Advanced Quantum Physics

F. Flicker

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These notes provide key results from the lectures. However, significant additional explanation will be provided in the lectures.

Notation

Eintein summation notation: denote component i of vector $\boldsymbol{v}$

$$[\boldsymbol{v}]_i = v_i. \tag{1}$$

Whenever an index appears twice, assume it is summed:

$$a_i b^i = \sum_i a_i b^i = \boldsymbol{a} \cdot \boldsymbol{b}. \tag{2}$$

I'll make an effort to keep track of upper/lower indices for additional bookkeeping. *E.g.*

$$\frac{\partial}{\partial x_i} = \nabla^i \tag{3}$$

(although strictly raised and lowered indices behave identically in Euclidean space).
I will use $\triangleq$ to mean 'equal by definition'.

1 The Lagrangian Formulation of Quantum Mechanics

1.1 Lagrangian Classical Mechanics

In Lagrangian mechanics we work with generalised co-ordinates $q_i(t)$ and generalised velocities $\dot{q}_i(t)$.
Define the Lagrangian

$$L = T - V \tag{4}$$

where T is the kinetic energy and V the potential energy. Specifically,

$$L(\{q_i\}, \{\dot{q}_i\}, t) = \frac{1}{2} m \dot{q}_i^2 - V(q_i). \tag{5}$$

Define the time integral of the Lagrangian to be the 'action' S:

$$S[q_i] = \int_{t_0}^{t_f} L \mathrm{d}t. \tag{6}$$

The action is a *functional*. Whereas a function takes a number as an argument and returns a number, a functional takes in an entire function as an argument, and again returns a number.

The **principle of least action**:
classical paths $q_i(t)$ extremise the action S.

To extremise:

$$\left(\frac{\partial S[q_i + \lambda \epsilon_i]}{\partial \lambda} \right)_{q_i, \epsilon_i} \Bigg|_{\lambda = 0} = 0. \tag{7}$$

Here, the subscripts to the parentheses indicate what is held constant in the partial derivative (always good practice!). Then λ is set to 0 after the differentiation.
The vector function $\epsilon_i(t)$ parameterises a variation away from the classical path $q_i(t)$. We require that the variation is zero at the start and end points of the trajectory:

$$\epsilon_i(t_0) = \epsilon_i(t_f) = 0. \tag{8}$$

(The vector index i is not to be confused with the subscript i = initial!)
Specifically:

$$S\left[q_i+\lambda\epsilon_i\right]=\int_{t_0}^{t_f} L\left(q_i+\lambda\epsilon_i,\dot{q}_i+\lambda\dot{\epsilon}_i,t\right)\mathrm{d}t \tag{9}$$

$$\Downarrow \text{ chain rule}$$

$$\left(\frac{\partial S\left[q_i+\lambda\epsilon_i\right]}{\partial\lambda}\right)_{q_i,\epsilon_i}=\int_{t_0}^{t_f}\left\{\left(\frac{\partial L}{\partial q_i}\right)_{\dot{q}_i,t}\left(\frac{\partial\left(q_i+\lambda\epsilon_i\right)}{\partial\lambda}\right)_{q_i,\epsilon_i}\right. \tag{10}$$

$$\left.+\left(\frac{\partial L}{\partial\dot{q}_i}\right)_{q_i,t}\left(\frac{\partial\left(\dot{q}_i+\lambda\dot{\epsilon}_i\right)}{\partial\lambda}\right)_{q_i,\epsilon_i}+\cancel{\left(\frac{\partial L}{\partial t}\right)_{q_i,\dot{q}_i}\left(\frac{\partial t}{\partial\lambda}\right)_{q_i,\epsilon_i}}\right\}\mathrm{d}t \tag{11}$$

$$=\int_{t_0}^{t_f}\left\{\left(\frac{\partial L}{\partial q_i}\right)_{\dot{q}_i,t}\epsilon_i+\left(\frac{\partial L}{\partial\dot{q}_i}\right)_{q_i,t}\dot{\epsilon}_i\right\}\mathrm{d}t \tag{12}$$

NB we are using Einstein summation notation here:

$$\frac{\partial L}{\partial q_i}\epsilon_i=\frac{\partial L}{\partial q_1}\epsilon_1+\frac{\partial L}{\partial q_2}\epsilon_2+\ldots \tag{13}$$

Now integrate the $\dot{\epsilon}$ term by parts in Eq 12:

$$\left(\frac{\partial S\left[q_i+\lambda\epsilon_i\right]}{\partial\lambda}\right)_{q_i,\epsilon_i}=\int_{t_0}^{t_f}\left\{\left(\frac{\partial L}{\partial q_i}\right)_{\dot{q}_i,t}-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}_i}\right)_{q_i,t}\right\}\epsilon_i\mathrm{d}t+\left[\left(\frac{\partial L}{\partial\dot{q}_i}\right)_{q_i,t}\epsilon_i\right]_{t_0}^{t_f} \tag{14}$$

but the boundary term vanishes by assumption (Eq 8). Applying the principle of least action, Eq 7, we require

$$\left(\frac{\partial S\left[q_i+\lambda\epsilon_i\right]}{\partial\lambda}\right)_{q_i,\epsilon_i}\Bigg|_{\lambda=0}=0=\int_{t_0}^{t_f}\left\{\left(\frac{\partial L}{\partial q_i}\right)_{\dot{q}_i,t}-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}_i}\right)_{q_i,t}\right\}\epsilon_i\mathrm{d}t. \tag{15}$$

This is true for all $\epsilon_i(t)$ (since this arbitrary function has not been specified). Therefore we have the

Euler Lagrange equations:

$$\left(\frac{\partial L}{\partial q_i}\right)_{\dot{q}_i,t}-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}_i}\right)_{q_i,t}=0. \tag{16}$$

The Euler Lagrange equations are obeyed by classical trajectories. *E.g.* with the general Lagrangian of Eq 5 we arrive at Newton's 2nd law:

$$-V'\left(q_i\right)=m\ddot{q}_i. \tag{17}$$

1.2 Hamiltonian Classical Mechanics

Hamiltonian mechanics uses generalised momenta p_i instead of generalised velocities $\dot{q}$. The 'momentum conjugate to $\dot{q}_i$' is defined to be

$$p^i \triangleq \frac{\partial L}{\partial \dot{q}_i}. \tag{18}$$

Then the 'Hamiltonian' is given by

$$H\left(q_i, p^i, t\right) \triangleq p^i \dot{q}_i - L \tag{19}$$

where L is the Lagrangian. Note that the classical Hamiltonian is simply a function. Dynamics can be identified using

Hamilton's equations of motion:

$$\dot{q}_i = \left(\frac{\partial H}{\partial p^i}\right)_{q_i,t}; \qquad \dot{p}^i = -\left(\frac{\partial H}{\partial q_i}\right)_{p_i,t}. \tag{20}$$

1.3 Connecting to Quantum Mechanics

For functions $f\left(q_i, p^i, t\right)$ define the

Poisson bracket:

$$\{f, g\} \triangleq \left(\frac{\partial f}{\partial q_i}\right)_{p^i,t}\left(\frac{\partial g}{\partial p^i}\right)_{q_i,t} - \left(\frac{\partial f}{\partial p^i}\right)_{q_i,t}\left(\frac{\partial g}{\partial q_i}\right)_{p^i,t} \tag{21}$$

from which Hamilton's equations of motion can be rewritten (exercise!):

$$\dot{q}_i = \{q_i, H\}; \qquad \dot{p}^i = \left\{p^i, H\right\}. \tag{22}$$

Applying the chain rule to the function f gives a general form for Hamilton's equation of motion:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{f, H\} + \left(\frac{\partial f}{\partial t}\right)_{q_i,p^i}. \tag{23}$$

Cf. the Heisenberg equation of motion in quantum mechanics:

$$\frac{\mathrm{d}\hat{A}_H}{\mathrm{d}t} = \frac{1}{i\hbar}\left[\hat{A}_H, \hat{H}\right] + \frac{\partial \hat{A}_H}{\partial t} \tag{24}$$

where the H subscript indicates that we are working in the Heisenberg picture, in which operators are time dependent. The final term only appears when the operator also has an explicit time dependence in the Schrödinger picture. The Heisenberg equation of motion plays the role of the Schrödinger equation in the Heisenberg picture.

Classical constants of motion obey

$$\frac{\mathrm{d}f}{\mathrm{d}t} = 0 \tag{25}$$

$$\downarrow$$

$$\{f, H\} = 0 \tag{26}$$

(assuming no explicit time dependence of the function) while quantum operators corresponding to good quantum numbers obey

$$\frac{\mathrm{d}\left\langle \hat{A} \right\rangle}{\mathrm{d}t} = 0 \tag{27}$$

$$\downarrow$$

$$\left[\hat{A}, \hat{H}\right] = 0 \tag{28}$$

(assuming no explicit time dependence of the operator).

