Exactly solvable systems

To get back into the habit of thinking about quantum system, to rekindle knowledge of the language and basic methods used, to introduce some new and key ideas that will be picked up on further down the line, and to recognze some deep truths, we start with a couple of systems that yield to analytic analysis.

1 Quantum linear harmonic oscillator

The simple harmonic oscillator is a familiar problem. How does the joke go?

> It is often said that the simple harmonic oscillator is the only problem that physicists understand. This is untrue... but a good approximation.

Here we take another look at the quantum harmonic oscillator, armed with a greater familiarity with quantum mechanics than when we first looked at it. We do so because it allows us to refamiliarise ourselves with important concepts and to practice key methods of quantum mechanics, but also because it has many applications, such as vibrations in molecules and solids, nuclear structure [1], the electromagnetic field, etc, etc. If we think of classical particles moving in a potential, and the potential has a minimum corresponding to stable equilibrium, then for small displacements away from the stable equilibrium we can use a truncated Taylor expansion

$$V(x) \simeq V(x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2$$

which is the potential of an oscillator. The corresponding force $F = -dV/dx$ is proportional to $x - x_0$ – hence the simple harmonic oscillator is often refered to as the linear harmonic oscillator by theoretical physicists. It provides a description of a variety of systems close to stable equilibrium. The same applies for quantum mechanical systems, such as the nuclear motion in a molecule responsible for the vibrational spectrum of molecular excitations. The motion is treated as that of an ideal oscillator where the potential is quadratic for all separations. Of course corrections become significant for larger distances when the truncated Taylor expansion of the exact potential is no longer accurate – for these one can apply perturbation theory, as previously studied, making use of the results of the following analysis.

The quantum linear harmonic oscillator problem, then, corresponds to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{\mathcal{H}}\psi(x,t) \tag{1.1}$$

with the Hamiltonian

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \tag{1.2}$$

The first term represents the kinetic energy and the second the potential energy $V(x) = \frac{1}{2}kx^2$ written in terms of a frequency ω which is that of a classical oscillator, mass m, experiencing a restoring force $-kx$. For that, $\omega^2 = k/m$. We take the minimum of the potential to be at $x_0 = 0$.

We will primarily focus on the stationary states of the quantum linear harmonic oscillator. These are the solutions of (1.1) of the form $\psi(x,t) = \exp(-i\varepsilon t/\hbar)\varphi_\varepsilon(x)$ where

$$\hat{\mathcal{H}}\varphi_\varepsilon(x) = \varepsilon\varphi_\varepsilon(x). \tag{1.3}$$

This is the time-independent Schrödinger equation for the quantum oscillator. We could use $\hat{\mathcal{H}}$ in the form of (1.2) and set about solving the Schrödinger equation as a differential equation. You can find this treatment in various quantum texts.[2] Alternatively, there is an elegant algebraic approach due to Dirac that we will adopt here.

[1] https://arxiv.org/pdf/2005.03134; not an application I know anything about, and the oscillator is relativistic — see later in this course for the necessary background.

[2] e.g. Schiff, p67; Shankar, p190; Griffiths, p48. It is a nice example of the application of methods you should be capable of. It is outside the scope of this course, but do give it a look.

1.1 Ladder operators and the eigenvalue spectrum

Recall the momentum operator which in the position representation is $\hat{p} = -i\hbar\frac{d}{dx}$. Using this, the Hamiltonian of the linear harmonic oscillator can equivalently be written as

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2. \tag{1.4}$$

Recall also the canonical commutation property of $\hat{p}$ and $\hat{x}$:[3]

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \tag{1.5}$$

Looking at (1.4) and motivated by the identity

$$(u - iv)(u + iv) = u^2 - i(vu - uv) + v^2 = u^2 + v^2 \tag{1.6}$$

satisfied by scalar numbers, we look to factorise the Hamiltonian. To this end, we define two new operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{1}{\sqrt{2m\hbar\omega}}\hat{p}, \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{1}{\sqrt{2m\hbar\omega}}\hat{p} \tag{1.7}$$

Now, $\hat{x}$ and $\hat{p}$ are Hermitian operators (they do, after all, correspond to physical observables) — evidently $\hat{a}$ and $\hat{a}^\dagger$ are not[4]. Instead $(\hat{a})^\dagger = \hat{a}^\dagger$ and $(\hat{a}^\dagger)^\dagger = \hat{a}$ as the notation implies. Because they are operators and not scalars we cannot assume $[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$ will be zero needed for (1.6) to hold for $\hat{a}$ and $\hat{a}^\dagger$, and indeed using the commutation properties of $\hat{x}$ and $\hat{p}$ one finds

