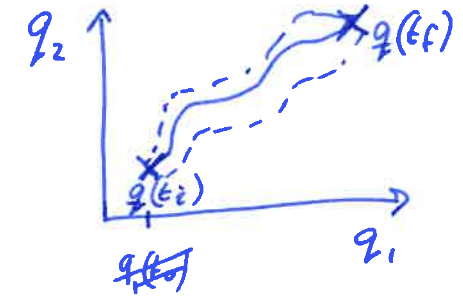
1. The Lagrangian formulation of Quantum Mechanics

1.1 Lagrangian classical mechanics



generalised coördinates $q_i(t) = \underline{q}(t)$

" velocities $\dot{q}_i(t) = \dot{\underline{q}}(t)$

Lagrangian $L = \underset{\text{kinetic}}{T} - \underset{\text{potential}}{V}$

$$L(\{q_i\},\{\dot{q}_i\},t) = \tfrac{1}{2}m\dot{q}_i^2 - V(\underline{q})$$

The 'principle of least action':

classical paths $\underline{q}$ extremise the 'action', S:

$$S[\underline{q}] \hat{=} \int_{t_i}^{t_f} L\,dt$$

(equivalent to Newton's laws)

'functional': ~ 'function of functions' $\underline{q}(t)$.

functional

To extremise:

$$\left(\frac{\partial S[\underline{q}+\lambda\underline{\epsilon}]}{\partial\lambda}\right)_{\underline{q},\underline{\epsilon}}\Bigg|_{\lambda=0} = 0 \quad . \qquad (\underline{\epsilon}(t_i) = \underline{\epsilon}(t_f) = 0)$$

$$\therefore \quad S[\underline{q}+\lambda\underline{\epsilon}] = \int_{t_i}^{t_f} L(\underline{q}+\lambda\underline{\epsilon},\, \dot{\underline{q}}+\lambda\dot{\underline{\epsilon}},\, t)\,dt$$

(chain rule)

$$\left(\frac{\partial S[\underline{q}+\lambda\underline{\epsilon}]}{\partial\lambda}\right)_{\underline{q},\underline{\epsilon}} = \int \frac{\partial L}{\partial \underline{q}}\frac{\partial(\underline{q}+\lambda\underline{\epsilon})}{\partial\lambda} + \frac{\partial L}{\partial\dot{\underline{q}}}\frac{\partial(\dot{\underline{q}}+\lambda\dot{\underline{\epsilon}})}{\partial\lambda} + \cancel{\frac{\partial L}{\partial t}\frac{\partial t}{\partial\lambda}}\,dt$$

$$= \int \frac{\partial L}{\partial\underline{q}}\cdot\underline{\epsilon} + \frac{\partial L}{\partial\dot{\underline{q}}}\cdot\dot{\underline{\epsilon}}\,dt$$

↓ by parts

$$= \underbrace{\int \underline{\epsilon}\cdot\left(\frac{\partial L}{\partial\underline{q}} - \frac{d}{dt}\frac{\partial L}{\partial\dot{\underline{q}}}\right)dt}_{=0\ \forall\,\underline{\epsilon}} .$$

PTO

Therefore $$\boxed{\frac{\partial L}{\partial \underline{q}} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\underline{q}}}\right) = 0}$$ "the Euler Lagrange Equation(s)".

E.g. if $L = \frac{1}{2} m \dot{\underline{q}}^2 - V(\underline{q})$

we get $-V'(\underline{q}) = m\ddot{\underline{q}}$ Newton's 2nd law.

NB what is $\frac{\partial L}{\partial \underline{q}}$?!

it's just a vector $\frac{\partial L}{\partial q_i} = \begin{pmatrix} \frac{\partial L}{\partial q_1} \\ \frac{\partial L}{\partial q_2} \\ \vdots \end{pmatrix}_i = \left(\frac{\partial L}{\partial \underline{q}}\right)_{\text{element } i}$

1.2 Hamiltonian mechanics

- uses $\{\underline{p}, \underline{q}\}$ instead of $\{\underline{q}, \dot{\underline{q}}\}$.

$\underline{p} \triangleq \frac{\partial L}{\partial \dot{\underline{q}}}$ 'the momentum conjugate to $\dot{\underline{q}}$'

then $\boxed{H \triangleq \underline{p}\cdot\dot{\underline{q}} - L}$ → (a 'Legendre transform')

the 'Hamiltonian'

& Hamilton's equations of motion:

$$\boxed{\dot{\underline{q}} = \frac{\partial H}{\partial \underline{p}} \; ; \; \dot{\underline{p}} = -\frac{\partial H}{\partial \underline{q}}}$$

1.3 Connecting to Quantum Mechanics

Define the 'Poisson bracket'

$f(\underline{p},\underline{q},t)$ → $$\boxed{\{f, g\} \triangleq \frac{\partial f}{\partial \underline{q}}\cdot\frac{\partial g}{\partial \underline{p}} - \frac{\partial f}{\partial \underline{p}}\cdot\frac{\partial g}{\partial \underline{q}}}$$

Therefore (Exercise): $$\boxed{\dot{\underline{q}} = \{\underline{q}, H\} \; ; \; \dot{\underline{p}} = \{\underline{p}, H\}}$$

For $f(p,q,t)$ the chain rule gives

$$\frac{df}{dt} = \frac{\partial f}{\partial q}\cdot\frac{\partial q}{\partial t} + \frac{\partial f}{\partial p}\cdot\frac{\partial p}{\partial t} + \frac{\partial f}{\partial t}$$

$$\therefore \boxed{\frac{df}{dt} = \{f, H\} + \left(\frac{\partial f}{\partial t}\right)_{p,q}}$$

"Hamilton's equation of motion"

But cf. the "Heisenberg equation of motion" from QM:

$$\boxed{\frac{d\hat{A}}{dt} = \frac{1}{i\hbar}[\hat{A}, \hat{H}] + \frac{\partial \hat{A}}{\partial t}}$$

(in the Heisenberg picture, operators $\hat{A}(t)$ are time dependent. This is Heisenberg's equivalent to the Schrödinger equation. Will see more of it later).

Classical constants of motion obey

$$\frac{df}{dt} = 0 \implies \{f, H\} = 0 \quad \text{(Liouville's equation)}$$

while the quantum operators corresponding to good quantum numbers obey

$$\frac{d\langle\hat{A}\rangle}{dt} = 0 \implies [\hat{A}, \hat{H}] = 0 .$$

(assuming no explicit t dependence $\frac{\partial A}{\partial t} = 0$).

1.4 Canonical Quantization

Classical observables become (necessarily) non-commuting operators in QM . . .

$$q \longrightarrow \hat{q} \quad (\text{more typically called } \hat{x})$$

$$p \rightarrow \hat{p} = -i\hbar\hat{\nabla}$$

$$H = T + V \rightarrow \hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V(\hat{x}) .$$

$$\& \quad H \rightarrow i\hbar\frac{\partial}{\partial t} \quad \ldots$$

1.5 Time evolution in QM

Recall the time dependent Schrödinger equation (TDSE):

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$$

or in Dirac notation (basis independent):

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle .$$

Therefore

$$\boxed{|\psi(t)\rangle = \hat{U}(t-t_0)|\psi(t_0)\rangle}$$

where

$$\boxed{\hat{U}(t-t_0) = e^{-i\hat{H}(t-t_0)/\hbar}}$$

the 'time translation operator'
or 'time evolution operator'.

Since $\hat{H}$ is <u>Hermitian</u>, $\hat{H}^\dagger = \hat{H}$, $\hat{U}$ is <u>unitary</u>, $\hat{U}^\dagger = \hat{U}^{-1}$.

Some people derive the TDSE from unitarity, finding the latter the more natural.

We will return to time evolution in detail in section 4.

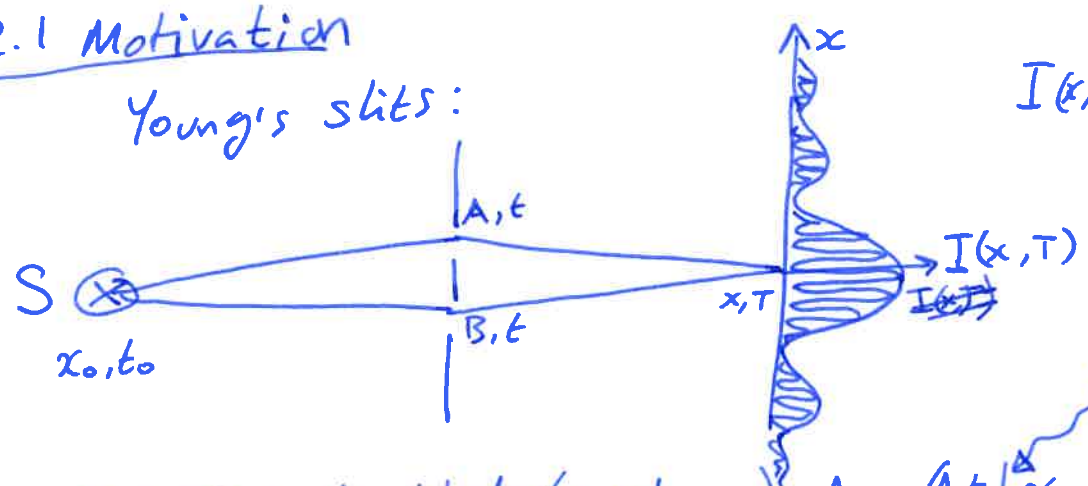
2. Path Integral QM

— Dirac 1934, Feynman 1948

2.1 Motivation

Young's slits:

$$I(x,T) = |\psi(x,T)|^2$$



'given'

$$\psi(x,T) = \text{Amplitude}(x,T\,|\,A,t)\cdot \text{Amp.}(A,t\,|\,x_0,t_0) + \text{Amp.}(x,T\,|\,B,t)\cdot\text{Amp.}(B,t\,|\,x_0,t_0)$$

