Part II Topics in Quantum Theory

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Preface

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Chapter 1

Quantum Dynamics

In this first chapter we're going to introduce some general ideas of quantum dynamics, using the two simplest quantum systems: the harmonic oscillator and a single spin-1/2.

1.1 The Quantum Harmonic Oscillator

There's an old crack from the late quantum field theorist Sidney Coleman to the effect that

> *The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.*

There's a large kernel of truth in this, for the simple reason that many systems in physics vibrate, from bridges to quantum fields, and within a certain approximation that vibration can be treated as harmonic. In this section we are going to remind ourselves about some features of quantum dynamics using this model as our basic example, as it allows most results to be expressed analytically. Along the way I'll try and point out which features generalise to more complicated systems (and which don't!).

1.1.1 Time Independent Case

The Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \tag{1.1}$$

where the position and momentum operators satisfy

$$[\hat{x}, \hat{p}] = i\hbar. \tag{1.2}$$

The state of the oscillator $\bar{\psi}$ evolves in time according to the (time dependent) Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\bar{\psi} = \hat{H}\bar{\psi}. \tag{1.3}$$

This is a first order differential equation, and so the evolution is fixed once the initial state $\bar{\psi}(0)$ is specified. We can write the solution as

$$\bar{\psi}(t) = \exp\Big(-i\hat{H}t/\hbar\Big)\bar{\psi}(0) \equiv \hat{U}(t)\bar{\psi}(0). \tag{1.4}$$

The operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ is called the *evolution operator*, as it evolves the state $\bar{\psi}(0)$ forward in time.

Functions of operators can be thought of as defined by their power series expansions, in this case

$$\hat{U}(t) = \mathbb{I} - i\frac{\hat{H}t}{\hbar} - \frac{1}{2}\left(\frac{\hat{H}t}{\hbar}\right)^2 + \cdots . \tag{1.5}$$

Alternatively, if an operator has a complete orthonormal eigenbasis $|n\rangle$ (as quantum observables do, being Hermitian operators), we can write any such function in terms of this basis and the corresponding function of the eigenvalues E_n

$$\hat{U}(t) = \sum_n e^{-iE_n t/\hbar} |n\rangle \langle n| . \tag{1.6}$$

This latter point of view then focuses attention on the eigenstates $|n\rangle$. To find these there are at least two approaches.

1. **Brute force:** Take the position representation $\hat{p} = -i\hbar\, \mathrm{d}/\mathrm{d}x$ and study the time independent Schrödinger equation in this representation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2 \psi_n = E_n \psi_n, \tag{1.7}$$

where $\langle x|n\rangle = \psi_n(x)$. The result is that the eigenfunctions have the form

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \tag{1.8}$$

with eigenvalues $E_n = \hbar\omega(n + 1/2)$, where $H_n(z)$ are the Hermite polynomials.

2. **More Sophisticated:** Define the hermitian conjugate pair

$$\begin{aligned} \hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right) \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right), \end{aligned} \tag{1.9}$$

which satisfy

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1. \tag{1.10}$$

The Hamiltonian is expressed as

$$\hat{H} = \frac{\hbar\omega}{2}\left[\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right] = \hbar\omega\left(N + \frac{1}{2}\right), \tag{1.11}$$

where $N \equiv \hat{a}^\dagger\hat{a}$. The commutation relation Eq. (1.10) implies

$$[N, \hat{a}] = -\hat{a}, \quad \left[N, \hat{a}^\dagger\right] = +\hat{a}^\dagger, \tag{1.12}$$

which in turn tells us that acting with $\hat{a}^\dagger(\hat{a})$ on an eigenstate $|n\rangle$ of N with eigenvalue n gives another eigenstate with eigenvalue increased (decreased) by 1.

Alternatively, we can try and find $\hat{U}(t)$ indirectly, from the effect it has on operators. Recall that in the *Heisenberg picture* operators acquire a time dependence

$$\hat{\mathcal{O}}(t) = \hat{U}^\dagger(t)\hat{\mathcal{O}}\hat{U}(t), \tag{1.13}$$

equivalent to the Heisenberg equation of motion

$$\frac{\mathrm{d}\hat{\mathcal{O}}(t)}{\mathrm{d}t} = \frac{i}{\hbar}\Big[\hat{H}, \hat{\mathcal{O}}(t)\Big]. \tag{1.14}$$

Let's see what this means for the Harmonic oscillator. Evidently $\hat{H} = \hat{U}^\dagger(t)\hat{H}\hat{U}(t)$, so

$$\hat{H} = \hat{U}^\dagger(t)\hat{H}\hat{U}(t) = \frac{\hat{p}(t)^2}{2m} + \frac{1}{2}m\omega^2\hat{x}(t)^2. \tag{1.15}$$

We have

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)] = \frac{\hat{p}(t)}{m} \tag{1.16}$$

$$\frac{\mathrm{d}\hat{p}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{p}(t)] = -m\omega^2\hat{x}(t). \tag{1.17}$$

You may recognize these equations as identical to *Hamilton's equations* for the SHO

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \frac{\partial\hat{H}}{\partial\hat{p}} = \frac{\hat{p}}{m} \tag{1.18}$$

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = -\frac{\partial\hat{H}}{\partial\hat{x}} = -m\omega^2\hat{x}. \tag{1.19}$$

Considering the case for the more general Hamiltonian,

$$\hat{H} = \hat{T}(\hat{p}) + \hat{V}(\hat{x}) = \sum_n \frac{t_n\hat{p}^n}{n!} + \sum_n \frac{v_n\hat{x}^n}{n!}, \tag{1.20}$$

we find the Heisenberg equation of motion

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}\sum_n \left[\frac{t_n\hat{p}^n}{n!}, \hat{x}\right] = \hat{T}'(\hat{p}), \tag{1.21}$$

which corresponds to Hamilton's equation $\dot{\hat{x}} = \partial\hat{H}\big/\partial\hat{p}$. The same proof works for $\mathrm{d}\hat{p}(t)/\mathrm{d}t = -\hat{V}'(\hat{x})$.

The general solution to Eqs. (1.18) and (1.19) is

$$\hat{x}(t) = \cos(\omega t)\hat{x}(0) + \sin(\omega t)\frac{\hat{p}(0)}{m\omega} \tag{1.22}$$

$$\hat{p}(t) = \cos(\omega t)\hat{p}(0) - m\omega\sin(\omega t)\hat{x}(0), \tag{1.23}$$

and corresponds to a point tracing out an ellipical trajectory centred at the origin in the $x-p$ plane (*phase space*). From this point of view the operators $\hat{a}$, $\hat{a}^\dagger$ in Eq. (1.9) can be seen as complex amplitudes whose phase changes linearly in time

$$\hat{a}(t) = e^{-i\omega t}\hat{a}(0), \quad \hat{a}^\dagger(t) = e^{+i\omega t}\hat{a}^\dagger(0). \tag{1.24}$$

This follows by writing the Hamiltonian as $\hat{H} = \omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$, such that $\dot{\hat{a}}(t) = -i\omega(t)$, which can be integrated to yield $\hat{a}(t)\exp(-i\omega t)\hat{a}(0)$.

1.1.2 Time Dependent Force

Mostly we don't leave quantum systems to get on with their own time evolution, but disturb them in some way. For example, an atom may experience an external radiation field. The prototype for this situation is the SHO subject to a time dependent force[1]

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - F(t)\hat{x}. \tag{1.25}$$

How does such a system evolve? The important thing to realise is that the solution of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}(t)|\psi\rangle \tag{1.26}$$

is *not*

$$\hat{U}(t) \neq \exp\Big(-i\hat{H}(t)t/\hbar\Big). \tag{1.27}$$

Let's consider the situation described by

$$F(t) = \begin{cases} F_1 & 0 \leq t < t_1 \\ F_2 & t_1 \leq t < t_2 \end{cases}. \tag{1.28}$$

The evolution operator is

$$\hat{U}(t) = \begin{cases} U_1(t) & 0 \leq t < t_1 \\ U_2(t-t_1)U_1(t_1) & t_1 \leq t < t_2 \end{cases}, \tag{1.29}$$

where $U_i = e^{-i\hat{H}_i t/\hbar}$ and $\hat{H}_i = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - F_i\hat{x}$. It's important to realise that $\hat{H}_1$ and $\hat{H}_2$ don't commute with each other,

$$[\hat{H}_1, \hat{H}_2] = -i\hbar\frac{\hat{p}}{m}(F_1 - F_2), \tag{1.30}$$

thus U_1 and U_2 don't commute and the product of U_1 and U_2 in Eq. (1.29) is not easily written in terms of a single exponential.

The evolution operator corresponding to a general force $F(t)$ can be understood by splitting the evolution up into many small stages

$$\begin{aligned}\hat{U}(t) &= \lim_{\Delta t\to 0} e^{-i\hat{H}(t-\Delta t)\Delta t/\hbar}e^{-i\hat{H}(t-2\Delta t)\Delta t/\hbar}\cdots e^{-i\hat{H}(\Delta t)\Delta t/\hbar}e^{-i\hat{H}(0)\Delta t/\hbar} \\ &= \lim_{\Delta t\to 0}\left(1 - \frac{i\hat{H}(t-\Delta t)\Delta t}{\hbar}\right)\left(1 - \frac{i\hat{H}(t-2\Delta t)\Delta t}{\hbar}\right)\cdots\left(1 - \frac{i\hat{H}(0)\Delta t}{\hbar}\right) \\ &= 1 - \frac{i}{\hbar}\int_0^t \mathrm{d}t_1\,\hat{H}(t_1) - \frac{1}{\hbar^2}\int_0^t \mathrm{d}t_2\int_0^{t_2}\mathrm{d}t_1\,\hat{H}(t_2)\hat{H}(t_1) + \cdots .\end{aligned} \tag{1.31}$$

Note that the time arguments of $\hat{H}(t)$ are increasing from right to left. The final expression for $\hat{U}(t)$ can be written in a dangerously compact fashion by using the notation

$$\mathcal{T}[\hat{H}(t_1)\hat{H}(t_2)] = \begin{cases} \hat{H}(t_1)\hat{H}(t_2) & t_1 \geq t_2 \\ \hat{H}(t_2)\hat{H}(t_1) & t_2 > t_1 \end{cases}, \tag{1.32}$$

[1] Recall that in the Heisenberg picture the Hamiltonian remained time independent. Now it has intrinsic time dependence.

and so on. The operation denoted by $\mathcal{T}$ is usually called *time ordering*. We have

$$\hat{U}(t) = 1 - \frac{i}{\hbar}\int_0^t \mathrm{d}t_1\, \hat{H}(t_1) - \frac{1}{2\hbar^2}\int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1\, \mathcal{T}[\hat{H}(t_1)\hat{H}(t_2)] + \cdots . \tag{1.33}$$

Allowing the integrals to range over $0 < t_i < t$ instead of ordering them necessitates the introduction of a factor $\frac{1}{n!}$ at the n^{th} order. This allows us to write

$$\hat{U}(t) = \mathcal{T}\exp\Big(-\frac{i}{\hbar}\int_0^t \mathrm{d}t'\, \hat{H}(t')\Big) \tag{1.34}$$

This expression should be handled with extreme care! It evidently reduces to $e^{-i\hat{H}t/\hbar}$ in the case of a time-independent Hamiltonian. In the general case, it is only really useful in the form of the expansion Eq. (1.33).

To make progress in the case of the driven oscillator, it's useful to once again consider the Heisenberg equations of motion

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)] = \frac{\hat{p}(t)}{m} \tag{1.35}$$

$$\frac{\mathrm{d}\hat{p}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{p}(t)] = -m\omega^2\hat{x}(t) + F(t). \tag{1.36}$$

In terms of $\hat{a}$ and $\hat{a}^\dagger$

$$\hat{H}(t) = \frac{\hbar\omega}{2}\Big(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\Big) - F(t)\sqrt{\frac{\hbar}{2m\omega}}\Big(\hat{a} + \hat{a}^\dagger\Big), \tag{1.37}$$

and we have

$$\frac{\mathrm{d}\hat{a}}{\mathrm{d}t} = -i\omega\hat{a} + iF(t)\sqrt{\frac{1}{2m\hbar\omega}}. \tag{1.38}$$

If we define $\tilde{\hat{a}}(t)e^{i\omega t}\hat{a}(t)$, we get

$$\frac{\mathrm{d}\tilde{\hat{a}}}{\mathrm{d}t} = +i\frac{F(t)e^{i\omega t}}{\sqrt{2m\hbar\omega}}, \tag{1.39}$$

with general solution

$$\tilde{\hat{a}}(t) = \tilde{\hat{a}}(0) + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega t'}\,\mathrm{d}t'\,, \tag{1.40}$$

and similarly

$$\tilde{\hat{a}}^\dagger(t) = \tilde{\hat{a}}^\dagger(0) - \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{-i\omega t'}\,\mathrm{d}t'\,. \tag{1.41}$$

From this we have

$$\hat{x}(t) = \frac{1}{2}\sqrt{\frac{2\hbar}{m\omega}}\Big(\hat{a}(t) + \hat{a}^\dagger(t)\Big) = \hat{x}(0) - \frac{1}{m\omega}\int_0^t F(t')\sin(\omega t')\,\mathrm{d}t'\,, \tag{1.42}$$

this is the same as for a classical harmonic oscillator (in the rotating frame).