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 \tag{1.8}$$

as well as

$$\hat{a}^\dagger\hat{a} = \frac{1}{\hbar\omega}\hat{\mathcal{H}} - \frac{1}{2}, \qquad \hat{a}\hat{a}^\dagger = \frac{1}{\hbar\omega}\hat{\mathcal{H}} + \frac{1}{2} \tag{1.9a}$$

or

$$\hat{\mathcal{H}} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \qquad \hat{\mathcal{H}} = \hbar\omega\left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right). \tag{1.9b}$$

These are expressions for the Hamiltonian of the quantum linear oscillator in terms of the new operators $\hat{a}$ and $\hat{a}^\dagger$. They are close as we can get to factorising the Hamiltonian.

The operators $\hat{a}$ and $\hat{a}^\dagger$ are known as `ladder operators`. To see why, suppose we have a stationary state of the linear oscillator with energy ε. In the position representation it satisfies the time-independent Schrödinger equation

$$\hat{\mathcal{H}}\varphi_\varepsilon(x) = \varepsilon\varphi_\varepsilon(x). \tag{1.10a}$$

Let us denote the corresponding ket $|\varepsilon\rangle$: $\langle x|\varepsilon\rangle = \varphi_\varepsilon(x)$ i.e.

$$\hat{\mathcal{H}}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle. \tag{1.10b}$$

The operators $\hat{a}$ and $\hat{a}^\dagger$ acting upon the ket $|\varepsilon\rangle$ will produce new kets, $\hat{a}|\varepsilon\rangle$ and $\hat{a}^\dagger|\varepsilon\rangle$ respectively. What can we deduce about them? Let us consider the effect of acting on each of these kets using the Hamiltonian. Firstly

$$\begin{aligned}
\hat{\mathcal{H}}\left(\hat{a}^\dagger|\varepsilon\rangle\right) &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hat{a}^\dagger|\varepsilon\rangle \qquad \text{using (1.9b)} \\
&= \hat{a}^\dagger\left[\hbar\omega\left(\hat{a}\hat{a}^\dagger + \frac{1}{2}\right)\right]|\varepsilon\rangle \qquad \text{pulling } \hat{a}^\dagger \text{ through} \\
&= \hat{a}^\dagger\left(\hat{\mathcal{H}} + \hbar\omega\right)|\varepsilon\rangle \qquad \text{using the second of (1.9b)} \\
&= (\varepsilon + \hbar\omega)\,\hat{a}^\dagger|\varepsilon\rangle \qquad \text{using (1.10b),}
\end{aligned} \tag{1.11a}$$

[3] Remember operators act on kets, so to identify $\hat{x}\hat{p} - \hat{p}\hat{x}$ we can for example use the position representation and let it act upon some wave function $\langle x|\psi\rangle = \psi(x)$:

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\,\psi(x) = x\left(-i\hbar\frac{d}{dx}\psi(x)\right) + i\hbar\frac{d}{dx}\left(x\psi(x)\right) = -i\hbar x\frac{d\psi(x)}{dx} + i\hbar\left(\psi(x) + x\frac{d\psi(x)}{dx}\right) = i\hbar\psi(x).$$

[4] But they are real differential operators:

$$\hat{a}\psi(x) = \left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\psi(x), \qquad \hat{a}^\dagger\psi(x) = \left(\sqrt{\frac{m\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\psi(x).$$

and similarly

$$\begin{aligned}
\hat{\mathcal{H}}\left(\hat{a}|\varepsilon\rangle\right) &= \hbar\omega\left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right)\hat{a}|\varepsilon\rangle \qquad \text{using (1.9b)} \\
&= \hat{a}\left[\hbar\omega\left(\hat{a}^\dagger\hat{a} - \frac{1}{2}\right)\right]|\varepsilon\rangle \qquad \text{pulling } \hat{a} \text{ through} \\
&= \hat{a}\left(\hat{\mathcal{H}} - \hbar\omega\right)|\varepsilon\rangle \qquad \text{using the first of (1.9b)} \\
&= \left(\varepsilon - \hbar\omega\right)\hat{a}|\varepsilon\rangle \qquad \text{using (1.10b).}
\end{aligned} \tag{1.11b}$$