1.4 Canonical quantization

Observable quantities in classical mechanics become (not necessarily commuting) operators in quantum mechanics. In the 'position basis' generalised co-ordinates become

$$q_i \to \hat{q}_i \tag{29}$$

(we more typically denote position operators $\hat{x}_i$) and generalised momenta become

$$p^i \to -i\hbar \frac{\partial}{\partial x_i} \tag{30}$$

where $\partial/\partial x_i$ is element i of ∇_i. The Hamiltonian function becomes the familiar Hamiltonian operator:

$$H = T + V \tag{31}$$

$$\downarrow$$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V\left(\hat{x}\right). \tag{32}$$

1.5 Time evolution in quantum mechanics

Recall the Time Dependent Schrödinger Equation (TDSE) (in the position basis, in 1D):

$$i\hbar\frac{\partial\psi\left(x,t\right)}{\partial t}=\hat{H}\psi\left(x,t\right) \tag{33}$$

or, in Dirac notation,

$$i\hbar\frac{\mathrm{d}|\psi\left(t\right)\rangle}{\mathrm{d}t}=\hat{H}|\psi\left(t\right)\rangle. \tag{34}$$

The equation admits the general solution

$$|\psi\left(t\right)\rangle=\hat{U}\left(t-t_{0}\right)|\psi\left(t_{0}\right)\rangle \tag{35}$$

where

$$\hat{U}\left(t-t_{0}\right)=\exp\left(-i\left(t-t_{0}\right)\hat{H}/\hbar\right) \tag{36}$$

is the 'time evolution operator'.

Since $\hat{H}$ is Hermitian, $\hat{U}$ is unitary:

$$\hat{U}^{\dagger}=\hat{U}^{-1}. \tag{37}$$

2 Path Integral Quantum Mechanics

2.1 Motivation: Young's Slits

Consider a particle departing from position x_0 at time t_0, passing through one of two slits located at positions A and B at time t, and continuing onto a screen. The amplitude to find the particle at position x on the screen at time T, which we can denote $\psi(x,T)$, is the sum of the amplitudes to take each of the two paths. That is:

$$\begin{aligned}\psi(x,T) = &\,\mathrm{Amp}(x,T|A,t)\,\mathrm{Amp}(A,t|x_0,t_0)\\ &+\mathrm{Amp}(x,T|B,t)\,\mathrm{Amp}(B,t|x_0,t_0)\end{aligned} \tag{38}$$

where $\mathrm{Amp}(x,T|A,t)$ denotes the amplitude to find the particle at position x at time T given that it was certainly at position A at time t. Eq 38 shows that amplitudes in quantum mechanics play the role that probabilities play in classical systems. We then find quantum probabilities using

the **Born rule**:

$$\text{Probability} = |\text{Amplitude}|^2 . \tag{39}$$

What if there are not two slits to pass through at time t, but an infinite number of slits with nothing between them? In that case, the sum must be replaced by an integral:

$$\psi(x,T) = \int \mathrm{d}y \mathrm{Amp}(x,T|y,t)\,\mathrm{Amp}(y,t|x_0,t_0) . \tag{40}$$

But this should be true at all times between t_0 and T. Imagine 'slicing' time into N discrete segments. Then the amplitude to find a particle at position x at time T, given it started at x_0 at time t_0, must be:

$$\psi(x,T) = \int \mathrm{d}y_{N-1} \int \mathrm{d}y_{N-2} \ldots \int \mathrm{d}y_1 \mathrm{Amp}(x,T|y_{N-1},t_{N-1})\,\mathrm{Amp}(y_{N-1},t_{N-1}|y_{N-2},t_{N-2}) \ldots \mathrm{Amp}(y_1,t_1|x_0,t_0) . \tag{41}$$

Eq 41 encodes the idea that a quantum particle can be thought of as taking every possible path between two points. This is the basic idea behind path integral quantum mechanics. The object

$$\int \mathscr{D}\boldsymbol{y} \triangleq \prod_{n=1}^{N} \int \mathrm{d}y_n \tag{42}$$

which, in the limit $N \to \infty$ contains an infinite number of independent integrals, is called a 'functional integral' or 'path integral' (not to be confused with the 1D 'line integrals' seen in first year).

Why use path integrals?

In many ways they are a more natural approach. E.g. $\int L\mathrm{d}t$ is a Lorentz scalar, allowing relativistic QM. Path integrals make certain calculations easier, e.g. the Aharonov Bohm effect. Finally, they suggest their own interpretation of QM which is perhaps the closest to classical mechanics. This is Feynman's sum over histories, which can be formulated with three axioms:

(i) The Born rule: probability $= |\psi|^2$.

(ii) ψ is given by a weighted sum over all possible classical trajectories $\boldsymbol{q}(t)$.

(iii) in this sum, each path is weighted by $\exp(iS[\boldsymbol{q}]/\hbar)$.

2.2 The Propagator

Quantum mechanics is unitary, meaning

$$|\psi(t)\rangle = \hat{U}(t-t_0)\,|\psi(t_0)\rangle. \tag{43}$$

Therefore

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t-t_0)\,|\psi(t_0)\rangle. \tag{44}$$

Inserting a

resolution of the identity (position basis):

$$\hat{\mathbb{I}} = \int \mathrm{d}x|x\rangle\langle x| \tag{45}$$

gives

$$\langle x|\psi(t)\rangle = \int \mathrm{d}x'\langle x|\hat{U}(t-t_0)\,|x'\rangle\langle x'|\psi(t_0)\rangle \tag{46}$$

or, in wavefunction notation,

$$\psi(x,t) = \int \mathrm{d}x' K(x,t;x',t_0)\,\psi(x',t_0) \tag{47}$$

where we have defined

the propagator:

$$K(x',t';x,t) \triangleq \langle x'|\hat{U}(t'-t)\,|x\rangle. \tag{48}$$

To get some intuition for the propagator, consider an initially perfectly localised wavepacket:

$$\psi\left(x', t_0\right) = A\delta\left(x' - x_0\right) \tag{49}$$

where δ is a Dirac delta-function and A is a constant required for the dimensions to match. Then Eq 47 tells us that

$$\psi\left(x, t\right) = A\int \mathrm{d}x' K\left(x, t; x', t_0\right)\delta\left(x' - x_0\right) \tag{50}$$

$$= AK\left(x, t; x_0, t_0\right). \tag{51}$$

That is, the propagator gives the amplitude to find the particle at position x at time t, given it was at position x' at time t': it propagates the particle from one point to another.

Given a potential, if you can find the propagator the you instantly have access to the quantum amplitude at all points in space and time. Hence, you know everything there is to know about the quantum problem. Of course, this turns out to be exceedingly difficult in almost all cases...

2.3 The Propagator: free space

In free space we can calculate the propagator exactly.

$$K\left(x, t; x_0, t_0\right) = \langle x|\exp\left(-i\hat{H}\left(t - t_0\right)/\hbar\right)|x_0\rangle. \tag{52}$$

In free space the potential $V = 0$ and so

$$\hat{H} = \hat{T} = \frac{\hat{p}^2}{2m}. \tag{53}$$

Therefore

$$K\left(x, t; x_0, t_0\right) = \langle x|\exp\left(-i\hat{p}^2\left(t - t_0\right)/2m\hbar\right)|x_0\rangle. \tag{54}$$

Inserting a

resolution of the identity (momentum basis):

$$\hat{\mathbb{I}} = \int_{-\infty}^{\infty} \mathrm{d}p|p\rangle\langle p| \tag{55}$$

gives

$$K\left(x, t; x_0, t_0\right) = \int_{-\infty}^{\infty} \mathrm{d}p\langle x|\exp\left(-i\hat{p}^2\left(t - t_0\right)/2m\hbar\right)|p\rangle\langle p|x_0\rangle. \tag{56}$$

By definition, $|p\rangle$ is an eigenstate of $\hat{p}$ with eigenvalue p:

$$\hat{p}|p\rangle = p|p\rangle \tag{57}$$

and so

$$K\left(x,t;x_0,t_0\right) = \int_{-\infty}^{\infty} \mathrm{d}p\langle x| \exp\left(-ip^2\left(t-t_0\right)/2m\hbar\right)|p\rangle\langle p|x_0\rangle \tag{58}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}p \exp\left(-ip^2\left(t-t_0\right)/2m\hbar\right)\langle x|p\rangle\langle p|x_0\rangle \tag{59}$$

(where the momentum operator has become simply a variable). Recalling that momentum eigenstates are plane waves:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(ipx/\hbar\right) \tag{60}$$

We find

$$K\left(x,t;x_0,t_0\right) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}p \exp\left(\frac{i}{\hbar}\left(p\left(x-x_0\right) - p^2\left(t-t_0\right)/2m\right)\right). \tag{61}$$

This is a Gaussian integral. It can be solved to give

the **propagator in free space**:

$$K\left(x,t;x_0,t_0\right) = \sqrt{\frac{m}{2\pi i\hbar}}\frac{1}{\sqrt{t-t_0}} \exp\left(\frac{im\left(x-x_0\right)^2}{2\hbar\left(t-t_0\right)}\right). \tag{62}$$

In free space, a particle can be thought as either taking a straight line between two points, or taking arbitrarily jagged paths between the same points. To see this, note that (for a free propagator only):

$$K\left(x_3,t_3;x_1,t_1\right) \equiv \int \mathrm{d}x_2 K\left(x_3,t_3;x_2,t_2\right) K\left(x_2,t_2;x_1,t_1\right). \tag{63}$$

Proof:

$$\int \mathrm{d}x_2 K\left(x_3,t_3;x_2,t_2\right) K\left(x_2,t_2;x_1,t_1\right) = \int \mathrm{d}x_2\langle x_3|\hat{U}\left(t_3-t_2\right)|x_2\rangle\langle x_2|\hat{U}\left(t_2-t_1\right)|x_1\rangle \tag{64}$$

remove the identity:

$$\int \mathrm{d}x_2 K\left(x_3,t_3;x_2,t_2\right)K\left(x_2,t_2;x_1,t_1\right) = \langle x_3|\hat{U}\left(t_3-t_2\right)\hat{U}\left(t_2-t_1\right)|x_1\rangle \tag{65}$$

$$= \langle x_3|\exp\left(-i\hat{T}\left(t_3-t_2\right)/\hbar\right)\exp\left(-i\hat{T}\left(t_2-t_1\right)/\hbar\right)|x_1\rangle \tag{66}$$

$$= \langle x_3|\exp\left(-i\hat{T}\left(t_3-t_1\right)/\hbar\right)|x_1\rangle \tag{67}$$

$$= K\left(x_3,t_3;x_1,t_1\right). \tag{68}$$

In this simplest case, we can break the propagator between two points into propagators between any intermediate number of points without introducing any approximation. The particle can either be thought of as following a straight line, or a sum over jagged lines.