What can we do with this solution? Suppose we start from the ground state, which satisfies

$$\hat{a}\,|0\rangle = 0. \tag{1.43}$$

Since $\hat{a}(t)\hat{U}^\dagger(t)\hat{a}\hat{U}(t)$ we have $\hat{a}\hat{U}(t) = \hat{U}(t)\hat{a}(t)$ and thus

$$\hat{a}\hat{U}(t)\,|0\rangle = \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}\,\mathrm{d}t'\,\hat{U}(t)\,|0\rangle\,, \tag{1.44}$$

we have that $\hat{U}(t)\,|0\rangle$ is an eigenstate of $\tilde{\hat{a}}(0) = \hat{a}$ with eigenvalue

$$\frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}\,\mathrm{d}t'\,, \tag{1.45}$$

in other words, it is a *coherent state*. Recall from AQP that a coherent state $|\alpha\rangle$ is defined as an eigenstate of $\hat{a}$ with eigenvalue α (generally complex, as $\hat{a}$ is not Hermitian)

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,. \tag{1.46}$$

The explicit form of a normalised coherent state is

$$|\alpha\rangle = e^{-|\alpha|^2/2}e^{\alpha\hat{a}^\dagger}\,|0\rangle\,, \tag{1.47}$$

where both the property Eq. (1.46) and the normalisation follow from the fundamental commutator $[\hat{a},\hat{a}^\dagger] = 1$. Given Eq. (1.47),

$$\hat{a}\,|\alpha\rangle = e^{-|\alpha|^2/2}\left[\hat{a}, e^{\alpha\hat{a}^\dagger}\right]|0\rangle = \alpha\,|\alpha\rangle\,. \tag{1.48}$$

For the normalisation, we have

$$\langle\alpha|\alpha\rangle = e^{-|\alpha|^2}\sum_{n,m}\langle 0|\frac{(\alpha^*\hat{a})^n}{n!}\frac{\left(\alpha\hat{a}^\dagger\right)^m}{m!}|0\rangle = e^{-|\alpha|^2}\sum_n\frac{|\alpha|^2}{n!} = 1. \tag{1.49}$$

Note that the ground state $|0\rangle$ is a coherent state with $\alpha = 0$.

Time-dependent perturbation theory (see AQP notes) gives

$$c_n^{(1)} = -\frac{i}{\hbar}\int_{t_0}^t \mathrm{d}t'\,e^{i\omega_{n,i}t'}V_{n,i}(t'). \tag{1.50}$$

In our case the energy different between $|0\rangle$ and $|1\rangle$ is $\hbar\omega$, and the matrix element $V_{1,0}(t') = -F(t')\hbar/(2m\omega)$. This coincides with (1.45), because

$$\langle 1|\hat{U}(t)|0\rangle = \langle 0|\hat{U}(t)\hat{a}(t)|0\rangle = \langle 0|\hat{U}(t)|0\rangle\frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}\,\mathrm{d}t'\,. \tag{1.51}$$

Then $\langle 0|\hat{U}(t)|0\rangle = 1 + \mathcal{O}(F^2)$.

1.2 A Spin in a Field

Two state systems abound in physics. Or rather, many physical situations can be approximated by considering only two states. Some important examples are the spin states of the electron, a pair of atomic states coupled by external radiation, and the two equivalent positions of the Nitrogen atom in the trigonal pyramid structure of Ammonia (NH_4).

Quantum two state systems are central to the field of *quantum computing*, where they replace the classical bit of information and are often known as *qubits*.

The simplest quantum system we can write down consists of just two states. The Hilbert space is then two dimensional, and any operator can be thought of as a 2×2 matrix. In this section, we'll see that there is a lot to be learnt from this seemingly elementary problem.

It's convenient to describe such a system using the language of spin-1/2, even though the two states may have nothing to do with real spin. The most general time dependent Hamiltonian can then be written using the spin-1/2 operators $\hat{S}_i = \frac{1}{2}\hat{\sigma}_i$ as

$$\hat{H}(t) = \mathbf{H}(t) \cdot \hat{\mathbf{S}}, \tag{1.52}$$

in terms of a time dependent 'magnetic field' $\mathbf{H}(t)$ (that again may have nothing to do with a real magnetic field). Using the Pauli matrices, we have the explicit form

$$\hat{H}(t) = \frac{1}{2}\begin{pmatrix} H_z(t) & H_x(t) - iH_y(t) \\ H_x(t) + iH_y(t) & -H_z(t) \end{pmatrix}. \tag{1.53}$$

The Schrödinger equation corresponding to Eq. (1.52) is

$$i\hbar \frac{\mathrm{d}\,|\Psi\rangle}{\mathrm{d}t} = \hat{H}(t)\,|\Psi\rangle\,, \tag{1.54}$$

where $|\Psi\rangle = (\psi_\uparrow, \psi_\downarrow)$.

As before, the formal solution to Eq. (1.54) can be written as

$$|\Psi(t)\rangle = \hat{U}(t,t')\,|\Psi(t')\rangle\,, \tag{1.55}$$

In the present case, $\hat{U}(t,t')$ is a 2×2 unitary matrix. It's perhaps a bit surprising that, for this most basic of all possible problems of quantum dynamics, there is no simple relationship between $\hat{H}(t)$ and $\hat{U}(t,t')$. If we think of $\hat{U}(t,t')$ as representing a kind of rotation in Hilbert space, $\hat{H}(t)$ corresponds to an instantaneous "angular velocity" describing an infinitesimal rotation. Because these rotations do not commute at different times, the relationship between the infinitesimal rotations and the finite rotation that results is complicated.

The same picture emerges if we look at the Heisenberg equation of motion for $\hat{\mathbf{S}}(t) = \hat{U}^\dagger(t,t')\hat{\mathbf{S}}(t')\hat{U}(t,t')$, which take the form

$$\begin{aligned} \frac{\mathrm{d}\hat{\mathbf{S}}}{\mathrm{d}t} &= \frac{i}{\hbar}[\mathbf{H}(t), \hat{\mathbf{S}}] \\ &= \frac{1}{\hbar}\mathbf{H}(t) \times \hat{\mathbf{S}} \end{aligned} \tag{1.56}$$

by virtue of the spin commutation relations $[\hat{S}_i, \hat{S}_j] = i\varepsilon_{ijk}\hat{S}_k$.[2] Thus $\hat{\mathbf{S}}$ precesses about $\mathbf{H}(t)$, which corresponds to the instantaneous angular velocity. Differential equations involving operators may make you uncomfortable, but this one is linear and first order, so

[2] The usual $\hbar$ is missing because we defined $\hat{\mathbf{S}} = \frac{1}{2}\hat{\boldsymbol{\sigma}}$

the solution must be expressible in the form of a matrix connecting the initial and final operators

$$\hat{\mathbf{S}}(t) = \mathrm{R}(t,t')\hat{\mathbf{S}}(t'). \tag{1.57}$$

R is a 3×3 matrix describing the rotation of the spin from time t' to time t. The formal expression for $\mathrm{R}(t,t')$ is

$$\mathrm{R}(t,t') = \mathcal{T}\exp\!\left(\int_{t'}^{t}\Omega(t_i)\,\mathrm{d}t_i\right), \tag{1.58}$$

where the matrix $\Omega(t)$ describing infinitesimal rotations has elements $\Omega_{jk}(t) = -(1/\hbar)H_i(t)\varepsilon_{ijk}$, i.e.

$$\Omega(t) = \begin{pmatrix} 0 & -H_z(t) & H_y(t) \\ H_z(t) & 0 & -H_x(t) \\ -H_y(t) & H_x(t) & 0 \end{pmatrix}. \tag{1.59}$$

$\mathrm{U}(t,t')$ and $\mathrm{R}(t,t')$ contain the same information, of course. We'll return to the relationship between these two in Chapter 6 on Lie Groups.

To find the $t\to t'$ time-evolution matrix for a magnetic field in the z-direction, and the matrix that maps the Heisenberg spin operator at time t' to the Heisenberg spin operator at t, we start from Eq. (1.53) to first yield the Hamiltonian

$$\hat{H} = \begin{pmatrix} H/2 & 0 \\ 0 & H/2 \end{pmatrix}. \tag{1.60}$$

This is independent of time, and therefore the time-ordered exponential is just an ordinary matrix exponential because the Hamiltonian cannot fail to commute with itself when evaluated at different times. Moreover it is diagonal in this basis and so the matrix exponential is also easily evaluated:

$$\begin{aligned}\hat{U}(t,t') &= \mathcal{T}\exp\!\left(-\frac{i}{\hbar}\int_{t'}^{t}H(t_i)\,\mathrm{d}t_i\right)\\ &= \exp\!\left(-\frac{i}{\hbar}\begin{pmatrix} H(t-t')/2 & 0 \\ 0 & -H(t-t')/2\end{pmatrix}\right)\\ &= \begin{pmatrix} \exp\!\left(-\frac{i}{\hbar}H(t-t')/2\right) & 0 \\ 0 & \exp\!\left(\frac{i}{\hbar}H(t-t')/2\right)\end{pmatrix}.\end{aligned} \tag{1.61}$$

Since $\Omega_{jk} = -H_i\varepsilon_{ijk}$ and $H_i = \delta_{iz}H$ we find that

$$\Omega(t) = \begin{pmatrix} 0 & -H & 0 \\ H & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{1.62}$$

which is not diagonal and therefore not trivial to exponentiate even though there is no problem time-ordering. We could perform a diagonalisation, but it is nicer to notice that $\Omega = iH\sigma_y \oplus 0$, and use $e^{i\theta\sigma_a} = \cos\theta + i\sigma_a\sin\theta$ (to prove this,use $\sigma_a^2 = 1$). Then

$$\begin{aligned}\mathrm{R}(t,t') &= \exp\big(iH(t-t')\sigma_y\big)\oplus\exp(0)\\ &= \big(\cos\big(H(t-t')\big) + i\sigma_y\sin\big(H(t-t')\big)\big)\oplus 1,\end{aligned} \tag{1.63}$$

with the matrix explicitly

$$\mathrm{R}(t,t') = \begin{pmatrix} \cos(H(t-t')) & -\sin(H(t-t')) & 0 \\ \sin(H(t-t')) & \cos(H(t-t')) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.64}$$

1.2.1 Rabi Oscillations

One time dependent situation that we can describe exactly is the rotating field

$$\hat{\mathbf{H}}(t) = \begin{pmatrix} \hat{H}_R \cos(\omega t) \\ \hat{H}_r \sin(\omega t) \\ \hat{H}_0 \end{pmatrix}, \tag{1.65}$$

corresponding to the Hamiltonian

$$\hat{H}(t) = \hat{H}_0 \hat{S}_z + \frac{\hat{H}_R}{2}\left(\hat{S}_+ e^{-i\omega t} + \hat{S}_- e^{i\omega t}\right), \tag{1.66}$$

where $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$. The key to solving the problem is to transform the Schrödinger equation Eq. (1.54) by multiplying by $\exp\left(i\omega t \hat{S}_z\right)$. Define

$$|\Psi_R(t)\rangle \equiv \exp\left(i\omega t \hat{S}_z\right)|\Psi(t)\rangle\,. \tag{1.67}$$

This transformed state satisfies

$$\begin{aligned} i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\Psi_R\rangle &= i\hbar e^{i\omega t \hat{S}_z}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle - \hbar\omega \hat{S}_z|\Psi_R\rangle \\ &= e^{i\omega t \hat{S}_z}\hat{H}(t)|\Psi\rangle - \hbar\omega \hat{S}_z|\Psi_R\rangle \\ &= e^{i\omega t \hat{S}_z}\hat{H}(t)e^{-i\omega t \hat{S}_z}|\Psi_R\rangle - \hbar\omega \hat{S}_z|\Psi_R\rangle \\ &= \hat{H}_{\text{Rabi}}|\Psi_R\rangle\,. \end{aligned} \tag{1.68}$$

In the last line we defined

$$\hat{H}_{\text{Rabi}} \equiv e^{i\omega t \hat{S}_z}\hat{H}(t)e^{-i\omega t \hat{S}_z} - \hbar\omega \hat{S}_z = (\hat{H}_0 - \hbar\omega)\hat{S}_z + \hat{H}_R \hat{S}_x. \tag{1.69}$$

To get the last equality you have to transform the Hamiltonian. You can use Eq. (**??**), or, since everything is a 2×2 matrix, you can multiply the matrices explicitly.

Physically, this corresponds to viewing things in a frame rotating with the field, so the Hamiltonian is now time independent. In this new frame the system precesses about a fixed axis $(\hat{H}_R, 0, \hat{H}_0 - \hbar\omega)$ at the **Rabi frequency**,

$$\omega_R = \frac{1}{\hbar}\sqrt{(\hat{H}_0 - \hbar\omega)^2 + \hat{H}_R^2}. \tag{1.70}$$

The amplitude of the oscillations in $\hat{S}_z$ due to this precession is maximal when $\hat{H}_0 = \hbar\omega$. In this case the rotation frequency of the field matches the frequency of precession about the z-axis that would occur if $\hat{H}_R = 0$.

