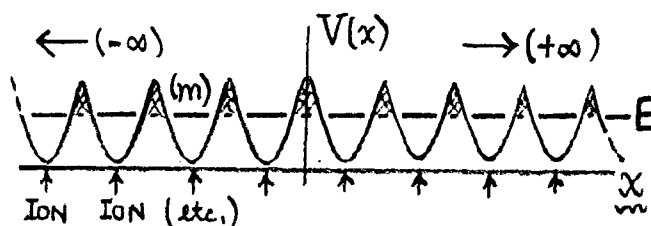
presentation frequency barrier penetration probability

The splitting of energy levels induced by coupling is a general feature of QM systems (e.g. the fs & hfs splitting in H-atom). Such splitting is dramatically illustrated in the solid state (i.e. for an electron interacting w/ a crystal lattice):

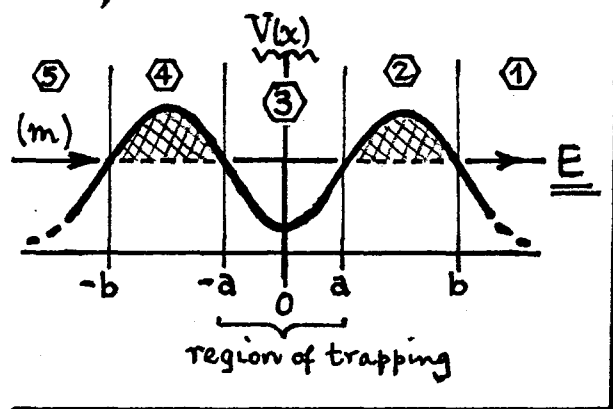


Each atomic level -- coupled to many other atoms in the lattice -- splits into a large # of perturbed levels to form an energy band.

The energy band structure could be estimated in the present context by model at right... (augmented Kronig - Penney model).



2) Another WKB elaboration is the double-hump (camel) problem.



The barrier of type ③ (dgm on p.W18) is reflected thru the origin to form a symmetric double-peaked barrier, with a well (region ③) in between. Particle (mass m , energy E) enters from left (⑤) and may tunnel all the way thru to right (①). Interesting features of this problem turn out to be:

- (i) m can get "trapped" in the well (region ③), forming a \sim bound (metastable) state;
- (ii) the normally small transmission coefficient $T \rightarrow 1$ at certain (resonant) energies.

1. The story of this problem is told in terms of T , which we can find as follows. As before (p.W15, Eq.(4)), we start in region ① \rightsquigarrow a rightward traveling transmitted wave:

$$\left[\psi_1(x) = \frac{A}{\sqrt{k(x)}} e^{+i \left[\int_b^x k(x') dx' + \frac{\pi}{4} \right]} \right] \leftarrow \text{rightward wave in region ①}; \quad (4)$$

$$\rightsquigarrow k(x) = \sqrt{2m[E - V(x)]}. \quad \text{Let: } k(x) = \sqrt{2m[V(x) - E]}. \quad (5)$$

Then $\psi_1 \rightarrow \psi_2 \rightarrow \psi_3$ as before, with the result (p.W15, Eq.(7))...

$$\left[\psi_3(x) = \frac{A}{\sqrt{k(x)}} \left\{ \frac{2}{Q} \sin \left[\int_x^a k(x') dx' + \frac{\pi}{4} \right] + \frac{iQ}{2} \cos \left[\int_x^a k(x') dx' + \frac{\pi}{4} \right] \right\}, \text{ in ③}; \right. \quad (6)$$

$$\left. \rightsquigarrow Q = \exp \left[- \int_a^b k(x) dx \right] \leftarrow \text{tunneling factor for righthand barrier ②} \right.$$

2. Now we must connect $\psi_3 \rightarrow \psi_4 \rightarrow \psi_5$. First, refer ψ_3 to the lefthand side of region ③, i.e. reference the integrals in Eq.(6) to $x = -a$. Get...