When a potential $\hat{V}$ is introduced, we will be forced to sum over jagged lines. The free space calculation is simple because the only operator appearing in Eq 66 and Eq 67 is the kinetic operator $\hat{T}$: if a potential is present, $\left[\hat{T},\hat{V}\right] \neq 0$ and the exponentials cannot combine.

2.4 Example: propagation through a finite-width slit

Consider a particle leaving a source at position x_0 at time t_0, passing through a slit $y \in [-b,b]$ at time t, and continuing to land on a screen at time T. The amplitude to arrive at point x on the screen is given by

$$\psi\left(x,T\right) \propto \int_{-b}^{b} \mathrm{d}y K\left(x,T;y,t\right)K\left(y,t;x_0,t_0\right) \tag{69}$$

where the proportionality is not an equality as there is a constant required for the dimensions to match. Inserting the free space propagator gives

$$\psi\left(x,T\right) \propto \frac{1}{\sqrt{T-t}}\frac{1}{\sqrt{t-t_0}}\int_{-b}^{b}\mathrm{d}y\exp\left(\frac{im}{2\hbar}\left(\frac{\left(x-y\right)^2}{T-t}+\frac{\left(y-x_0\right)^2}{t-t_0}\right)\right). \tag{70}$$

This can be rewritten in terms of Fresnel integrals

$$\mathrm{Fr}\left(x\right) = \int_0^x \exp\left(iy^2\right)\mathrm{d}y. \tag{71}$$

Plotting $\mathrm{Fr}(x)$ in the Argand plane results in the 'Cornu spiral' (Fig. 1). This shows that the principal contribution to the amplitude comes from the paths near the centre of the slit.

2.5 Equivalence between Feynman and Schrödinger

This is implicit in the construction:

$$K\left(x,t;x_0,t_0\right) = \langle x|\exp\left(-i\hat{H}\left(t-t_0\right)/\hbar\right)|x_0\rangle \tag{72}$$

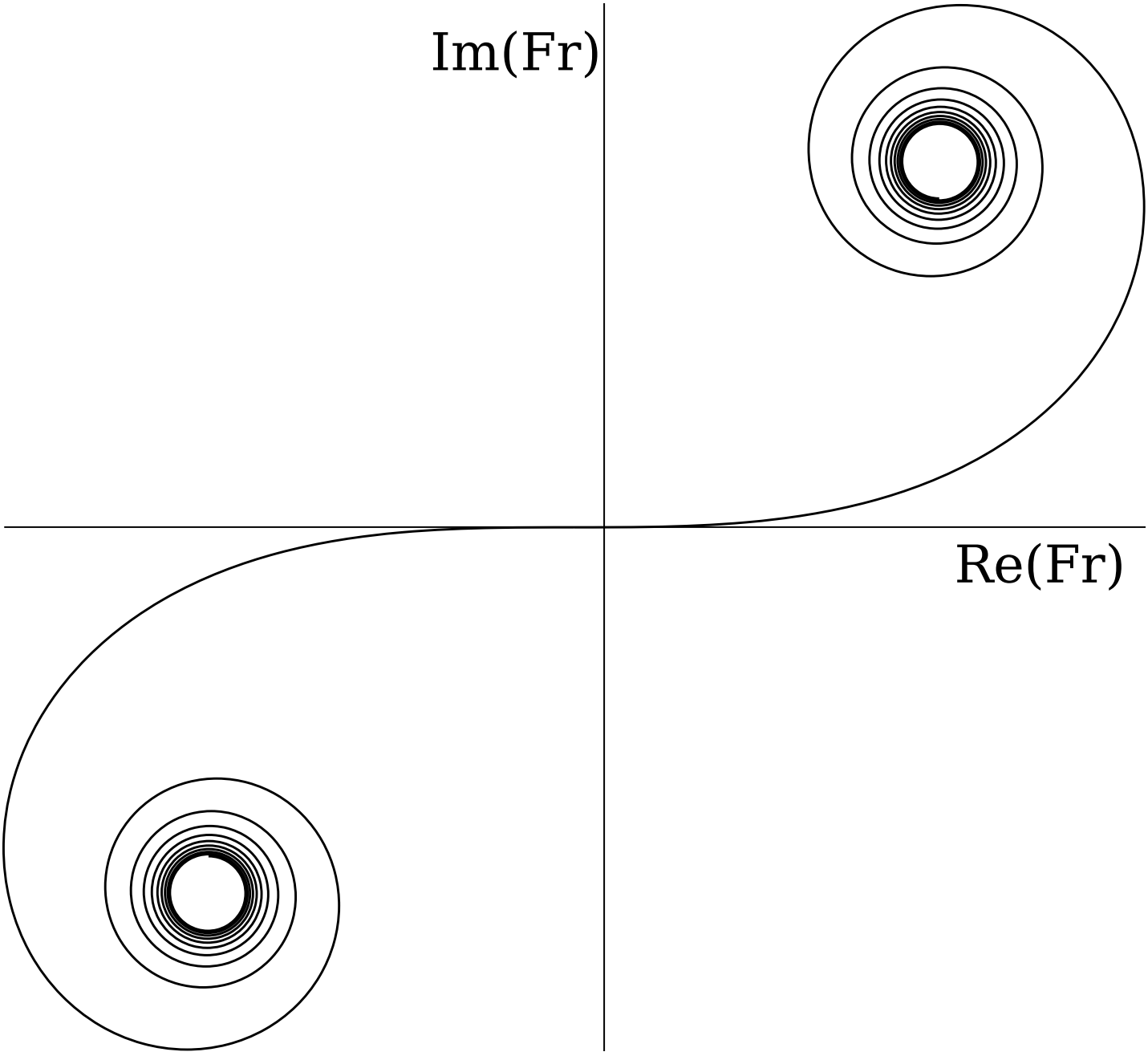

Figure 1: The Cornu Spiral.

which means states evolve unitarily. This is equivalent to the TDSE. Some prefer to derive the TDSE explicitly using the limit

$$\lim_{\delta t \to 0} K\left(x, t+\delta t; x, t\right) \tag{73}$$

but the result is equivalent.

2.6 The propagator in a general potential: Deriving Feynman (iii)

In general,

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V\left(\hat{x}\right) \tag{74}$$

and so

$$K\left(x, t; x_0, t_0\right) = \langle x| \exp\left(-i\left(\hat{T}+\hat{V}\right)\left(t-t_0\right)/\hbar\right)|x_0\rangle. \tag{75}$$

The problem with evaluating this is that $\hat{T}$ and $\hat{V}$ do not commute, and

$$\exp\left(A+B\right) \neq \exp\left(A\right)\exp\left(B\right) \tag{76}$$

unless $[A, B] = 0$. Hence we cannot just insert an identity as in the case of a free particle.
The solution is to use *time slicing*. Break the path into tiny slices $\delta t = t/N$ with N large. Then,

$$\exp\left(-i\hat{H}t/\hbar\right) = \left(\exp\left(-i\hat{H}\delta t/\hbar\right)\right)^N \tag{77}$$

and

$$\exp\left(-i\left(\hat{T}+\hat{V}\right)\delta t/\hbar\right) \approx \exp\left(-i\hat{T}\delta t/\hbar\right)\exp\left(-i\hat{V}\delta t/\hbar\right) \tag{78}$$

which becomes exact in the limit $\delta t \to 0$ (equivalently $N \to \infty$). Using time slicing we have:

$$K\left(x_N, t; x_0, t=0\right) = \langle x_N| \exp\left(-i\hat{H}\delta t/\hbar\right) \times \ldots |x_0\rangle \tag{79}$$

where '...' signifies there are N identical copies within the bracket. Now we can insert $N-1$ resolutions of the identity into the position basis:

$$K\left(x_N, t; x_0, t=0\right) = \int \mathrm{d}x_{N-1} \ldots \int \mathrm{d}x_1 \langle x_N| \exp\left(-i\hat{H}\delta t/\hbar\right)|x_{N-1}\rangle \ldots \langle x_1| \exp\left(-i\hat{H}\delta t/\hbar\right)|x_0\rangle. \tag{80}$$