From (1.11a) we recognise $\hat{a}^\dagger|\varepsilon\rangle$ is a stationary state of the linear oscillator with energy $\varepsilon + \hbar\omega$, and from (1.11b) that $\hat{a}|\varepsilon\rangle$ is a stationary state with energy $\varepsilon - \hbar\omega$. It follows that applying repeatedly

$$\hat{\mathcal{H}}(\hat{a}^\dagger)^m|\varepsilon\rangle = (\varepsilon + m\hbar\omega)(\hat{a}^\dagger)^m|\varepsilon\rangle, \qquad \hat{\mathcal{H}}(\hat{a})^m|\varepsilon\rangle = (\varepsilon - m\hbar\omega)(\hat{a})^m|\varepsilon\rangle, \tag{1.12}$$

and we see that in this way $\hat{a}^\dagger$ and $\hat{a}$ repeatedly acting upon a state ket generate a heirarchy of stationary states, stepping up or down the energy spectrum in steps $\hbar\omega$. Hence the name ladder operators.

Since we know kinetic energy is never negative, and the potential of our linear oscillator has a minimum value of zero, we expect the spectrum to have a lower bound, which is not evident from (1.12). Let us therefore assume the existence of a state of minimum energy, using $|\varepsilon_0\rangle$ denote the corresponding ket and ε_0 the value of this minimum energy, also known as the ground state energy. We recognise that this must satisfy

$$\hat{a}|\varepsilon_0\rangle = 0 \tag{1.13}$$

otherwise (1.11b) shows $\hat{a}|\varepsilon_0\rangle$ is an eigenstate with energy $\varepsilon_0 - \hbar\omega$, which is lower than the ground state energy ε_0, which would be a contradiction. So $\hat{a}|\varepsilon_0\rangle = 0$ must indeed hold. Using this

$$\begin{aligned}
\hat{\mathcal{H}}|\varepsilon_0\rangle &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|\varepsilon_0\rangle \qquad \text{using (1.9b)} \\
&= \frac{1}{2}\hbar\omega|\varepsilon_0\rangle \qquad \text{using (1.13),}
\end{aligned} \tag{1.14}$$

from which we can read off that the ground state ket $|\varepsilon_0\rangle$ is an eigenstate of the Hamiltonian $\hat{\mathcal{H}}$ with ground state energy $\varepsilon_0 = \hbar\omega/2$. Notably, this is not zero, which would be the case for a classical oscillator. The non-zero least amount of energy of the quantum oscillator is known as "zero-point" energy. Since $\hat{a}^\dagger$ acting upon an ket moves us up the spectrum one rung of the ladder, applying it n times to the ground state gives the $n'th$ excited state. Therefore, from (1.12) we can write for the energy eigenstates of the harmonic oscillator

$$|n\rangle \propto (\hat{a}^\dagger)^n|0\rangle, \qquad \text{where} \qquad \hat{\mathcal{H}}|n\rangle = \varepsilon_n|n\rangle, \qquad \text{with} \qquad \varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{1.15}$$

where we now use integer n and not energy $\varepsilon_n = (n + \frac{1}{2})\hbar\omega$ to label the states. Notice we have established this using operators alone. We have not adopted a specific representation.

1.2 Creation and annhiliation

The operators $\hat{a}$ and $\hat{a}^\dagger$ are also known as `annihilation` and `creation` operators respectively. This originates from their effect being to create and annihiliate a quantum of energy $\hbar\omega$. The monikers raising and lowering are also used.

We have seen that, apart from a zero-point energy $\frac{1}{2}\hbar\omega$, a characteristic state of the quantum oscillator has an integer number of such energy quanta.[5] The number operator

$$\hat{\mathcal{N}} = \hat{a}^\dagger\hat{a} \tag{1.16}$$

counts how many: $\hat{\mathcal{N}}|n\rangle = n|n\rangle$. The Hamiltonian expressed in terms of the number operator is $\hat{\mathcal{H}} = \hbar\omega(\hat{\mathcal{N}} + 1/2)$. Instead of thinking of the oscillator moving up and down the ladder of energy states, we can instead picture the

[5] singular quantum; plural quanta

oscillator as an object comprising an increasing or decreasing number of quanta. Interaction with the oscillator corresponds to excitation/deexcitation and a transfer in and out of an integer number of the elementary unit of energy. We could attach a physical significance to these energy quanta. The modern theory of particles envisages particles as excitations, quanta, of an underlying quantum field. In the context of the lattice vibrations in solids, they are phonons; spin excitations in a solids are magnons; for the electomagnetic field they are photons. The zero-point energy then represents e.g. the energy in the electromagnetic field when no photons are present.