$$\left[\psi_3 = \frac{A}{\sqrt{k}} \left\{ \left[\frac{2}{Q} \sin \phi + \frac{iQ}{2} \cos \phi \right] \sin \left(\int_{-a}^x k dx' + \frac{\pi}{4} \right) + \right. \right. \quad (7)$$

$$\left. \left. \rightsquigarrow \phi = \int_{-a}^a k(x) dx \sim \text{net phase in well ③} \right. \left. + \left[\frac{2}{Q} \cos \phi - \frac{iQ}{2} \sin \phi \right] \cos \left(\int_{-a}^x k dx' + \frac{\pi}{4} \right) \right\} \right.$$

Ψ_3 in Eq. (7) contains both rightward and leftward traveling waves $e^{\pm i \int k dx'}$, so the connection $\Psi_3 \rightarrow \Psi_4 \rightarrow \Psi_5$ is more complicated than $\Psi_1 \rightarrow \Psi_2 \rightarrow \Psi_3$, where we start with Ψ_1 = rightward only. Results are...

$$\left[\begin{aligned} \Psi_4 &= \frac{A}{\sqrt{k}} \left\{ [M] \frac{Q}{2} e^{\int_{-b}^x k dx'} + [N] \frac{1}{Q} e^{-\int_{-b}^x k dx'} \right\}, \text{ in barrier } \textcircled{4}; \\ \text{or } [M] &= \frac{2}{Q} \sin \phi + \frac{iQ}{2} \cos \phi, \quad [N] = \frac{2}{Q} \cos \phi - \frac{iQ}{2} \sin \phi. \end{aligned} \right. \quad (8)$$

Note that we are carrying along the phase ϕ accumulated in the well region $\textcircled{3}$; this ϕ did not appear in the tunneling calculation for a single barrier. Finally:

$$\left[\begin{aligned} \Psi_5 &= \frac{A}{\sqrt{k}} \left\{ \left[\sin \phi + \frac{iQ^2}{4} \cos \phi \right] \cos \left(\int_x^{-b} k dx' + \frac{\pi}{4} \right) + \left[\frac{4}{Q^2} \cos \phi - i \sin \phi \right] \sin \left(\int_x^{-b} k dx' + \frac{\pi}{4} \right) \right\}, \text{ in } \textcircled{5}; \\ \text{put in form of traveling waves} \\ \text{i.e. } \Psi_5 &= \frac{A}{\sqrt{k}} \left\{ \left[\frac{1}{2} \left(\frac{4}{Q^2} + \frac{Q^2}{4} \right) \cos \phi - i \sin \phi \right] e^{+i \left(\int_{-b}^x k dx' + \frac{\pi}{4} \right)} + \left[\frac{1}{2} \left(\frac{4}{Q^2} - \frac{Q^2}{4} \right) \cos \phi \right] e^{-i \left(\int_{-b}^x k dx' + \frac{\pi}{4} \right)} \right\}. \end{aligned} \right. \quad (9)$$

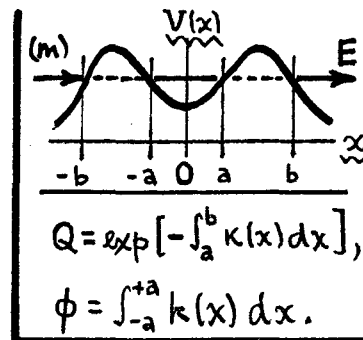
rightward wave
leftward wave

3. Ψ_5 is the incident (rightward) wave + reflected (leftward) wave. Comparing Ψ_5 with the transmitted wave Ψ_1 in Eq. (4), we see that the transmission coeff. is

$$\rightarrow T = \frac{|\Psi_1(\text{right})|^2}{|\Psi_5(\text{right})|^2} = 1 / \left| \frac{1}{2} \left(\frac{4}{Q^2} + \frac{Q^2}{4} \right) \cos \phi - i \sin \phi \right|^2 \quad (10)$$

$$\text{or } T = 1 / \left[1 + \frac{4}{Q^4} \left(1 - \frac{Q^4}{16} \right)^2 \cos^2 \phi \right] \approx 1 / \left[1 + \frac{4}{Q^4} \cos^2 \phi \right] \quad Q \ll 1$$

