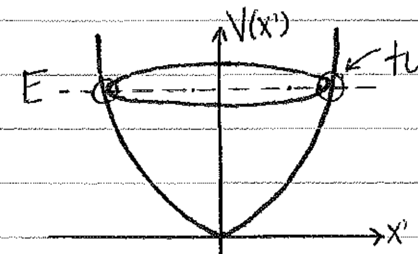
Lecture 23 - Bound States & Propagators

1. WKB - Bound States (2.5 SAK)
2. Propagators (2.6 SAK)

1. WKB (applications): Bound States

$$\psi(x) = \frac{1}{(E-V(x))^{1/4}} \exp\left[\frac{\pm i}{\hbar} \underbrace{\int^{x} dx' \sqrt{2m(E-V(x'))}}_{\int p(x')dx'}\right]$$

*Wavefunction must be single-valued



turning points

The wavefunction must be the same regardless of which turning point is analyzed.

→ $\pi/2$ phase shift @ turning points

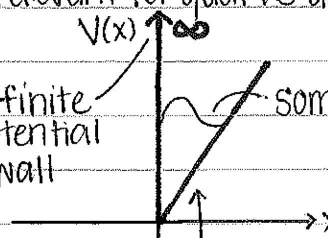
quantized orbits

$$\oint p(x', E_n)\,dx' = (n+\tfrac{1}{2})\pi\hbar$$ to achieve correct shift

→ This is incredibly similar to the Bohr-Sommerfeld quantization condition, which was derived from the above wavefunction and its requirement to be single-valued

Wedge potential:

(relevant for quarks and QCD)



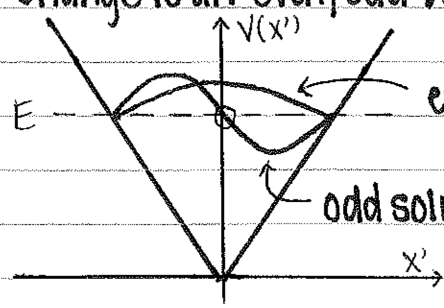
infinite potential wall

some bound states

Above $\pi/2$ phase shift assumed to be a smooth potential at the turning points.

quarks are confined here (infinitely)
- you can't pull them apart

→ Change to an even/odd wedge potential



even solution: $\psi(x') = \psi(-x')$

odd solution: $\psi(x') = -\psi(-x')$; $\underbrace{\psi(0) = 0}_{\text{Solution vanishes @ 0}}$

Choose the odd solution!

Now: **Solve the momentum integral**

$$\oint \sqrt{2m(E-\underbrace{|x'|\lambda}_{V(x')})}\,dx' = (n+\tfrac{1}{2})\pi\hbar$$

↑ n <u>must</u> be odd (odd solutions)

Where $V(x) \equiv mg|x| = \lambda|x|$ with turning points @ $-E/\lambda$, E/λ

integrate to the turning points

$$4\int_0^{E/\lambda} \sqrt{2m(E-x'\lambda)}\,dx' = (n+\tfrac{1}{2})\pi\hbar$$

└ origin → right T.P. → origin → left T.P. → origin

→ Integral yields quantized energy levels

$$E_n = \left(\frac{[3(m-\frac{1}{4})\pi]^{2/3}}{2}\right)(\lambda^2\hbar^2)^{1/3} \quad \text{for } \overbrace{n = 2m-1}^{\text{guarantees odd}}$$

$$\Rightarrow n+\tfrac{1}{2} = 2(m-\tfrac{1}{4})$$

└ analytic solution for bound states energies

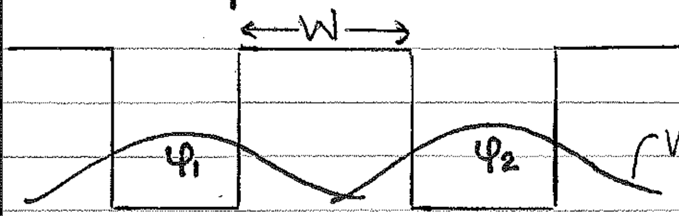
Bound states - approximating discrete energy levels