1.3 Normalised eigenstates

Let us return to the state kets. These must be normalised if they are to be used to calculate expectation values in order to predict the results of measurements performed on the quantum oscillator. A normalised ket $|\psi\rangle$ satisfies $\langle\psi|\psi\rangle = 1$ where $\langle\psi| = (|\psi\rangle)^\dagger$.

That $|n\rangle$ is proportional to $(\hat{a}^\dagger)^n|0\rangle$ (we just showed that! see (1.15)) implies $\hat{a}^\dagger|n\rangle = c_n|n+1\rangle$ where c_n is a constant that ensures that $|n\rangle$ is normalised if $|n+1\rangle$ is. We see then that

$$\begin{aligned}\langle n|\hat{a}\hat{a}^\dagger|n\rangle &= \left(\langle n|\hat{a}\right)\left(\hat{a}^\dagger|n\rangle\right)\\ &= \left(\hat{a}^\dagger|n\rangle\right)^\dagger\left(\hat{a}^\dagger|n\rangle\right)\\ &= \left(c_n|n+1\rangle\right)^\dagger\left(c_n|n+1\rangle\right)\\ &= \left(c_n^*\langle n+1|\right)\left(c_n|n+1\rangle\right) = |c_n|^2 \end{aligned} \tag{1.17}$$

since $|n+1\rangle$ is normalised. But

$$\begin{aligned}\hat{a}\hat{a}^\dagger|n\rangle &= \left(\frac{1}{\hbar\omega}\hat{\mathcal{H}} + \frac{1}{2}\right)|n\rangle \qquad \text{using (1.9a)}\\ &= \left(\frac{1}{\hbar\omega}\left(n+\frac{1}{2}\right)\hbar\omega + \frac{1}{2}\right)|n\rangle \qquad \text{using (1.15)}\\ &= (n+1)\,|n\rangle. \end{aligned} \tag{1.18}$$

So $\langle n|\hat{a}\hat{a}^\dagger|n\rangle = n+1 = |c_n|^2$. Choosing c_n real and positive,

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{1.19}$$

Rearranging this equation with $n \to n-1$:

$$\begin{aligned}|n\rangle &= \frac{1}{\sqrt{n}}\hat{a}^\dagger|n-1\rangle\\ &= \frac{1}{\sqrt{n(n-1)}}\left(\hat{a}^\dagger\right)^2|n-2\rangle \qquad \text{inserting corresponding expression for } |n-1\rangle\\ &= \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n|0\rangle \qquad \text{repeating a further } n-2 \text{ times.}\end{aligned} \tag{1.20}$$

This is an expression for correctly-normalised ket $|n\rangle$ in terms of the normalised ground state ket $|0\rangle$.

If we want an explicit expression we have to choose the representation we want. Let us choose the position representation. Recall that acting upon the ground state ket with the annihilation operator gives zero: $\hat{a}|0\rangle = 0$. Hence in the position representation

$$a|0\rangle = 0 \qquad \Rightarrow \qquad \left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\psi_0(x)$$

(see footnote 4). Tidying

$$\begin{aligned} & \frac{d}{dx}\psi_0(x) = -\frac{m\omega x}{\hbar}\psi_0(x)\\ \Rightarrow \qquad & \frac{1}{\psi_0}\frac{d\psi_0}{dx} = \frac{d}{dx}(\ln\psi_0) = -\frac{m\omega x}{\hbar} \qquad \text{assuming } \psi_0 > 0\\ \Rightarrow \qquad & \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + A \qquad A \text{ constant}\\ \Rightarrow \qquad & \psi_0(x) = \tilde{A}e^{-\frac{m\omega}{2\hbar}x^2}, \qquad \tilde{A} = e^A, \text{ another constant.}\end{aligned} \tag{1.21}$$