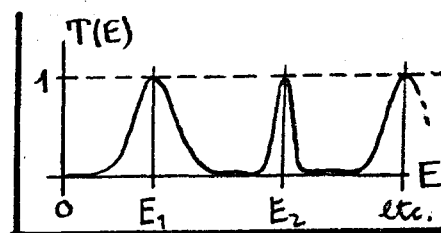
REMARKS



- (1) $Q \ll 1$ ensures WKB approxn OK. But now phase ϕ plays big role: $T \rightarrow 1$ when $\cos \phi = 0$.
- (2) If the well vanishes, $\phi \rightarrow 0$ and: $T \approx (Q^2/2)^2$. This is similar to previous tunneling result... this T = tunneling prob. for two successive (each $\frac{Q^2}{2}$) barriers.
- (3) $T \rightarrow 1$ when $\cos \phi \rightarrow 0$ means in tunnels thru no matter how wide or tall the barrier.

3) Graph T of Eq. (10) vs. energy E . You see resonances whenever $\cos \phi \rightarrow 0$, i.e. when...

$$\left[\begin{aligned} \cos \phi \rightarrow 0 &\Rightarrow \phi \rightarrow (n + \frac{1}{2})\pi, \text{ i.e.} \\ \int_{-a}^a \sqrt{2m[E - V(x)]} dx &= (n + \frac{1}{2})\pi \hbar. \quad (11) \end{aligned} \right. \quad \text{Same as B-S quantization.}$$



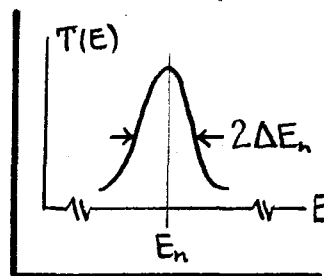
This is just the condition for the formation of (quasi) bound states E_n in the well ("quasi" because ultimately the state leaks away) -- m gets "trapped" in the well. A resonance occurs because the oscillating wave trapped in the well is exactly in phase with the incident wave, and so is resonantly reinforced by the small wave amplitude leaking thru the (lefthand) barrier [phenomenon \sim driving a damped SHO at or near its natural frequency].

We can estimate the widths of the above resonances in the following way...

$$\left[\begin{aligned} \text{When } \phi \sim \phi_n = (n + \frac{1}{2})\pi, \text{ let: } \phi - \phi_n &\approx \left(\frac{\partial \phi}{\partial E} \right) \Delta E_n, \quad \text{w/ } \Delta E_n = E - E_n. \\ \text{But: } \phi &= \frac{1}{\hbar} \int_{-a}^a \sqrt{2m[E - V(x)]} dx, \text{ so...} \\ \rightarrow \hbar \frac{\partial \phi}{\partial E} &= \int_{-a}^a \frac{1}{2} (2m[E - V(x)])^{-\frac{1}{2}} 2m dx = \int_{-a}^a \frac{dx}{p(x)/m} = \frac{\tau}{2}, \\ &\quad \text{natural period for oscillation of } m \text{ in well} \\ \text{thus } \phi &\approx \phi_n + \left(\frac{E - E_n}{\hbar} \right) \frac{\tau_n}{2}, \quad \text{w/ } \tau_n = \tau(E = E_n), \\ \text{and } \cos \phi &\approx \sin \left[\left(\frac{E - E_n}{\hbar} \right) \frac{\tau_n}{2} \right] \approx \left(\frac{E - E_n}{\hbar} \right) \frac{\tau_n}{2}, \text{ as } E \rightarrow E_n \text{ (resonance).} \quad (12) \end{aligned} \right.$$