1.3 The Adiabatic Approximation

The idea of *separation of scales*, be they in length, time, or energy, is endemic in science. If we are interested in studying processes on one scale (such as the weather, say) we hope that they don't depend on the details of processes at another (the motion of molecules).

Rather, we hope that these latter processes can be described in an average way, involving only a few parameters and dynamical quantities (density, local velocity).

The adiabatic approximation is a special case of this idea. Let's suppose that in our two level system, the field $\hat{\mathbf{H}}(t)$ is changing very slowly (we'll make this idea precise in a moment). If this motion is truly glacial, we'd expect to be able to forget about it altogether, and just solve the problem by finding the energy eigenstates and eigenvalues in the present epoch

$$\hat{H}(t)\,|\pm_t\rangle = E_\pm(t)\,|\pm_t\rangle\,. \tag{1.71}$$

We put the t in a subscript on the states to emphasise that they depend on time as a *parameter*. We refer to the $|\pm_t\rangle$ as the **instantaneous energy eigenstates**. Although we can always define these states for any $\hat{\mathbf{H}}(t)$, we have no reason in general to expect that this t-dependence has anything to do with the other kind of t-dependence that arises by solving the time dependent Schrödinger equation.

The **adiabatic theorem** is roughly the statement that these two t dependences *do* in fact coincide, in the limit that $\hat{H}(t)$ changes very slowly. To make this more precise, let's expand the state of the system, evolving in time *according to the Schrödinger equation*, in the instantaneous eigenbasis

$$|\Psi(t)\rangle = c_+(t)\,|+_t\rangle + c_-(t)\,|-_t\rangle\,. \tag{1.72}$$

Thus, some of the t dependence is "carried" by the $|\pm_t\rangle$, and by substituting into the Schrödinger equation we are going to find the time dependence of the $c_\pm(t)$. This involves finding $\mathrm{d}\,|\pm_t\rangle/\mathrm{d}t$.

Now the following idea you may find a bit odd. Since the time dependence of $|\pm_t\rangle$ is parametric, we can view the problem of calculating $\mathrm{d}\,|\pm_t\rangle/\mathrm{d}t$ as an exercise in *time independent* perturbation theory.[3] Going from t to $t+\delta t$ changes the Hamiltonian by an amount

$$\delta\hat{H}(t) = \frac{\mathrm{d}\hat{H}(t)}{\mathrm{d}t}\delta t. \tag{1.73}$$

Treating this as a perturbation, the state $|+_t\rangle$ changes by an amount

$$\delta\,|+_t\rangle = \frac{\langle -_t|\delta\hat{H}(t)|+_t\rangle}{E_+(t)-E_-(t)}\,|-_t\rangle\,, \tag{1.74}$$

so that

$$\frac{\mathrm{d}\,|+_t\rangle}{\mathrm{d}t} = \frac{\langle -_t|\dot{\hat{H}}(t)|+_t\rangle}{E_+(t)-E_-(t)}\,|-_t\rangle\,. \tag{1.75}$$

Using Eq. (1.75) and the corresponding result for $\mathrm{d}\,|-_t\rangle/\mathrm{d}t$, we find that the Schrödinger equation gives the following pair of equations for the $c_\pm(t)$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}c_+\\ c_-\end{pmatrix} = \begin{pmatrix}E_+(t) & i\hbar\frac{\langle +_t|\dot{\hat{H}}(t)|-_t\rangle}{E_+-E_-}\\ i\hbar\frac{\langle -_t|\dot{\hat{H}}(t)|+_t\rangle}{E_--E_+} & E_-(t)\end{pmatrix}\begin{pmatrix}c_+(t)\\ c_-(t)\end{pmatrix}. \tag{1.76}$$

[3] It's a bit like the interaction representation in time dependent perturbation theory.

If $\hat{H}(t)$ is changing slowly enough, the off-diagonal terms can be neglected and the solution is[4]

$$\boxed{c_\pm(t) = \exp\left(-\frac{i}{\hbar}\int_0^t E_\pm(t')\,\mathrm{d}t'\right)c_\pm(0).} \tag{1.77}$$

Thus the amplitudes evolve independently, and there are no transitions between the instantaneous eigenstates. The phase factor is a generalization of the familiar $e^{-iE_\pm t/\hbar}$ for stationary states, which accounts for the slowing varying instantaneous eigenenergy.

When is this approximation valid? The off-diagonal matrix element in Eq. (1.76) must be small compared to $E_1(t) - E_2(t)$, which corresponds to the condition

$$\hbar\left|\langle -_t|\dot{\hat{H}}|+_t\rangle\right| \ll [E_+(t) - E_-(t)]^2. \tag{1.78}$$

Degeneracy must be avoided, because the eigenbasis becomes undefined within the degenerate subspace. You can't remain in an eigenstate if you don't know what it is. The approximation is a *semiclassical* one, meaning that it improves at smaller $\hbar$.

1.3.0.1 Adiabatic

Adiabatic is a peculiar term that appears in two related contexts in physics, both referring to slow changes to a system. In thermodynamics, it describes changes without a change in entropy. For reversible changes, this corresponds to no flow of heat, which is the origin of the name (from the Greek for 'impassable').

Later, the idea entered mechanics when it was realized that a mechanical system with one degree of freedom undergoing periodic motion, and subject to slow changes, has an **adiabatic invariant**. This turns out to be the **action**

$$S = \oint p\,\mathrm{d}x\,. \tag{1.79}$$

($\oint$ indicates that we integrate for one period of the motion) Largely due to the work of Paul Ehrenfest (1880-1933), the invariant played a major role in the "old" quantum theory that predated Schrödinger, Heisenberg, et al.. If the motion of a system is quantised, slow changes to the system's parameters presumably do not lead to sudden jumps. Thus the quantity that comes in quanta must be an adiabatic invariant – and conveniently Planck's constant has the right units. This line of reasoning eventually gave rise to the **Bohr–Sommerfeld quantisation condition**

$$\oint p\,\mathrm{d}x = nh, \quad n \in \mathbb{N}. \tag{1.80}$$

1.3.1 Landau–Zener Tunnelling

The picture of adiabatic evolution described above is extremely simple, and it's natural to ask how it breaks down when the condition Eq. (1.78) is not satisfied. Let's consider

[4] Note the resemblance to the WKB wavefunction, with energy and time taking the roles of momentum and position. WKB is a kind of adiabatic approximation in space.

Fig. 1.1: The action of a periodic trajectory is equal to the area enclosed in the phase plane. For a simple harmonic oscillator the curve is an ellipse and the action is the product of the energy and the period. If the period of the oscillator is altered slowly (by changing the length of a pendulum, say) the ellipse will distort but the area will remain fixed.

time evolution with the Hamiltonian

$$\hat{H}(t) = \begin{pmatrix} \beta t & \Delta \\ \Delta & -\beta t \end{pmatrix}. \tag{1.81}$$

The instantaneous eigenvalues are

$$E_{\pm}(t) = \pm\sqrt{(\beta t)^2 + \Delta^2}. \tag{1.82}$$

We denote the corresponding eigenvalues $|\pm_t\rangle$. As a function of t, the eigenvalues show an **avoided crossing**. The adiabatic theorem tells us that if we start in the state corresponding to the lower energy $E_-(t)$, and β is sufficiently small, the state at time t is

$$\exp\left(-\frac{i}{\hbar}\int_0^t E_-(t')\,\mathrm{d}t'\right)|-_t\rangle\,, \tag{1.83}$$

where $|-_t\rangle$ is the corresponding eigenstate. We're integrating from $t = 0$ because the integral diverges at $-\infty$ as the phase whizzes faster and faster.

Fig. 1.2: Instantaneous eigenvalues of the Landau–Zener problem. The dotted line schematically illustrates what happens when we pass over the branch point.

How small should β be? We use the condition Eq. (1.78), and the fact that the minimum splitting of the energy levels is 2Δ to arrive at the requirement

$$\frac{\hbar\beta}{\Delta^2} \ll 1. \tag{1.84}$$

We are interested in the situation where this is not the case.

In fact, we can do better than this, via an ingenious excursion into the complex plane. The functions $E_{\pm}(t)$ have branch cuts starting at $t = \pm i\Delta/\beta$. We can think of adiabaticity failing because the branch points are too close to the real axis.

Fig. 1.3: (Top) Branch cut and contour of time evolution in the complex t plane. (Bottom) Riemann surface of $\sqrt{(\beta t)^2 + \Delta^2}$ (real part).

But who said t had to be real? There is nothing to stop us integrating the Schrödinger equation along an arbitrary contour. Then we can be as far away from the branch points as we like (Fig. 1.3), and the adiabatic approximation should be valid once more. We can use Eq. (1.83): the exponent now acquires a real part, which describes the decay of the amplitude. Having made the adiabatic approximation, we can deform the contour of integration in Eq. (1.83). The real part of the exponent arising during evolution from $t = -\infty$ to $t = +\infty$ can then be written

$$\frac{2i}{\hbar}\int_0^{i\Delta/\beta}\sqrt{(\beta t)^2 + \Delta^2}\,\mathrm{d}t = -\frac{\pi\Delta^2}{2\hbar\beta}, \tag{1.85}$$

Fig. 1.4: Comparison of Eq. (1.87) with the probability of a superconducting qubit to remain in the ground state. The two states correspond to different values of the magnetic flux trapped in a superconducting ring, and the bias ir provided by ramping another flux.

giving the modulus of the amplitude

$$|c_-(-\infty \to +\infty)| = \exp\left(-\frac{\pi\Delta^2}{2\hbar\beta}\right). \tag{1.86}$$

Note, however, that our state is now evolving with an instantaneous energy $E_+(t)$, because we passed onto the other sheet of the Riemann surface. We are now in the *upper* state $|+_t\rangle$, see Fig. 1.2.

Thus the square of Eq. (1.86) actually gives the probability to make the transition to the upper state. The probability to remain in the lower state is therefore

$$\boxed{P_{\text{ground}} = 1 - \exp\left(-\frac{\pi\Delta^2}{2\hbar\beta}\right).} \tag{1.87}$$

To verify the Landau-Zener result to lowest non-vanishing order in time-dependent perturbation theory, since the result is perturbative in Δ, so we take for our unperturbed Hamiltonian $\hat{H}_0$

$$\hat{H}_0 = \begin{pmatrix} \beta t & 0 \\ 0 & \beta t \end{pmatrix}, \tag{1.88}$$

and our perturbation $\hat{V}$

$$\hat{V} = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}. \tag{1.89}$$

Since our unperturbed Hamiltonian carries an explicit time dependence, we have to remember to integrate it up when converting between the interaction and Schrödinger pictures:

$$\hat{V}_I(t) = \exp\left(i\int_{t_0}^{t} \hat{H}_0(t')\,\mathrm{d}t'\,/\hbar\right)\hat{V}_S(t_0)\exp\left(-i\int_{t_0}^{t} \hat{H}_0(t')\,\mathrm{d}t'\,/\hbar\right). \tag{1.90}$$

The Landau-Zener tunnelling appears in this formulation as the transition from the $-\beta t$ eigenstate to the $+\beta t$ eigenstate. Using the result of first-order time dependent perturbation theory

$$c_+^{(1)} = -\frac{i}{\hbar}\int_{-\infty}^{\infty} \exp\left(i\int_0^{t'}\left(E_0^+(t'') - E_0^-(t'')\right)\mathrm{d}t''\right)V_{+-}(t')\,\mathrm{d}t'\,, \tag{1.91}$$

we find

$$\begin{aligned} c_+^{(1)} &= -\frac{i\Delta}{\hbar}\int_{-\infty}^{\infty} e^{i(\beta-(-\beta))t'^2/2}\,\mathrm{d}t' \\ &= -\frac{i\Delta}{\hbar}\sqrt{\frac{\pi\hbar}{i\beta}}. \end{aligned} \tag{1.92}$$

Therefore the transition probability $P_{-\to+}$ is given by

$$\left|c_+^{(1)}\right|^2 = \frac{\pi\Delta^2}{\beta\hbar}, \tag{1.93}$$

in agreement with the Landau-Zener result to order Δ^2.

1.4 Berry's Phase

There is a surprise lurking in our derivation of the adiabatic theorem, one that remained hidden until 1984. We found the change in the instantaneous eigenstates in a small interval δt to be

$$\delta\left|+_t\right\rangle = \frac{\langle -_t|\delta\hat{H}(t)|+_t\rangle}{E_+(t) - E_-(t)}\left|-_t\right\rangle. \tag{1.94}$$

This change is in the direction of $|-_t\rangle$ i.e. *orthogonal* to $|+_t\rangle$. The usual justification for this in the context of perturbation theory is that any change parallel to $|+_t\rangle$ is no change at all, amounting only to a modification of the magnitude or phase of the state, neither or which is physically meaningful. For example, a small change in the phase of $|+_t\rangle$ gives

$$\left|+_t\right\rangle \to e^{i\delta\theta}\left|+_t\right\rangle \sim (1 + i\delta\theta)\left|+_t\right\rangle. \tag{1.95}$$

Suppose now that $\hat{H}(t)$ is subject to some adiabatic *cyclic* change around some closed path γ in the space of matrices. If after time T we have $\hat{H}(T) = \hat{H}(0)$, then after evolving $|+_t\rangle$ according to Eq. (1.94) it would be natural to expect that it will return to its original value. That is,

$$\left|+_T\right\rangle \stackrel{?}{=} \left|+_0\right\rangle. \tag{1.96}$$

Berry's remarkable discovery was that *this does not happen*. Rather,

$$\left|+_T\right\rangle = e^{i\theta_B[\gamma]}\left|+_0\right\rangle, \tag{1.97}$$

where the phase $\theta_B[\gamma]$ that now bears his name is a functional of the path γ.