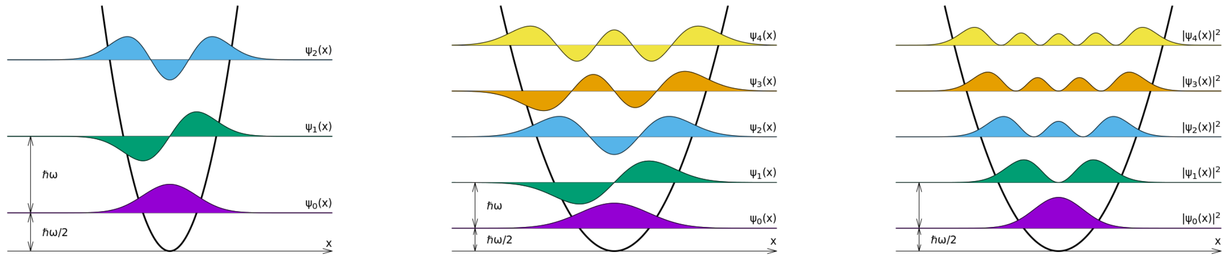

Figure 1: Left and middle: Potential $1/2kx^2$ and first few wave functions $\langle x|n\rangle = \psi_n(x)$ of the harmonic oscillator for two different values of k. Right: Probability densities $|\psi_n(x)|^2$ corresponding to the middle case.

$\tilde{A}$ normalises ψ_0:

$$1 = \int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = |\tilde{A}|^2 \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2} dx = |\tilde{A}|^2 \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} e^{-y^2} dy \quad \text{using} \quad y = \sqrt{\frac{m\omega}{\hbar}}x$$
$$= |\tilde{A}|^2 \sqrt{\frac{\pi\hbar}{m\omega}} \qquad \text{using tables.} \tag{1.22}$$

Making the natural choice (real, positive)

$$\langle x|0\rangle = \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} = \frac{1}{(\pi\lambda^2)^{1/4}} e^{-x^2/(2\lambda^2)}.$$

The ground state wave function is a Gaussian, with characteristic width $\lambda = \sqrt{\hbar/(m\omega)}$. For the other wave functions we use (1.20),

$$\langle x|n\rangle = \psi_n(x) = \frac{1}{\sqrt{n!}} \left(\sqrt{\frac{m\omega}{2\hbar}} x + \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} \right)^n \psi_0(x)$$
$$= \frac{1}{(2^{2n}(n!)^2\pi\lambda^2)^{1/4}} e^{-x^2/(2\lambda^2)} H_n(x/\lambda) \qquad \text{after a bit of work!} \tag{1.23}$$

where $H_n(x)$ is a Hermite polynomial.[6] See Fig. 1. With the exception of the ground state the wave functions oscillate within the classical turning points of the potential, changing sign n times. The wave functions extend slightly into the classically forbidden region, decaying exponentially as they do.

The probability distribution of higher lying states continues to oscillate, unlike the probability of finding a classical oscillator at x. The quantum probability is enhanced near the classical turning point, like that of the classical oscillator where it increases as the mass slows down to rest and then reverses. See Fig. 2.

Class examples

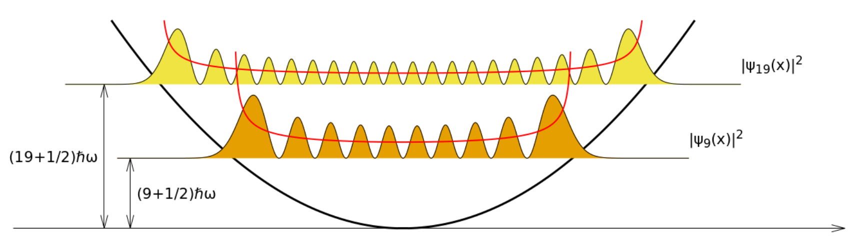

Figure 2: Probability densities of two states of the quantum linear oscillator with higher energy. The classical probability distribution is shown in red.

[6] e.g. `https://en.wikipedia.org/wiki/Hermite_polynomials`. I am not expecting you to be familiar with these functions!

2 The Aharonov-Bohm effect

When studying the dynamics of charged particles using classical Newtonian mechanics, forces enter due to electric and magnetic fields $\vec{E}$ and $\vec{B}$ respectively. The equation of motion is

$$m\frac{d^2\vec{r}}{dt^2} = q\left(\vec{E}+\vec{v}\times\vec{B}\right), \qquad \text{where} \qquad \vec{v} = \frac{d\vec{r}}{dt}. \tag{2.1}$$

Here, m is the mass and q the charge of the particle. These fields are tangible: we can measure them experimentally[7].