Amplitudes act like probabilities in QM; then

$$\text{Probability} = |\text{Amp.}|^2.$$

$$\text{Amp.}(x,T\,|\,x_0,t_0) \triangleq K(x,T;x_0,t_0)$$

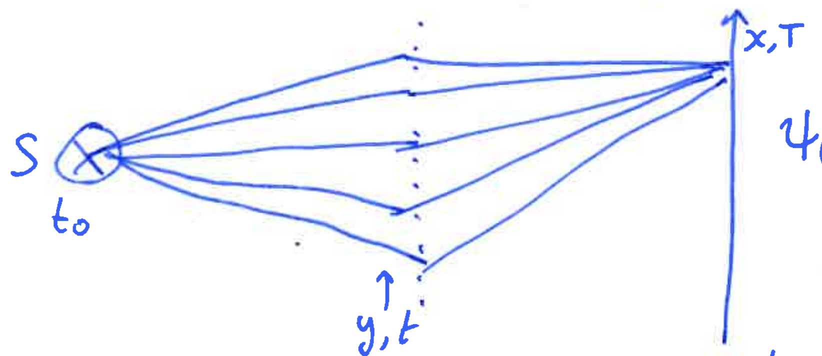
(NB I use $\triangleq$ to mean 'equal by definition')

'the propagator'.

$$K(x,T;x_0,t_0) = \langle x|\hat{U}(T-t_0)|x_0\rangle.$$

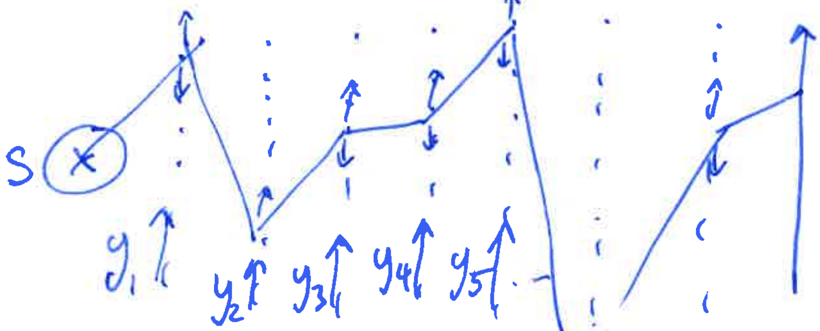
(we will return to this shortly).

What if there are no slits / ∞ slits? → (Depending on how you look at it!)



$$\psi(x,T) = \int dy\, \text{Amp}(x,T\,|\,y,t)\,\text{Amp.}(y,t\,|\,S)$$

True @ all points — path integral: $\underbrace{\text{'}\mathcal{D}y\text{'}}$ 'functional integral'



$$\psi(x,T) = \overbrace{\int dy_1 \cdots dy_N}\, \text{Amp}(x,T\,|\,y_N,t_N)\cdot \text{Amp}(y_N,t_N\,|\,y_{N-1},t_{N-1})\cdot\ldots\,\text{Amp}(y_1,t_1\,|\,S)$$

NB paths are everywhere continuous, nowhere differentiable.

Why use path integrals?

- In many senses more fundamental. E.g. $\int L\,dt$ can be a Lorentz scalar $\rightarrow$ relativistic QM.
- useful for some calculations, e.g Aharonov Bohm effect (see later in course)
- Gives its own interpretation of QM: [Feynman 1948]
  - (i) Prob. $= |\psi|^2$
  - (ii) $\psi = \sum_{\text{paths}}$ configuration space
  - (iii) paths weighted by $e^{iS_{cl}[x]/\hbar}$ ← classical action.

2.2 The propagator

Recall: $|\psi(t)\rangle = \hat{U}(t-t_0)|\psi(t_0)\rangle$ (equivalent to TDSE).

$$\therefore \langle x|\psi(t)\rangle = \langle x|\hat{U}(t-t_0)|\psi(t_0)\rangle$$

Insert a 'resolution of the identity': $\int dx'\,|x'\rangle\langle x'| = \hat{\mathbb{1}}$

where $\hat{\mathbb{1}}|a\rangle = |a\rangle \quad \forall\, |a\rangle$.

$$\therefore \underbrace{\langle x|\psi(t)\rangle}_{\psi(x,t)} = \int dx'\,\underbrace{\langle x|\hat{U}(t-t_0)|x'\rangle}_{\substack{K(x,t;x',t_0)\\ \text{the propagator.}}}\underbrace{\langle x'|\psi(t_0)\rangle}_{\psi(x',t_0)}$$

Imagine a completely localised initial wavepacket:

$$\psi(x',t_0) = \delta(x'-x_0) \rightarrow (\text{Dirac } \delta)$$

$$\therefore \psi(x,t) = K(x,t;x_0,t_0).$$

the propagator <u>is</u> the amplitude to find the particle @ x,t given it was @ x_0,t_0.

2.3 The propagator: free space

Recall $K(x,t;x_0,t_0) = \langle x| e^{-i\hat{H}(t-t_0)/\hbar} |x_0\rangle$.

In free space $V=0$

$\therefore \hat{H} = \hat{T} = \hat{p}^2/2m$.

$$\therefore K(x,t;x_0,t_0) = \langle x| e^{-i\hat{p}^2(t-t_0)/2m\hbar} |x_0\rangle.$$

Insert $\hat{\mathbb{1}} = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|$ (we'll use this trick a lot!)

$$K(x,t;x_0,t_0) = \int_{-\infty}^{\infty} dp \langle x| e^{-i\hat{p}^2(t-t_0)/2m\hbar} |p\rangle\langle p|x_0\rangle.$$

But $\hat{p}|p\rangle = \overbrace{p}^{\text{number}}|p\rangle$

& $f(\hat{p})|p\rangle = f(p)|p\rangle$ (functions are defined by their Taylor series).

$$\therefore K(x,t;x_0,t_0) = \int dp\, e^{-ip^2(t-t_0)/2m\hbar} \underbrace{\langle x|p\rangle}_{\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}} \underbrace{\langle p|x_0\rangle}_{\frac{1}{\sqrt{2\pi\hbar}} e^{-ipx_0/\hbar}}$$

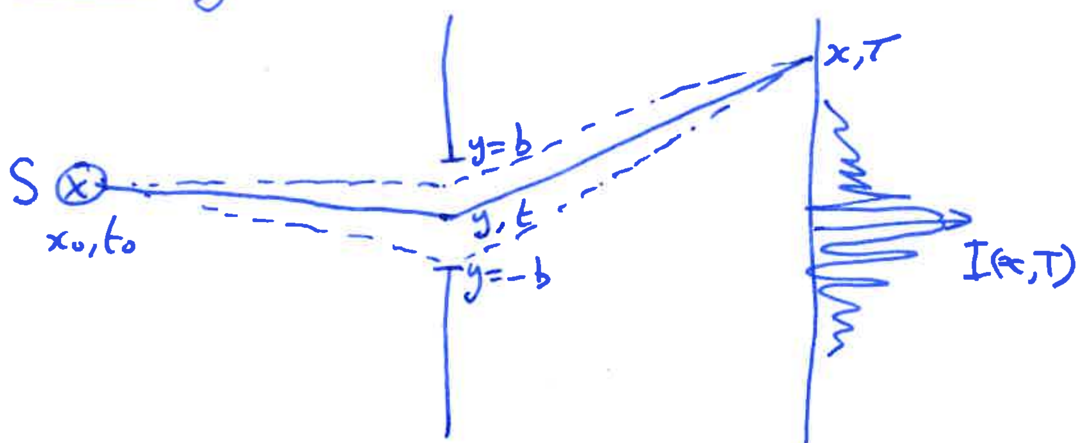
$$\therefore K(x,t;x_0,t_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, e^{\frac{i}{\hbar}\left(p(x-x_0) - p^2(t-t_0)/2m\right)}$$

– Gaussian integral.

Show in problem set:

$$K(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi i\hbar}}\frac{1}{\sqrt{t-t_0}}\, e^{i(x_0-x)^2 m/2\hbar(t-t_0)}$$

2.4 E.g. Finite width slit



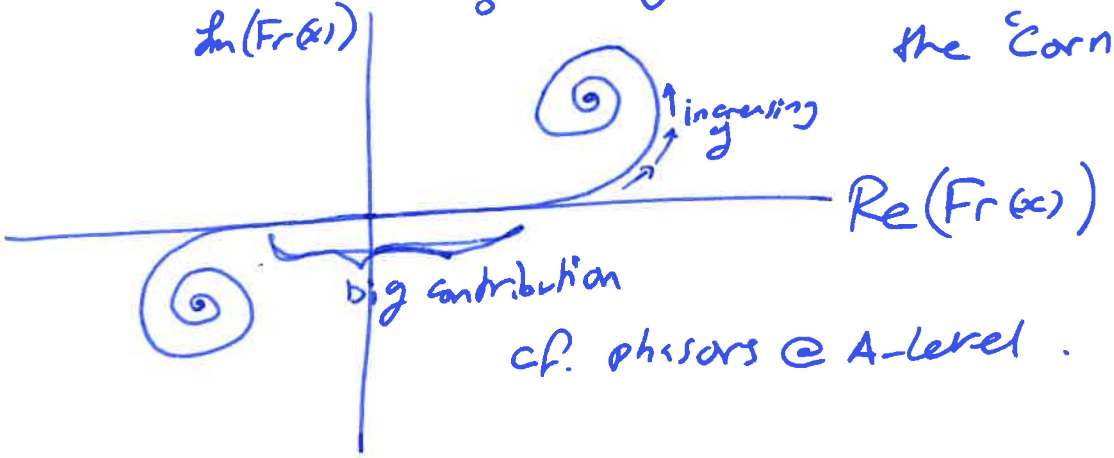
$$\psi(x,T) = \int_{-b}^{b} dy\, K(x,T;y,t)\,K(y,t;x_0,t_0) \qquad (\delta(x'-x_0) \text{ at } t=t_0)$$

$$= \text{const.}\ \frac{1}{\sqrt{T-t}}\frac{1}{\sqrt{t-t_0}}\int_{-b}^{b} e^{i(x-y)^2 m/2\hbar(T-t)}\, e^{i(y-x_0)^2 m/2\hbar(t-t_0)}\, dy$$

Can be written as a 'Fresnel integral':

$$Fr(x) = \int_0^x e^{iy^2} dy \,.$$

the 'Cornu spiral'



cf. phasors @ A-level.

2.5 Equivalence between Feynman & Schrödinger

– Explicit in the construction:

$$K(x,T;x_0,t_0) = \langle x|\hat{U}(T-t_0)|x_0\rangle$$

$$= \langle x|e^{-i\hat{H}(T-t_0)/\hbar}|x_0\rangle. \Big\} \equiv \text{TDSE}.$$

('equivalent to')

– Some prefer to derive TDSE using the limit

$$\lim_{\delta t\to 0} K(x, t+\delta t; x, t)$$

but it's equivalent.