We must evaluate N integrals of the form

$$K_n \triangleq K\left(x_{n+1}, \delta t; x_n, 0\right) = \langle x_{n+1}| \exp\left(-i\hat{H}\delta t/\hbar\right)|x_n\rangle = \langle x_{n+1}| \exp\left(-i\left(\hat{T}+\hat{V}\right)\delta t/\hbar\right)|x_n\rangle. \tag{81}$$

We use the fact that the exponent is small to approximate

$$K_n \approx \langle x_{n+1}| \exp\left(-i\hat{T}\delta t/\hbar\right) \exp\left(-i\hat{V}\delta t/\hbar\right)|x_n\rangle \tag{82}$$

and we can now treat this slice like a free particle. That is, we insert a resolution of the identity into the momentum basis:

$$\begin{aligned}
K_n &\approx \int \mathrm{d}p \langle x_{n+1}| \exp\left(-i\hat{T}\delta t/\hbar\right)|p\rangle\langle p| \exp\left(-i\hat{V}\delta t/\hbar\right)|x_n\rangle && (83)\\
&= \frac{1}{2\pi\hbar}\int \mathrm{d}p \exp\left(-ip^2\delta t/2m\hbar\right)\langle x_{n+1}|p\rangle \exp\left(-iV\left(x_n\right)\delta t/\hbar\right)\langle p|x_n\rangle && (84)\\
&= \exp\left(-iV\left(x_n\right)\delta t/\hbar\right) K_n^{\text{free}} && (85)\\
&= \exp\left(-iV\left(x_n\right)\delta t/\hbar\right)\sqrt{\frac{m}{2\pi i\hbar\delta t}} \exp\left(im\left(x_{n+1}-x_n\right)^2/2\hbar\delta t\right). && (86)
\end{aligned}$$

Putting it all together gives

$$K\left(x_N, t; x_0, 0\right) = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{N/2}\int \mathrm{d}x_{N-1}\ldots\int \mathrm{d}x_1 \exp\left(i\frac{\delta t}{\hbar}\sum_{n=1}^{N-1}\left(\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\delta t}\right)^2 - V\left(x_n\right)\right)\right). \tag{87}$$

The exponent in this limit simply becomes an integral:

$$\begin{aligned}
\lim_{N\to\infty}\delta t\sum_{n=1}^{N-1}\left(\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\delta t}\right)^2 - V\left(x_n\right)\right) &= \int_0^t \mathrm{d}t'\left(\frac{m}{2}\dot{x}^2 - V\left(x\right)\right) && (88)\\
&= \int_0^t \mathrm{d}t' L && (89)\\
&= S\left[x\right] && (90)
\end{aligned}$$

where $S\left[x\right]$ is the action of the classical trajectory x. Therefore

$$K\left(x, t; x_0, t_0\right) = \int \mathscr{D}x \exp\left(iS\left[x\right]/\hbar\right) \tag{91}$$

where $\int \mathscr{D}x$ denotes a path integral. This is Feynman's postulate (iii): all classical paths, no matter how crazy, appear in the quantum sum over trajectories ('histories') with equal magnitude. All that changes is the phase.

2.7 What about commutators?

The non-commutation of operators can be recovered in the path integral approach. The details of the calculation are beyond the scope of this course (involving a Wick rotation to imaginary time) and will be omitted here to avoid confusion. I will however outline the approach in the lectures.

3 Semiclassics

A strength of path integral quantum mechanics is that classical paths typically dominate the sum over histories (recall the Cornu spiral, Section 2.4). Other paths can be thought of as 'quantum corrections' or 'quantum fluctuations' (the latter is a slight misnomer as nothing is really fluctuating). Semiclassics is a process of including these corrections systematically as a series expansion.

3.1 Mathematical background

3.1.1 Gaussian integrals (1D)

Recall the form of a Gaussian integral:

$$I(a) = \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(-\frac{1}{2}ax^2\right), \quad a \in \mathbb{C},\ \mathfrak{Re}(a) \geq 0. \tag{92}$$

This can be evaluated using an elegant trick:

$$\begin{aligned} I(a)^2 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}x\mathrm{d}y \exp\left(-\frac{1}{2}a\left(x^2+y^2\right)\right) && (93)\\ &= \int_0^{2\pi} \mathrm{d}\theta \int_0^{\infty} \mathrm{d}r r \exp\left(-\frac{1}{2}ar^2\right) && (94)\\ &= \frac{2\pi}{a} && (95) \end{aligned}$$

and so

$$I(a) = \sqrt{\frac{2\pi}{a}}. \tag{96}$$

3.1.2 Gaussian integrals (ND)

Now consider an N-dimenional Gaussian integral

$$I(A) = \int \mathrm{d}^N \boldsymbol{x} \exp\left(-\frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x}\right) \tag{97}$$

where A is a symmetric positive definite matrix (meaning all its eigenvalues are strictly positive). To do this integral, note that we can diagonalise A:

$$A = ODO^T \tag{98}$$

where O is an orthogonal matrix:

$$O^T O = \mathbb{I} \tag{99}$$

and

$$D = \mathrm{diag}\left(a_1, a_2, \ldots a_N\right). \tag{100}$$

Therefore, defining

$$\tilde{\boldsymbol{x}} \triangleq O^T \boldsymbol{x} \tag{101}$$

gives

$$\boldsymbol{x}^T A \boldsymbol{x} = \tilde{\boldsymbol{x}}^T D \tilde{\boldsymbol{x}} \tag{102}$$

$$= \sum_{i=1}^{N} a_i \tilde{x}_i^2. \tag{103}$$

In this diagonal basis the integral reduces to

$$I\left(A\right) = \prod_{i=1}^{N} \int \mathrm{d}\tilde{x}_i \exp\left(-\frac{1}{2} a_i \tilde{x}_i^2\right) \tag{104}$$

where the orthogonality condition, Eq 99, ensures that the Jacobian of the transformation (the equivalent of the r that appeared when switching to plane polar co-ordinates in 1D) is unity. Eq 104 is just a product of 1D Gaussian integrals, and so

$$I\left(A\right) = \left(2\pi\right)^{N/2} \left(a_1 a_2 \ldots a_N\right)^{-1/2}. \tag{105}$$

Recalling that the determinant of a matrix is the product of its eigenvalues, this gives

$$I\left(A\right) = \sqrt{\frac{\left(2\pi\right)^N}{\det\left(A\right)}}. \tag{106}$$

3.1.3 Gaussian integrals (∞D)

The infinite limit can be taken without issue. Recalling that functions are infinite-dimensional vectors, and differential operators can be thought of as infinity-by-infinity matrices, we have

$$I\left(\hat{A}\right) = \int \mathscr{D}x \exp\left(-\frac{1}{2} \int_0^t x\left(t'\right) \hat{A} x\left(t'\right) \mathrm{d}t'\right) \tag{107}$$

$$= \sqrt{\frac{\left(2\pi\right)^\infty}{\det\left(\hat{A}\right)}} \tag{108}$$

where the determinant of an operator is again the product of its eigenvalues. The infinity does not prove to be a problem in practice, and can be handled through a clever use of normalisation.

3.1.4 Functional calculus

In Chapter 1 we saw how to derive the Euler Lagrange equation (Eq. 16) from the principle of least action (Eq. 7). This can also be done using functional calculus. To do so, we must vary the action $S[\boldsymbol{x}]$, which is a functional (function of functions), with respect to the function $\boldsymbol{x}(t)$. Using Einstein summation notation:

$$S[x_i] = \int_0^T L(x_i, \dot{x}_i)\,\mathrm{d}t' \tag{109}$$

(neglecting any explicit time dependence of the Lagrangian). Any variation in the action, using the chain rule, is:

$$\delta S[x_i] = \int_0^T \left(\frac{\partial L}{\partial x_i}\delta x_i + \frac{\partial L}{\partial \dot{x}_i}\delta \dot{x}_i\right)\mathrm{d}t' \tag{110}$$

and integrating the second term by parts:

$$\delta S[x_i] = \int_0^T \left(\frac{\partial L}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t'}\left(\frac{\partial L}{\partial \dot{x}_i}\right)\right)\delta x_i \mathrm{d}t' + \cancel{\left[\frac{\partial L}{\partial \dot{x}_i}\delta x_i\right]_0^t} \tag{111}$$

where the boundary term is zero as we assume that the paths do not vary at the start and end points:

$$\delta x_i(0) = \delta x_i(T) = 0. \tag{112}$$

We can now take the 'functional derivative' of the action simply by dividing through by a small variation in the path:

$$\frac{\delta S[x_i]}{\delta x_j(t)} = \int_0^T \left(\frac{\partial L}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t'}\left(\frac{\partial L}{\partial \dot{x}_i}\right)\right)\frac{\delta x_i(t')}{\delta x_j(t)}\mathrm{d}t'. \tag{113}$$

Finally, we use the useful fact that

$$\frac{\delta x_i(t')}{\delta x_j(t)} = \delta_i^j \delta(t - t') \tag{114}$$

where δ_i^j is the Kroencker delta (one if $i = j$, zero otherwise) and $\delta(t - t')$ is a Dirac delta function.

