QUANTUM MECHANICS

(cont'd)

3. Successes

Quantum Mechanics is an enormously successful theory. Although the calculations are generally very difficult, once they are performed (with appropriate assumptions) the results agree very well with reality.

Furthermore, the theory explains many phenomena of the subatomic world that cannot be explained by classical physics. These include:

- superposition
- tunneling
- spin and the Pauli exclusion principle for fermions

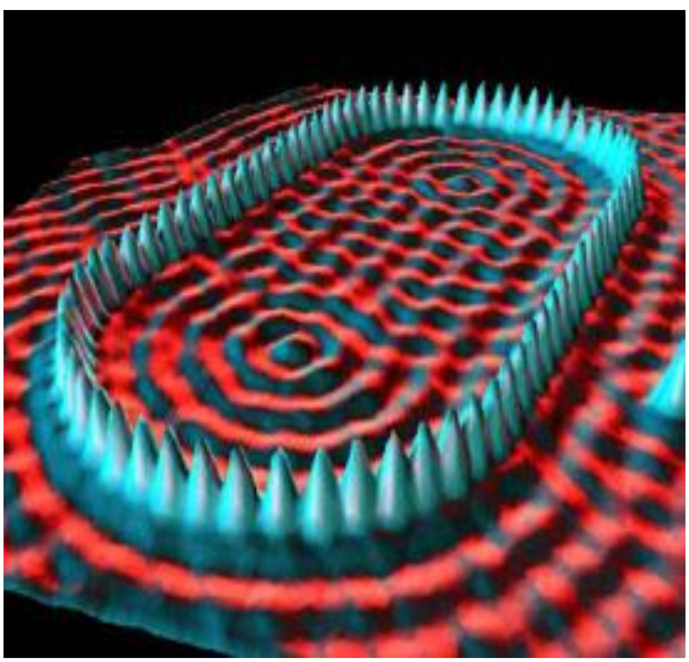
which are essential concepts for our understanding of the physical world.

3.1 Superposition

The Schrodinger equation is a *linear* differential equation.

Mathematically, this means that if ψ_1 and ψ_2 are solutions, then so is any linear combination of the two, ie. wave-functions of the form $A\,\psi_1 + B\,\psi_2$, where A and B are constants.

Physically, this implies the existence of "mixed" states in addition to the "classically acceptable" solutions.



In the above STM image, the shape of the "corral" gives two possible positions of the single atom placed inside.

The scan shows the "mixed state" where the atom has a 50% probability of being at either location.
Superposition also forms the basis of the chemical bond as it is understood today.

If two atoms, each with one electron, are brought close to one another, then a valid solution to the combined Schrodinger equation will be a *molecular orbital* which is a linear combination of the two atomic orbitals.

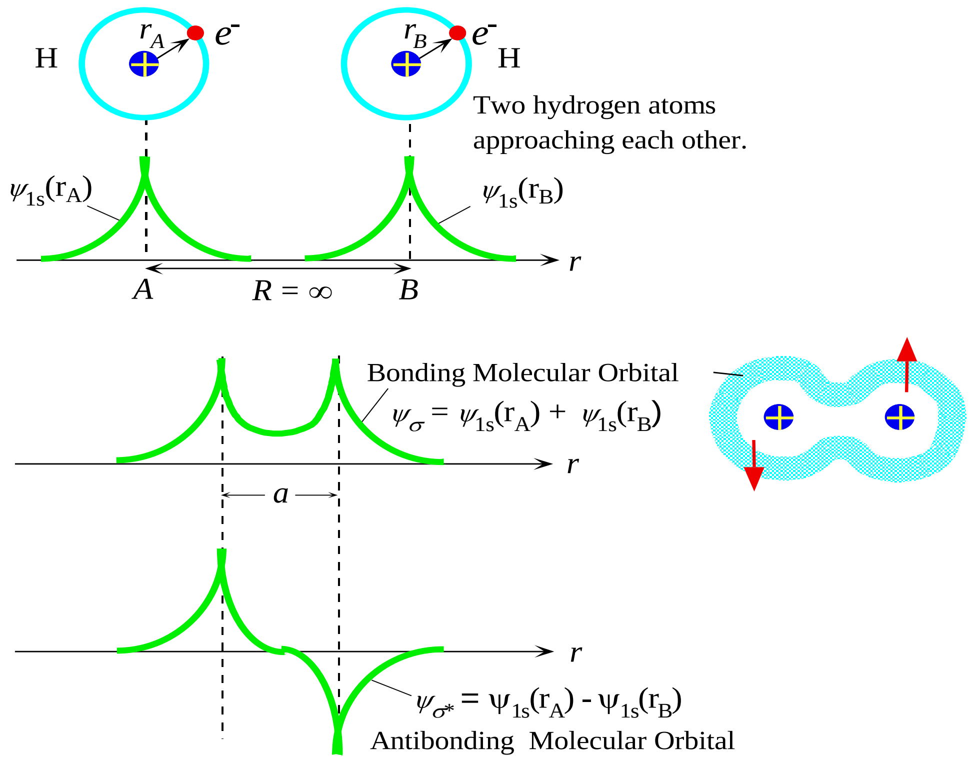


Fig. 4.1: Formation of molecular orbitals, bonding and antibonding (ψ_σ and $\psi_{\sigma*}$) when two H atoms approach each other. The two electrons pair their spins and occupy the bonding orbital ψ_σ.