Then, near a resonance, $E \sim E_n$, the transmission coeff. of Eq. (10) is approx'ly...

$$\boxed{T(E) \approx 1 / \left[1 + \left(\frac{E - E_n}{\Delta E_n} \right)^2 \right]}, \quad \text{w/ } \Delta E_n = Q^2 \hbar / \tau_n, \quad (13)$$



$T(E)$ is a Lorentzian near E_n . The incident particle (with $E \sim E_n$) gets trapped in the well for a time $\Delta t_n \sim \tau_n / Q^2 \gg \tau_n$ (many oscillations) but ultimately leaks thru the barrier with $T \sim 1$ certainty.

ASIDE #1 Trapping in the double-hump well.

To show more graphically that the particle gets "trapped" in a double-hump well near a transmission resonance, we analyse the relative intensities of the incident vs. trapped wave. From Eq.(6) & Eq.(9) above, we have...

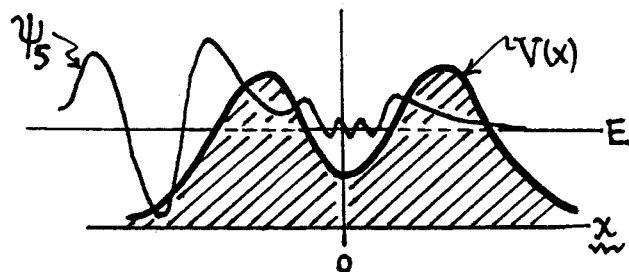
$$\left\{ \begin{array}{l} \text{intensity in well} \\ \text{incident intensity} \end{array} \right\} \begin{array}{l} |\psi_3|^2 \\ |\psi_5|^2 \end{array} = \frac{|A|^2}{k_3} \left[\frac{4}{Q^2} \sin^2 \left(\int_x^a k_3 dx' + \frac{\pi}{4} \right) + \frac{Q^2}{4} \cos^2 \left(\int_x^a k_3 dx' + \frac{\pi}{4} \right) \right], \quad (14)$$

$Q = \text{tunneling factor, Eq.(6);}$
 $\Phi = \text{phase in well, Eq.(7).}$

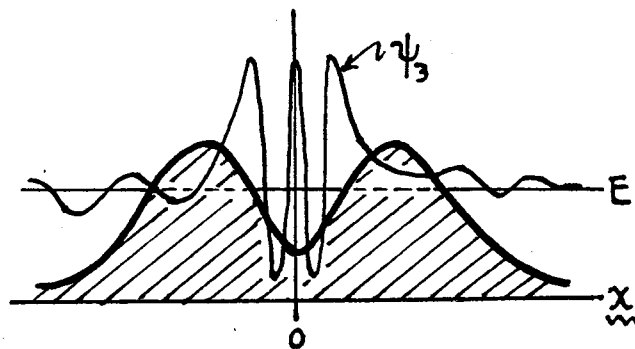
$k_3 = \sqrt{\frac{2m}{\hbar^2} [E - V(x)]}$ in region ③: $-a \leq x \leq a$; likewise $k_5 = k$ (region ⑤). By assumption, the wave oscillates "many" times inside the well (see p. WKB 19), and so we take a space average of $|\psi_3|^2$, using $\langle \sin^2(\cdot) \rangle = \langle \cos^2(\cdot) \rangle = 1/2$. If we also assume that the tunneling factor $Q \ll 1$, then the relative intensity in (14) is:

$$\frac{\text{in well}}{\text{incident}} = \frac{|\psi_3|^2}{|\psi_5|^2} \underset{Q \ll 1}{\approx} \frac{k_5}{k_3} \left(\frac{2Q^2}{4\cos^2\phi + Q^4} \right) \sim \begin{cases} Q^2 \ll 1, & \text{for } \cos\phi \neq 0; \\ 1/Q^2 \gg 1, & \text{when } \cos\phi = 0. \end{cases} \quad (15)$$

So the (in well)/(incident) intensity ratio is a sensitive fun of the resonance factor $\cos\phi$. In pictures, we have...



off-resonance: $\cos\phi \neq 0$.



near resonance: $\cos\phi \rightarrow 0$.