There are no forces or fields in the corresponding Schrödinger equation. Instead[8],

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{\mathcal{H}}\Psi \qquad \text{where} \qquad \hat{\mathcal{H}} = \frac{1}{2m}\left(\vec{p}-q\vec{A}\right)^2 + q\phi \tag{2.2}$$

where $\phi = \phi(\vec{r},t)$ and $\vec{A} = \vec{A}(\vec{r},t)$ are the electromagnetic scalar and vector potentials[9]. The fields and potentials are related:

$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial\vec{A}}{\partial t}, \qquad \vec{B} = \vec{\nabla}\times\vec{A} \tag{2.4}$$

— it then follows that

$$\begin{aligned}\vec{\nabla}\cdot\vec{B} &= \vec{\nabla}\cdot\left(\vec{\nabla}\times\vec{A}\right) = 0\\ \vec{\nabla}\times\vec{E} &= \vec{\nabla}\times\left(-\vec{\nabla}\phi - \frac{\partial\vec{A}}{\partial t}\right) = -\frac{\partial}{\partial t}\left(\vec{\nabla}\times\vec{A}\right) = -\frac{\partial\vec{B}}{\partial t},\end{aligned}$$

which we recognise as two of the Maxwell equations.

Class discussion

Note that the potentials ϕ and $\vec{A}$ overdescribe the physics. The transformation

$$\vec{A}\to\vec{A}' = \vec{A}+\vec{\nabla}\Lambda, \qquad \phi\to\phi' = \phi - \frac{\partial\Lambda}{\partial t} \tag{2.5}$$

for scalar function $\Lambda(\vec{r},t)$ leaves the measurable electric and magnetic fields unchanged. A transformation that leaves physical observables unchanged is known as a `Gauge transformation`. Gauge transformations are a major concept in modern theoretical physics.

So which is more fundamental? The measurable fields, entering the classical theory, or the potentials that over-describe the physics but which enter the quantum theory. The Aharanov-Bohm effect tells us. It was one of the "Seven wonders of the Quantum World" in a New Scientist feature[10].

2.1 Electron orbiting a magnetic flux tube

Class example

[7] How?

[8] This is often refered to as **minimal coupling**

[9] Note $\vec{p}$ is a differential operator and so does not commute with $\vec{A}$, which in general depends upon position. We have

$$\left(\vec{p}-q\vec{A}\right)^2 = \left(\vec{p}-q\vec{A}\right)\cdot\left(\vec{p}-q\vec{A}\right) = p^2 - q\left(\vec{p}\cdot\vec{A}+\vec{A}\cdot\vec{p}\right) + q^2A^2 \tag{2.3}$$

which is more obviously Hermitian.

[10] M. Brooks, *Seven wonders of the quantum world*, New Scientist May 5, 2010. Available to subscribers so you will need to access via the University Library link.

Figure 3: Left: Yakir Aharonov (1932-); Right: David Bohm (1917-1992). Government warning: Smoking kills.

2.2 Aharonov-Bohm experiment

The Aharonov-Bohm effect, named after Bristol-based physicists Yakir Aharonov and David Bohm[11] (Fig. 3) is the name given to quantum-mechanical phenomena where a charged particle is influenced by the electromagnetic potentials, φ and $\vec{A}$, despite moving exclusively through regions of space where the electric and magnetic fields $\vec{E}$ and $\vec{B}$ are zero. The previous thought-experiment illustrates the effect but the original proposal and subsequent experimental verification were based on interference effects.

If $f = f(x)$ and $g = g(x)$, then

$$\frac{d}{dx}\left(fe^{ig}\right) = \left(\frac{df}{dx}\right)e^{ig} + f\left(i\frac{dg}{dx}\right)e^{ig}. \tag{2.6}$$

Similarly, if $\psi = \psi(\vec{r})$ and $\chi = \chi(\vec{r})$,

$$\vec{\nabla}\left(\psi e^{i\chi}\right) = \left(\vec{\nabla}\psi\right)e^{i\chi} + \psi\left(i\vec{\nabla}\chi\right)e^{i\chi}. \tag{2.7}$$

Rearranging,

$$\left(\vec{\nabla} - i\left(\vec{\nabla}\chi\right)\right)\left(\psi e^{i\chi}\right) = \left(\vec{\nabla}\psi\right)e^{i\chi}. \tag{2.8}$$

So

$$\left(\vec{\nabla} - i\left(\vec{\nabla}\chi\right)\right)\cdot\left(\vec{\nabla} - i\left(\vec{\nabla}\chi\right)\right)\left(\psi e^{i\chi}\right) = \left(\vec{\nabla} - i\left(\vec{\nabla}\chi\right)\right)\cdot\left(\left(\vec{\nabla}\psi\right)e^{i\chi}\right) = \left(\vec{\nabla}\left(\vec{\nabla}\psi\right)\right)e^{i\chi}. \tag{2.9}$$