	Exact	WKB
n=1	2.2338	2.320
↓	⋮	⋮
n=10	12.829	12.828

the higher the state level, the more accurate your approximation becomes

<u>Tunneling</u>

Double-well potential



well potentials

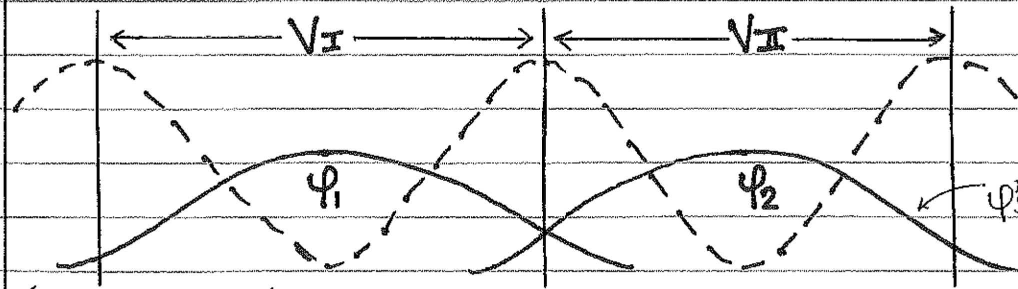
$$\psi_\pm = \frac{\varphi_1 \pm \varphi_2}{\sqrt{2}}$$

$$\mathcal{E}_\pm = E_0 \pm \delta \rightsquigarrow \sim e^{iW/\hbar}$$

But potential wells are rarely so perfectly square and the potentials are not so neatly defined...

— best just to describe potentials in terms of regions that may be defined as classically allowable or classically forbidden where the WKB approximation is applicable in the semiclassical realm and the entirely quantum realm.

→



φ's are just individual potentials in a single well

(let $\hbar=1$, $m=1/2$)

$\varphi_{1,2}$ correspond to the $E=0$ eigenstates

↳ satisfy $\begin{cases} (-\partial_{x'}^2 + V_I)\varphi_1 = 0 \\ (-\partial_{x'}^2 + V_{II})\varphi_2 = 0 \end{cases}$

Excited states in well $\gg 0$ (i.e. very far apart)

$$\Psi = c_1\varphi_1 + c_2\varphi_2 + \ldots \underbrace{f(\,)\cancel{\varphi_1^{ex}}}_{0} + \ldots \underbrace{f(\,)\cancel{\varphi_2^{ex}}}_{0}$$

there are excited state contributions, but their probabilities are incredibly small so we ignore them

What is the effective Hamiltonian of these two potentials?

$\langle\varphi_1|H|\varphi_2\rangle$ is the Bardeen tunneling formula (the overlap between the two wavefunctions)

$$H_{eff}^{(\varphi_1,\varphi_2)} = \begin{pmatrix} 0 & \overbrace{\langle\varphi_1|\hat{H}|\varphi_2\rangle} \\ \langle\varphi_2|\hat{H}|\varphi_1\rangle & 0 \end{pmatrix}$$

→ Use WKB to solve for φ_1, φ_2

$$\langle\varphi_1|\hat{H}|\varphi_2\rangle = \int dx'\,\varphi_1^*(-\partial_{x'}^2 + V(x'))\varphi_2$$

$$= \int_I dx'\,\varphi_1^*(-\partial_{x'}^2 + V_I(x'))\varphi_2 + \int_{II} dx'\,\varphi_1^*\underbrace{(-\partial_{x'}^2 + V_{II}(x'))\varphi_2}_{0}$$

↑ focus on region I

$$= \int_I dx'\,\varphi_1^*(-\partial_{x'}^2 + V_I(x'))\varphi_2$$

⟶ Solve using integration by parts

$$= \int_I dx'\left[-\partial_{x'}(\varphi_1^*\partial_{x'}\varphi_2) + (\partial_{x'}\varphi_1^*\partial_{x'}\varphi_2) + V_I(x')\varphi_1^*\varphi_2\right]$$

$$= \int_I dx'\left[-\partial_{x'}(\varphi_1^*\partial_{x'}\varphi_2) + \partial_{x'}[(\partial_{x'}\varphi_1^*)\varphi_2] \underbrace{- \partial_{x'}^2\varphi_1^*\varphi_2 + V_I\varphi_1^*\varphi_2}_{=0}\right]$$