2.6 The propagator: general case — Deriving Feynman (iii)

In general, $\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V(\hat{x})$.

$$\therefore\ K(x,t;x_0,t_0) = \langle x|e^{-i(\hat{T}+\hat{V})(t-t_0)/\hbar}|x_0\rangle.$$

<u>Problem</u>: $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}e^{\hat{B}}$ unless $[\hat{A},\hat{B}]=0$.

otherwise we could separate $e^{-i\hat{T}(t-t_0)/\hbar}\, e^{-i\hat{V}(t-t_0)/\hbar}$ & insert identities...

Solution : 'time slicing'.

Break path into tiny slices using $\delta t = t/N$, N large.

Then, $e^{-i\hat{H}t/\hbar} = \left(e^{-i\hat{H}\delta t/\hbar}\right)^N$

& $e^{-i(\hat{T}+\hat{V})\delta t/\hbar} \simeq e^{-i\hat{T}\delta t/\hbar} e^{-i\hat{V}\delta t/\hbar}$ (exact for $\delta t \to 0$).

We have: $K(x_N, t; x_0, t=0) = \langle x_N | \underbrace{e^{-i\hat{H}\delta t/\hbar} \times \cdots}_{N \text{ identical copies.}} | x_0 \rangle$

for ease of notation(!)

Insert $N-1$ copies of $\hat{1} = \int dx_i |x_i\rangle\langle x_i|$:

$$K = \int dx_1 \cdots \int dx_{N-1} \underbrace{\langle x_N | e^{-i\hat{H}\delta t/\hbar} | x_{N-1}\rangle}\langle x_{N-1} | e^{-i\hat{H}\delta t/\hbar} | x_{N-2}\rangle \cdots$$

$\therefore$ N copies of $K_n \triangleq K(x_{n+1}, \delta t; x_n, 0) = \langle x_{n+1} | e^{-i\hat{H}\delta t/\hbar} | x_n\rangle$

Now use that δt is small:

$$K_n \simeq \langle x_{n+1} | e^{-i\hat{T}\delta t/\hbar} e^{-i\hat{V}\delta t/\hbar} | x_n \rangle$$

& insert $\hat{1} = \int dp |p\rangle\langle p|$ as with the free particle:

$$K_n \simeq \int \underbrace{\langle x_{n+1} | e^{-i\hat{T}\delta t/\hbar} | p \rangle}_{e^{-ip^2\delta t/2m\hbar} \cdot \underbrace{\langle x_{n+1} | p\rangle}_{\frac{1}{\sqrt{2\pi\hbar}} e^{ipx_{n+1}/\hbar}}} \underbrace{\langle p | e^{-i\hat{V}\delta t/\hbar} | x_n \rangle}_{e^{-iV(x_n)\delta t/\hbar} \cdot \underbrace{\langle p | x_n\rangle}_{\frac{1}{\sqrt{2\pi\hbar}} e^{-ipx_n/\hbar}}} dp$$

$$\therefore K_n \simeq e^{-iV(x_n)\delta t/\hbar} \cdot K_n^{\text{free}}$$

$$= e^{-iV(x_n)\delta t/\hbar} \cdot e^{im(x_{n+1}-x_n)^2/2\hbar\delta t} \cdot \sqrt{\frac{m}{2\pi i\hbar\delta t}}.$$

All together...

$$K(x_N, t; x_0, 0) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\delta t}\right)^{N/2} \int dx_1 \cdots dx_{N-1} \exp\left(\frac{i\delta t}{\hbar} \sum_{n=1}^{N-1} \frac{m}{2}\left(\frac{x_{n+1}-x_n}{\delta t}\right)^2 - V(x_n)\right).$$

But $\lim_{N\to\infty} \delta t \sum_{n=1}^{N-1} \frac{m}{2}\left(\frac{x_{n+1}-x_n}{\delta t}\right)^2 - V(x_n)$

$$= \int_0^t dt' \, \frac{m}{2}\dot{x}^2 - V(x)$$

$$= \int_0^t dt' \, L(x,\dot{x},t')$$

$$= S_{cl}[x] \; !$$

$\rightarrow$ (the classical action)

$$\therefore \; K(x,t;x_0,t_0) = \int \mathcal{D}x \, e^{iS[x]/\hbar}$$

Feynman's (iii)-rd postulate of QM.

Paths weighted with equal magnitude (however crazy) but varying phase.

NB check this intermediate step:

$$K(x_{n+1},\delta t; x_n, 0) = \underbrace{e^{-iV(x_n)\delta t/\hbar}}_{} K^{\text{free}}(x_{n+1},\delta t; x_n, 0)$$

interaction simply modifies phase of intermediate paths.

This motivates the 'interaction picture', to which we return shortly.

2.7 What about commutators?!

– An advanced diversion (non-examinable!)

Time slicing uses $e^{-i(\hat{T}+\hat{V})\delta t/\hbar} \simeq e^{-i\hat{T}\delta t/\hbar} e^{-i\hat{V}\delta t/\hbar}$

How do you get the non-commutation of operators back?

One way to see this is via a curious connection between QM & statistical mechanics...

Note: $$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$$

bears a formal resemblance to the heat/diffusion equation:

$$\frac{\partial \rho(x,\tau)}{\partial \tau} = D\frac{\partial^2 \rho}{\partial x^2}$$

ρ = density of diffusing material, or heat
τ = time.

~~Thus~~ $\therefore$ Substituting $\boxed{t \to -i\tau}$ in the TDSE gives diffusion.

This is called a 'Wick rotation' to 'imaginary time' (!).

~~As a result~~ ~~More generally, we have~~

Similarly, in QM we have:

$$\langle x_f | e^{-i\hat{H}t/\hbar} | x_i \rangle = \int \mathcal{D}x \, e^{iS[x]/\hbar}$$

where $S[x] = \int_{t_i}^{t_f} dt' \, \frac{1}{2}m\dot{x}^2 - V(x)$.

Whereas in statistical mechanics we have:

$$\langle x_f | e^{-\beta\hat{H}} | x_i \rangle = \int \mathcal{D}x \, e^{-S_E[x]/\hbar}$$

where $\beta = 1/k_B T$

& $S_E[x] = \int_0^{\beta\hbar} d\tau \, \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)$.

Again, $t \to -i\tau$. (τ has units of $\beta\hbar$, or time).

This gives the result:

$\boxed{\text{QM in } \underbrace{N}_{\text{space}} + \underbrace{1}_{\text{time}} \text{ D is statistical mechanics in } N+0 \text{ D!}}$

NB S_E is called the 'Euclidean action'.

This is because the Lorentz metric $x^2 - c^2t^2$ becomes the Euclidean metric $x^2 + c^2\tau^2$ under Wick rotation.

Back to commutation:

whether the path integral is well defined depends on the action.

In general it works better in the Euclidean metric, where paths are suppressed exponentially by $e^{-\beta \hat{H}}$.

So: surely $[q, \dot{q}] = 0$, violating the Heisenberg uncertainty principle...

but it doesn't.

$$[q, \dot{q}] = q(t+\delta t) \frac{q(t+\delta t) - q(t)}{\delta t} - q(t) \frac{q(t+\delta t) - q(t)}{\delta t}$$

operator order becomes time order in path integrals.

$$\text{So } [q, \dot{q}] = (q(t+\delta t) - q(t))^2 / \delta t = \left(\frac{q(t+\delta t) - q(t)}{\delta t}\right)^2 \cdot \delta t$$

But surely this is still zero: $\dot{q}^2 \cdot \delta t$ ...

No! In Stat. Mech. this is Brownian motion.

For that, we know $\underline{\delta q^2 \sim \delta t}$ (cf. random walk). This is formalised as 'Itô's Lemma'.

$\therefore [q, \dot{q}] = 1$ not 0!

Wick rotate back...

$$[x, p] = i\hbar .$$

The trick is that $\dot{q}^2 \delta t$ is not zero if $\dot{q}^2 \to \infty$ as $\delta t \to 0$.

Non-commutation arises from the jaggedness of the paths.

Recall: paths are everywhere continuous, but nowhere differentiable.

3. Semiclassics

A strength of the path integral approach is that the classical path is typically dominant (recall the Cornu Spiral). Other paths are thought of as 'quantum corrections' or 'quantum fluctuations' (a slight misnomer).

Here we will see this idea in more detail.

Why do semiclassics?

— If you think classically, it gives an intuitive view of QM (perhaps outdated)

— It's invaluable to some fields, e.g quantum chaos.
(quantum = linear (TDSE), chaos = nonlinear ...)
→ Look up the Berry Keating conjecture: ~~Solving~~ Proving the Riemann Hypothesis (£1M prize) may be ≡ to finding $\hat{H}$ whose classical limit is xp ...

— Useful in optics

— gives analytical approximate solutions (not just numerical)

— Most importantly: it's how we do QFT.
'Free particles' are governed by the classical action.

3.1 Mathematical background

3.11 Gaussian integrals (1D)

Recall the trick.

$$I = \int_{-\infty}^{\infty} dx\, e^{-ax^2} \qquad a \in \mathbb{C},\ Re(a) \geq 0.$$

to solve: $I^2 = \iint_{-\infty}^{\infty} dx\,dy\, e^{-a(x^2+y^2)}$

Use polar coörds:

$$I^2 = \int_0^\infty r\,dr \int_0^{2\pi} d\theta\, e^{-ar^2}$$

$$= 2\pi \left[\frac{e^{-ar^2}}{-2a} \right]_0^\infty$$

$$= \pi/a$$

$$\therefore I = \sqrt{\pi/a}. \qquad \text{or for } a \to \tfrac{a}{2},\ I = \int_{-\infty}^{\infty} e^{-\frac{1}{2}ax^2} dx = \sqrt{\frac{2\pi}{a}}.$$

3.12 Gaussian Integrals (ND)

$$I(\underline{\underline{A}}) = \int d^n\underline{x}\, e^{-\frac{1}{2}\underline{x}^T \underline{\underline{A}}\, \underline{x}}$$

$\underline{\underline{A}}$ a symmetric, $\underbrace{\text{+ve definite}}_{\equiv x^T \underline{\underline{A}} x > 0 \ \forall \underline{x} \in \mathbb{R}^N.}$ matrix.

Use $\underline{\underline{A}} = \underline{\underline{O}}\,\underline{\underline{D}}\,\underline{\underline{O}}^T$

$\underline{\underline{D}} \to \operatorname{diag}(a_1, a_2 \cdots, a_N)$ $\to$ eigvals all +ve.