Similarly, if an electron can be in either of two distinct orbitals, then it can also be in a *hybrid* orbital that is a linear combination of the two, which may have a different geometry to either of the two "pure" states.

3.2 Tunneling

When a particle travels in a region of higher potential enererergy, conservation of energy dictates that it must lose kinetic energy ($E=T+V$)

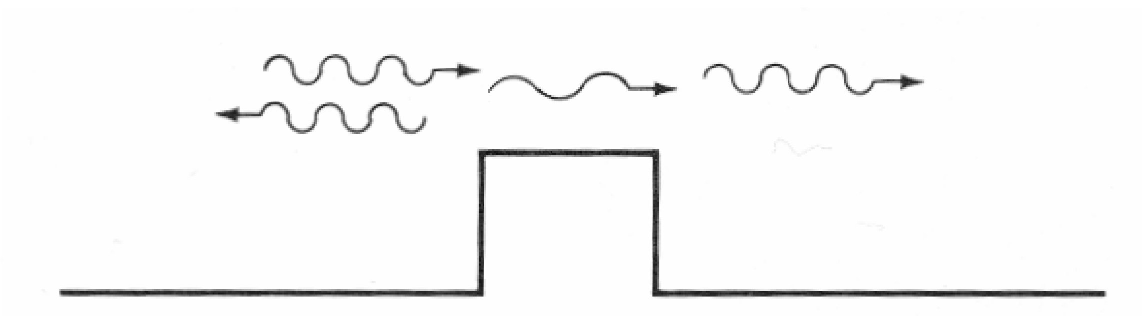
If the wave-function has a plane-wave form:

$$\Psi = A\exp i(kx-\omega t)$$

where:

$$k = \hbar(mv) = \left(\hbar\sqrt{2m}\right)\sqrt{\tfrac{1}{2}mv^2}$$

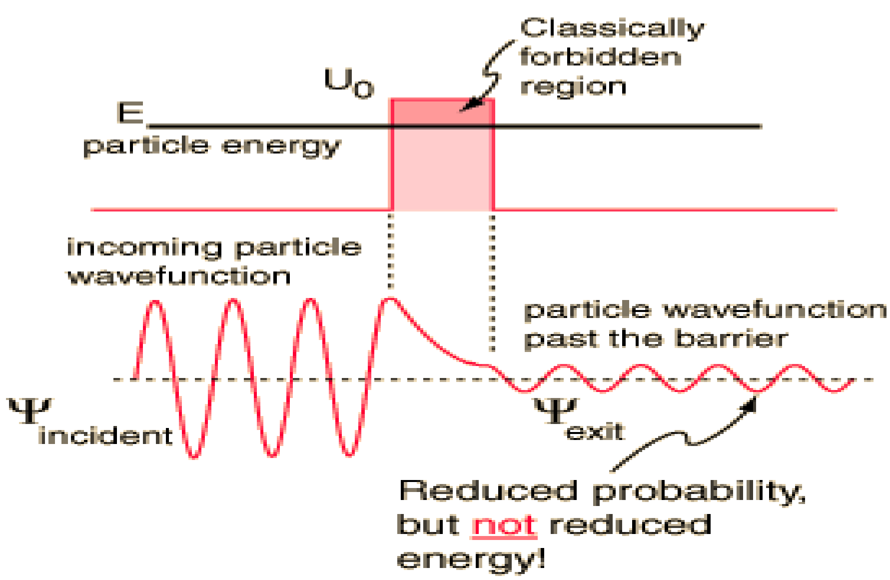
Thus, in the region of high potential, k becomes smaller and the wave-function has a longer wavelength.



What happens if $V>E$? Then, in the region of the potential, T is negative, which is classically impossible.

However, quantum-mechanically, this merely corresponds to *k* being imaginary and so the wave-function is an exponential decay rather than an oscillating function. This is called an *evanescent wave*.

Furthermore, if this decay has a non-zero value at the far end of the potential region, the solution is again oscillating. The particle has *tunneled* trough a barrier of greater energy than the particle has!



Note that having tunneled through the barrier, the particle has the *same* energy as it had before it met the barrier.