This gives

$$\frac{\delta S\left[x_i\right]}{\delta x_j\left(t\right)} = \int_0^T \left(\frac{\partial L}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t'}\left(\frac{\partial L}{\partial \dot{x}_i}\right)\right) \delta_i^j \delta\left(t - t'\right) \mathrm{d}t' \tag{115}$$

$$= \left(\frac{\partial L}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i}\right)\right) \delta_i^j \tag{116}$$

$$= \frac{\partial L}{\partial x_j} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_j}\right). \tag{117}$$

The principle of least action dictates that the left hand side is zero, from which the Euler Lagrange equations follow.

3.2 The method of stationary phase

3.2.1 1D

Consider the familiar integral

$$I\left(\epsilon\right) = \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(if\left(x\right)/\epsilon\right) \tag{118}$$

where ϵ is small. Consider the saddle points x_b defined by

$$f'\left(x_b\right) \triangleq \left.\frac{\mathrm{d}f\left(x\right)}{\mathrm{d}x}\right|_{x=x_b} = 0. \tag{119}$$

These points dominate the integral, as the phase winds the slowest at these points (recall the Cornu spiral, Fig. 1). Therefore a decent approximation to the integral can be found by Taylor expanding around x_b:

$$f\left(x\right) \approx f\left(x_b\right) + \cancel{\left(x - x_b\right) f'\left(x_b\right)} + \frac{\left(x - x_b\right)^2}{2} f''\left(x_b\right) + \mathcal{O}\left(x^3\right) \tag{120}$$

giving

$$I_b\left(\epsilon\right) \approx \exp\left(if\left(x_b\right)/\epsilon\right) \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(i\frac{1}{2}\left(x - x_b\right)^2 f''\left(x_b\right)/\epsilon\right). \tag{121}$$

This is a Gaussian integral, which gives

$$I_b\left(\epsilon\right) \approx \sqrt{\frac{2\pi i\epsilon}{f''\left(x_b\right)}} \exp\left(if\left(x_b\right)/\epsilon\right). \tag{122}$$

A convenient way to write this is

$$I_b\left(\epsilon\right) \approx \sqrt{\frac{2\pi\epsilon}{\left|f''\left(x_b\right)\right|}} \exp\left(if\left(x_b\right)/\epsilon + \nu_b \pi i/4\right) \tag{123}$$

where

$$\nu_b \triangleq \operatorname{sign}\left(f''\left(x_b\right)\right). \tag{124}$$

More generally there will be multiple saddle points to sum over:

$$I\left(\epsilon\right) \approx \sum_b I_b\left(\epsilon\right). \tag{125}$$

This 'method of stationary phase' becomes the 'method of steepest descent' for integrals of the form

$$I\left(\epsilon\right) = \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(-\epsilon f\left(x\right)\right). \tag{126}$$

3.2.2 ND

$$I\left(\epsilon\right) = \int_{-\infty}^{\infty} \mathrm{d}^N \boldsymbol{x} \exp\left(if\left(\boldsymbol{x}\right)/\epsilon\right) \tag{127}$$

as before,

$$f\left(\boldsymbol{x}\right) \approx f\left(x_{i,b}\right) + \cancel{\left(x_i - x_{i,b}\right)\frac{\partial f\left(x_{i,b}\right)}{\partial x_i}} + \frac{\left(x_i - x_{i,b}\right)\left(x_j - x_{j,b}\right)}{2}\frac{\partial^2 f\left(x_b\right)}{\partial x_i \partial x_j} + \mathcal{O}\left(x^3\right) \tag{128}$$

and

$$I_b\left(\epsilon\right) \approx \sqrt{\frac{\left(2\pi\epsilon\right)^N}{\left|\det\left(\frac{\partial^2 f\left(x_b\right)}{\partial x_i \partial x_j}\right)\right|}} \exp\left(if\left(\boldsymbol{x}_b\right)/\epsilon + \nu_b \pi i/4\right) \tag{129}$$

where

$$\nu_b = \operatorname{sign}\left(\det\left(\frac{\partial^2 f\left(x_b\right)}{\partial x_i \partial x_j}\right)\right). \tag{130}$$

3.2.3 ∞D

$$K\left(x_f, t_f; x_i, t_i\right) = \int \mathscr{D}x \exp\left(iS\left[x\right]/\hbar\right) \tag{131}$$

$$\approx \sum_b \sqrt{\frac{\left(2\pi\hbar\right)^\infty}{\left|\det\left(\frac{\delta^2 S\left(x_b\right)}{\delta x_i\left(t_f\right)\delta x_j\left(t_i\right)}\right)\right|}} \exp\left(iS\left[x_b\right]/\hbar + \nu_b \pi i/4\right) \tag{132}$$

where $x_b\left(t\right)$ are paths satisfying

$$\left.\frac{\delta S\left[x\right]}{\delta x\left(t\right)}\right|_{x(t)=x_b(t)} = 0 \tag{133}$$

i.e. classical trajectories. This method becomes one of the key tools in quantum field theory. In quantum mechanics it is perhaps easiest to understand at the wavefunction level, where it becomes...

3.3 The WKB Approximation

Uses:

- gives an approximate analytical form of $\psi(x)$ for any potential $V(x)$.
- Allows an approach to the classical limit, historically important in establishing the correspondence principle.
- Sets up QFT.

The idea: $\psi(x,t)$ is treated as a plane wave with a wavelength which varies slowly across space: $\lambda(x)$. Specifically, we require $\lambda \ll L_{\text{system}}$, and $|\lambda'| \ll 2\pi$. We work semi-classically by approximating $[x,p]=0$. Therefore we can write

$$E = \frac{p(x)^2}{2m} + V(x). \tag{134}$$

$p(x)$ would usually be meaningless in quantum mechanics, but here it is

$$p(x) = \pm\sqrt{2m(E - V(x))} \tag{135}$$

and we choose the + sign by convention. Then the wavelength is

$$\lambda(x) = 2\pi\hbar/p(x). \tag{136}$$

We seek plane waves, so define

$$\psi(x,t) = \exp(iS(x,t)/\hbar). \tag{137}$$

The function S is chosen to be suggestive of an action. To motivate this, consider:

$$\begin{aligned} S &= \int L\mathrm{d}t && (138)\\ &= \int (p\cdot\dot{q} - H)\,\mathrm{d}t && (139)\\ &= \int p\cdot\frac{\mathrm{d}q}{\mathrm{d}t}\mathrm{d}t - \int H\mathrm{d}t && (140)\\ &= \int p\mathrm{d}q - Et && (141) \end{aligned}$$

assuming in the last line that the Hamiltonian function has no explicit time dependence. [Please forgive the switching back and forth between q and x; different conventions are used in classical and quantum mechanics!] Therefore

$$\psi(x,t) = \exp(-iEt/\hbar)\exp\left(i\int p\mathrm{d}q/\hbar\right). \tag{142}$$

That is, we've factored out the time dependence. This is usual in quantum mechanics, where we typically write

$$\psi(x,t) = \exp(-iEt/\hbar)\,\phi(x) \tag{143}$$

before finding $\phi(x)$ which solves the Time Independent Schrödinger Equation (TISE). We will follow this convention here.

Define

$$\phi(x) = \exp(i\sigma(x)/\hbar) \tag{144}$$

where

$$\sigma(x) = \int p(x)\,\mathrm{d}x. \tag{145}$$

Provided $\sigma \in \mathbb{C}$ there is no approximation so far: ϕ can have a varying magnitude and phase.

Now substitute Eq. 144 into the TISE:

$$\hat{H}\phi = E\phi \tag{146}$$

$$-\frac{\hbar^2}{2m}\phi'' + V\phi = E\phi \tag{147}$$

$$-\hbar^2\left(\frac{i\sigma''}{\hbar} + \left(\frac{i\sigma'}{\hbar}\right)^2\right)\phi = 2m(E-V)\,\phi. \tag{148}$$

Therefore σ obeys the equation

$$-i\hbar\sigma'' + (\sigma')^2 = p(x)^2. \tag{149}$$

The key step in the WKB approximation is to now expand σ in powers of $\hbar$:

$$\sigma(x) \approx \sigma_0(x) + \frac{\hbar}{i}\sigma_1(x) + \left(\frac{\hbar}{i}\right)^2\sigma_2(x) + \mathcal{O}\left(\hbar^3\right). \tag{150}$$

This is confusing for a number of reasons. First, while $\hbar$ is small in SI units, it is a dimensionful quantity and so its 'size' depends on the choice of units. Second, following on, if $\hbar$ is not 'small' the expansion doesn't obviously make sense. Third, the units of the different terms look wrong.

The way to understand the expansion is to note that σ_0, σ_1,and σ_2 must have different dimensions to one another. Hence, you see that we're not exactly expanding in powers of $\hbar$: we're identifying some quantity with the same units as $\hbar$ (the action $\sigma = \int p\mathrm{d}q$), and are expanding in powers of the dimensionless quantity

$\hbar/\sigma$. This is small provided the action is large compared to $\hbar$.
We proceed in the expansion order-by-order.