$\underline{\underline{O}}$ orthogonal: $\underline{\underline{O}}^T\underline{\underline{O}} = \underline{\underline{1}}$.

$$\therefore \underline{x}^T \underline{\underline{A}}\,\underline{x} = \underline{\tilde{x}}^T \underline{\underline{D}}\,\underline{\tilde{x}} \quad \text{where } \underline{\tilde{x}} = \underline{\underline{O}}\,\underline{x}$$

$$= \sum_{i=1}^N a_i \tilde{x}_i^2.$$

$$|\det(\underline{\underline{O}})| = 1 \quad \therefore \text{Jacobian} = 1.$$

$$\therefore I(\underline{\underline{A}}) = \prod_{i=1}^N \int d\tilde{x}_i\, e^{-\frac{1}{2}a_i \tilde{x}_i^2}$$

$$= (2\pi)^{N/2} (a_1 \cdots a_N)^{-1/2}$$

$$I(\underline{\underline{A}}) = \sqrt{\frac{(2\pi)^N}{\det(\underline{\underline{A}})}}.$$

3.13 Gaussian Integrals (∞D)

$$I(\hat{A}) = \int \mathcal{D}x\, e^{-\frac{1}{2}\int_0^t x(t')\hat{A}\,x(t')dt'}$$

$$= \sqrt{\frac{(2\pi)^\infty}{\det(\hat{A})}}.$$

Recall: functions $\to x(t)$ are ∞D vectors

differential operators $\to \hat{A}$ are $\infty \times \infty$ matrices.

& $\det(\hat{A}) = \prod$ eigenvalues of $\hat{A}$.

E.g. $\frac{1}{2}\int_0^t x(t')\hat{A}\,x(t')\,dt' = S_E[x]$

$$= \int_0^{\beta\hbar} \tfrac{1}{2}m\dot{x}^2 + V(x)\,d\tau\ .$$

3.14 Functional calculus

We've seen the functional integral $\int \mathcal{D}x = \int dx_1 \int dx_2 \cdots \int dx_N$ $(N\to\infty)$.

Recall page ①: classical paths extremise the action.

$$\left.\left(\frac{\partial S[\underline{x}+\lambda\underline{\varepsilon}]}{\partial\lambda}\right)\right|_{\lambda=0} = 0$$

* sorry, quick ink change...

giving the Euler Lagrange equations:

$$\frac{\partial L}{\partial \underline{x}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\underline{x}}} = 0\ .$$

We can also do this with functional differentiation:

Vary $S[\underline{x}]$, a function of functions, with respect to the function $\underline{x}(t)$.

Switch to full Einstein Σ notation: $x_i = [\underline{x}]_{\text{element } i}$.

$x_i x^i = \underline{x}\cdot\underline{x}$

$$S[x_i] = \int_0^t L(x_i, \dot{x}_i)\,dt' \quad \text{(neglect explicit } t \text{ dependence)}$$

*inky fingerprints...

$$\delta S[x_i] = \int_0^t \left(\frac{\partial L}{\partial x_i}\,\delta x_i + \frac{\partial L}{\partial \dot{x}_i}\,\delta\dot{x}_i\right)dt'$$

usual notation for a small change

chain rule.

By parts on 2nd term:

$$\delta S = \int_0^t \left(\frac{\partial L}{\partial x_i}\,\delta x_i - \frac{d}{dt'}\left(\frac{\partial L}{\partial \dot{x}_i}\right)\delta x_i\right)dt'$$

$$\delta S = \int_0^t \left(\frac{\partial L}{\partial x_i} - \frac{d}{dt'}\frac{\partial L}{\partial \dot{x}_i}\right)\delta x_i\,dt'$$

$$\therefore \quad \frac{\delta S}{\delta x_j(t)} = \int_0^t \left(\frac{\partial L}{\partial x_i} - \frac{d}{dt'} \frac{\partial L}{\partial \dot{x}_i} \right) \frac{\delta x_i}{\delta x_j} \, dt'$$

Now use : $\boxed{\dfrac{\delta x_i(t')}{\delta x_j(t)} = \delta_i^j \, \delta(t'-t)}$

← Kronecker δ, keeping track of upper / lower indices

$$\therefore \quad \frac{\delta S}{\delta x_j(t)} = \frac{\partial L}{\partial x_j(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_j(t)}$$

& this $= 0$.

3.2 the method of stationary phase

3.21 1D

Consider the familiar integral

$$I(\varepsilon) = \int_{-\infty}^{\infty} dx \, e^{i f(x)/\varepsilon} \quad \text{where } \varepsilon \text{ is small (cf. } \hbar\text{).}$$

The integral is dominated by the saddle points, x_b, defined by $\left.\dfrac{df}{dx}\right|_{x=x_b} = 0$.

(I will use the notation $f'(x_b)$ to mean $\left.\dfrac{df(x)}{dx}\right|_{x=x_b}$).

This is because the phase winds slowest here. (Recall the Cornu spiral again!)

At these saddle points we can Taylor expand f:

$$I_b(\varepsilon) \simeq e^{i f(x_b)/\varepsilon} \int_{-\infty}^{\infty} dx \, e^{\frac{i}{2\varepsilon}(x-x_b)^2 f''(x_b)}$$

Since $f(x) \simeq f(x_b) + \cancel{(x-x_b) f'(x_b)} + \dfrac{(x-x_b)^2}{2} f''(x_b) + \dots$

0   neglect.

Therefore $I_b(\varepsilon) \simeq \sqrt{\dfrac{2\pi i \varepsilon}{f''(x_b)}} \, e^{i f(x_b)/\varepsilon}$

or $I_b(\varepsilon) \simeq \sqrt{\frac{2\pi\varepsilon}{|f''(x_b)|}}\, e^{i f(x_b)/\varepsilon + \nu_b \pi i/4}$

$\nu_b = \mathrm{Sign}(f''(x_b))$.

In general there are multiple saddle points to sum over:

$$I(\varepsilon) = \sum_b I_b(\varepsilon).$$

N.B. the classical path is actually a saddle point of $S[x]$ in general — not just an extremum.

N. Molto B.: 'the method of stationary phase' becomes 'the method of steepest descent' for integrals of the form $\int dx\, e^{-f(x)\cdot\varepsilon}$.

3.22 ND

$$I(\varepsilon) = \int d^N\underline{x}\, e^{i f(\underline{x})/\varepsilon}$$

as before, $f(\underline{x}) \simeq f(\underline{x}_b) + \frac{1}{2}(x_i - x_{b,i})(x_j - x_{b,j}) \frac{\partial^2 f(\underline{x})}{\partial x_i \partial x_j}$

as $\left.\frac{\partial f}{\partial x_i}\right|_{x_{b,i}} = 0$ at a saddle point.

$$\therefore\ I(\varepsilon) = \sum_b \sqrt{\frac{(2\pi\varepsilon)^N}{\left|\det\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)\right|}}\, e^{i f(\underline{x}_b)/\varepsilon + \nu_b \pi i/4}$$

$\nu_b = \mathrm{Sgn}\left(\det\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)\right)$.

3.23 ∞D

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}x\, e^{iS[x]/\hbar}$$

$$\simeq \sum_b \sqrt{\frac{(2\pi\hbar)^\infty}{\left|\det\left(\frac{\delta^2 S}{\delta x(t_f)\,\delta x(t_i)}\right)\right|}}\, e^{iS[x_b]/\hbar + \nu_b \pi i/4}$$

where $x_b(t)$ are paths satisfying $\left.\frac{\delta S[x]}{\delta x(t)}\right|_{x(t)=x_b(t)} = 0$. $\Rightarrow$ classical trajectories!

This method becomes invaluable in QFT.
In QM it is perhaps easiest to understand at the wavefunction level, where it becomes...

3.3 The WKB approximation

uses:
- gives an approximate analytical form for $\psi(x)$ for any potential $V(x)$.
- allows an approach to the classical limit
  - ↳ historically important in establishing the 'correspondence principal'.
- Sets up QFT.

the idea: $\psi(x,t)$ is treated as a plane wave with a slowly varying wavelength $\lambda(x)$.
(in space)

Specifically, λ ~~variations~~ $\ll L_{system}$.
& $|\lambda'| \ll 2\pi$.

(Semi) classical, so $[x,p]=0$.

$\therefore$ we can write

normally meaningless in QM

$$E = \frac{p(x)^2}{2m} + V(x)$$

$$\& \quad p(x) = \pm\sqrt{2m(E-V(x))}$$

& we choose + by convention.

NB $p(x) = 2\pi\hbar/\lambda(x)$.

As we seek plane waves, use

$$\psi(x,t) = e^{iS(x,t)/\hbar}$$

suggestive nomenclature!

if we say S is an action:

$$S = \int L\,dt = \int (p\cdot\dot{q} - H)\,dt \quad \text{(Legendre transform)}$$

$$= \int p\cdot\frac{dq}{dt}\,dt - \int H\,dt$$

$\therefore\ S = \int p\,dq - Et$. (assuming H is t-independent?) 10

$\therefore\ \psi(x,t) = e^{-iEt/\hbar} e^{i\int p\,dq/\hbar}$

this is the usual t dependence of an energy eigenstate.

We typically write $\psi(x,t) = e^{-iEt/\hbar}\phi(x)$.

Then solve the time independent S.E. for ϕ.

Do the same here.

$$\therefore\ \psi(x,t) = e^{-iEt/\hbar}\phi(x)$$

& work with $\phi(x)$ from now on.

We have

$$\phi(x) = e^{i\sigma(x)/\hbar}$$

where $\sigma(x) = \int p(x)\,dx$.

If $\sigma \in \mathbb{C}$ there is no approximation yet — ϕ can have varying magnitude & phase.

Subs. into TISE:

$$\hat{H}\phi = E\phi$$

$$-\frac{\hbar^2}{2m}\phi'' + V\phi = E\phi$$

$$-\frac{\hbar^2}{2m}\left(\frac{i\sigma''}{\hbar} + \left(\frac{i\sigma'}{\hbar}\right)^2\right)\phi + V\phi = E\phi.$$

$\therefore\ \sigma$ obeys $\boxed{-i\hbar\sigma'' + (\sigma')^2 = 2m(E-V) = p(x)^2}$

Now the key step:

<u>expand in powers of $\hbar$.</u>

$$\sigma(x) \simeq \sigma_0(x) + \frac{\hbar}{i}\sigma_1(x) + \left(\frac{\hbar}{i}\right)^2\sigma_2(x) + \dots$$

0^{th} order

Start from $\quad -i\hbar\sigma'' + (\sigma')^2 = p^2$.

to 0^{th} order in $\hbar$, the first term (linear in $\hbar$) is 0.

$\therefore\ (\sigma')^2 = p^2$

& to 0^{th} order $\sigma = \sigma_0$.