Swapping left and right, multiplying by $(-i\hbar)^2 e^{-i\chi}$ and introducing $\vec{\hat{p}} = -i\hbar\vec{\nabla}$

$$\vec{\hat{p}}^2\psi = e^{-i\chi}\left(\vec{\hat{p}} - \hbar\vec{\nabla}\chi\right)^2\left(\psi e^{i\chi}\right). \tag{2.10}$$

It follows then that if wave function ψ satisfies

$$i\hbar\frac{\partial\psi}{\partial t} = \left(\frac{1}{2m}\vec{\hat{p}}^2 + q\varphi\right)\psi \tag{2.11}$$

then

$$i\hbar\frac{\partial(\psi e^{i\chi})}{\partial t} = \left(\frac{1}{2m}\left(\vec{\hat{p}} - \hbar\vec{\nabla}\chi\right)^2 + q\varphi\right)\left(\psi e^{i\chi}\right). \tag{2.12}$$

Choosing

$$\chi(\vec{r}) = \frac{q}{\hbar}\int_{\vec{r}_0}^{\vec{r}}\vec{A}(\vec{r}\,')\cdot d\vec{r}\,' \tag{2.13}$$

where $\vec{r}_0$ is some fixed origin means $\vec{\nabla}\chi = (q/\hbar)\vec{A}$ and we finally see that the solutions of the Schrödinger equation (2.2) with vector potential $\vec{A}$ is $\Psi = \psi_0 e^{i\chi}$ where ψ_0 is the solution in the absence of the vector potential.

In an experiment, Fig. 4, an electron beam is split and passes to either side ($+$ and $-$) of a solenoid before coming together where the two parts (ψ_+ and ψ_-) combine and create an interference pattern. If the $\vec{B}$-field within the

[11] Phys. Rev. **115**, 485 (1959); the effect had actually been predicted by Werner Ehrenberg and Raymond Siday a decade earlier: Proc. Phys. Soc. B**62**, 8 (1949).

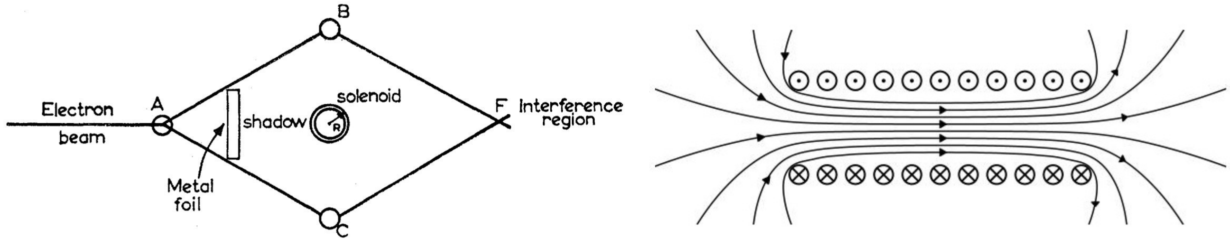

Figure 4: Left: Schematic experiment to demonstrate interference with time-independent vector potential. An electron beam is split and passes around a solenoid taking either path $C_+ \equiv ABF$ or path $C_- \equiv ACF$. [From Aharonov & Bohm, Phys. Rev. **115**, 485 (1959).] Right: Magnetic field lines of an 11-turn solenoid. As the length of the solenoid increases, the strength of the field outside decreases.

solenoid is zero then the vector potential $\vec{A}$ outside is zero and $\psi_+ = \psi_- = \psi_0$. If the $\vec{B}$-field within the solenoid is not zero then the vector potential $\vec{A}$ outside does not vanish outside, and

$$\psi_\pm = \psi_0 e^{i\chi_\pm}, \qquad \chi_\pm = \frac{q}{\hbar}\int_{C_\pm} \vec{A}\cdot d\vec{r}\,'. \tag{2.14}$$