3.3.1 0^{th} order

To 0^{th} order in $\hbar$ the WKB epansion, Eq. 150, reads

$$\sigma(x) = \sigma_0(x) + \mathcal{O}(\hbar). \tag{151}$$

To 0^{th} order in $\hbar$ the main WKB equation, Eq. 149, reads:

$$(\sigma_0')^2 = p(x)^2 \tag{152}$$

and so we get the result

$$\sigma_0'(x) = \pm p(x) \tag{153}$$

with solution

$$\sigma_0(x) = \pm \int p(x)\,\mathrm{d}x. \tag{154}$$

Hence, to 0^{th} order in $\hbar$ the WKB approximation to the wavefunction is

$$\phi^{(0)}(x) = \exp\left(\pm i \int p(x)\,\mathrm{d}x/\hbar\right). \tag{155}$$

Good – this was the starting assumption!

3.3.2 1^{st} order

We now repeat the process iteratively, using the result of the previous level.
To 1^{st} order in $\hbar$ the WKB epansion, Eq. 150, reads

$$\sigma(x) = \sigma_0(x) + \frac{\hbar}{i}\sigma_1(x) + \mathcal{O}\left(\hbar^2\right). \tag{156}$$

The main WKB equation, Eq. 149, reads:

$$-i\hbar\left(\sigma_0'' + \left(\frac{\hbar}{i}\right)\sigma_1''\right) + \left(\sigma_0' + \left(\frac{\hbar}{i}\right)\sigma_1'\right)^2 = p(x)^2 \tag{157}$$

$$-i\hbar\sigma_0'' - \hbar^2\sigma_1'' + (\sigma_0')^2 - \hbar^2(\sigma_1')^2 + \frac{2\hbar}{i}\sigma_0'\sigma_1' = p(x)^2 \tag{158}$$

Keeping terms to 1^{st} order in $\hbar$ gives

$$-i\hbar\sigma_0'' + (\sigma_0')^2 + \frac{2\hbar}{i}\sigma_0'\sigma_1' = p(x)^2 . \tag{159}$$

Inserting the 0^{th} order result, Eq. 152, gives

$$-i\hbar\sigma_0'' + \frac{2\hbar}{i}\sigma_0'\sigma_1' = 0 \tag{160}$$

or

$$\sigma_1' = -\frac{1}{2}\frac{\sigma_0''}{\sigma_0'}. \tag{161}$$

Again using the 0^{th} order result, that

$$\sigma_0' = \pm p(x) \tag{162}$$

gives

$$\sigma_1' = -\frac{1}{2}\frac{p'}{p} \tag{163}$$

with solution

$$\sigma_1(x) = -\frac{1}{2}\ln(p(x)) . \tag{164}$$

Hence, to 1^{st} order in $\hbar$ the WKB approximation to the wavefunction is

$$\phi^{(1)}(x) = \exp\left(\pm i\int p(x)\,\mathrm{d}x/\hbar - \frac{1}{2}\frac{\hbar}{i}\frac{i}{\hbar}\ln(p(x))\right) \tag{165}$$

or

$$\phi^{(1)}(x) = \frac{1}{\sqrt{p(x)}}\exp\left(\pm i\int p(x)\,\mathrm{d}x/\hbar\right). \tag{166}$$

This is the WKB approximation:

$$\phi_{\text{WKB}}(x) = \frac{A_+}{\sqrt{p(x)}}\exp\left(i\int p(x)\,\mathrm{d}x/\hbar\right) + \frac{A_-}{\sqrt{p(x)}}\exp\left(-i\int p(x)\,\mathrm{d}x/\hbar\right). \tag{167}$$

Since $p \in \mathbb{C}$ we can find evanescent solutions as well as sinusoidal solutions, as is familiar from earlier quantum courses. The prefactor $1/\sqrt{p}$ can be understood intuitively by analogy to pass-the-parcel, in which you hang on to the parcel for as long as possible. If p is smaller in given region, the velocity v is smaller, so the probability to find the particle, $|\phi|^2 \sim 1/p$, is bigger.

Note the connection between the WKB wavefunction and the result of the method of stationary phase, Eq 132:

$$\psi(x,t) = \frac{A}{\sqrt{\left|\det\left(\frac{\delta^2 S(x_b)}{\delta x_i(t_f)\delta x_j(t_i)}\right)\right|}} \exp\left(iS\left[x_{\text{classical}}\right]/\hbar + \nu_b \pi i/4\right). \tag{168}$$

This is no coincidence!

3.4 WKB for bound states

3.4.1 Failure of the WKB method

Consider an arbitrary potential satisfying

$$V(x) - E > 0,\ x < a \text{ (region I)} \tag{169}$$

$$V(x) - E < 0,\ a < x < b \text{ (region II)} \tag{170}$$

$$V(x) - E > 0,\ x > b \text{ (region III)}. \tag{171}$$

That is, regions I and III are classically forbidden, and region II is classically allowed. Classically, the particle would be trapped in region II. Without specifying the potential any further, we can already get a good approximation for the wavefunction using WKB. This is a big deal! The number of potentials which admit exact solutions is limited to about two cases (the square well and harmonic oscillator).
In principle the approach is the same as the one you saw in 2nd year quantum mechanics. Specifically, we solve for the wavefunction in each of the regions separately, then match the wavefunctions at the meeting points.

$$\phi_I(x) = \frac{A_I}{\sqrt{p(x)}} \exp\left(\int_x^a |p(x')|\,\mathrm{d}x'/\hbar\right) \tag{172}$$

$$\phi_{II}(x) = \frac{A_{II}}{\sqrt{p(x)}} \cos\left(\int_a^x |p(x')|\,\mathrm{d}x'/\hbar - \pi/4\right) \equiv \frac{A_{II}}{\sqrt{p(x)}} \cos\left(\int_x^b |p(x')|\,\mathrm{d}x'/\hbar - \pi/4\right) \tag{173}$$

$$\phi_{III}(x) = \frac{A_{III}}{\sqrt{p(x)}} \exp\left(-\int_b^x |p(x')|\,\mathrm{d}x'/\hbar\right) \tag{174}$$

and

$$\phi_I(a) = \phi_{II}(a) \tag{175}$$

$$\phi_{II}(b) = \phi_{III}(b). \tag{176}$$

Within region II, consistency is required between the two expressions (one heading up from a, the other heading down from b).

However, the WKB approximation fails terrible exactly where it is needed most, at a and b. This is because these are classical turning points. Hence, $E = V$, and $p = 0$, so the wavelength $\lambda \to \infty$. But WKB assumes $\lambda \ll L_{\text{system}}$.

3.4.2 Airy function regularisation

To deal with this problem, note that, sufficiently close to the classical turning points, the potential is approximately linear:

$$V(x) - E \approx \begin{cases} F_a(a - x), & x \approx a \\ F_b(x - b), & x \approx b. \end{cases} \tag{177}$$

The TISE for a linear potential actually provides a third exactly solvable case beyond the square well and harmonic oscillator.

$$-\frac{\hbar^2}{2m}\phi'' + Fx\phi = E\phi \tag{178}$$

is a rescaling of 'Airy's equation'

$$y'' - xy = 0 \tag{179}$$

which is solved by the 'Airy function'

$$\mathrm{Ai}(x) \triangleq \frac{1}{\pi}\int_0^\infty \mathrm{d}t \cos\left(\frac{t^3}{3} + xt\right). \tag{180}$$

This remarkable function was originally introduced in Airy's study of supernumerary rainbows. It models a quantum particle in a linear potential, as in a semiconductor heterojunction or a constant gravitational field. It also models quark confinement, and is the basis of Witten's conjecture in string theory.

The Airy function features underdamped sinusoidal oscillations for $x < 0$, and decays exponentially for $x > 0$. Using the Airy function we can regularise the WKB wavefunction, smoothing it across the classical turning points.

In the lectures we will see the key features of the WKB approximation. Interestingly, the wavefunction is higher towards the edges of the well. This seems counterintuitive at first: any well is quadratic to the coarsest approximation, so shouldn't the eigenfunctions resemble harmonic oscillator solutions? Actually they do, but the WKB wavefunctions resemble harmonic oscillator solutions with large energy quantum numbers. These are more likely to be found near the energetically costly edges of the well. This is the correspondence principle: WKB is semiclassical, and the classical regime is returned in the limit of large quantum numbers.

3.4.3 Bohr Sommerfeld quantization

Using Airy function regularisation we can match the WKB wavefunctions between the regions. Consistency of the wavefunction leads to the condition

$$\frac{1}{\hbar}\int_a^b p\mathrm{d}x = \left(n+\frac{1}{2}\right)\pi,\ n\in\mathbb{Z}. \tag{181}$$

[Simons / Fowler follow Landau and Lifshitz in the derivation, which is a little complex.] The action accrued over an entire period $a \to b \to a$ can be written in the neat form:

This is the Bohr-Sommerfeld quantization condition:

$$\oint p\mathrm{d}x/\hbar = 2\pi\left(n+\frac{1}{2}\right). \tag{182}$$

This was a major result of 'old quantum theory'.

3.5 Phase space Quantization

In fact, the Bohr-Sommerfeld quantization condition is incredibly durable, and proves to be exactly correct beyond the approximations introduced by WKB. In general, the integral $\oint p\mathrm{d}x$ gives the area enclosed by an orbit in 'phase space', (x, p). The Bohr-Sommerfeld condition states that quantum orbits enclose quantized areas in phase space: the area between successive allowed orbits is exactly $2\pi\hbar$.