$\therefore\ \sigma_0' = \pm p(x)$

$\therefore\ \sigma_0(x) = \pm\int p(x)\,dx$

$\therefore\ \phi^{(0)}(x) = e^{\pm i\int p(x)dx}$. (Good – assumed!).

1^{st} order

Again, $\quad -i\hbar\sigma'' + (\sigma')^2 = p^2$

$$-i\hbar\left(\sigma_0'' + \frac{\hbar}{i}\sigma_1''\right) + \left(\sigma_0' + \frac{\hbar}{i}\sigma_1'\right)^2 = p^2$$

$$\therefore\ -i\hbar\sigma_0'' - \underbrace{\cancel{\hbar^2\sigma_1''}}_{0\ \mathcal{O}(\hbar^2)} + \underbrace{\cancel{(\sigma_0')^2}}_{=} + 2\sigma_0'\sigma_1'\frac{\hbar}{i} + \underbrace{\cancel{\left(\frac{\hbar}{i}\right)^2(\sigma_1')^2}}_{0\ \mathcal{O}(\hbar^2)} = \underbrace{\cancel{p^2}}_{=}$$

$$\therefore\ \sigma_0'' + 2\sigma_0'\sigma_1' = 0$$

but $\sigma_0' = \pm p(x)$ from 0^{th} order. ?

$$\therefore\ \sigma_1' = -\frac{1}{2}\frac{\sigma_0''}{\sigma_0'} = \frac{-p'}{2p} = -\frac{1}{2}\frac{d\ln p}{dx}$$

$$\therefore\ \sigma_1(x) = -\tfrac{1}{2}\ln(p(x)).$$

$$\therefore\ \phi^{(1)}(x) = e^{\pm\frac{i}{\hbar}\int p\,dx - \frac{1}{2}\ln(p)\cdot\frac{\hbar}{i}\cdot\frac{i}{\hbar}}$$

$$= \frac{1}{\sqrt{p}}\,e^{\pm i\int p\,dx/\hbar}.$$

This gives the WKB approximation:

$$\boxed{\phi_{WKB}(x) = \frac{A_+}{\sqrt{p}}e^{i\int p\,dx/\hbar} + \frac{A_-}{\sqrt{p}}e^{-i\int p\,dx/\hbar}}$$

N.B. p can be complex.

If $E > V$, $p = \sqrt{2m(E-V)} \in \mathbb{R}$.

If $E < V$, $p = \sqrt{2m(E-V)}$ is purely imaginary.

This case, $E<V$, is the 'classically forbidden region'.

Just like in QM, we can write

$$p = i\underbrace{\hbar\kappa}_{\mathbb{R}} = i\cdot\underbrace{\sqrt{2m|E-V|}}_{\mathbb{R}}.$$

Then if $E<V$ we have

$$\phi_{WKB}(x) = \frac{A_+}{\sqrt{\hbar\kappa}}e^{-\int\kappa dx + \pi i/4} + \frac{A_-}{\sqrt{\hbar\kappa}}e^{\int\kappa dx + \pi i/4}.$$

Exponentially decaying/growing solutions — evanescent waves.

N. Molto B.: the $\frac{1}{\sqrt{p}}$ can be understood like pass-the-parcel.

If p is smaller, v is smaller, so $|\phi|^2 \propto \frac{1}{p}$ is bigger.

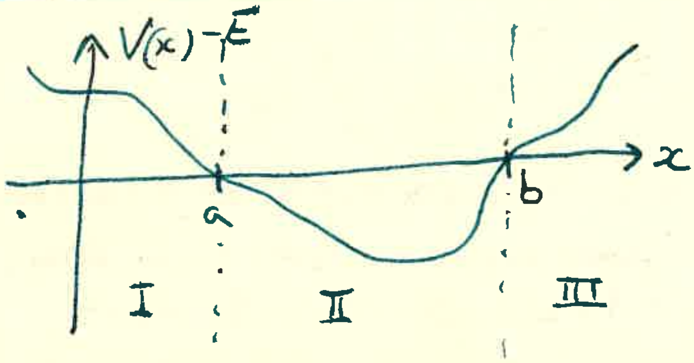
There's a higher probability to find the particle where it moves slower.

Hang onto the parcel as long as you can...

N. Benissimo: Recall the method of stationary phase:

$$\psi(x,t) = \sqrt{\frac{(2\pi\hbar)^{\infty}}{\left|\det\left(\frac{\delta^2 S}{\delta x^2}\right)\right|}}\, e^{iS[x_{classical}]/\hbar + 4\pi i/4}.$$

3.4 WKB for bound states



asymmetric.

I, III classically forbidden.

Solution scheme same as QM:

Solve for ϕ_I, ϕ_{II}, ϕ_{III}, then ensure consistency @ meeting points.

$$\phi_I(x) = \frac{A_I}{\sqrt{|P(x)|}} e^{\int_x^a |P| dx'/\hbar}$$

$$\phi_{III}(x) = \frac{A_{III}}{\sqrt{|P(x)|}} e^{-\int_b^x |P| dx'/\hbar} \qquad (A \in \mathbb{C})$$

$$\phi_{II}(x) = \frac{A_{II}^+}{\sqrt{P}} e^{i\int_a^b p\,dx'/\hbar} + \frac{A_{II}^-}{\sqrt{P}} e^{-i\int_a^b p\,dx'/\hbar}$$

Match $\phi_I(a) = \phi_{II}(a)$

$\phi_{II}(b) = \phi_{III}(b)$.

<u>However</u>, WKB fails terribly @ a, b!

Here (classical turning points)

$$E = V \therefore p = 0 \therefore \lambda \to \infty$$

but we assumed $\lambda << L_{system}$.

Solution: close to a, b the potential is approximately linear.

$$E - V(x) \simeq \begin{cases} F_a(a-x), & x \simeq a \\ F_b(x-b), & x \simeq b \end{cases}.$$

TISE for linear potential:

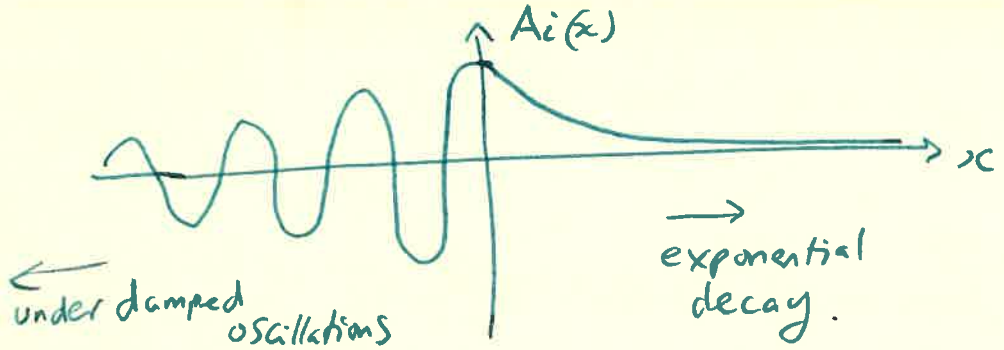
$$-\frac{\hbar^2}{2m}\phi'' + Fx\phi = E\phi$$

can be solved exactly using an 'Airy function':

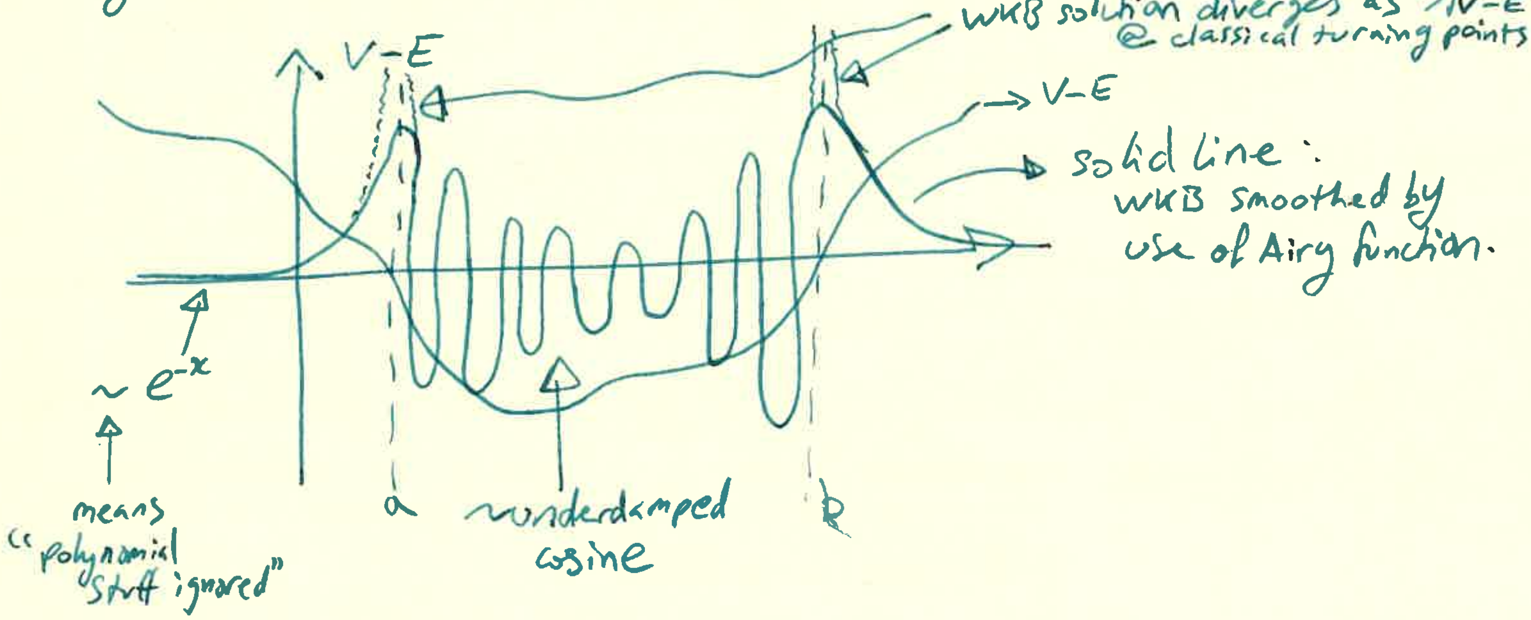
Airy's eq^n $\quad y'' - xy = 0$

Solved by $\quad Ai(x) \triangleq \frac{1}{\pi}\int_0^\infty dt \cos\left(\frac{t^3}{3} + xt\right)$

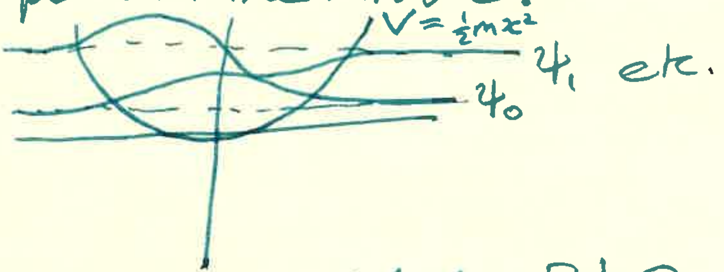
- Originally introduced to explain supernumerary rainbows
- Also models QM particle in a semiconductor heterojunction, particle in a constant gravitational field, quark confinement
- Also the basis of Witten's conjecture in string theory.