Near resonance, the relatively large intensity of ψ_3 in the well \Rightarrow the particle is most likely to be found there -- so indeed it is "trapped" in the well.

ASIDE #2 Lifetime of the trapped state.

The analysis of Eqs.(12)-(13) for the transmission coefficient $T(E)$ near resonance, $E \approx E_n$, shows that the trapped state has an energy width $2\hbar Q^2/\tau_n$. By inference, that state should have a finite lifetime $\Delta t_n \approx \frac{1}{2} \tau_n / Q^2$.

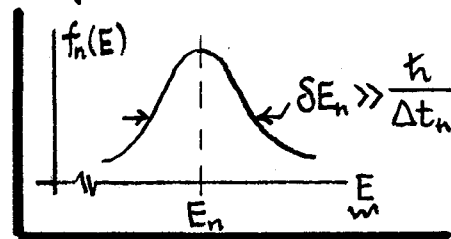
WKB : Lifetime of a trapped state in the double-hump well.

W24

Here $\tau_n = 2m \int_a^b dx / p_n(x)$ is the natural oscillation period of m in the well at energy E_n , and the tunneling factor [Eq.(6)] $Q \ll 1$. We now show how Δt_n appears dynamically in the wave fun for the trapped particle.

We put a wavepacket in the well, with a spread of energies δE_n about the resonant energy E_n , i.e. we look at the superposition of well states...

$$\rightarrow \underline{\Psi_n(x,t) = \int_{-\infty}^{\infty} \Psi_3(x,E) f_n(E) e^{-\frac{i}{\hbar} E t} dE.} \quad (16)$$



The spectral fun $f_n(E)$ is peaked near $E = E_n$, but-- by assumption-- has an energy width δE_n which is broad w.r.t. the width $\hbar / \Delta t_n$ of the trapped state, i.e. $\delta E_n \gg \hbar / \Delta t_n$. So Ψ_n contains "many" possible well states $\Psi_3(x,E)$, and Ψ_n is well-localized in time compared to the Ψ_3^s , since: $\delta t_n \approx \hbar / \delta E_n \ll \Delta t_n$.

The well states are specified by Eq.(6). For $Q \ll 1$, we take...

$$\rightarrow \Psi_3(x,E) \approx \frac{A}{\sqrt{k_3(x)}} \frac{2}{Q} \sin \left[\int_x^a k_3(x') dx' + \frac{\pi}{4} \right]. \quad (17)$$

The const A is free for normalisation. We choose A so that the incoming wave is a unit WKB plane wave: $\Psi_5 \approx (1/\sqrt{k_5}) \exp[i(\int_b^x k_5 dx' + \frac{\pi}{4})]$, near resonance ($\cos \phi \rightarrow 0$). From Eq.(9), this requires...

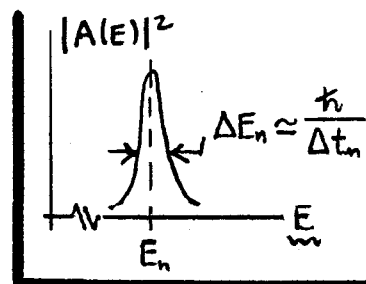
$$\rightarrow A = 1 / \left[\frac{1}{2} \left(\frac{4}{Q^2} + \frac{Q^2}{4} \right) \cos \phi - i \sin \phi \right], \quad \phi = \int_a^b k_3(x) dx = \text{well phase.} \quad (18)$$