An electron acquires a phase $\oint p\mathrm{d}x/\hbar$ when traversing an orbit.

The extra 1/2 in Eq. 182 is called the 'Maslov index'. It is an extra phase change picked up by the particle upon turning. In general, a particle picks up a phase of $\pi/2$ at a 'soft' turning point (V' small, in units such that this makes sense) and π at a hard turning point (such as the wall of an infinite potential well).

We can say that a transition from orbit n to orbit $n-1$ released a photon of energy $\Delta E = \hbar\omega$, where $\omega = 2\pi/T$ with T the time to complete the orbit. To see this:

$$T = \oint \mathrm{d}t = \oint \frac{\mathrm{d}x}{v} \tag{183}$$

where

$$v = \frac{\partial E}{\partial p} \tag{184}$$

is the velocity. Then

$$\Delta E \cdot \oint \frac{\mathrm{d}p}{\mathrm{d}E}\mathrm{d}x = \oint p\mathrm{d}x = 2\pi\hbar \tag{185}$$

and so

$$\Delta E = \frac{2\pi\hbar}{T}. \tag{186}$$

4 Magnetic Fields in Quantum Mechanics

$c = 1$ throughout.

4.1 Vector potential recap

Maxwell's equations in free space:

$$\nabla \cdot \boldsymbol{E} = 0 \tag{187}$$

$$\nabla \times \boldsymbol{E} = -\dot{\boldsymbol{B}} \tag{188}$$

$$\nabla \cdot \boldsymbol{B} = 0 \tag{189}$$

$$\nabla \times \boldsymbol{B} = \dot{\boldsymbol{E}}. \tag{190}$$

Eq 189, which says that magnetic monopoles do not exist, means that we can always define a field $\boldsymbol{A}(\boldsymbol{x}, t)$ such that

$$\boldsymbol{B}(\boldsymbol{x}, t) = \nabla \times \boldsymbol{A}(\boldsymbol{x}, t) \tag{191}$$

$$\boldsymbol{E}(\boldsymbol{x}, t) = -\nabla\phi(\boldsymbol{x}, t) - \dot{\boldsymbol{A}}(\boldsymbol{x}, t) \tag{192}$$

where ϕ is the electric potential / voltage. Then

$$\nabla \cdot \boldsymbol{B} = \nabla \cdot \nabla \times \boldsymbol{A} = 0 \tag{193}$$

and

$$\nabla \times \boldsymbol{E} = -\nabla \times \nabla\phi - \nabla \times \dot{\boldsymbol{A}} \tag{194}$$

$$= -\partial_t \nabla \times \boldsymbol{A} \tag{195}$$

$$= -\dot{\boldsymbol{B}} \tag{196}$$

as required. However, there remains an arbitrariness in the definition of $\boldsymbol{A}$. Specifically, Maxwell's equations are equally well obeyed by the transformed fields

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \nabla\lambda\left(\boldsymbol{x}, t\right) \tag{197}$$

$$\phi \to \phi' = \phi - \lambda\left(\dot{\boldsymbol{x}}, t\right). \tag{198}$$

This is 'gauge invariance'. While often described as a symmetry, this is not quite accurate: a symmetry is something physical, but gauge invariance describes a redundancy in a mathematical description, and therefore cannot cause any physical consequences (just as there can be no physical consequences of counting in a different base).

It is convenient to define

$$A^{\mu} \triangleq \begin{pmatrix} \phi \\ \boldsymbol{A} \end{pmatrix}^{\mu} \tag{199}$$

and

$$F^{\mu\nu} \triangleq \partial^{\mu} A^{\nu} - \partial^{\nu} A^{\mu} \tag{200}$$

where

$$\partial^{\mu} \triangleq \begin{pmatrix} \partial_t \\ \nabla \end{pmatrix}^{\mu} \tag{201}$$

and

$$\partial_t \triangleq \frac{\partial}{\partial t}. \tag{202}$$

We can then rewrite the full set of Maxwell's equations in the simpler form

$$\partial_{\mu} F^{\mu\nu} = 0. \tag{203}$$

Gauge invariance then means invariance of this equation to the change

$$A^{\mu} \to A^{\mu'} = A^{\mu} + \partial^{\mu}\lambda. \tag{204}$$

4.2 Magnetic fields in Lagrangian quantum mechanics

In Eq. 5 we saw the Lagrangian

$$L = T - V. \tag{205}$$

However, a magnetic field does no work on an electron: it changes neither T nor V. Yet it does change the motion of the electron. The previous description of the Lagrangian was therefore incomplete. In the presence of a magnetic field, we have

$$L = \frac{1}{2}m\dot{\boldsymbol{x}}^2 + q\left(\dot{\boldsymbol{x}} \cdot \boldsymbol{A}\left(\boldsymbol{x}, t\right) - \phi\left(\boldsymbol{x}, t\right)\right) \tag{206}$$

where q is the charge on the particle. The proof of this form is to show that it leads to the appropriate Euler Lagrange equations. These are the equations of motion of an electron in an electromagnetic field: the Lorentz force law

$$m\ddot{\boldsymbol{x}} = q\left(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right). \tag{207}$$

This derivation is do-able but tricky, and is beyond the syllabus.

In Chapter 2 we saw that the propagator takes the form

$$K\left(\boldsymbol{x}_f, t_f; \boldsymbol{x}_i, t_i\right) = \int \mathscr{D}\boldsymbol{x} \exp\left(iS\left[\boldsymbol{x}\right]/\hbar\right). \tag{208}$$

This remains the case in electromagnetic fields, provided we update the Lagrangian to that in Eq. 206:

$$S\left[\boldsymbol{x}\right] = \int_{t_i}^{t_f} \left\{\frac{1}{2}m\dot{\boldsymbol{x}}^2 + q\left(\dot{\boldsymbol{x}} \cdot \boldsymbol{A} - \phi\right)\right\} \mathrm{d}t'. \tag{209}$$

4.3 The Aharonov Bohm Effect

This remarkable effect was theorised by Aharonov and Bohm in Bristol in 1959. It was experimentally confirmed by Chambers in Bristol in 1961.

Consider the two-slit experiment conducted with electrons. Now replace the partition between the slits with a solenoid of infinite length. Recall that the magnetic field is uniform within the solenoid, running along its axis, and is exactly zero outside. Experimentally this can be done in such a way that the electron is perfectly shielded from the magnetic field. What happens as the magnetic field is turned on within the solenoid?

The obvious answer would be that nothing happens. The field is zero everywhere that the electron can travel, so it is natural to suggest that it cannot induce a phase along any classical trajectory. Hence, the path integral is unchanged.

However, this is not what is seen. Instead, the 2-slit interference pattern shifts along the screen as the field is increased. This is the Aharonov Bohm effect. The easiest way to understand it is with path integrals.

The wavefunction at position $\boldsymbol{x}$ on the screen, up to an overall normalisation, is

$$\psi\left(\boldsymbol{x}, t\right) = K\left(\boldsymbol{x}, t; 0, 0\right) = \int \mathscr{D}\boldsymbol{x} \exp\left(iS\left[\boldsymbol{x}\right]/\hbar\right). \tag{210}$$

Take the electric potential ϕ to be zero. The change in the action accrued along each path upon turning on

the magnetic field is given by

$$S_{\boldsymbol{A}}\left[\boldsymbol{x}\right]-S_{\boldsymbol{0}}\left[\boldsymbol{x}\right]=q\int_{0}^{t}\dot{\boldsymbol{x}}\cdot\boldsymbol{A}\mathrm{d}t'=q\int_{\boldsymbol{0}}^{\boldsymbol{x}}\boldsymbol{A}\cdot\mathrm{d}\boldsymbol{x} \tag{211}$$

and so the wavefunction acquires a phase

$$\psi_{\boldsymbol{A}}\left(\boldsymbol{x},t\right)=\psi_{\boldsymbol{0}}\left(\boldsymbol{x},t\right)\exp\left(iq\int_{\mathcal{C}}\boldsymbol{A}\cdot\mathrm{d}\boldsymbol{x}/\hbar\right). \tag{212}$$

The global phase of a wavefunction is meaningless (a gauge choice). However, we can look to see if there is a relative phase shift between two paths $\mathcal{C}_R$ and $\mathcal{C}_L$ travelling right and left around the solenoid, respectively. The phase difference is

$$\begin{aligned}\Delta\theta&=\frac{q}{\hbar}\left(\int_{\mathcal{C}_R}-\int_{\mathcal{C}_L}\right)\boldsymbol{A}\cdot\mathrm{d}\boldsymbol{x} &(213)\\ &=\frac{q}{\hbar}\oint\boldsymbol{A}\cdot\mathrm{d}\boldsymbol{x} &(214)\\ &=\frac{q}{\hbar}\iint\boldsymbol{B}\cdot\mathrm{d}\boldsymbol{S} &(215)\\ &=q\Phi/\hbar &(216)\end{aligned}$$

where Φ is the flux through the solenoid. The trick is that $\oint$ is an integral around any path enclosing Φ: the electron doesn't actually need to visit the region of the magnetic flux in order to feel its effect.