Using this form we can work out how to connect the regions despite the divergence of $1/\sqrt{p}$:



NB amplitude is <u>larger</u> near edges. But shouldn't it look like a finite potential well, or harmonic oscillator? Don't they peak in the middle?

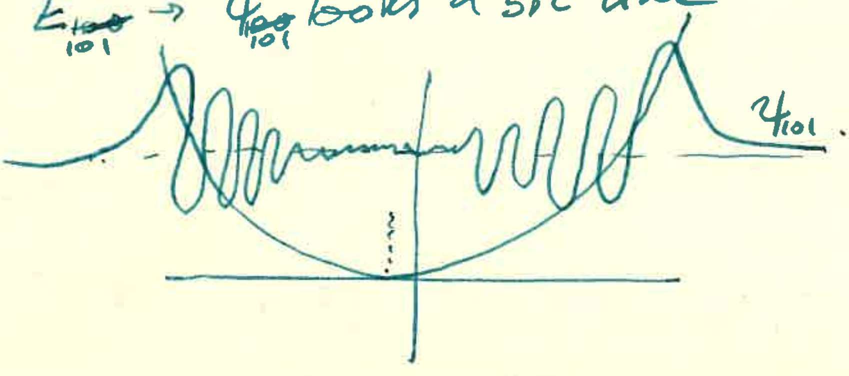


Yes... for low eigenstates. But @ large E_n, the ψ spends more time in the energetically <u>costly</u> regions

↓

edge of the classically allowed region!

So $E_{\cancel{100}\,101} \rightarrow \psi_{\cancel{100}\,101}$ looks a bit like



This is the correspondence principle: WKB is semiclassical, & higher energies are 'more classical'. $\therefore$ WKB better there.

<u>Matching conditions</u>

Using the Airy form, we can match @ a, b:

$$\phi_{I}(a) = \phi_{II}(a)$$
$$\phi_{II}(b) = \phi_{III}(b).$$

Then, consistency of ϕ_{II} at the two ends of the classically allowed region leads to:

$$\frac{1}{\hbar}\int_a^b p\,dx = (n+\tfrac{1}{2})\pi \quad , n \in \mathbb{Z}.$$

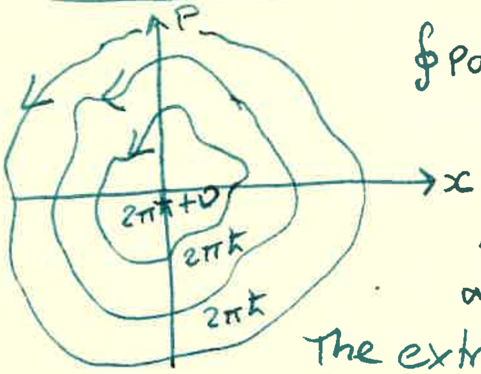
[* As far as I can tell, Simons / Fowler get this calculation from Landau & Lifshitz — But I can't make sense of them...]

Then if we double the length of the integral to go $a \to b \to a$, we can write the neat form

$$\boxed{\oint p\,dx = 2\pi\hbar\,(n+\tfrac{1}{2})}.$$

This is the Bohr-Sommerfeld quantization condition — part of 'old quantum theory' (pre-Schrödinger/Heisenberg).

3.5 Phase space quantization



$\oint p\,dx$ = area enclosed in phase space (x, p).

Bohr-Sommerfeld says quantum orbits enclose area $2\pi\hbar$ between contours.

E.g. an electron acquires a phase $\oint p\,dx/\hbar$ along an orbit.

The extra $+\frac{1}{2}$ is called the 'Maslov index' ν in general. It is an extra phase of $-\pi/2$ picked up at a 'soft' turning point. At 'hard' turning points (V' large) $\Delta\Phi = \pi$ instead. Cf. a waggling rope.

Finally, we can say that a transition from orbit n to $n-1$ releases a photon of energy $\Delta E = \hbar\omega$, where $\omega = 2\pi/T$, with T the time to complete the circuit:

$$T = \oint dt = \oint \frac{dx}{v}; \quad \Delta E \cdot \oint \frac{dp}{dE}\,dx = \oint p\,dx = 2\pi\hbar; \quad \frac{\partial E}{\partial p} = v; \quad \therefore \Delta E = \frac{2\pi\hbar}{T}.$$

4. Time evolution

Recap of 3rd year:

In the 'Schrödinger picture', states are time dependent & operators are time independent:

$$\underbrace{\hat{H}_S}_{\text{Schrödinger}} |\psi_S(t)\rangle = E|\psi_S(t)\rangle.$$

In the 'Heisenberg picture', states are time independent & operators are time dependent:

$$\underbrace{\hat{H}_H(t)}_{\text{Heisenberg}} |\psi_H\rangle = E|\psi_H\rangle$$

We can write

$$|\psi_S(t)\rangle = e^{-i\hat{H}t/\hbar} \underbrace{|\psi_S(0)\rangle}_{\text{could choose to be } |\psi_H\rangle}.$$

$$\hat{A}_H(t) = e^{-i\hat{H}t/\hbar} \underbrace{\hat{A}_H(0)}_{\text{could choose to be } \hat{A}_S} e^{i\hat{H}t/\hbar}.$$

(choice of $|\psi_S(0)\rangle = |\psi_H\rangle$ is a phase choice).

The pictures are equivalent. E.g.

$$\langle\psi_H|\hat{A}_H|\varphi_H\rangle = \underbrace{\langle\psi_H|e^{i\hat{H}t/\hbar}}_{\langle\psi_S(t)|}\underbrace{e^{-i\hat{H}t/\hbar}\hat{A}_H e^{i\hat{H}t/\hbar}}_{\hat{A}_S}\underbrace{e^{-i\hat{H}t/\hbar}|\varphi_H\rangle}_{|\varphi_S(t)\rangle}$$

- Measurable properties independent of picture.

Time evolution equations:

$$i\hbar\,\partial_t|\psi_S(t)\rangle = \hat{H}|\psi_S(t)\rangle \quad \text{(TDSE)}$$

$$\frac{d\hat{A}_H(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}_H(t), \hat{A}_H(t)\right] \quad \text{Heisenberg eq}^n.$$

(assuming no explicit time dependence: $\frac{\partial A_S}{\partial t} = 0$).

Also recall:

Schrödinger : $\psi(x,t)$ waves

Heisenberg : $\underline{\underline{H}}\,\underline{\psi} = E\underline{\psi}$ matrices

then : <u>Dirac</u> : $|\psi(t)\rangle$ kets!

- unified the approaches.

Dirac also has a 'picture'.

As he notoriously disliked the use of his name, it is called the...

4.1 <u>Interaction picture</u>

- particularly useful when interactions only occur for a limited time.
- But that's always the case! E.g. experiments involve interacting with the system for a finite time', or collisions at CERN...

Write $\hat{H} = \hat{H}_0 + \hat{V}(t)$

then $\underset{\text{Interaction}}{|\psi_I(t)\rangle} = e^{i \overset{\text{not } \hat{H}}{\hat{H}_0} t/\hbar} \underset{\text{Schrödinger}}{|\psi_S(t)\rangle}$

New equation of motion:

$$i\hbar \partial_t |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle.$$

(Prove in problem set).

Summary:

	Schrödinger	Heisenberg	Interaction
States	$\lvert\psi_S(t)\rangle = e^{-i\hat{H}t/\hbar} \lvert\psi_S(0)\rangle$	$\lvert\psi_H\rangle$	$\lvert\psi_I(t)\rangle = e^{-i\hat{H}_0 t/\hbar} \lvert\psi_I(0)\rangle$
Operators	$\hat{A}_S$	$\hat{A}_H(t) = e^{-i\hat{H}t/\hbar} \hat{A}_H(0) e^{i\hat{H}t/\hbar}$	$\hat{A}_I(t) = e^{-i\hat{H}_0 t/\hbar} \hat{A}_I(0) e^{i\hat{H}_0 t/\hbar}$
E.O.M.	$i\hbar \partial_t \lvert\psi_S(t)\rangle = \hat{H} \lvert\psi_S\rangle$	$i\hbar \frac{d\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}_H]$	$i\hbar \partial_t \lvert\psi_I\rangle = \hat{V}_I(t) \lvert\psi_I\rangle$

NB $|\psi_I(0)\rangle = |\psi_S(0)\rangle$ like Schrödinger

& if $V=0$, $|\psi_I(t)\rangle = |\psi_I(0)\rangle$ like Heisenberg.

$$\langle \psi_I | \hat{A}_I | \varphi_I \rangle = \langle \psi_S | \hat{A}_S | \varphi_S \rangle = \langle \psi_H | \hat{A}_H | \varphi_H \rangle.$$

4.2 Time evolution operator

Integrate E.O.M. wrt time:

$$|\psi_I(t)\rangle = |\psi_I(0)\rangle - \frac{i}{\hbar} \int_0^t dt' \, \hat{V}_I(t') |\psi_I(t)\rangle$$

(Exact).