To get a better grip on this slippery concept, recall that the Hamiltonian of our two state system (Eq. (1.52)) is parametrised in terms of the field $\mathbf{H}(t)$. Suppose we fix the states $|\mathbf{H}, \pm\rangle$ for each value of the field at the outset. That is, there is no ambiguity in the phase as in Eq. (1.97). We can then use these states to write the state of the system in the instantaneous eigenbasis (c.f. Eq. (1.72))

$$|\Psi(t)\rangle = c_+(t)\,|\mathbf{H}(t), +\rangle + c_-(t)\,|\mathbf{H}(t), -\rangle. \tag{1.98}$$

If $|\mathbf{H}, +\rangle$ changes smoothly as $\mathbf{H}$ changes, we will see that Eq. (1.94) cannot be obeyed: there is always some contribution in the direction of $|\mathbf{H}, +\rangle$ corresponding to a change of phase. This defines a vector field in the space of $\mathbf{H}$ by

$$\mathbf{A}_+(\mathbf{H}) \equiv -i\,\langle \mathbf{H}, +|\,(\boldsymbol{\nabla}_{\mathbf{H}}\,|\mathbf{H}, +\rangle), \tag{1.99}$$

and likewise for $|\mathbf{H}, -\rangle$.

To show that using normalised states guarantees $\mathbf{A}_+(\mathbf{H})$ is real, we start by considering the norm of the state $|\mathbf{H}+\delta\mathbf{H},+\rangle$:

$$\langle \mathbf{H}+\delta\mathbf{H},+|\mathbf{H}+\delta\mathbf{H},+\rangle = \langle \mathbf{H},+|\mathbf{H},+\rangle + \delta\mathbf{H}\cdot\Big(\boldsymbol{\nabla}(\langle \mathbf{H},+|)\,|\mathbf{H},+\rangle + \langle \mathbf{H},+|\,\boldsymbol{\nabla}(|\mathbf{H},+\rangle)\Big) + \mathcal{O}\Big(\delta^2\Big), \tag{1.100}$$

which vanishes to $\mathcal{O}(\delta^2)$ if

$$0 = \Big(\boldsymbol{\nabla}\,\langle \mathbf{H},+|\Big)\,|\mathbf{H},+\rangle + \langle \mathbf{H},+|\,\Big(\boldsymbol{\nabla}\,|\mathbf{H},+\rangle\Big). \tag{1.101}$$

Now using the definition of $\mathbf{A}_+ = -i\,\langle \mathbf{H},+|\,(\boldsymbol{\nabla}\,|\mathbf{H},+\rangle)$ we find that

$$\begin{aligned}\mathbf{A}_+^* &= \mathbf{A}_+^\dagger \\ &= i\Big(\boldsymbol{\nabla}\,\langle \mathbf{H},+|\Big)\,|\mathbf{H},+\rangle \\ &= -i\,\langle \mathbf{H},+|\,\Big(\boldsymbol{\nabla}\,|\mathbf{H},+\rangle\Big) \\ &= \mathbf{A}_+.\end{aligned} \tag{1.102}$$

This reflects the anti-Hermitian nature of the gradient operator.

Things become a lot clearer with a concrete example. Let's write $\mathbf{H} = H_0\hat{\mathbf{n}}$, with $\hat{\mathbf{n}}$ a unit vector. Introducing spherical polar coordinates in the usual way,

$$\hat{\mathbf{n}} = \begin{pmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{pmatrix}. \tag{1.103}$$

The Hamiltonian $\hat{H} = \mathbf{H}\cdot\hat{\mathbf{S}}$ takes the form

$$\hat{H} = \frac{H_0}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}. \tag{1.104}$$

You can then easily check that the eigenstate $|\mathbf{H},+\rangle$ is

$$|\mathbf{H},+\rangle = \begin{pmatrix}\cos(\theta/2)e^{-i\phi/2}\\ \sin(\theta/2)e^{i\phi/2}\end{pmatrix}. \tag{1.105}$$

Computing $\mathbf{A}_+(\mathbf{H})$ defined by Eq. (1.99) gives[5]

$$\mathbf{A}_+(\mathbf{H}) = -\hat{\boldsymbol{\phi}}\frac{\cot\theta}{2H_0}. \tag{1.107}$$

In order to find the Berry connection $\mathbf{A}_-$, we can write first down $|\mathbf{H},-\rangle$ by demanding orthogonality with the E_+ eigenstate, so that in the basis with $\hat{S}_z$ diagonal,

$$|\mathbf{H},-\rangle = \begin{pmatrix}-\sin\frac{\theta}{2}e^{-i\phi/2}\\ \cos\frac{\theta}{2}e^{i\phi/2}\end{pmatrix}. \tag{1.108}$$

[5]The gradient operator in spherical polars is

$$\boldsymbol{\nabla} = \hat{\mathbf{r}}\partial_r + \hat{\boldsymbol{\theta}}\frac{1}{r}\partial_\theta + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\partial_\phi, \tag{1.106}$$

we'll often use the notation $\partial_i = \partial/\partial x_i$, $\partial_i^2 = \partial^2/\partial x_i^2$, etc. in these notes.

Taking the **H**-space gradient of this state gives

$$\boldsymbol{\nabla}\left|\mathbf{H},-\right\rangle = \frac{\hat{\boldsymbol{\theta}}}{2r}\begin{pmatrix}-\cos\frac{\theta}{2}e^{-i\phi/2}\\ -\sin\frac{\theta}{2}e^{i\phi/2}\end{pmatrix} - \frac{i\hat{\boldsymbol{\phi}}}{2r\sin\theta}\begin{pmatrix}-\sin\frac{\theta}{2}e^{-i\phi/2}\\ -\cos\frac{\theta}{2}e^{i\phi/2}\end{pmatrix}, \tag{1.109}$$

and noticing that the projection onto $\hat{\boldsymbol{\theta}}$ is proportional to $|\mathbf{H},+\rangle$ we can write down

$$\begin{aligned}\langle\mathbf{H},-|\boldsymbol{\nabla}|\mathbf{H},-\rangle &= \frac{i\hat{\boldsymbol{\phi}}}{2r\sin\theta}\Big(-\sin\tfrac{\theta}{2}e^{i\phi/2}, \quad \cos\tfrac{\theta}{2}e^{-i\phi/2}\Big)\begin{pmatrix}\sin\frac{\theta}{2}e^{-i\phi/2}\\ \cos\frac{\theta}{2}e^{i\phi/2}\end{pmatrix}\\ &= i\hat{\boldsymbol{\phi}}\frac{\cos^2\frac{\theta}{2}-\sin^2\frac{\theta}{2}}{2r\sin\theta}\\ &= \hat{\boldsymbol{\phi}}\frac{i\cot\theta}{2r},\end{aligned} \tag{1.110}$$

and so

$$\begin{aligned}\mathbf{A}_- &= -i\left\langle\mathbf{H},-|\boldsymbol{\nabla}|\mathbf{H},-\right\rangle\\ &= +\hat{\boldsymbol{\phi}}\frac{i\cot\theta}{2r}.\end{aligned} \tag{1.111}$$

We now use Eq. (1.98) in the derivation of the adiabatic theorem as before. Instead of Eq. (1.94) we get

$$\delta\left|\mathbf{H},+\right\rangle = \frac{\langle\mathbf{H},-|\delta\hat{H}|\mathbf{H},+\rangle}{H_0}\left|\mathbf{H},-\right\rangle + i\mathbf{A}_+(\mathbf{H})\cdot\delta\mathbf{H}\left|\mathbf{H},+\right\rangle, \tag{1.112}$$

where we have used $E_+ - E_- = H_0$. After making the adiabatic assumption we get

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}c_+\\ c_-\end{pmatrix} = \begin{pmatrix}E_+(t)+\hbar\mathbf{A}_+(\mathbf{H})\cdot\dot{\mathbf{H}} & 0\\ 0 & E_-(t)+\hbar\mathbf{A}_-(\mathbf{H})\cdot\dot{\mathbf{H}}\end{pmatrix}\begin{pmatrix}c_+(t)\\ c_-(t)\end{pmatrix}, \tag{1.113}$$

and the solution is now

$$c_\pm(t) = \exp\left(-\frac{i}{\hbar}\int_0^t\Big[e_\pm(t')+\hbar\mathbf{A}_\pm(\mathbf{H})\cdot\dot{\mathbf{H}}\Big]\,\mathrm{d}t'\right)c_\pm(0). \tag{1.114}$$

Moving around a closed loop, we see that the states acquires an additional phase

$$\boxed{\theta_{B,\pm}[\gamma] = -\oint_\gamma \mathbf{A}_\pm(\mathbf{H})\cdot\mathrm{d}\mathbf{H}\,,} \tag{1.115}$$

which depends only on the path, and not on the way it is traversed (i.e. the parametrisation $\mathbf{H}(t)$).

Clearly, $\mathbf{A}_\pm$ depends on how we chose our states $|\mathbf{H},\pm\rangle$ in the first place. So you could be forgiven for thinking that $\theta_{B,\pm}$ does too. However, any other choice can be obtained by multiplying $|\mathbf{H},\pm\rangle$ by some **H** dependent phase factor. Then

$$\begin{aligned}\left|\mathbf{H},\pm\right\rangle &\to \exp(i\Lambda_\pm(\mathbf{H}))\left|\mathbf{H},\pm\right\rangle\\ \mathbf{A}_\pm(\mathbf{H}) &\to \mathbf{A}_\pm + \boldsymbol{\nabla}_{\mathbf{H}}\Lambda_\pm(\mathbf{H}),\end{aligned} \tag{1.116}$$

and the line integral in Eq. (1.115) is unchanged. Thus $\theta_{B,\alpha}$ is a property of the path γ in the **H** space, not of how the phases of the eigenstates are chosen.

You should recognise Eq. (1.116) as a *gauge transformation*, with $\mathbf{A}_\pm(\mathbf{H})$ playing the role of the vector potential (sometimes called the **Berry potential**). We have just shown that $\theta_{B,\pm}$ is a gauge invariant quantity.

To get to the geometric meaning of $\theta_{B,\pm}$, we compute the "magnetic field" associated with $\mathbf{A}_\pm$

$$\mathbf{B}_\pm(\mathbf{H}) \equiv \boldsymbol{\nabla}_\mathbf{H} \times \mathbf{A}_\pm(\mathbf{H}) = \pm\frac{\hat{\mathbf{n}}}{2H_0^2}, \tag{1.117}$$

which corresponds to a **magnetic monopole** of charge $\pm\frac{1}{2}$ at the origin. This field is a gauge invariant quantity, which provides another way of seeing the gauge invariance of $\theta_{B,\pm}$. Using Stokes' theorem to convert the loop integral in Eq. (1.115) into a surface integral over a surface Σ bounded by γ gives

$$\boxed{\theta_{B,\pm}[\gamma] = -\sum_\Sigma \mathbf{B}_\pm \cdot \mathrm{d}\mathbf{S} = \mp\frac{1}{2}\Omega,} \tag{1.118}$$

where Ω is the solid angle enclosed by Σ.[6]

Note that the singularities appearing the gauge field in Eq. (1.106) at the north and south poles have no physical meaning. It is better to focus on the field $\mathbf{B}_\pm$ which is well behaved there.

1.4.1 Classical Analogue [*non-examinable*]

A beautiful *classical* analogue of Berry's phase can be demonstrated using a gyroscope. Imagine holding one end of its axle, and moving it around so that a unit vector parallel to the axle traces out a closed curve on the unit sphere. When you return the axle to its original orientation, you will find – provided the bearings are nice and smooth – that the wheel has rotated! Remarkably, the angle of rotation turns out to be the solid angle enclosed within the curve traced out on the unit sphere.

It sounds like this must be connected to Berry's phase, and indeed it is. Though the physics of this situation is very different, the mathematics is almost identical. To deal with the physics first: the key point is that, by holding the gyroscope by the axle, we never apply any torque parallel to the axle. Thus the angular momentum in this direction is fixed (to zero, say). However, this direction is changing in time

Let's denote by θ the angular orientation of the wheel on the axle. Imagine marking out the angle in degree increments on the axle, and measuring θ using some mark on the wheel. It's natural to write the condition of vanishing angular momentum as

$$L_{\text{axle}} \stackrel{?}{=} I\dot{\theta} = 0. \tag{1.119}$$

Actually, this won't quite do, because the whole point is that the axle itself is going to move. Imagine twisting the axle back and forth, keeping it pointing in the same direction.