By Eq.(12), the trapped state occurs near $\phi \approx (n + \frac{1}{2})\pi + \frac{1}{2} \left(\frac{E - E_n}{\hbar} \right) \tau_n$, so...

$$\cos \phi \approx -(-1)^n \frac{1}{2} \left(\frac{E - E_n}{\hbar} \right) \tau_n, \quad \sin \phi \approx (-1)^n, \quad \text{to 1st order in } (E - E_n);$$

$$\text{and} \rightarrow \underline{A \approx (-1)^n i / \left[1 - i \left(\frac{E - E_n}{\hbar / 2 \Delta t_n} \right) \right]}, \quad \Delta t_n = \frac{1}{2} \tau_n / Q^2. \quad (19)$$

A is sharply peaked near E_n -- its width $\Delta E_n \approx \hbar / \Delta t_n$ is small compared to that of the above spectral fun $f_n(E)$.



Consequently, in Eq. (17), we can evaluate $k_3(x)$ at $E = E_n$, and thus get an approximate form for the well states ψ_3 near resonance...

$$\left. \begin{aligned} \psi_3(x, E) &\approx \frac{2i(-)^n}{Q\sqrt{k_n(x)}} \sin\left[\int_x^a k_n(x') dx' + \frac{\pi}{4}\right] / \left[1 - i\left(\frac{E - E_n}{\hbar/2\Delta t_n}\right)\right], \\ \text{w// } k_n(x) &= \frac{1}{\hbar} [2m(E_n - V(x))]^{1/2} \leftarrow k_n \text{ is independent of } E. \end{aligned} \right\} (20)$$

Now put ψ_3 of Eq. (20) into the superposition of Eq. (16)...

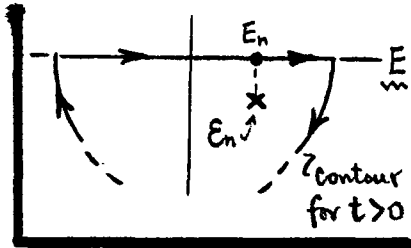
$$\left. \begin{aligned} \Psi_n(x, t) &\approx \Phi_n(x) \int_{-\infty}^{\infty} \frac{f_n(E) e^{-i(E/\hbar)t}}{1 - i(E - E_n)/(\hbar/2\Delta t_n)} dE, \\ \text{w// } \Phi_n(x) &= \frac{2i(-)^n}{Q\sqrt{k_n(x)}} \sin\left[\int_x^a k_n(x') dx' + \frac{\pi}{4}\right] \end{aligned} \right\} (21)$$

The integral gives the time-dependence for the wavepacket Ψ_n . Since the integral denominator is resonant over an energy range $\Delta E_n \sim \hbar/\Delta t_n$, while $f_n(E)$ does not vary appreciably over $\Delta E_n \gg \Delta E_n$, we can evaluate $f_n(E)$ at $E = E_n$, and take it outside the integral. Then...

$$\rightarrow \Psi_n(x, t) \approx \Phi_n(x) f_n(E_n) \cdot \underbrace{\frac{i\hbar}{2\Delta t_n} \int_{-\infty}^{\infty} \frac{e^{-i(E/\hbar)t} dE}{E - (E_n - i\hbar/2\Delta t_n)}}_{I_n}. \quad (22)$$

The remaining integral can be done by contour integration...

$$\left. \begin{aligned} &\dots \text{integrand has a simple pole at } E_n = E_n - i\hbar/2\Delta t_n \dots \\ &\dots \text{for } t > 0, \text{ close contour in } \underline{\text{lower}} \text{ half-plane:} \\ &\Rightarrow I_n = (-) 2\pi i \text{Res}(@ E_n) = -2\pi i e^{-\frac{i}{\hbar} E_n t}; \\ &\dots \text{for } t < 0, \text{ close contour in } \underline{\text{upper}} \text{ half-plane} \Rightarrow I_n = 2\pi i \text{Res}(\text{no pole}) = 0; \end{aligned} \right\}$$