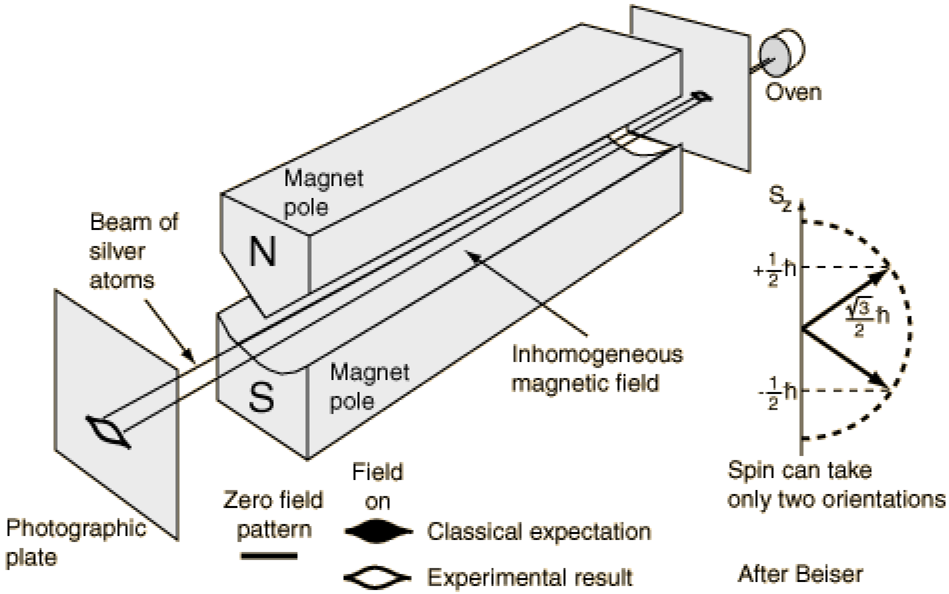
Applications of this principle include the Scanning Tunneling Microscope and several phenomena in electronic devices, Radioactive decay can also be interpreted as a particle tunneling through a potential barrier.

3.3 Spin

One of the results of applying special relativity to quantum mechanics is the appearance of two solutions distinguished by the sign of the wave-function (as a result of a square root).

Since most particle properties are dependent on the value of ψ^2 rather than Ψ, the two solutions are generally indistinguishable unless some symmetry-breaking field (such as a magnetic field) is present.

Because this gives a charged particle a magnetic moment similar to a spinning charge object, the effect is called *spin*. In the Stern-Gerlach experiment, a strong magnetic field gradient spins a randomly oriented beam of electrons into two components of opposing spin.



The most important consequence of spin is the distinguishing of particles into two groups called *bosons* and *fermions*, depending on the symmetry (*parity*) of their wavefunctions. This distinction becomes important when more than one particle is considered.

The combination of two identical particles with wave-functions Ψ_1 and Ψ_2 is given by $\Psi_1\Psi_2 \pm \Psi_2\Psi_1$, where the + sign applies to symmetric wavefunctions and the – sign to antisymmetric wavefunctions.

The combination of two identical symmetric wavefunctions merely gives another valid wavefunction (which is also symmetric). Thus there are no restrictions on the combination of symmetric (bosonic) wave-functions. At very low temperatures bosons can be made to occupy the same energy state. The Bose-Einstein condensate, predicted in 1924, was first experimentally created in 1995.

However, a combination of two identical antisymmetric wave-functions gives a zero solution and is therefore not permitted. This is the *Pauli Exclusion principle* which states that two fermions can not occupy the same quantum state.

Two antisymmetric wave functions that are identical but *of opposite sign* can however combine to give a valid (symmetric) solution. Thus, if energy levels are calculated without regard to spin (as they usually are), as many particles as there are spin states can occupy that level.

Electrons are fermions with two possible spin states. Thus two electrons can occupy each energy level.

This has important consequences in many areas of physics and chemistry, such as:

- electron population of atomic energy levels and atomic spectra

- the periodic table

- electron energies in solids

Furthermore, the combination of two sign-reversed but otherwise identical antisymmetric wave-functions is symmetric. This has important consequences in effects such as superconductivity.

4. and problems

Successful in explaining things as quantum mechanics is, there are grave problems when one uses it to try and explain “what is really happening”.

The macroscopic world is just a combination of a large number of microscopic phenomena. Why, then, don’t we see quantum effects in the “real” world?