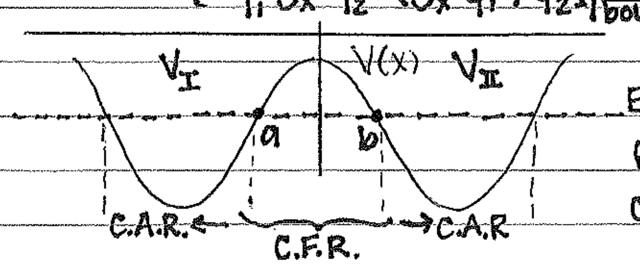
$$\Longrightarrow (-\partial_{x'}^2\varphi_1^* + V_I(x')\varphi_1)\varphi_2 = 0$$

└ Recall $(-\partial_{x'}^2 + V_I)\varphi_1 = 0$

$$\langle\varphi_1|\hat{H}|\varphi_2\rangle = \int_I dx'\,\partial_{x'}\left[-\varphi_1^*\partial_{x'}\varphi_2 + (\partial_{x'}\varphi_1^*)\varphi_2\right]$$

$$= \left[-\varphi_1^*\partial_{x'}\varphi_2 + (\partial_{x'}\varphi_1^*)\varphi_2\right]\Big|_{boundary}$$

*Answer does not depend on the boundary



C.A.R. - Classically allowed Region

C.F.R. - Clasically forbidden region

normalization constants

$$\varphi_1 = \frac{N_1}{\sqrt{V(x)-E}} \exp\left[-\int_a^x \sqrt{V(x')-E}\,dx'\right]$$

$$\varphi_2 = \frac{N_2}{\sqrt{V(x)-E}} \exp\left[+\int_b^x \sqrt{V(x')-E}\,dx'\right]$$

⇒ The Overlap Integral

$$\langle \varphi_1 | \hat{H} | \varphi_2 \rangle = N_1^* N_2 \exp\left(-\int_a^b \sqrt{V(x')-E}\,dx'\right)$$

2. **Propagators** (2.6 SAK)

The path integral – classical intuition + quantum features

$K \sim \langle x | e^{iH(t-t_0)/\hbar} | x' \rangle$

└ the propagator = the time evolution operator in real space

Start with the standard time evolution operator:

$$|\alpha; t\rangle = e^{iH(t-t_0)/\hbar} \underbrace{|\alpha; t_0\rangle}_{|\alpha\rangle \text{ – initial state}}$$

→ Introduce an entirely new set of states in the x-basis

$$\underbrace{\langle x' | \alpha; t\rangle}_{\psi_\alpha(x',t)} = \int dx'' \langle x' | e^{-iH(t-t_0)/\hbar} | x''\rangle \underbrace{\langle x'' | \alpha, t_0\rangle}_{\psi_\alpha(x'',t_0)}$$

$$K(x',t;x'',t_0) = \langle x' | e^{iH(t-t_0)/\hbar} | x''\rangle$$

└ Schrödinger equation equivalent for the unitary translation operator

$$\psi_\alpha(x',t) = \int dx'' K(x',t;x'',t_0)\,\psi_\alpha(x'',t_0)$$

↳ $K_{\text{observable}} = \sum_{aa'} \langle x' | a\rangle \langle a | \underbrace{e^{-iH(t-t_0)/\hbar} | a'\rangle}_{e^{-iE_a(t-t_0)/\hbar}\,\delta_{aa'}} \langle a' | x''\rangle$

$$= \sum_a \langle x' | a\rangle \langle a | x''\rangle \exp(-iE_a t/\hbar)$$

Propagator gives solution to the Schrödinger eq. → Propagator satisfies the S.E.

$$\Rightarrow \left[\frac{-\hbar^2}{2m}\partial_{x'}^2 + V(x') - i\hbar\partial_t\right] K(x',t;x'',t_0) \sim 0$$