[6] While there is an ambiguity of $\Omega \leftrightarrow 4\pi - \Omega$ in the solid angle enclosed by a curve, this is harmless because (accounting for the change in the sense of the curve) it amounts to a change of the phase by 2π.

The wheel will not move, though the angle θ will be going up and down because the axle is moving.

To include this effect, imagine defining an orthonormal triad of vectors $(\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{n}})$, where $\hat{\mathbf{n}}$ is parallel to the axle, and $\hat{\mathbf{a}} \times \hat{\mathbf{b}} = \hat{\mathbf{n}}$. The motion we just described corresponds to a rotation in the $a - b$ plane. Rotating the axle by ϕ corresponds to

$$\begin{aligned} \hat{\mathbf{a}} &\to \cos\phi\hat{\mathbf{a}} + \sin\phi + \hat{\mathbf{b}} \\ \hat{\mathbf{b}} &\to \cos\phi\hat{\mathbf{b}} - \sin\phi\hat{\mathbf{a}}. \end{aligned} \tag{1.120}$$

Now notice that

$$\mathrm{d}\phi = -\hat{\mathbf{a}} \cdot \mathrm{d}\hat{\mathbf{b}} = \hat{\mathbf{b}} \cdot \mathrm{d}\hat{\mathbf{a}}\,. \tag{1.121}$$

Thus Eq. (1.119) should really be

$$\dot{\theta} + \dot{\phi} = \dot{\theta} + \frac{1}{2}\left[\hat{\mathbf{b}} \cdot \dot{\hat{a}} - \hat{\mathbf{a}} \cdot \dot{\hat{b}}\right] = 0. \tag{1.122}$$

To make the connection to Berry's phase, we introduce the complex vector $\boldsymbol{\psi} = (\hat{\mathbf{a}} + i\hat{\mathbf{b}})/\sqrt{2}$. Then Eq. (1.122) can be written

$$\dot{\theta} + i\boldsymbol{\psi}^\dagger \frac{\mathrm{d}\boldsymbol{\psi}}{\mathrm{d}t} = 0. \tag{1.123}$$

Now for each direction $\hat{\mathbf{n}}$, fix $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$. We have some freedom here, as we can always choose them differently by rotating in the plane normal to $\hat{\mathbf{n}}$ as in Eq. (1.120). This is entirely analogous to the freedom to choose a gauge that we had in the quantum problem. Once we have done this, we can find the angle of rotation by

$$\Delta\theta = \int \dot{\theta}\,\mathrm{d}t = \int -i\boldsymbol{\psi}^\dagger \frac{\mathrm{d}\boldsymbol{\psi}}{\mathrm{d}t}\,\mathrm{d}t = \int \mathbf{A}_{\hat{\mathbf{n}}} \cdot \mathrm{d}\hat{\mathbf{n}}\,, \tag{1.124}$$

where we defined $\mathbf{A}_{\hat{\mathbf{n}}} = -i\boldsymbol{\psi}^\dagger \boldsymbol{\nabla}_{\hat{\mathbf{n}}} \boldsymbol{\psi}$. Just as with Berry's phase, this angle is independent of the arbitrary choice we just made.

Now we just have to compute it. We first fix an explicit form for the triad

$$\hat{\mathbf{a}} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \tag{1.125}$$

$$\hat{\mathbf{b}} = (-\sin\phi, \cos\phi, 0) \tag{1.126}$$

$$\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{1.127}$$

and then compute

$$\mathbf{A}_{\hat{\mathbf{n}}} = -\cos\theta \boldsymbol{\nabla}_{\hat{\mathbf{n}}}\phi. \tag{1.128}$$

We get

$$\Delta\theta = \oint \mathbf{A}_{\hat{\mathbf{n}}} \cdot \mathrm{d}\hat{\mathbf{n}} = \int (\boldsymbol{\nabla}_{\hat{\mathbf{n}}} \times \mathbf{A}_{\hat{\mathbf{n}}}) \cdot \mathrm{d}\mathbf{S} = \int \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = \Omega, \tag{1.129}$$

which is the result stated above.

$\boldsymbol{\nabla}_{\hat{\mathbf{n}}} \times \mathbf{A}_{\hat{\mathbf{n}}}$ can be found in a slicker way without introducing an explicit parametrisation of the triad. To evaluate the antisymmetric tensor

$$\partial_i\hat{\mathbf{a}} \cdot \partial_j\hat{\mathbf{b}} - \partial_j\hat{\mathbf{a}} \cdot \partial_i\hat{\mathbf{b}}, \tag{1.130}$$

we first notice that $\partial_i \hat{\mathbf{a}}$ must lie in the $b-n$ plane (to preserve normalisation) and likewise $\partial_j \hat{\mathbf{b}}$ must lie in the $a-n$ plane. Thus Eq. (1.130) can be written

$$\partial_i \hat{\mathbf{a}} \cdot \partial_j \hat{\mathbf{b}} - \partial_j \hat{\mathbf{a}} \cdot \partial_i \hat{\mathbf{b}} = (\hat{\mathbf{n}} \cdot \partial_i \hat{\mathbf{a}})\Big(\hat{\mathbf{n}} \cdot \partial_j \hat{\mathbf{b}}\Big) - (\hat{\mathbf{n}} \cdot \partial_j \hat{\mathbf{a}})\Big(\hat{\mathbf{n}} \cdot \partial_i \hat{\mathbf{b}}\Big). \tag{1.131}$$

Now using the property $\hat{\mathbf{n}} \cdot \partial_i \hat{\mathbf{a}} = -\hat{\mathbf{a}} \cdot \partial_i \hat{\mathbf{n}}$, which follows from preserving the orthogonality of the triad under differentiation, we have

$$\begin{aligned}(\hat{\mathbf{n}} \cdot \partial_i \hat{\mathbf{a}})\Big(\hat{\mathbf{n}} \cdot \partial_j \hat{\mathbf{b}}\Big) - (\hat{\mathbf{n}} \cdot \partial_j \hat{\mathbf{a}})\Big(\hat{\mathbf{n}} \cdot \partial_i \hat{\mathbf{b}}\Big) &= (\hat{\mathbf{a}} \cdot \partial_i \hat{\mathbf{n}})\Big(\hat{\mathbf{b}} \cdot \partial_j \hat{\mathbf{n}}\Big) - (\hat{\mathbf{n}} \cdot \partial_j \hat{\mathbf{n}})\Big(\hat{\mathbf{b}} \cdot \partial_i \hat{\mathbf{n}}\Big) \\ &= (\hat{\mathbf{a}} \times \hat{\mathbf{b}}) \cdot (\partial_i \hat{\mathbf{n}} \times \partial_j \hat{\mathbf{n}}) \\ &= \hat{\mathbf{n}} \cdot (\partial_i \hat{\mathbf{n}} \times \partial_j \hat{\mathbf{n}}). \end{aligned} \tag{1.132}$$

In polar coordinates,

$$\hat{\mathbf{n}} \cdot (\partial_i \hat{\mathbf{n}} \times \partial_j \hat{\mathbf{n}}) = \sin\theta \partial_i \theta \partial_j \phi, \tag{1.133}$$

which is just what we found before.

Chapter 2

Introduction to Path Integrals

2.1 The Languages of Quantum Theory

From the outset, quantum mechanics was written in two apparently different languages. Schrödinger's equation, published in 1926, describes the time evolution of the wave function $\Psi(\mathbf{r}, t)$ of the system

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right]\Psi(\mathbf{r}, t). \tag{2.1}$$

It is historically the *second* formulation of modern quantum theory, the first having been given a year earlier by Heisenberg. In Heisenberg's version it is the matrix elements of observables that evolve in time: hence this way of doing things is sometimes known as *matrix mechanics*. Schrödinger quickly proved the equivalence of the two approaches, and in Dirac's formulation of operators acting in Hilbert space, this equivalence is rather evident. The evolution of a state can be written using the unitary operator of time evolution $\hat{U}(t) \equiv^{-i\hat{H}t/\hbar}$, where $\hat{H}$ is the Hamiltonian, as

$$|\Psi(t)\rangle = \hat{U}(t)\,|\Psi(0)\rangle\,. \tag{2.2}$$

For any operator $\hat{A}$ and pair of states $|\Phi\rangle$, $|\Psi\rangle$, we then have

$$\langle\Psi(t)|\hat{A}|\Phi(t)\rangle = \langle\Psi(0)|\hat{A}(t)|\Phi(0)\rangle\,, \tag{2.3}$$

where $\hat{A}(t) \equiv e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}$ defines the time evolution of $\hat{A}$. To put it another way, $\hat{A}(t)$ obeys the Heisenberg equation of motion

$$\frac{\mathrm{d}\hat{A}}{\mathrm{d}t} = \frac{i}{\hbar}\big[\hat{H}, \hat{A}\big]. \tag{2.4}$$

In contrast to the Schrödinger equation, which allowed physicists trained to solve the partial differential equations of classical physics to go to work on the problems of the atom, Heisenberg's formulation is practically useless. It took the genius of Wolfgang Pauli to solve the Hydrogen atom using matrix mechanics, a calculation we will discuss in Chapter 6

Eqs. (2.1) and (2.4) embody a radical departure from classical ideas. In particular, the notion of a trajectory $\mathbf{r}(t)$ of a particle in time is nowhere to be seen. It is surprising, then, that there is a way to describe quantum mechanics in terms of trajectories, and more surprising still that it did not emerge until more than 20 years after the above formulations.[1] This is **Feynman's path integral**.

[1] Coincidentally, around the same time a fourth formulation of quantum theory was given by Groenewold and Moyal. This **phase space formulation** makes contact with classical mechanics through the Hamiltonian, rather than Lagrangian, viewpoint. We'll meet it briefly in Chapter 5.

2.2 The Propagator

The path integral is a tool for calculating the *propagator*. Since this is an idea of wider utility, we'll take a moment to get acquainted. In fact, we already have, for the propagator is just a representation of the time evolution operator

$$K(\mathbf{r},t|\mathbf{r}',t') \equiv \theta(t-t')\,\langle \mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle\,, \tag{2.5}$$

where $|\mathbf{r}\rangle$ denotes a position eigenstate.[2] $\theta(t)$ is the step function

$$\theta(t) \equiv \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}. \tag{2.6}$$

As the name implies, $K(\mathbf{r},t|\mathbf{r}',t')$ is used to propagate the state of a system forward in time. Thus Eq. (2.2) may be written, for $t > t'$

$$\begin{aligned} \Psi(\mathbf{r},t) = \langle \mathbf{r}|\Psi(t)\rangle &= \langle \mathbf{r}|\hat{U}(t-t')|\Psi(t')\rangle \\ &= \int \mathrm{d}\mathbf{r}'\ \langle \mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle\,\langle \mathbf{r}'|\Psi(t')\rangle \\ &= \int \mathrm{d}\mathbf{r}'\, K(\mathbf{r},t|\mathbf{r}',t')\Psi(\mathbf{r}',t'), \end{aligned} \tag{2.7}$$

where in the second line we inserted a complete set of states. Equivalently, $K(\mathbf{r},t|\mathbf{r}',t')$ is the *fundamental solution* of the time dependent Schrödinger equation, which means that it satisfies both of

$$\begin{gathered} \left[i\hbar\frac{\partial}{\partial t} - \hat{H}\right] K(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \\ K(\mathbf{r},t|\mathbf{r}',t') = 0 \quad \text{for} \quad t < t' \end{gathered} \tag{2.8}$$

To explain why these two definitions are equivalent, if we integrate Eq. (2.8) with respect to t from $t'-\varepsilon$ to $t'+\varepsilon$ we find

$$i\hbar K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t') - \int_{t'-\varepsilon}^{t'+\varepsilon} \mathrm{d}t\, \hat{H}K(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}'). \tag{2.9}$$

Using the fact that we know $K = 0$ for $t < t'$ we may approximate the integral for small ε as

$$K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}') - \varepsilon\frac{i}{\hbar}\hat{H}K(\mathbf{r},t|\mathbf{r}',t'). \tag{2.10}$$

We can see that this is equivalent to the first definition (2.5) by Taylor expanding (2.5) in t about t' and using the fact that $\partial_t\hat{U} = -\frac{i}{\hbar}\hat{H}\hat{U}$ as well as $\hat{U}(0) = 1$,

$$\begin{aligned} K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t') &\approx \langle \mathbf{r}|\hat{U}(0)|\mathbf{r}'\rangle + \varepsilon\,\langle \mathbf{r}|\partial_t\hat{U}(0)|\mathbf{r}'\rangle \\ &\approx \delta(\mathbf{r}-\mathbf{r}') - \varepsilon\frac{i}{\hbar}\,\langle \mathbf{r}|\hat{H}\hat{U}(0)|\mathbf{r}'\rangle \\ &\approx \delta(\mathbf{r}-\mathbf{r}') - \varepsilon\frac{i}{\hbar}\hat{H}K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t'). \end{aligned} \tag{2.11}$$

[2] The weird notation $K(\mathbf{r},t|\mathbf{r}',t')$ is to emphasize that $\mathbf{r}'$ and t' are to be treated as parameters. In particular, when we apply the Hamiltonian, it will operate on the $\mathbf{r}$ variable only.