At the detector

$$\begin{aligned} |\Psi|^2 &= |\psi_+ + \psi_-|^2 \\ &= |\psi_0|^2 |e^{i\chi_+} + e^{i\chi_-}|^2 \\ &= |\psi_0|^2 |e^{i\chi_-}|^2 |e^{i(\chi_+ - \chi_-)} + 1|^2 \\ &= |\psi_0|^2 \left(2 + 2\cos(\chi_+ - \chi_-)\right) \\ &= 4|\psi_0|^2 \cos^2\left(\frac{\chi_+ - \chi_-}{2}\right) \\ &\propto \cos^2\left(\frac{q\Phi}{2\hbar}\right) \end{aligned} \tag{2.15}$$

using

$$\chi_+ - \chi_- = \int_{C_+} \vec{A}(\vec{r}\,')\cdot d\vec{r}\,' - \int_{C_-} \vec{A}(\vec{r}\,')\cdot d\vec{r}\,' = \oint \vec{A}(\vec{r}\,')\cdot d\vec{r}\,' = \Phi. \tag{2.16}$$

Varying the magnetic field inside the solenoid causes variations in the interference pattern, *even though the electrons never move through a region of space where $\vec{B}$ differs from zero*.

Note that once again it is the enclosed flux Φ that the interference pattern depends upon, so that the interference pattern is gauge invariant. $\vec{A}$ itself is not measurable.

Bra–Ket Notation Summary Table

Notation	Name	Mathematical Meaning	Physical Interpretation	Notes / Properties
$\vert\psi\rangle$	Ket	Column vector $\begin{bmatrix}\psi_1\\ \psi_2\\ \vdots\end{bmatrix}$	State vector of a quantum system	Represents a state in Hilbert space
$\langle\phi\vert$	Bra	Conjugate transpose of $\vert\phi\rangle$	Dual vector to a ket	$\langle\phi\vert = (\vert\phi\rangle)^\dagger$
$\langle\phi\vert\psi\rangle$	Inner product	Complex number	Probability amplitude	$\vert\langle\phi\vert\psi\rangle\vert^2$ = transition probability
$\Vert\psi\Vert$ or $\sqrt{\langle\psi\vert\psi\rangle}$	Vector norm	Non-negative real scalar	Length (magnitude) of state vector $\vert\psi\rangle$	States are normalized: $\Vert\psi\Vert = 1$
$\vert\psi\rangle\langle\phi\vert$	Outer product	Operator / matrix	Maps $\vert\chi\rangle \to \vert\psi\rangle\langle\phi\vert\chi\rangle$	Rank-1 linear operator
$\langle A\rangle = \langle\psi\vert\hat{A}\vert\psi\rangle$	Expectation value	Scalar	Average measurement outcome of $\hat{A}$	Real if $\hat{A}$ is Hermitian
$\langle\psi\vert\hat{A}\vert\phi\rangle$	Matrix element	Scalar (complex number)	Transition amplitude via operator $\hat{A}$	Equals $(\langle\phi\vert\hat{A}^\dagger\vert\psi\rangle)^*$ if $\hat{A}$ is not Hermitian
$\hat{A}\vert\psi\rangle$	Operator on ket	New ket	Effect of observable or transformation $\hat{A}$	Linear operator acting on state
$\langle\psi\vert\hat{A}$	Operator on bra	New bra	Conjugate of operator acting on ket	$\langle\psi\vert\hat{A} = (\hat{A}\vert\psi\rangle)^\dagger$
$\vert\psi\rangle\otimes\vert\phi\rangle$	Tensor product	Kronecker (tensor) product of vectors	Composite state of two subsystems	Used for entangled/multi-particle systems
$\vert\psi\rangle\vert\phi\rangle$ or $\vert\psi,\phi\rangle$	Tensor product	Abbreviated notation		Used when the context is clear

Additional Notes:

- Linear operators like position $\hat{x}$, momentum $\hat{p}$, and Hamiltonian $\hat{H}$ act on kets.
- In practice, physical quantum states are always unit vectors: $\|\psi\| = 1 \quad \Rightarrow \quad \langle\psi|\psi\rangle = 1$.
- In an orthonormal basis: $\langle m|n\rangle = \delta_{mn}$.
- Completeness relation: $\sum_n |n\rangle\langle n| = \mathbb{1}$, the identity operator.
- Matrix elements like $\langle\psi|\hat{A}|\phi\rangle$ are used in time evolution, perturbation theory and Fermi's golden rule.
- The tensor product combines vectors from different Hilbert spaces: $|\psi\rangle \in \mathcal{H}_A,\ |\phi\rangle \in \mathcal{H}_B \quad \Rightarrow \quad |\psi\rangle\otimes|\phi\rangle \in \mathcal{H}_A\otimes\mathcal{H}_B$.