But if V is small (meaning $\int V dt/\hbar \ll 1$), which is usual, we can define a perturbation series:

$$0^{th} \text{ order}: \quad |\psi_I^{(0)}(t)\rangle = |\psi_I^{(0)}(0)\rangle$$

$$1^{st} \text{ order}: \quad |\psi_I^{(1)}(t)\rangle = |\psi_I^{(0)}(0)\rangle - \frac{i}{\hbar}\int_0^t dt' \, \hat{V}_I(t')|\psi_I^{(0)}(0)\rangle$$

2^{nd} order:

$$|\psi_I^{(2)}(t)\rangle = |\psi_I^{(0)}(0)\rangle - \frac{i}{\hbar}\int_0^t dt' \hat{V}_I(t')\left(|\psi_I^{(0)}(0)\rangle - \frac{i}{\hbar}\int_0^{t'} dt'' \hat{V}_I(t)|\psi_I^{(0)}(0)\rangle\right)$$

$$\downarrow$$

$$|\psi_I^{(2)}(t)\rangle = |\psi_I^{(0)}(0)\rangle - \frac{i}{\hbar}\int_0^t dt' \hat{V}_I(t')|\psi_I^{(0)}(0)\rangle + \left(\frac{-i}{\hbar}\right)^2 \underbrace{\int_0^t dt' \int_0^{t'} dt''}_{\text{time ordering vital - check limits.}} \hat{V}_I(t')\hat{V}_I(t'')|\psi_I^{(0)}(0)\rangle$$

The ∞ order solution simplifies:

$$\boxed{|\psi_I(t)\rangle = \hat{U}_I(t,0)|\psi_I(0)\rangle}$$

where

$$\boxed{\hat{U}_I(t,0) = \hat{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt' \hat{V}_I(t')\right)}$$

the 'time ordering operator' – orders events from past (right) to future (left).

How it works:

recall, $e^{\hat{x}} \triangleq \hat{\mathbb{1}} + \hat{x} + \frac{1}{2}\hat{x}^2 + \frac{1}{3!}\hat{x}^3 + \dots$

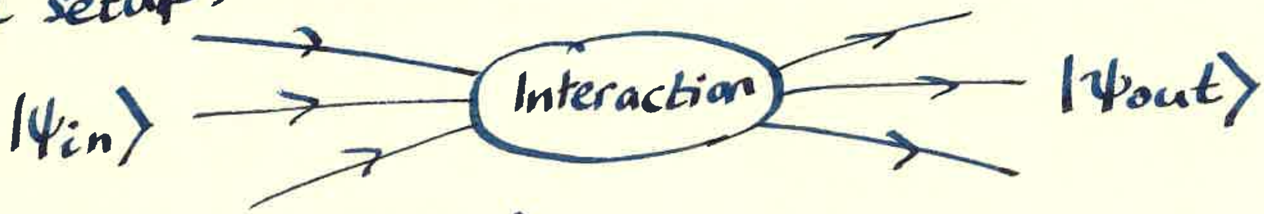
$$\therefore \hat{U}_I(t,0)|\psi_I(0)\rangle = \hat{\mathbb{1}}|\psi_I(0)\rangle + \hat{T}\left(\frac{-i}{\hbar}\right)\int_0^t dt' \hat{V}_I(t')|\psi_I(0)\rangle$$

$$+ \frac{1}{2}\hat{T}\underbrace{\int_0^t dt' \hat{V}_I(t') \int_0^{t'} dt'' \hat{V}_I(t'')}_{2 \text{ orderings of the form } \int_0^t\int_0^{t'} \hat{V}_I(t')\hat{V}_I(t'')dt'dt''}|\psi_I(0)\rangle$$

cancel

4.3 Putting I to work

Typical setup:



(Basic LHC schematic)

∴ Imagine $V(t)$ turning on for a limited time.
What's the probability of initial state $|i\rangle$ becoming Energy eigenstate $|n\rangle$?

$$|i(t)\rangle = \hat{U}_I(t)\underbrace{|i(0)\rangle}_{\hat{=}|i\rangle} = \sum_n |n\rangle\underbrace{\langle n|\hat{U}_I(t)|i\rangle}_{\hat{=}\,c_n(t)}$$

Using the series expansion of $\hat{U}$:

$$c_n(t) = \underbrace{\langle n|i\rangle}_{\delta_{ni} = c_n^{(0)}(t)} + \underbrace{\left(\frac{-i}{\hbar}\right)\int_0^t dt' \langle n|\hat{V}_I(t')|i\rangle}_{c_n^{(1)}(t)} + \ldots$$

Use $\hat{V}_I(t) = e^{i\hat{H}_0 t/\hbar}\,\hat{V}_I\, e^{-i\hat{H}_0 t/\hbar}$

If $|i\rangle$ is also an energy eigenstate

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_0^t dt'\, e^{i\omega_{ni}t'}\, V_{ni}(t')$$

where $\omega_{ni} = \dfrac{E_n - E_i}{\hbar}$

$V_{ni}(t) = \langle n|\hat{V}_I(t)|i\rangle$

$$\text{Prob.}\left(|i\rangle \to |n\rangle\right) = |c_n(t)|^2$$
$$= |c_n^{(0)}(t) + c_n^{(1)}(t) + \ldots|^2.$$

Easiest to see with an example ...

E.g. (Ben Simons' notes): Kicked oscillator

Initial state is the simple harmonic oscillator ground state @ $t=-\infty$: $|i\rangle = |0, t=-\infty\rangle$

i.e. $|n\rangle = |0\rangle$.

State is 'kicked' by potential

$$\hat{V}(t) = -eE\hat{x}e^{-t^2/\tau^2}$$

What is the probability the final state is $|1\rangle$ @ $t=+\infty$

i.e. $|f\rangle = |1, t=+\infty\rangle$?

Answer:

Work to 1st order.

$$\text{Prob}\left(|0,-\infty\rangle \to |1,\infty\rangle\right) \simeq \Big|\underbrace{C^{(0)}_{n=1}(t=\infty)}_{\delta_{10}=0} + C^{(1)}_{n=1}(t=\infty)\Big|^2$$

$$\therefore \quad C^{(1)}_1(\infty) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt'\, e^{i\omega_{10}t'} \langle 1|\hat{V}_I(t')|0\rangle.$$

recall some SHO facts:

$$E_n = \hbar\omega(n+1/2)$$

$$\therefore \omega_{10} = \frac{E_1 - E_0}{\hbar} = \omega.$$

Ladder operators: $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger)$

where $|1\rangle = \hat{a}^\dagger|0\rangle$.

$$\therefore \quad \langle 1|\hat{V}_I(t)|0\rangle = -eEe^{-t^2/\tau^2}\underbrace{\langle 1|\hat{x}|0\rangle}$$

independent of picture; easiest is 'S' here.

$$\langle 1|\hat{x}|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle 1|\hat{a}+\hat{a}^\dagger|0\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\underbrace{\langle 0|\hat{a}}(\hat{a}+\hat{a}^\dagger)|0\rangle$$

Since $|1\rangle = \hat{a}^\dagger|0\rangle$

& $\langle 1| = (|1\rangle)^\dagger = (\hat{a}^\dagger|0\rangle)^\dagger$

$= \langle 0|\hat{a}$.

$$\therefore \langle 1|\hat{x}|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle 0|\hat{a}\hat{a}|0\rangle + \langle 0|\hat{a}\hat{a}^\dagger|0\rangle\right)$$

$\langle 0|\hat{a}\hat{a}|0\rangle \to 0$ as $\hat{a}|0\rangle = 0$.

recall $\quad [\hat{a},\hat{a}^\dagger] = \hat{\mathbb{1}}$

$$\therefore \langle 0|\hat{a}\hat{a}^\dagger|0\rangle = \langle 0|\hat{\mathbb{1}} + \hat{a}^\dagger\hat{a}|0\rangle$$

$$= \langle 0|0\rangle$$

$$= 1.$$

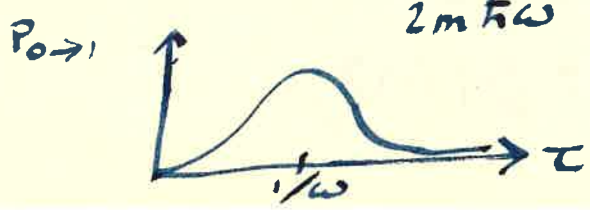
$$\therefore \langle 1|\hat{V}_I(t)|0\rangle = -eEe^{-t^2/\tau^2}\sqrt{\frac{\hbar}{2m\omega}}$$

$$\therefore c_1^{(1)}(\infty) = -\frac{i}{\hbar}(-eE)\sqrt{\frac{\hbar}{2m\omega}}\underbrace{\int_{-\infty}^{\infty}dt'\, e^{i\omega t'}e^{-t'^2/\tau^2}}$$

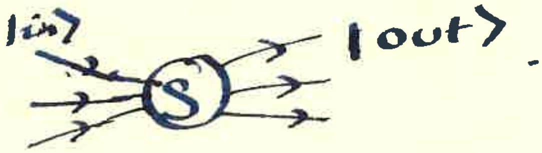
Gaussian, after completing the square

$$\therefore c_1^{(1)}(\infty) = ieE\sqrt{\frac{\pi}{2m\hbar\omega}}\,\tau e^{-\omega^2\tau^2/4}$$

$$\therefore \text{Prob}(0\to 1) = \frac{\tau^2 e^2 E^2\pi}{2m\hbar\omega}e^{-\omega^2\tau^2/2}.$$



4.4 The S-matrix

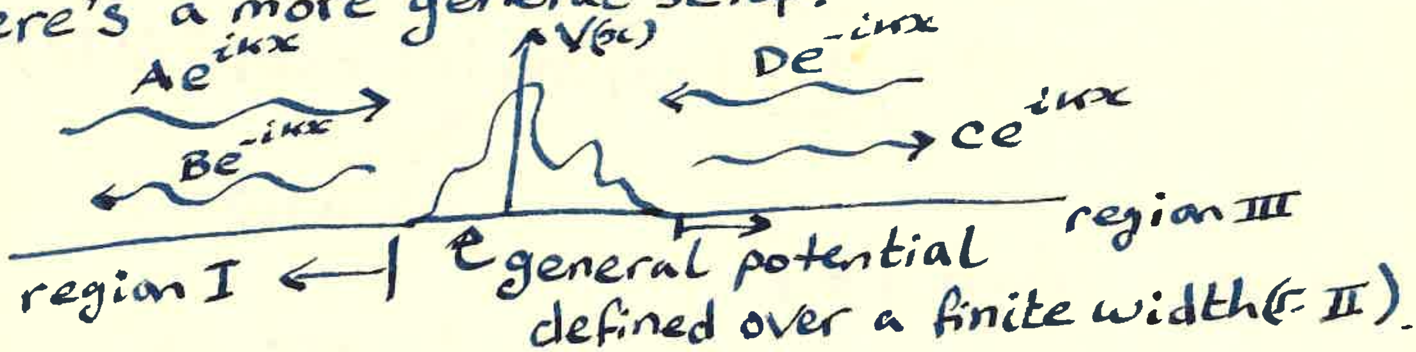
- S stands for 'scattering'.
- Central to particle physics: 

- Allows us to define 'free particles', e.g. electrons, as asymptotic states at $t = \pm\infty$.