Aharonov and Bohm concluded that in quantum mechanics it is potentials that are important, not forces (which are zero in this problem), in contrast to classical mechanics where forces are real and potentials merely a mathematical convenience. This is remarkable, as the potential $\boldsymbol{A}$ is gauge dependent!

Alternatively we might note that it is not $\boldsymbol{A}$ that appears, but $\oint\boldsymbol{A}\cdot\mathrm{d}\boldsymbol{x}$. This is gauge independent. But it is also non-local. This is an early appearance of topology in physics.

4.4 Magnetic Monopoles

A precursor to the Aharonov Bohm effect was Dirac's quantum theory of magnetic monopoles (1931). The motivation is to make Maxwell's equations (in the presence of charges) symmetric. Specifically,

$$\begin{aligned}\nabla\cdot\boldsymbol{E}&=\rho_E &(217)\\ \nabla\times\boldsymbol{E}&=j_M-\dot{\boldsymbol{B}} &(218)\\ \nabla\cdot\boldsymbol{B}&=\rho_B &(219)\\ \nabla\times\boldsymbol{B}&=j_E+\dot{\boldsymbol{E}}. &(220)\end{aligned}$$

These differ from the usual Maxwell's equations only because Eq. 219 usually has $\rho_M = 0$, meaning the magnetic charge density is strictly zero. A magnetic monopole, if discovered, would violate this: it would be an elementary particle charged under the magnetic field – that is, it would feature the north pole of a magnet, say, without the south.

Magnetic monopoles would be sources or sinks of magnetic field, in exact analogy to electrons and positrons for electric field. Any closed surface enclosing a magnetic monopole would obey

$$\oiint \boldsymbol{B} \cdot \mathrm{d}\boldsymbol{S} = \pm g \tag{221}$$

where g is the magnetic charge of a north monopole.

Dirac noted that the existence of magnetic monopoles would explain the quantization of electric charge (otherwise still unexplained). His argument was as follows. Imagine creating a monopole-antimonopole pair and separating them. Any surface enclosing the north monopole has a flux g passing through it. We can imagine for simplicity this flux passing through at a single point. Then, the flux follows a 'Dirac string' connecting the north monopole to the south. If an electron were to pass around this string it would pick up an Aharonov Bohm phase (in modern terminology):

$$\psi = \psi_0 \exp\left(ie \oint \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{x}/\hbar \right). \tag{222}$$

For the wavefunction to remain single-valued, and therefore well-defined, it must be the case that

$$e \oint \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{x}/\hbar = 2\pi\mathbb{Z}. \tag{223}$$

By Gauss' theorem this states that

$$eg = h\mathbb{Z}. \tag{224}$$

Hence, both e and g must be quantized (integers, in appropriate units).

4.5 Magnetic fields in Hamiltonian quantum mechanics

In Chapter 1 (Eq. 18) we saw that the momentum in classical mechanics is given by

$$\boldsymbol{p} \triangleq \frac{\partial L}{\partial \dot{\boldsymbol{x}}} \tag{225}$$

and the Hamiltonian is defined by

$$H = \boldsymbol{p} \cdot \dot{\boldsymbol{q}} - L. \tag{226}$$

This remains true in the presence of magnetic fields. However, the Lagrangian has to be updated, and now

takes the form of Eq. 206. This gives

$$\boldsymbol{p} = m\dot{\boldsymbol{x}} + q\boldsymbol{A} \tag{227}$$

$$H = \frac{1}{2m}\left(\boldsymbol{p} - q\boldsymbol{A}\right)^2 + V\left(\boldsymbol{x}\right). \tag{228}$$

As before, we can use canonical quantization to obtain quantum mechanics from classical. In the position basis,

$$\boldsymbol{x} \to \hat{\boldsymbol{x}} \tag{229}$$

$$\boldsymbol{p} \to -i\hbar\nabla \text{ 'canonical momentum'} \tag{230}$$

without change. The vector potential behaves in the same way as the usual potential:

$$V\left(\boldsymbol{x}\right) \to \hat{V} = V\left(\hat{\boldsymbol{x}}\right) \tag{231}$$

$$\boldsymbol{A}\left(\boldsymbol{x}\right) \to \hat{\boldsymbol{A}} = \boldsymbol{A}\left(\hat{\boldsymbol{x}}\right) \tag{232}$$

where we have assumed no explicit time dependence, for simplicity. In quantum field theory $\boldsymbol{A}$ becomes a dynamical field; its particle content is the photon.

However, the canonical momentum is no longer gauge invariant. Instead, we must introduce the

$$\hat{\boldsymbol{p}} - q\hat{\boldsymbol{A}} \text{ 'kinetic momentum'.} \tag{233}$$

Note that

$$\left[\hat{\boldsymbol{p}}, \hat{\boldsymbol{A}}\right] \neq 0 \tag{234}$$

in general.

4.6 Probability currents in magnetic fields

In second year you saw the expression for the probability current density (in the position basis)

$$\boldsymbol{j}\left(\boldsymbol{x}, t\right) = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) \tag{235}$$

which obeys the continuity equation

$$\nabla \cdot \boldsymbol{j} = -\dot{\rho} \tag{236}$$

where

$$\rho = \psi^* \psi. \tag{237}$$

In the presence of a magnetic field this becomes

$$\boldsymbol{j}(\boldsymbol{x}, t) = \frac{i\hbar}{2m} \left(\psi \nabla \psi^* - \psi^* \nabla \psi + 2q\boldsymbol{A}\rho / i\hbar \right) \tag{238}$$

and the continuity equation remains unchanged. Note that this is not simply Eq. 235 with the canonical momentum replaced by the kinetic momentum: the full derivation must instead be carried out with the new Hamiltonian.

If we define

$$\psi(\boldsymbol{x}, t) = \sqrt{\rho(\boldsymbol{x}, t)} \exp\left(i\theta(\boldsymbol{x}, t) \right) \tag{239}$$

with $\rho,\ \theta \in \mathbb{R}$,we find that

$$\boldsymbol{j}(\boldsymbol{x}, t) = \rho \frac{\hbar}{m} \left(\nabla\theta - q\boldsymbol{A}/\hbar \right) \tag{240}$$

$$= \rho \boldsymbol{v} \tag{241}$$

where $\boldsymbol{v}$ can be thought of as similar to a velocity. The current density is gauge invariant (as befits an observable quantity). However, neither $\boldsymbol{A}$ nor $\nabla\theta$ are individually gauge invariant. This means that a gauge choice directly affects the phase of the wavefunction.

Worse, when $\boldsymbol{B} = \boldsymbol{0}$, $\psi(\boldsymbol{x}, 0)$ determines $\psi(\boldsymbol{x}, t)$ (this is the purpose of the TDSE!). But this is no longer true in the presence of a $\boldsymbol{B}$ field. Two initial conditions must be specified: these could be $\rho(\boldsymbol{x}, 0)$ and $\boldsymbol{j}(\boldsymbol{x}, 0)$, except along lines of $\rho = 0$.

4.7 Landau Levels

4.7.1 Quantum result

A solvable example of electronic behaviour in a magnetic field is the case of a uniform $\boldsymbol{B}$, with $V = 0$. This was first solved by Lev Landau. We may choose $\boldsymbol{B} = B\hat{z}$ without loss of generality: we can anticipate that this will move electrons in circles in the xy plane.

To proceed we must make a gauge choice. One option is

$$\boldsymbol{A} = xB\hat{y}. \tag{242}$$

The Hamiltonian is

$$\hat{H} = \frac{1}{2m}\left(\hat{\boldsymbol{p}} - q\hat{\boldsymbol{A}}\right)^2 \tag{243}$$

$$= \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_z^2\right) + \frac{1}{2m}\left(\hat{p}_y - q\hat{x}B\right)^2. \tag{244}$$

In the position basis,

$$\hat{H} = \frac{-\hbar^2}{2m}\left(\partial_x^2 + \partial_z^2\right) + \frac{1}{2m}\left(-i\hbar\partial_y - qxB\right)^2. \tag{245}$$

Since

$$\left[\hat{H}, \hat{p}_y\right] = \left[\hat{H}, \hat{p}_z\right] = 0 \tag{246}$$

these three operators share a set of eigenstates. Hence, we can write

$$\psi_n\left(\boldsymbol{x}, t\right) = \exp\left(iE_n t/\hbar\right)\exp\left(ik_y y\right)\exp\left(ik_z z\right) f_n\left(x\right) \tag{247}$$

and the TISE becomes

$$\hat{H}\psi_n = \left\{\frac{\hbar^2 k_z^2}{2m} - \frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2m}\left(\hbar k_y - qBx\right)^2\right\}\psi_n = E_n\psi_n. \tag{248}$$

But this should be familiar – it's just a 1D harmonic oscillator centred on $x_0 = \hbar k_y/qB$. Hence, the energy eigenvalues are

$$E_n = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c\left(n + \frac{1}{2}\right) \tag{249}$$

where

$$\omega_c \triangleq \frac{|q|\,B}{m} \tag{250}$$

is the 'cyclotron frequency'.

- In a uniform $\boldsymbol{B}$, the energies of a free electron become quantized into 'Landau levels'.
- The energies E_n are gauge independent, but the eigenstates ψ_n are not.
- Each E_n is highly degenerate (labelled by the choices of x_0).