Berry's phases

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Abstract

Berry's phases, a geometric feature of quantum mechanics, were proposed by M.V. Berry in 1983. Since then they were identified in various fields and they are now understood to be a fundamental aspect of quantum systems. Basic concepts will be discussed, as well as a few examples from electrodynamics (Aharanov-Bohm effect) and condensed matter theory, focusing on the observable consequences.

1. Definitions

Let's consider a Hamiltonian H dependent on a parameter R: H(R(t)) and suppose that at t=0 the system is in its non-degenerate ground state |G(R(0));t=0>=|G>. If we change R with time, the state ket will evolve in a function Ψ(t). If |G> is well separated in energy from the excited states and the evolution is slow, we can suppose that Ψ is proportional to the ground state at time t:

$$\Psi(t)= \exp(-i\int E(t')dt'/\hbar) \exp(ig(t))\, |G(R(t));t=0> \qquad (1)$$

where g is real for the normalization condition and the first term is the temporal evolution.

The g is called Berry's phase.

By imposing that (1) satisfies Schroedinger's equation one finds g:

$$\frac{dg}{dt} = i < G(t) \mid \nabla_R G(t) > \frac{dR}{dt}$$

from which

$$g(t) - g(0) = g(t) = i\int < G(R) \mid \nabla_R G(R) > dR$$

One can check that g is real by differentiating the normalization condition with respect to R.

The interesting case is when H(T)=H(0); the final state is not equal to the initial one; the additional Berry's phase is expressed only in terms of geometrical properties of the parameter space. By applying Stokes' theorem one can transform the line integral in a surface integral; this will be very important in the applications, because it will be then allowed to use the formalism of electrodynamics even when there is no applied field. For the sake of simplicity I shall restrict the discussion to the case when R is a 3-D parameter, so that the curvature is just the rotor:

$$g(t) = i\oint < G(R) | \nabla_R G(R) > dR = -\operatorname{Im}\iint < \nabla_R G(R) | \times | \nabla_R G(R) >$$

So i$< G(R) | \nabla_R G(R) >$ is a kind of vector potential (Berry's connection) and the vector product (curvature) is the analogous of the magnetic field. The analogy is not only formal, we shall see that in some cases it affects the dynamics as if it was a real vector potential.
Now we go on to see some situations in which Berry's phases play a fundamental role.

2. Aharanov-Bohm effect
   Consider an electron confined in a box centered in the origin (infinite potential well). Let χ be the ground state. If you move the box in R, the ground state is χ(r-R). Now put a solenoid in the origin, with the the box outside. The current creates a magnetic field only inside the solenoid. Outside the solenoid the magnetic field B vanishes, but in general the vector potential does not vanish anywhere. Classically the electron would not feel the presence of the electromagnetic field, since the particle and the field live in different regions of space. Quantum mechanically the new eigenfunction is:

$$| G(R) >= \exp\left\{ \frac{ie}{hbar * c} \int_R^r A(r')dr' \right\} * c(r - R)$$

Now let the box wind around the solenoid one time.

Berry's connection is:

$i < G(t) | \nabla_R G(t) >$ =-ieA(R)/(hbar*c)

hence

$$g = \frac{e}{hbar * c}\oint A \cdot dR = \frac{e}{hbar * c}\Phi_B$$

The geometric phase is proportional to the magnetic flux. There is a measurable effect of the magnetic field on the electron, even though the latter is zero where the particle is!

3. Ionic motion in molecules

Consider the Hamiltonian of a molecule:

$$H = \frac{1}{2}\sum_{nuclei}\frac{p_i^2}{2M_i} + h(R;x)$$

where R are the coordinates of the nuclei and x the electronic degrees of freedom.
The usual Ansatz of Born-Oppenheimer approximation is that the wavefunction can be written as:

$\Psi(R)\chi(r;R)$

By putting this expression in the Hamiltonian and integrating over the electronic coordinates one gets:

$$[\sum \frac{\left(-ihbar\nabla_R - ihbar < c\,|\nabla_R c >\right)}{2M_i} + e(R)]\Psi(R) = E\Psi(R)$$

So Berry’s connection of the electrons acts as an electromagnetic field on the nuclei. In fact, if one is interested only in the classical motion of the nuclei, one should take care to calculate if the curvature of this connection is non-zero. This is a first step to take into account the coupling between slow and fast degrees of freedom: the first correction to the Born-Oppenheimer approximation is given by a Berry’s connection.

Conclusions

Experimental verification of these effects was found already in the ’50 and ’60, but the importance of Berry’s phase is to give a unitary description of a large variety of situations. Here I have only touched some examples, but there are many more (nuclei with half integer z-component angular momentum, dependence of the resistivity of nanotubes on the magnetic flux) and many more are still to come.

Bibliography

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