Many properties of the S matrix can already be identified at the single particle level.

NB You might like to recap scattering from a finite-width step from 2nd year.

Here's a more general setup:



I.e send in A & D, get out B & C.

$$\phi_I = Ae^{ikx} + Be^{-ikx}$$

$$\phi_{III} = Ce^{ikx} + De^{-ikx}.$$

[In yr 2, $V(x)$ was a step; $A=1$, $D=0$, $B=r$, $C=t$.]

The S-matrix is defined as:

$$\underbrace{\begin{pmatrix} B \\ C \end{pmatrix}}_{\text{outgoing}} = \underline{\underline{S}} \underbrace{\begin{pmatrix} A \\ D \end{pmatrix}}_{\text{ingoing}}.$$

I.e. $|out\rangle = \underline{\underline{S}}|in\rangle$ //

4.5 Properties of $\underline{\underline{S}}$

Property 1: S is <u>Unitary</u>.

This one's quite obvious – time evolution is always unitary in QM (in the absence of measurement). Some take it as a definition/postulate.

Specifically,

$$\langle in | in \rangle = \langle out | out \rangle \quad (=1)$$

$$|out\rangle = \underline{\underline{S}}\,|in\rangle$$

$$\therefore \langle in | in \rangle = \langle in | \underline{\underline{S}}^{\dagger}\underline{\underline{S}}\,| in \rangle$$

$$\& \quad \underline{\underline{S}}^{\dagger}\underline{\underline{S}} = \hat{\mathbb{1}}$$

Property 2: if $\underline{V(x) \in \mathbb{R}}$, S is <u>symmetric</u>.

NB you can always choose $V(x) \in \mathbb{R}$ in the absence of a magnetic field.

Proof:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \underline{\underline{S}} \begin{pmatrix} A \\ D \end{pmatrix} \quad (A)$$

$\downarrow$ complex conjugate

– the same picture, with

$$\begin{matrix} A \\ B \\ C \\ D \end{matrix} \longrightarrow \begin{matrix} B^* \\ A^* \\ D^* \\ C^* \end{matrix} \quad \therefore \begin{pmatrix} A^* \\ D^* \end{pmatrix} = \underline{\underline{S}} \begin{pmatrix} B^* \\ C^* \end{pmatrix}$$

(Same S!)

$\therefore$ (* again) $\quad \begin{pmatrix} A \\ D \end{pmatrix} = \underline{\underline{S}}^* \begin{pmatrix} B \\ C \end{pmatrix} \quad$ (B)

Subs. (A) into (B):

$$\begin{pmatrix} A \\ D \end{pmatrix} = \underline{\underline{S}}^* \underline{\underline{S}} \begin{pmatrix} A \\ D \end{pmatrix}$$

$$\therefore \quad \underline{\underline{S}}^* \underline{\underline{S}} = \hat{\mathbb{1}}$$

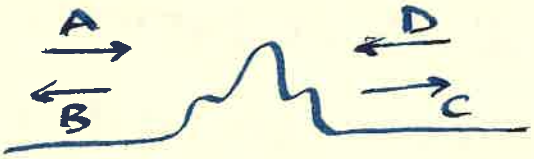
But property 1 already says $\underline{\underline{S}}^\dagger \underline{\underline{S}} = \hat{\mathbb{1}}$.

$$\therefore \quad \underline{\underline{S}}^* = \underline{\underline{S}}^\dagger$$

$$\& \quad \underline{\underline{S}} = \underline{\underline{S}}^T \;//$$

Property 3: if $\underline{V(x) = V(-x)}$, $\underline{\underline{\underline{S}} = \underline{\underline{\sigma_x}}\, \underline{\underline{S}}\, \underline{\underline{\sigma_x}}}$

Proof:



(or symmetric in general if not centred @ $x=0$)

Symmetric, $\therefore \begin{pmatrix} A \\ B \end{pmatrix} \leftrightarrow \begin{pmatrix} D \\ C \end{pmatrix}$ enacts no change.

$$\therefore \text{(A)} \Rightarrow \begin{pmatrix} C \\ B \end{pmatrix} = \underline{\underline{S}} \begin{pmatrix} D \\ A \end{pmatrix} \quad \text{(C)}$$

Recall: $\underline{\underline{\sigma_x}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $\quad \underline{\underline{\sigma_x}} \begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} B \\ C \end{pmatrix}$ etc.

& $\underline{\underline{\sigma_x}}^2 = \mathbb{1}$ So we can insert $\underline{\underline{\sigma_x}}^2$ anywhere.

$\underline{\underline{\sigma_x}}$ (C): $\quad \begin{pmatrix} B \\ C \end{pmatrix} = \underline{\underline{\sigma_x}}\, \underline{\underline{S}}\, \underbrace{\underline{\underline{\sigma_x}}}_{\text{having inserted } \sigma_x^2.} \begin{pmatrix} A \\ D \end{pmatrix}$

$$\therefore \text{(A)}, \underline{\underline{\sigma_x}}\text{(C)} \Rightarrow \quad \underline{\underline{S}} = \underline{\underline{\sigma_x}}\, \underline{\underline{S}}\, \underline{\underline{\sigma_x}} \;//$$

NB if $V=0$, $\underline{\underline{S}} = \underline{\underline{\sigma_x}}$ (check).

this makes sense as $\underline{\underline{\sigma_x}}^3 = \underline{\underline{\sigma_x}}$.

An interesting result of properties 1 & 3:

Since $\underline{\underline{S}} = \underline{\underline{\sigma_x}}\,\underline{\underline{S}}\,\underline{\underline{\sigma_x}}$

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} S_{22} & S_{21} \\ S_{12} & S_{11} \end{pmatrix} \quad (S_{ij} \in \mathbb{C})$$

& we can write $S = \begin{pmatrix} S_{11} & S_{12} \\ S_{12} & S_{11} \end{pmatrix}$ when $V(x) = V(-x)$.

But unitarity tells us

$$\underline{\underline{S}}^{-1} = \underline{\underline{S}}^{\dagger}$$

therefore $\begin{pmatrix} S_{11}^* & S_{12}^* \\ S_{12}^* & S_{11}^* \end{pmatrix} = \dfrac{1}{S_{11}^2 - S_{12}^2} \begin{pmatrix} S_{11} & S_{12} \\ S_{12} & S_{11} \end{pmatrix}$

i.e. $S_{11}^* = \dfrac{S_{11}}{S_{11}^2 - S_{12}^2}$; $S_{12}^* = \dfrac{-S_{12}}{S_{11}^2 - S_{12}^2}$

re-arrange: $S_{11}^2 - S_{12}^2 = \dfrac{S_{11}}{S_{11}^*} = -\dfrac{S_{12}}{S_{12}^*}$.

writing $S_{ij} = |S_{ij}| e^{i\vartheta_{ij}}$

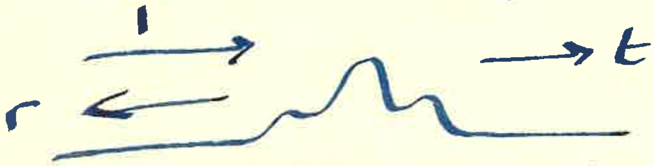
we see $\vartheta_{11} = \vartheta_{12} + \pi/2$:

$$\frac{|S_{11}| e^{i\vartheta_{11}}}{|S_{11}| e^{-i\vartheta_{11}}} = \frac{|S_{12}| e^{i\vartheta_{12} + i\pi}}{|S_{12}| e^{-i\vartheta_{12}}}$$

$$\therefore\ e^{2i\vartheta_{11}} = e^{2i\vartheta_{12} + \pi i}$$

$$\therefore\ \vartheta_{11} = \vartheta_{12} + \tfrac{\pi}{2} \quad (+\pi\mathbb{Z}).$$

Consider the usual setup, with one incident wave:



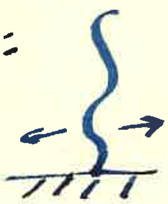
$$\begin{pmatrix} r \\ t \end{pmatrix} = \underline{\underline{S}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} S_{11} \\ S_{12} \end{pmatrix}$$

$$\therefore \quad \frac{r}{t} = \frac{S_{11}}{S_{12}} = \frac{|S_{11}|}{|S_{12}|} e^{\pi i/2} .$$

$\therefore$ r & t are always $\frac{\pi}{2}$ out of phase!

- holds only for symmetric potentials, but most familiar settings — e.g. windows — have that.

- recall also the 'Maslov index' on page 12 (2nd side). A 'soft' potential induces a $\pi/2$ phase shift on reflection, while a 'hard' potential induces a π shift.

  Think again of waggling a rope with a free end:  vs fixed end: 

4.6 Time reversal

The properties of $\underline{\underline{S}}$ are really just the properties of QM in general.

Let's take a closer look at property 2.

Complex conjugation, $*$, enacts 'time reversal' in QM.

There are a few ways to see this.

E.g. the propagator

$$K(x_f, t_f; x_i, t_i) = \langle x_f | \hat{U}(t_f - t_i) | x_i \rangle$$

$$\therefore \; K^*(x_f, t_f; x_i, t_i) = \langle x_i | \hat{U}^\dagger(t_f - t_i) | x_f \rangle$$

$$= \langle x_i | \hat{U}(t_i - t_f) | x_i \rangle$$

$$= K(x_i, t_i; x_f, t_f)$$

which means that if K propagates a state forwards in time from x_i, t_i to x_f, t_f, then K^* propagates a state backwards in time from x_f, t_f to x_i, t_i.

Equivalently we can see this symmetry in the TDSE:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \psi''(x,t) + V(x)\psi(x,t)$$

$$\downarrow *$$

$$-i\hbar \frac{\partial \psi^*(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \psi^{*''}(x,t) + V(x)\psi^*(x,t)$$

$$\downarrow \text{relabel } t \to t' = -t$$

$$i\hbar \frac{\partial \psi^*(x,-t')}{\partial t'} = \frac{-\hbar^2}{2m} \psi^{*''}(x,-t') + V(x)\psi^*(x,-t')$$

$\therefore$ if $\psi(x,t)$ solves the TDSE,

then $\psi^*(x,-t)$ also solves it.

This is the basis of certain interpretations of QM, such as the transactional interpretation.

It is also the basis of the 'Feynman - Wheeler absorber theory', which inspired Feynman's development of Lagrangian / Path integral QM. It also led to the film Tenet ...

NB classical mechanics also has a similar time reversal symmetry.