The idea of representing the solution of a partial differential equation (PDE) should be familiar to you from your study of Green's functions. Indeed, 'Green's function' and 'propagator' are often used interchangeably.

The fact that the wavefunction at later times can be expressed in terms of $\Psi(\mathbf{r},0)$ is a consequence of the Schrödinger equation being first order in time (and linearity naturally implies the relationship is a linear one). To see the generality of the idea, let us first discuss how it works for the heat equation, another PDE first order in time. The fundamental solution satisfies

$$\left[\frac{\partial}{\partial t} - D\nabla^2_{\mathbf{r}}\right] K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{2.12}$$

$$K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = 0 \quad \text{for} \quad t < t'. \tag{2.13}$$

To show that the fundamental solution of the heat equation is

$$K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = \frac{\theta(t-t')}{(4\pi D(t-t'))^{3/2}} \exp\left(-\frac{(\mathbf{r}-\mathbf{r})^2}{4D(t-t')}\right), \tag{2.14}$$

we must first note that the Heaviside step function θ takes care of the second demanded property (2.13). We must also consider that

$$\frac{\partial}{\partial t}\theta(t-t') = \delta(t-t'), \tag{2.15}$$

which can be verified by integrating both sides with respect to time along the interaval $(-\infty, t)$. Armed with this it is a simple matter of applying the operator $\left[\frac{\partial}{\partial t} - D\nabla^2_{\mathbf{r}}\right]$ to (2.14) for K_{heat}. Doing this we find

$$\left[\frac{\partial}{\partial t} - D\nabla^2_{\mathbf{r}}\right] K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = \delta(t-t')\frac{1}{(4\pi D(t-t'))^{3/2}} \exp\left(-\frac{(\mathbf{r}-\mathbf{r})^2}{4D(t-t')}\right) \tag{2.16}$$

where in the above we have made use of the identity

$$\nabla^2_{\mathbf{r}} \exp\left(\frac{\alpha}{2}\mathbf{r}^2\right) = \left(3\alpha + \alpha^2\mathbf{r}^2\right) \exp\left(\frac{\alpha}{2}\mathbf{r}^2\right) \tag{2.17}$$

for the spatial derivatives, and we find that all of the terms involving Heaviside functions cancel.

We should now examine the right hand side of the formula (2.16) excluding the $\delta(t-t')$ term; let

$$f(\mathbf{r},t|\mathbf{r}',t') = \frac{1}{(4\pi D(t-t'))^{3/2}} \exp\left(-\frac{(\mathbf{r}-\mathbf{r})^2}{4D(t-t')}\right). \tag{2.18}$$

We only need to worry about the case where $t-t'=0$ since there is a temporal delta function multiplying it in (2.16). In the limit that $t-t' \to 0$ we can see that the function vanishes everywhere where $\mathbf{r}-\mathbf{r}'$ is non-zero. However, we can also see from the standard Gaussian formula

$$\int \mathrm{d}^N\mathbf{r} \exp\left(-\frac{\mathbf{r}^2}{2\sigma^2}\right) = \left(\sigma\sqrt{2\pi}\right)^N, \tag{2.19}$$

thus

$$\int f(\mathbf{r},t|\mathbf{r}',t')\,\mathrm{d}^3\mathbf{r} = 1. \tag{2.20}$$

These are the exact properties of a delta function in $\mathbf{r}-\mathbf{r}'$, so we see that

$$\lim_{t\to t'} f(\mathbf{r},t|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}'), \tag{2.21}$$

and thus (2.14) is the fundamental solution of the heat equation.

Thus if $\Theta(\mathbf{r},0)$ describes the initial temperature distribution within a uniform medium with thermal diffusivity D, then at some later time we have

$$\Theta(\mathbf{r},t) = \int \mathrm{d}\mathbf{r}'\, K_{\mathrm{heat}}(\mathbf{r},t|\mathbf{r}',0)\Theta(\mathbf{r},0). \tag{2.22}$$

Eqs. (2.14) and (2.22) have the following meaning. We can represent the initial continuous temperature distribution as an array of hot spots of varying temperatures. The evolution of a hot spot is found by solving Eq. (2.14), with the right hand side representing a unit amount of heat injected into the system at point $\mathbf{r}'$ and time t'. As time progresses, each hot spot diffuses outwards with a Gaussian profile of width $\sqrt{D(t-t')}$, independently of the others by virtue of the linearity of the equation.

Fig. 2.1: Spreading of a hot spot.

What can be accomplished in one time step can equally well be done in two. Thus the propagator must have the property

$$K(\mathbf{r},t|\mathbf{r}',t') = \int \mathrm{d}^3\mathbf{r}''\, K(\mathbf{r},t|\mathbf{r}'',t'')K(\mathbf{r}'',t''|\mathbf{r}',t'). \tag{2.23}$$

To verify this for $K_{\mathrm{heat}}(\mathbf{r},t|\mathbf{r}',t')$, we must substitute its form into (2.14) and show both sides are equivalent. If we concentrate on the exponent of the integrand, we should complete the square in order to perform the Gaussian Integral,

$$-\frac{(\mathbf{r}-\mathbf{r}'')^2}{4D(t-t'')} - \frac{(\mathbf{r}''-\mathbf{r}')^2}{4D(t''-t')} = -\frac{t-t'}{4D(t-t'')(t''-t'}\left(\mathbf{r}'' + \frac{(t''-t')\mathbf{r}-(t-t'')\mathbf{r}'}{t-t'}\right)^2 - \frac{(\mathbf{r}-\mathbf{r}')^2}{4D(t-t')}. \tag{2.24}$$

When multiplying the time-dependant prefactors of equation (2.14), we find a product of Heaviside θ functions. Since we know that $t<t''<t'$, we find

$$\theta(t-t') = \theta(t-t'')\theta(t''-t'). \tag{2.25}$$

The standard N-dimensional Gaussian integral says that

$$\int \mathrm{d}^N\mathbf{r}\exp\left(-\frac{\mathbf{r}^2}{2\sigma^2}\right) = \left(\sigma\sqrt{2\pi}\right)^N. \tag{2.26}$$

Applying this to the integrand of equation (2.23) with it's exponent in the completed square form (2.24), we find that the time-dependant prefactors cancel out. The entire RHS just simplifies down to (2.14), which is the same as the LHS.

With this in hand, it's a small leap to find the propagator for the free particle Schrödinger equation. The Hamiltonian is $\hat{H} = -\frac{\hbar^2\nabla^2}{2m}$, so by taking $D \to \frac{\hbar}{2m}$ and $t \to it$, we get[3]

$$\boxed{K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left(-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}\right).} \tag{2.27}$$

2.2.1 The Propagator in Momentum Space

We originally defined the propagator in Eq. (2.5) as a real space representation of the time evolution operator. We could just as well choose to take matrix elements in another basis. Since the free particle Hamiltonian $\hat{H} = -\frac{\hbar^2\nabla^2}{2m}$ is diagonal in momentum space, it makes sense to look at[4]

$$\begin{aligned} K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') &= \theta(t-t') \langle \mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle \\ &= \theta(t-t') \exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{t-t'}{\hbar}\right)\delta(\mathbf{p}-\mathbf{p}') \end{aligned} \tag{2.28}$$

We can confirm that Eqs. (2.27) and (2.28) are related by a change of basis (Fourier transform) using

$$\langle \mathbf{r}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar). \tag{2.29}$$

The definitions of the respective propagators are

$$K(\mathbf{r}, t|\mathbf{r}', t') = \langle \mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle \tag{2.30}$$

$$K(\mathbf{p}, t|\mathbf{p}', t') = \langle \mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle\,. \tag{2.31}$$

We may transform from one to the other by inserting two resolutions of the identity

$$\begin{aligned} \langle \mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle &= \langle \mathbf{r}|\left[\int \mathrm{d}\mathbf{p}\, |\mathbf{p}\rangle \langle \mathbf{p}|\right]\hat{U}(t-t')\left[\int \mathrm{d}\mathbf{p}'\, |\mathbf{p}'\rangle \langle \mathbf{p}'|\right]|\mathbf{r}'\rangle \\ &= \int \mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}' \langle \mathbf{r}|\mathbf{p}\rangle \langle \mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle \langle \mathbf{p}'|\mathbf{r}'\rangle \\ &= \int \frac{\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'}{(2\pi\hbar)^3} \exp(i(\mathbf{p}\cdot\mathbf{r} - \mathbf{p}'\cdot\mathbf{r}')/\hbar) \langle \mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle\,. \end{aligned} \tag{2.32}$$

We know from Eqs. (2.27) and (2.28) that

$$K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left(-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}\right) \tag{2.33}$$

$$K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\delta(\mathbf{p}-\mathbf{p}') \exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{t-t'}{\hbar}\right), \tag{2.34}$$

[3] In d dimensions the 3/2 power in the prefactor becomes $d/2$.

[4] Don't forget that with the normalisation used here, $|\mathbf{r}\rangle$ has units of $[\text{Length}]^{-d/2}$, while $|\mathbf{p}\rangle$ has units $[\text{Momentum}]^{-d/2}$. A δ-function $\delta(x)$ in d-dimensions has units of $[\text{x}]^{-d}$.

so the answer amounts to putting expression (2.34) into the left hand side of (2.32) and showing that this is equivalent to (2.33). If we do this, we can integrate over $\mathbf{p}'$ and apply the properties of the δ-function to set $\mathbf{p}' = \mathbf{p}$. We now have an exponent in the integrand on which we may complete the square

$$i\mathbf{p}\cdot\frac{\mathbf{r}-\mathbf{r}'}{\hbar} - i\frac{\mathbf{p}^2(t-t')}{2m\hbar} = -\frac{i(t-t')}{2m\hbar}\left(\mathbf{p} - m\frac{\mathbf{r}-\mathbf{r}'}{t-t'}\right)^2 - \frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}. \tag{2.35}$$

Now we have completed the square we may apply our N-dimensional Gaussian integral formula (2.26). Performing this gives the required LHS.

This idea generalises to any time independent Hamiltonian with a complete set of energy eigenfunctions $\{\varphi_\alpha(\mathbf{r})\}$ and eigenvalues $\{E_\alpha\}$

$$K(\mathbf{r},t|\mathbf{r}',t') = \theta(t-t')\sum_\alpha \varphi_\alpha(\mathbf{r})\varphi_\alpha^*(\mathbf{r}')e^{-iE_\alpha(t-t')/\hbar}. \tag{2.36}$$

For a time dependent Hamiltonian, we have the complication that the time evolution operator must be thought of as a function of two variables – the initial and final times, say – rather than just the *duration* of evolution.[5]

$$|\Psi(t)\rangle = \hat{U}(t,t')\,|\Psi(t')\rangle\,. \tag{2.38}$$

Nevertheless, the propagator $K(\mathbf{r},t|\mathbf{r}',t') = \theta(t-t')\,\langle\mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle$ obeys the same basic equation Eq. (2.8).

2.3 The Path Integral

By using the reproducing property of the kernel (2.23) we can subdivide the evolution from time t_i to t_f into N smaller intervals of length $\Delta t = (t_\mathrm{f}-t_\mathrm{i})/N$, each characterised by its own propagator

$$K(\mathbf{r}_\mathrm{f},t_\mathrm{f}|\mathbf{r}_\mathrm{i},t_\mathrm{i}) = \int \mathrm{d}\mathbf{r}_1\cdots\mathrm{d}\mathbf{r}_{N-1}\,K(\mathbf{r}_\mathrm{f},t_\mathrm{f}|\mathbf{r}_{N-1},t_{N-1})\cdots K(\mathbf{r}_1,t_1|\mathbf{r}_\mathrm{i},t_\mathrm{i}). \tag{2.39}$$

This is not totally perverse: as we will see shortly the apparent increase in complexity is countered by the simplification of the propagator for small propagation intervals. The idea is that in the limit[6] the integration over the variables $\{\mathbf{r}_i\}$ becomes an *integral over paths* $\mathbf{r}(t)$, with a continuous index – time – rather than a discrete one. This is the path integral.

[5] In terms of the Hamiltonian $\hat{H}(t)$, $\hat{U}(t,t')$ has the deceptively simple form,

$$\hat{U}(t,t') = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t'}^{t}\mathrm{d}t_i\,\hat{H}(t_i)\right), \tag{2.37}$$

where $\mathcal{T}$ denotes the time ordering operator. The time ordering is essential because the commutator of the Hamiltonian evaluated at two different times is in general nonzero.

[6] These three words are terribly glib. Spare a thought for the mathematicians who had to try and make something respectable out of this!

Fig. 2.2: Slicing the propagation time into many small intervals.