└ constraint #1

$$\psi_\alpha(x',t\to t_0) = \int dx'' \delta(x'-x'')\,\psi_\alpha(x'',t_0)$$

$$\lim_{t\to t_0} K(x',t;x'',t_0) = \delta(x'-x'')$$

└ constraint #2

boundary conditions needed for unique solution

↳ yields $K(x',t;x'',t_0) = 0$ for $\underbrace{t < t_0}$

Causality – the preference of moving forward in time (though backwards is not forbidden)

Applying constraints:

$$\left[\frac{-\hbar^2}{2m}\partial^2_{x'} + V(x') - i\hbar\partial_t\right] K(x',t;x'',t_0) = -i\hbar\delta(x'-x'')\delta(t-t_0)$$

$$-i\hbar\partial_t K(x',t;x'',t_0) = -i\hbar\delta(x'-x'')\delta(t-t_0)$$ goes to 0 everywhere except very close to t_0 where it blows up

$\Rightarrow K(x',t_0+\delta;x'',t_0) = \delta(x'-x'')$, our boundary condition!

just the Green's function for the propagator

Reminder: Compare with Coulomb's Law

$$\nabla^2\varphi(x') = \rho(x')$$

$$\hookrightarrow \int dx''\delta(x'-x'')\rho(x'')$$

Boundary conditions: $\nabla^2 K(x',x'') = \delta(x'-x'')$

(!) You can break the initial wavefunction into tiny bits and then solve IF you know how to solve it (a lot of times, this is not the case)

Free Particle Solution: $(V=0)$

$$K(x't,x''t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\, e^{\frac{im(x'-x'')^2}{2\hbar(t-t_0)}}$$

In the Case of the Time-Independent Schrödinger Equation:

MIDTERM – PROBLEM 3

$$\left[\frac{-\hbar^2}{2m}\partial^2_{x'} + V(x') - E\right] K(x',x'';E) = \overbrace{\underbrace{-i\hbar}_{\text{convention}}\delta(x'-x'')}^{f(x')}$$

$i\hbar\partial_t$ becomes the energy in this case

$$\left[\frac{-\hbar^2}{2m}\partial^2_{x'} + V(x') - E\right]\psi_\alpha(x',E) = \left[\int dx''\delta(x'-x'')f(x'')\right] f(x')$$

As defined,

Fourier transform from time domain $\rightarrow$ energy domain

$$K(x',x'';E) = \int_{-\infty}^{\infty} dt\, \underbrace{\Theta(t-t_0)}_{\text{step function}} K(x',t;x'',t_0)\, e^{-iE(t-t_0)/\hbar}$$

$$= \int_{t_0}^{\infty} dt\, K(x',t;x'',t_0)\, e^{-iE(t-t_0)/\hbar}$$

step function expressed as explicit lower bound

For the free particle: $V=0$, time-independent S.W.E.

(the Mathematica solution)

$$K(x',x'';E) = \frac{m}{i\hbar}\frac{1}{\sqrt{2mE}}\exp\left[i\sqrt{\frac{2mE}{\hbar^2}}\,|x'-x''|\right]$$

Perturbation & the Midterm Problem

$$\left[\frac{-\hbar^2}{2m}\partial_x^2 + V(x) - E\right]\psi(x) = 0$$

↳ perturbation allows you to shift this out

$$\left[\frac{-\hbar^2}{2m}\partial_x^2 - E\right]\psi(x) = -\underbrace{V(x)}_{V(x)=V_0\delta(x)}\psi(x)$$

$$= -V_0\delta(x)\psi(x)$$

$$= -V_0\underbrace{\delta(x)\psi(0)}_{\delta(x)\psi(x)\text{ non-zero only @ }\psi(0)}$$

$$= (PF)f(x)$$

↑ can treat this prefactor. Some function of x to describe this propagator with respect to the wavefunction

$$\psi_\alpha(x',E) = (PF)\int dx''\, K(x',x'';E)\, f(x'')$$

where K here is the propagator of the Time-Independent Schrödinger Equation free particle

*Note: $f(x'')$ does not solve any Schrödinger Wave Eq. because it is usually some combination of $V(x'')\psi(x'')$, which is not terribly informative except under Born Approximation conditions