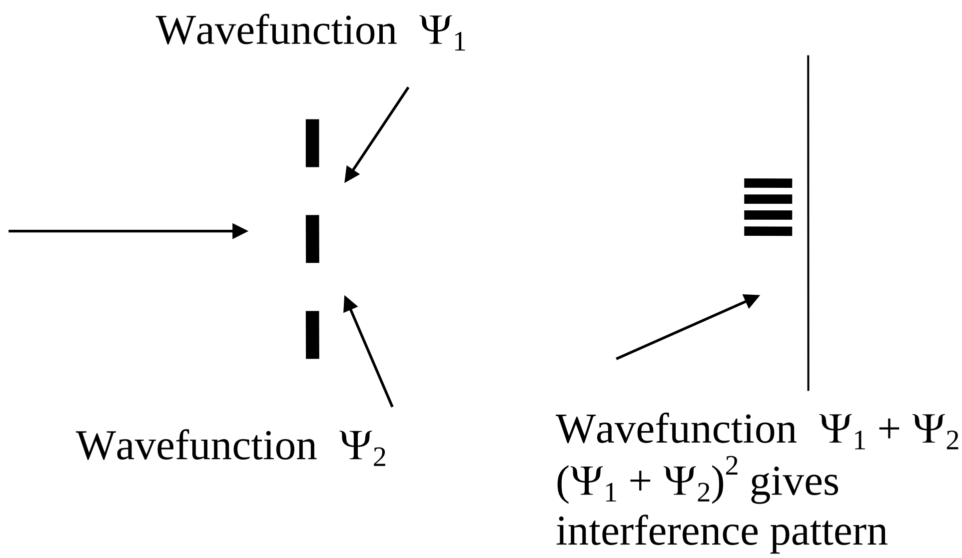
For some effects – uncertainty principle, tunneling – the numbers are just too small to be effective on “our” scale.

However, the Schrodinger equation predicts that any complex system will be in a complicated superposition of several states. But a system is always observed to be in just *one* state (though repeating the experiment gives the various states in the calculated probabilities).

Taken to extremes, this leads to paradoxes such as that Schrodinger’s cat, where if the life or death of a cat is linked to a quantum process which is represented by a superposition, then the cat is itself in a superposition of “alive” and “dead” until it is observed.

But what is an observation?

The paradox does not exist only at a macroscopic level. Consider the two-slit interference experiment.



At the screen, only whole electrons are observed at certain points (the *wavefunction* shows the interference pattern, not the electron itself).

If we insist that the electron has a physical existence between the emitter and the screen, it must obviously pass through one just one the slits. But it must be in some way “aware” of the other slit, since if the other slit was not there then there would be no interference!

Discussions such as these, based on “thought experiments”, since the experiments themselves could not be performed, raged between Bohr and Einstein in the 1920’s and 30’s. Einstein refused to accept the probabilistic nature of quantum mechanics and thought that it was incomplete – ie. an approximation to a full theory.

A popular approach to the problem was to postulate “hidden variables”, ie. the existence of variables within a system that completely determine its outcome, even if the current theory can only make statistical predictions on these outcomes. Einstein was expressing a preference for theories of this type when he made his famous comment “God does not play dice”.

To counteract this, Bohr introduced the “Copenhagen Interpretation” – that the wave-function has no physical reality, but is merely a tool for computing the results of measurements. Like this QM works excellently.

But, what is a measurement?

And, what happens between measurements?

Bohr’s answer: don’t ask the questions. You only see the world through “measurements”, whatever they are. Just do the calculations and get the results!

In 1935, Einstein and others postulated the "EPR" paradox which showed that QM is non-local (violates special relativity). According to QM, two particles can be in unknown but related states. A measurement on one particle *immediately* determines the state of the other particle, even if it is far away.

In 1964, attempting to vindicate Einstein, John Bell obtained inequalities whereby experimental results can distinguish between non-local and local theories. Bell's Theorem states that any "complete" theory of quantum mechanics must be non-local, and therefore, he thought, incorrect.

However, in 1982, Alain Aspect and actually performed experiments that could measure the variables in Bell's theorem. The results were in favour of Quantum Mechanics not Einstein. This conclusion has since been verified in many different ways and to great accuracy.

Today, Bell's Theorem and Aspect's results are interpreted as saying that "any realistic theory of quantum mechanics is non-local". Here, "realistic" means a theory that insists on the real existence of the particle at all times (hidden variables).

Thus, either the real world is non-realistic (particles do not exist until they are observed) – or it is non-local (violates special relativity).

The problem centres around the reality (or otherwise) of the wave-function.

If particles form the basis of reality, then the wave-function is just a mathematical tool as proposed by the Copenhagen Interpretation. Unfortunately, this means that on the microscopic scale, nature is non-local. There is thus a fundamental philosophical conflict between the two great theories of the 20^{th} Century.

On the other hand, if the wave-function is the basis of reality, then particles as commonly understood do not exist. Particles are observed because our measuring apparatus gives the results that we attribute to particles.

Nature is not only stranger than we imagine, but stranger than we *can* imagine. The subject is still open.