So what is the integrand? A clue is provided by the observation that in the presence of a constant potential $V(\mathbf{r}) = V_0$, the propagator is a simple modification of Eq. (2.27)

$$K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left(-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')} - i\frac{V_0(t-t')}{\hbar}\right), \tag{2.40}$$

as may be verified by direct substitution into the Schrödinger equation. Now as the propagation time $t - t'$ goes to zero, we know that the propagator is going to approach a δ-function. Therefore, Eq. (2.40) should still hold if we take V_0 to be the value of the potential at the midpoint $\frac{\mathbf{r}+\mathbf{r}'}{2}$ (say)[7].

Putting this into Eq. (2.39), for $N \to \infty$, $(\mathbf{r}_{i+1})^2/(t_{i+1} - t_i) \to \dot{\mathbf{r}}^2 \Delta t$,

$$\boxed{K(\mathbf{r}_\text{f}, t_\text{f}|\mathbf{r}_\text{i}, t_\text{i}) = \int_{\substack{\mathbf{r}(t_\text{f})=\mathbf{r}_\text{f} \\ \mathbf{r}(t_\text{i})=\mathbf{r}_\text{i}}} \mathcal{D}\mathbf{r}(t) \exp\left(\frac{i}{\hbar}\int_{t_\text{i}}^{t_\text{f}} \left[\frac{m\dot{\mathbf{r}}^2}{2} - V(\mathbf{r}(t))\right] \mathrm{d}t\right).} \tag{2.41}$$

The symbol $\mathcal{D}\mathbf{r}(t)$, which corresponds to a "volume element" in the space of paths, is presumed to contain the appropriate normalization, including a horribly divergent factor $\left(\frac{m}{2i\pi\hbar\Delta t}\right)^{3/2}$. The subscript on the $\int \mathcal{D}\mathbf{r}(t)$ integral indicates that all paths must begin at $\mathbf{r}_\text{i}$ and end at $\mathbf{r}_\text{f}$.

One may wonder how Eq. (2.41), beset by such mathematical vagaries, can be of any use at all. One thing we have going for us is that all of these difficulties have nothing to do with $V(\mathbf{r})$, and are therefore unchanged in going from the free particle case to something more interesting. We can therefore use the free particle result to provide the normalisation, and calculate the effect of introducing $V(\mathbf{r})$ relative to this

2.3.1 Enter the Lagrangian

It's a historical oddity that the Hamiltonian is one of the last things you meet in classical mechanics and one of the first in quantum mechanics. Eq. (2.41) represents the first appearance in quantum mechanics of the *Lagrangian*

$$L(\mathbf{r}, \dot{\mathbf{r}}) \equiv \frac{m\dot{\mathbf{r}}^2}{2} - V(\mathbf{r}), \tag{2.42}$$

and its time integral, the *action*[8]

$$S[\mathbf{r}(t)] \equiv \int_{t_\text{i}}^{t_\text{f}} L(\mathbf{r}(t), \dot{\mathbf{r}}(t))\, \mathrm{d}t\,. \tag{2.43}$$

[7] The particular choice is unimportant here, but the midpoint prescription turns out to be vital when a vector potential is included (See Chapter 4).

[8] The square brackets are used to indicate that S is a *functional* of the path. A functional is a machine that takes a function and produces a number

As you know very well, variations of the path $\mathbf{r}(t)$ with fixed endpoints (i.e $\mathbf{r}(t_\mathrm{i}) = \mathbf{r}_\mathrm{i}$, $\mathbf{r}(t_\mathrm{f}) = \mathbf{r}_\mathrm{f}$) leave the action unchanged to first order if (and only if) the *Euler–Lagrange equations* are satisfied

$$\frac{\partial L}{\partial \mathbf{r}} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{r}}}\right) = 0. \tag{2.44}$$

As we'll see shortly, the path integral provides a natural explanation of how these equations and the action principle arise in the classical limit.

2.4 Path Integral for the Harmonic Oscillator

To show that this all works we at least have to be able to solve the harmonic oscillator. Confining ourselves to one dimension, the Lagrangian is

$$L_\mathrm{SHO}(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2. \tag{2.45}$$

The propagator is therefore expressed as the path integral

$$K_\mathrm{SHO}(x_\mathrm{f}, t_\mathrm{f}|x_\mathrm{i}, t_\mathrm{i}) = \int_{\substack{x(t_\mathrm{f})=x_\mathrm{f}\\ x(t_\mathrm{i})=x_\mathrm{i}}} \mathcal{D}x(t) \exp\left(\frac{i}{\hbar}\overbrace{\int_{t_\mathrm{i}}^{t_\mathrm{f}} \left[\frac{m\dot{x}^2}{2} - \frac{m\omega^2 x^2}{2}\right] \mathrm{d}t}^{S_\mathrm{SHO}[x(t)]}\right). \tag{2.46}$$

This form is reminiscent of a Gaussian integral. Before we can use this insight, we first have to deal with the feature that the paths $x(t)$ satisfy the boundary conditions $x(t_\mathrm{i}) = x_\mathrm{i}$, $x(t_\mathrm{f}) = x_\mathrm{f}$. We can make things simpler by substituting $x(t) = x_0(t) + \eta(t)$, where $x_0(t)$ is some function satisfying these same conditions. Then $\eta(t)$, the new integration variable, satisfies $\eta(t_\mathrm{i}) = \eta(t_\mathrm{f}) = 0$.

What should we take for $x_0(t)$? Making the substitution in the action gives

$$S_\mathrm{SHO}[x_0(t) + \eta(t)] = S_\mathrm{SHO}[x_0(t)] + S_\mathrm{SHO}[\eta(t)] + \int_{t_\mathrm{i}}^{t_\mathrm{f}} \Big[m\dot{x}_0(t)\dot{\eta}(t) - m\omega^2 x_0(t)\eta(t)\Big]\,\mathrm{d}t\,. \tag{2.47}$$

Integrating the last term by parts, and bearing in mind that $\eta(t)$ vanishes at the endpoints, puts it in the form

$$-\int_{t_\mathrm{i}}^{t_\mathrm{f}} \Big[m\ddot{x}_0(t) + m\omega^2 x_0(t)\Big]\eta(t)\,\mathrm{d}t\,. \tag{2.48}$$

We recognize the quantity in square brackets as the equation of motion of the simple harmonic oscillator. Thus if we choose $x_0(t)$ to satisfy this equation, the cross term in Eq. (2.47) vanishes[9] and the propagator takes the from

$$K_\mathrm{SHO}(x_\mathrm{f}, t_\mathrm{f}|x_\mathrm{i}, t_\mathrm{i}) = \exp\left(\frac{i}{\hbar}S_\mathrm{SHO}[x_0(t)]\right)\times \int_{\eta(t_\mathrm{f})=\eta(t_\mathrm{i})=0} \mathcal{D}\eta(t) \exp\left(\frac{i}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \left[\frac{m\dot{\eta}^2}{2} - \frac{m\omega^2\eta^2}{2}\right] \mathrm{d}t\right). \tag{2.49}$$

[9] Choosing $x_0(t)$ to be the classical trajectory eliminates the linear term in η in general. This is after all exactly what the action principle tells us that classical trajectories do (note the condition of fixed endpoints, vital in the derivation of the Euler–Lagrange equations, arises naturally here). The action for $\eta(t)$ will not be independent of $x_0(t)$ for more complicated – i.e. non-quadratic – Lagrangians, however.

To find the classical action of the trajectory of a harmonic oscillator with $x(t_\mathrm{i}) = x_\mathrm{i}$ and $x(t_\mathrm{f}) = x_\mathrm{f}$, we first let $T \equiv t_\mathrm{f} - t_\mathrm{i}$ and shift things to be symmetrical around $t = 0$. Then we can write the classical motion as

$$x(t) = A\cos\omega t + B\sin\omega t \tag{2.50}$$

with

$$A = \frac{x_\mathrm{f} + x_\mathrm{i}}{2\cos\omega T}, \quad B = \frac{x_\mathrm{f} - x_\mathrm{i}}{2\sin\omega T}. \tag{2.51}$$

Evaluating the Lagrangian gives

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2\Big[\Big(B^2 - A^2\Big)\cos 2\omega T + 2AB\sin 2\omega T\Big]. \tag{2.52}$$

When we calculate the action integral the term in AB vanishes (being odd), leaving

$$\begin{aligned} S_\mathrm{SHO} = \int_{-T/2}^{T/2} L\,\mathrm{d}t &= \frac{1}{2}m\omega\Big(B^2 - A^2\Big)\sin\omega T \\ &= \frac{m\omega}{2\sin\omega T}\Big[\Big(x_\mathrm{i}^2 + x_\mathrm{f}^2\Big)\cos\omega T - 2x_\mathrm{i}x_\mathrm{f}\Big]. \end{aligned} \tag{2.53}$$

As a check, let $\omega \to 0$ and see that the free particle action is recovered.

Now we turn our attention to the η path integral in Eq. (2.49). Because the action for $\eta(t)$ is independent of time, and $\eta(t)$ vanishes at the endpoints, it cries out to be expanded in a Fourier series

$$\eta(t) = \sum_{n=1}^{\infty} \eta_n \sin\left(\frac{\pi n(t - t_\mathrm{i})}{t_\mathrm{f} - t_\mathrm{i}}\right). \tag{2.54}$$

In terms of the Fourier coefficients $\{\eta_n\}$ the action takes the form

$$S_\mathrm{SHO}[\eta(t)] = \frac{m(t_\mathrm{f} - t_\mathrm{i})}{4}\sum_{n=1}^{\infty}\left[\frac{\pi^2 n^2}{(t_\mathrm{f} - t_\mathrm{i})^2} - \omega^2\right]\eta_n^2. \tag{2.55}$$

The η integral now begins to look like a product of Gaussian integrals, provided that we are free to interpret $\mathcal{D}\eta(t) = \prod_i^\infty \mathrm{d}\eta_n$ (we are).

The Gaussian integral we can do

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-bx^2/2} = \sqrt{\frac{2\pi}{b}}. \tag{2.56}$$

So we take a wild guess and write

$$K_\mathrm{SHO}(x_\mathrm{f}, t_\mathrm{f}|x_\mathrm{i}, t_\mathrm{i}) \stackrel{?}{=} \exp\left(\frac{i}{\hbar}S_\mathrm{SHO}[x_0(t)]\right) \times \prod_{n=1}^{\infty}\sqrt{\frac{4\pi i\hbar}{m}\frac{(t_\mathrm{f} - t_\mathrm{i})}{\pi^2 n^2 - \omega^2(t_\mathrm{f} - t_\mathrm{i})^2}}. \tag{2.57}$$

Does it work? No. But then we didn't expect it to, because of the difficulties in defining the path integral in the first place. However, as we noted in the previous section, the fudge factor required is independent of the potential, so the overall normalization can be deduced from the free particle result that must apply when $\omega = 0$. Adapting the result Eq. (2.27) to one dimension, we find

$$K_\mathrm{SHO}(x_\mathrm{f}, t_\mathrm{f}|x_\mathrm{i}, t_\mathrm{i}) = \left(\frac{m}{2i\pi\hbar(t_\mathrm{f} - t_\mathrm{i})}\right)^{1/2}\exp\left(\frac{i}{\hbar}S_\mathrm{SHO}[x_0(t)]\right) \times \prod_{n=1}^{\infty}\left(1 - \frac{\omega^2(t_\mathrm{f} - t_\mathrm{i})^2}{\pi^2 n^2}\right)^{-1/2}. \tag{2.58}$$

The infinite product was found by Leonhard Euler (1707 – 1783)

$$\prod_{n=1}^{\infty}\left(1-\frac{\omega^2(t_\mathrm{f}-t_\mathrm{i})^2}{\pi^2 n^2}\right)=\frac{\sin(\omega(t_\mathrm{f}-t_\mathrm{i}))}{\omega(t_\mathrm{f}-t_\mathrm{i})}. \tag{2.59}$$

We arrive at the final result

$$\boxed{K_{\mathrm{SHO}}(x_\mathrm{f},t_\mathrm{f}|x_\mathrm{i},t_\mathrm{i})=\left(\frac{m\omega}{2i\pi\hbar\sin(\omega(t_\mathrm{f}-t_\mathrm{i}))}\right)^{1/2}\exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}[x_0(t)]\right).} \tag{2.60}$$

To show that Eq. (2.60) satisfies the free particle Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K=-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 K, \tag{2.61}$$

for short times, $\omega(t_\mathrm{f}-t_\mathrm{i})\ll 1$, we may use the short time approximation to simplify the form of K_{SHO}. Working to first order in $\omega(t_\mathrm{f}-t_\mathrm{i})$, we may simplify the cosine and sine terms to give

$$K_{\mathrm{SHO}}(x_\mathrm{f},t_\mathrm{f}|x_\mathrm{i},t_\mathrm{i})=\left(\frac{m\omega}{2i\pi\hbar\omega(t_\mathrm{f}-t_\mathrm{i})}\right)^{1/2}\exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}[x_0(t)]\right), \tag{2.62}$$

where we expand the action detailed in equation (2.53) to first order in $\omega(t_\mathrm{f}-t_\mathrm{i})$,

$$\begin{aligned}S_{\mathrm{SHO}}[x_0(t)]&=\frac{m\omega}{2\sin(\omega(t_\mathrm{f}-t_\mathrm{i}))}\left[\left(x_\mathrm{i}^2+x_\mathrm{f}^2\right)\cos(\omega(t_\mathrm{f}-t_\mathrm{i}))-2x_\mathrm{i}x_\mathrm{f}\right]\\&=\frac{m\omega(x_\mathrm{i}-x_\mathrm{f})^2}{2\omega(t_\mathrm{f}-t_\mathrm{i})}.\end{aligned} \tag{2.63}$$

If we apply this reduced form of K_{SHO} to the free-particle Schrödinger equation (2.61), where the $\nabla_{\mathbf{r}}^2$ is interpreted to act on x_f, we can see that (2.61) is satisfied.