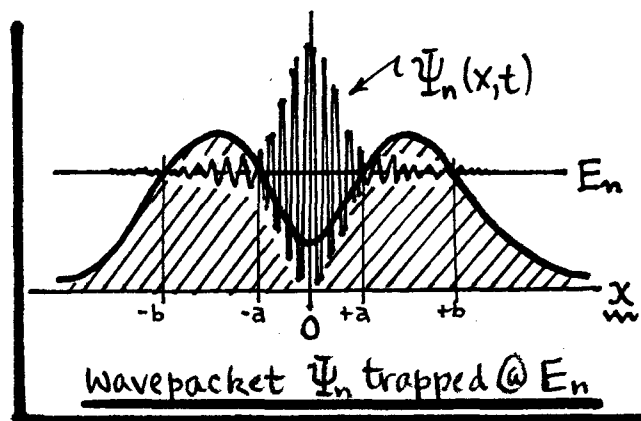


$$\text{so// } \rightarrow I_n = \left(\frac{2\pi}{i}\right) e^{-\frac{i}{\hbar} (E_n - \frac{i\hbar}{2\Delta t_n}) t}, \text{ for } t > 0; I_n \equiv 0, \text{ for } t < 0. \quad (23)$$

WKB: Final disposition of packet Ψ_n trapped in a well.

W(26)

When (23) is used in (22), we have the result for how an initially well-localized wavepacket Ψ_n behaves when trapped in the well near one of the well's bound state energies E_n . The analysis shows...



$$\left\{ \begin{array}{l} \Psi_n(x, t < 0) \equiv 0, \text{ prior to trapping;} \\ \Psi_n(x, t > 0) = \left[\frac{\pi \hbar}{\Delta t_n} f_n(E_n) \Phi_n(x) e^{-\frac{i}{\hbar} E_n t} \right] e^{-t/2\Delta t_n}, \text{ afterwards;} \\ \text{w// } \Delta t_n = \tau_n / 2Q^2 \quad \tau_n = 2m \int_{-a}^{+a} dx / p_n(x), \text{ natural period;} \\ \quad Q = \exp \left[-\int_a^b K(x) dx \right], \text{ tunneling factor.} \end{array} \right\} \quad (24)$$

The [] in $\Psi_n(x, t > 0)$ is just the (oscillatory) WKB bound state at energy E_n . But, because the "leakage" Q out of this state is putatively nonzero, the [WKB] state is modified by the additional "exponential decay factor", as noted. Ultimately Ψ_n becomes extinct, as $t \gg \Delta t_n$, because of "leakage", so Ψ_n can at most be called a "quasi-stationary" or "metastable" state.

Evidently, the intensity of Ψ_n decays as: $|\Psi_n|^2 \propto e^{-\Gamma_n t}$, w// decay rate:

$$\left\{ \begin{array}{l} \# \text{ decays/sec : } \Gamma_n = 1/\Delta t_n = \left(\frac{1}{\tau_n/2} \right) \cdot Q^2 \\ \quad \left(\begin{array}{l} \# \text{ times/sec particle} \\ \text{appears at a barrier} \end{array} \right) \quad \left(\begin{array}{l} \text{probability of barrier penetration} \\ \text{per presentation (transmission coeff.)} \end{array} \right) \end{array} \right\} \quad (25)$$

The factors entering Γ_n make physical sense, as labelled.

REMARKS

1. Whenever a QM stationary state can communicate with (i.e. is coupled to) other states, it will tend to make a transition, i.e. "decay", to the new states;
2. Whenever the emitted energy spectrum is Lorentzian ($|A(E)|^2$ in (19) is Lorentzian), the decay will be exponential: $|\Psi|^2 \propto e^{-\Gamma t}$, in lowest order.