2.4.1 What Can You Actually Do With a Path Integral?

- Gaussian integrals (like the simple harmonic oscillator);
- Err...
- That's it.

Bear in mind, however, that the number of problems that can be solved exactly by the other formulations of quantum mechanics is also rather limited. Apart from the harmonic oscillator, the other Hamiltonian you all know how to solve exactly is the Hydrogen atom. Can it be done with a path integral? The answer is yes[10]. Furthermore, the special features of the Hydrogen atom that make it amenable to exact solution – we'll discuss them in Chapter 6 – are precisely the same features that make it possible to calculate the path integral.

[10] This illustrates the principle of *conservation of troubles*, according to which a problem is no easier or harder in a different language; the difficulties are just moved around (and sometimes out of sight!).

The value of the path integral is firstly to provide a new language for quantum theory, one that has given rise to many new insights. New effects can arise when the *topology* of paths is important, e.g. the Aharonov–Bohm effect.

A new formulation can also suggest new approximate methods to solve problems that have no exact solution. The most obvious approach is to expand the integrand in the path integral in powers of the potential $V(\mathbf{r})$. This turns out to be equivalent to time-dependent perturbation theory, as you can easily check.

A more useful line of attack is to try to evaluate the path integral *numerically*, using the same discretisation of time that we used to derive it. For Eq. (2.41) this is in fact a terrible idea, as the integrand is complex, and oscillates wildly, leading to very poor convergence. However, as we'll see in Chapter 5, it is possible to formulate the partition function of quantum statistical mechanics as a path integral in imaginary time. We've already seen the form of the propagator in imaginary time, when we discussed the heat equation (2.14). Notice that it is real and positive, so we can think of it as a probability distribution. Evaluating the partition function by sampling the probability distribution of paths is the basis of the *path integral Monte Carlo* method.

2.5 Semiclassics and the Method of Stationary Phase

The other great insight provided by the path integral concerns the emergence of classical mechanics from quantum mechanics. The appearance of the Lagrangian and action in the integrand should already have us asking what role the condition of stationary action plays in quantum theory. A clue is provided by a method of approximating ordinary integrals that goes by the names **steepest descent**, **stationary phase**, **saddle point**, or occasionally **Laplace's method**.

In order to illustrate an application of the method of stationary phase, we depart from the consideration of the propagator – evaluated by the path integral – and discuss the semiclassical method for solving for energy eigenstates of the Schrödinger equation.

2.5.1 JWKB Method

The JWKB (Jeffreys, Wentzel, Kramers, Brillouin) method is a semiclassical technique for obtaining approximate solutions to the one-dimensional Schrödinger equation. It is mainly used in calculating bound-state energies and tunnelling rates through potential barriers, and is valid in the semiclassical limit $\lambda = \frac{h}{p} = \frac{h}{mv}$ or $\hbar \to 0$ or $m \to \infty$ where m is the mass of the particle, p its momentum, etc.

The key idea is as follows. Imagine a particle of energy E moving through a region where the potential $V(x)$ is *constant*. If $E > V$, the wave function is of the form

$$\psi(x) = Ae^{\pm ikx} \tag{2.64}$$

$$k = \frac{\sqrt{2m(E-V)}}{\hbar}. \tag{2.65}$$

The plus sign indicates particles travelling to the right etc. The wave function is oscillatory, with constant wavelength $\lambda = 2\pi/k$, and has constant amplitude, A. Consider now the case where $V(x)$ is not a constant but varies rather slowly in comparison to λ (so that in a region containing many wavelengths the potentially is essentially constant). Then it is reasonable to suppose that ψ remains practically sinusoidal except that the wavelength and the amplitude change slowly with x. This is the central theme of the JWKB method: rapid oscillations are modulated by gradual variation in amplitude and wavelength.

Similarly, if $E < V$ (with V a constant), then ψ is exponential

$$\psi(x) = Ae^{\pm Kx} \tag{2.66}$$

$$K = \frac{\sqrt{2m(V-E)}}{\hbar}. \tag{2.67}$$

Now, if $V(x)$ is not constant but again varies slowly in comparison to $1/K$, the solution remains practically exponential except that A and K are now slowly varying functions of x.

There are of course places where this idea breaks down, e.g. in the vicinity of a classical turning point where $E \approx V$. Here, λ (or $1/K$) goes to infinity and $V(x)$ can hardly be said to vary "slowly"! Proper handling of this is the most difficult aspect of the JWKB approximation but the final results are simple and easy to implement.

2.5.2 Derivation

We seek to solve

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2(x)\psi(x) = 0 \tag{2.68}$$

$$k^2(x) = \frac{2m}{\hbar^2}(E - V(x)) \tag{2.69}$$

The semiclassical limit corresponds to k large. If k were constant, then of course the solutions would just be $e^{\pm ikx}$. This suggests that we try $\psi(x) = e^{iS(x)}$, where in general $S(x)$ is a complex function. Then,

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = iS'e^{iS} \tag{2.70}$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = (iS'' - S'^2)e^{iS}, \tag{2.71}$$

and the Schrödinger equation reduces to $(iS'' - S'^2 + k^2)e^{iS} = 0$, or

$$\begin{aligned} S' &= \pm\sqrt{k^2(x) + iS''(x)} \\ &= \pm k(x)\sqrt{1 + iS''(x)/k^2} \end{aligned} \tag{2.72}$$

(Note that if k were a constant, $S'' = 0$ and $S' = \pm k$.)

We now attempt to solve the above equation by iteration, using $S' = \pm k$ as the first guess, and as a second guess we use

$$\begin{aligned} S' &= \pm k\sqrt{1 \pm ik'(x)/k^2} \\ &\approx k\left(1 \pm \frac{i}{2}\frac{k'(x)}{k^2}\right) \\ &\approx \pm k + \frac{i}{2}\frac{k'(x)}{k} \end{aligned} \tag{2.73}$$

where we have assumed that the corrections are small. Then, we have

$$\begin{aligned} \frac{\mathrm{d}S}{\mathrm{d}x} &= \pm k + \frac{i}{2}\frac{k'}{k} \\ S(x) &\sim \pm \int^x k(x')\,\mathrm{d}x' + \frac{i}{2}\int^x \frac{k'(x')}{k(x')}\,\mathrm{d}x' + c \end{aligned} \tag{2.74}$$

The second integral is a perfect differential ($d \ln k$), so

$$\begin{aligned} S(x) &= \pm \int^x k(x')\,\mathrm{d}x' + \frac{i}{2}\ln k + c \\ \psi &= e^{iS} \\ &= Ce^{\pm i\int^x k(x')\mathrm{d}x'}e^{-\frac{1}{2}\ln k} \\ &= \frac{C}{\sqrt{k(x)}}e^{\pm i\int^x k(x')\mathrm{d}x'} \end{aligned} \tag{2.75}$$

Note that in making the expansion, we have assumed that $\frac{k'}{k^2} \ll 1$ or $\frac{\lambda}{2\pi}\frac{\mathrm{d}k}{\mathrm{d}x} \ll k$, i.e. that the change in k in one wavelength is much smaller than k. Alternatively, one has $\lambda\frac{\mathrm{d}V}{\mathrm{d}x} \ll \frac{\hbar^2k^2}{m}$ so that the change in V in one wavelength is much smaller than the local kinetic energy.

Note that in the classically forbidden regions, $k^2 < 0$, one puts $k = iK(x)$ and carries through the above derivation to get

$$\psi(x) = \frac{C}{\sqrt{K(x)}}e^{\pm i\int^x K(x')\mathrm{d}x'} \tag{2.76}$$

$$K^2 = \frac{2m}{\hbar^2}(V - E) > 0. \tag{2.77}$$

2.5.3 Connection Formulae

In our discussion above, it was emphasised that the JWKB method works when the short wavelength approximation holds. This of course breaks down when we hit the classical turning points where $k^2(x) = 0$ (which happens when $E = V$). To overcome this problem, we will derive below equations relating the forms of the solution to both sides of the turning point.

If the potential can be approximated by an increasing linear potential near the turning point $x = a$ (the region $x > a$ being classically forbidden), we can write in the vicinity of the turning point

$$k^2(x) = \frac{2m}{\hbar^2}\left(-\frac{\mathrm{d}V}{\mathrm{d}x}\right)_{x=a}(x - a). \tag{2.78}$$

The Schrödinger equation near the turning point becomes

$$\psi'' - \left.\frac{\mathrm{d}V}{\mathrm{d}x}\right|_{x=a} \frac{2m}{\hbar^2}(x-a)\psi = 0. \tag{2.79}$$

If we let

$$z = \alpha(x-a) \tag{2.80}$$

$$\alpha^3 = \frac{2m}{\hbar^2}\frac{\mathrm{d}V}{\mathrm{d}x} \geq 0, \tag{2.81}$$

then the above differential equation becomes equivalent to **Airy's equation**

$$f''(z) - zf(z) = 0. \tag{2.82}$$

The solution of this equation is a non-elementary function called the *Airy function* (in fact, there are two linearly independent solutions, as this is a second order equation), and we are particularly interested in its behaviour at large $|z|$. As is often the case with special functions, there is an integral representation of the Airy function, and we can use this to find the large $|z|$ behaviour in a controlled way.

The first thing to note is that the Fourier transform of the equation

$$i'(k) + k^2\tilde{f}(k) = 0 \tag{2.83}$$

is *first* order, and may be solved easily

$$\tilde{f}(k) = A\exp\Big(ik^3/3\Big), \tag{2.84}$$

with A some constant. Thus all we have to do to find the solution $f(z)$ is compute the Fourier integral[11]

$$f(z) = \frac{1}{2\pi}\int e^{ikz}\tilde{f}(k)\,\mathrm{d}k = \frac{A}{2\pi}\exp\Big(ik^3/3 + ikz\Big)\,\mathrm{d}k\,. \tag{2.85}$$

But wait! A linear second order equation has two independent solutions, and it looks like we have only found one. However, we didn't yet specify the contour of integration in Eq. (2.85), and our freedom to choose this allows us to generate more than one solution.

To show that $f(z)$ defined by Eq. (2.85) satisfies Airy's equation , we have

$$\begin{aligned} f''(x) - xf(x) &= A\int\Big(-k^2 - x\Big)\exp\Big(ik^3/3 + ikx\Big)\,\mathrm{d}k \\ &= iA\int\frac{\mathrm{d}}{\mathrm{d}k}\exp\Big(ik^3/3 + ikx\Big)\,\mathrm{d}k \\ &= 0, \end{aligned} \tag{2.86}$$

as long as the integrand vanishes at the endpoints.

[11] Using the convention $f(z) = \int_{-\infty}^{\infty} e^{ikz}\tilde{f}(k)\frac{\mathrm{d}k}{2\pi}$. Overall numerical factors aren't important here: it's a linear equation.

Where does the integrand vanish? We have to go to large $|k|$ in such a way that the dominant term $ik^3/3$ term in the exponent has a negative real part. Writing $k = |k|e^{i\theta}$, we can see that this happens as $|k| \to \infty$ in the three wedges

$$\begin{aligned} \text{I}: \quad & 0 < \theta < \pi/3 && (2.87)\\ \text{II}: \quad & 2\pi/3 < \theta < \pi && (2.88)\\ \text{III}: \quad & 4\pi/3 < \theta < 5\pi/3. && (2.89)\\ & && (2.90) \end{aligned}$$

Different choices for the starting and ending wedge give different solutions[12].

Fig. 2.3: A possible contour in the plane of complex k, passing through one of the stationary points of the integrand.

Now comes the key idea. Because the integrand is an exponential, it quickly becomes negligible as we move off into a wedge. The largest contribution should come from the largest value of the real part of the exponent. The stationary points[13] satisfy $k^2 + z = 0$ and lie at

2.6 The Classical Limit

[12] Use Cauchy's theorem to convince yourself that only two are independent.

[13] Why do we look at a stationary point if we only want to maximise the real part of the exponent? Think about the Cauchy-Riemann equations.

Chapter 3

Scattering Theory

Chapter 4

Identical Particles in Quantum Mechanics

Chapter 5

Density Matrices

Chapter 6

Lie Groups [*non-examinable*]

Chapter 7

Relativistic Quantum Physics [*non-examinable*]

Appendix **A**

Appendix: Operator Algebra

A.1 General Operator Algebra

Some properties of the **commutator** $[A, B] = AB - BA$ of operators[1] A and B

$$[A, BC] = [A, B]C + B[A, C] \tag{A.1}$$

[1] In AQP operators wore hats: we'll omit them unless there is a danger of ambiguity