The mathematics of 2-state systems

Sourendu Gupta

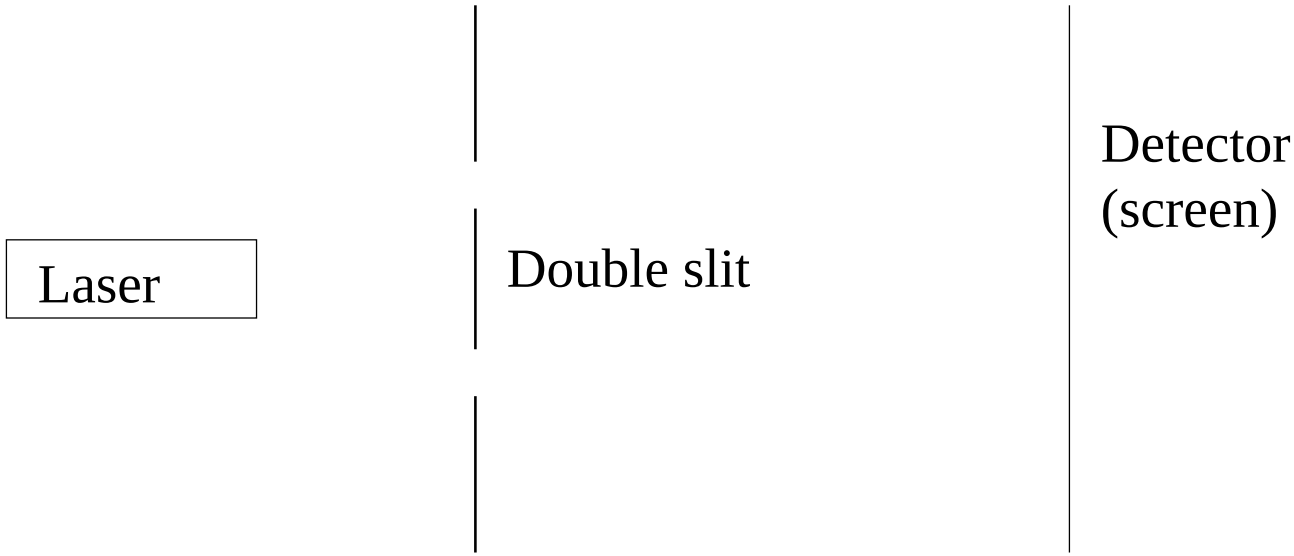
TIFR, Mumbai, India

Quantum Mechanics 1 2013
13 August, 2013

Outline

Outline

The two-slit experiment

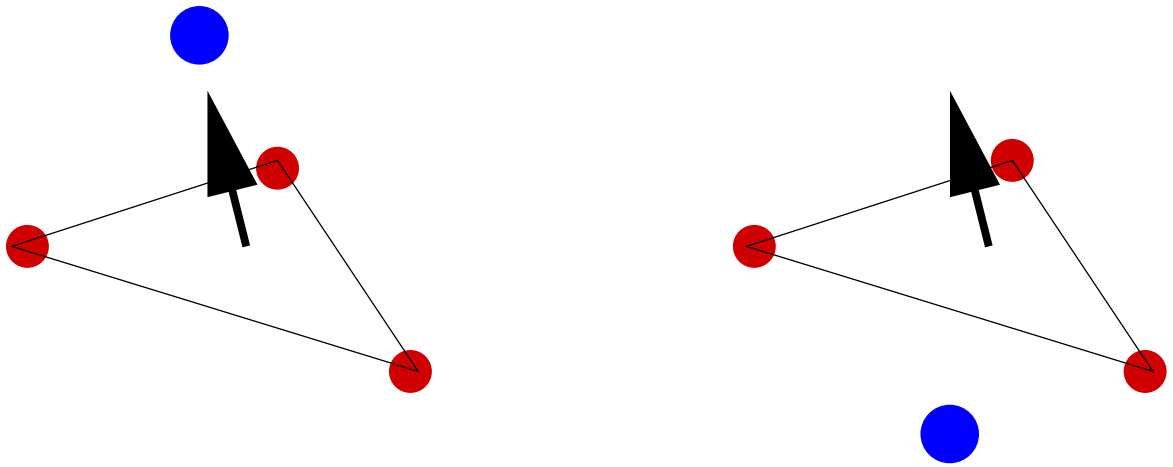


One can label the slits in many ways: the labelling can be arbitrary or physical). Clearly there is an identifiable quantum state corresponding to the photon coming from slit 1, and another for the photon coming from slit 2. The interference phenomenon is seen whenever the quantum state relevant to the measurement is a superposition of the two.

The H_2^+ molecule

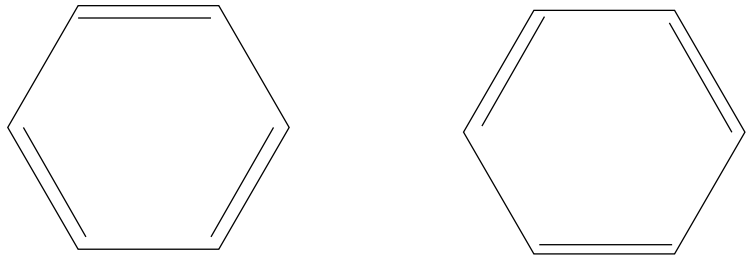
The two hydrogen atoms can be labelled (either arbitrarily, or physically by taking one of the nuclei to be of Hydrogen, the other to be of Deuterium). The electron can be in orbit around one or the other nucleus. The molecule does not form unless the electron state can be a linear superposition of the two.

The ammonia molecule



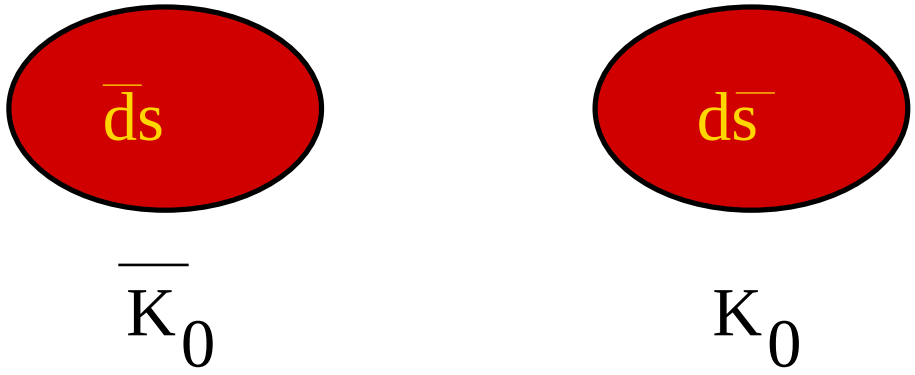
The three hydrogen atoms define a plane. The ammonia molecule has a magnetic moment, and its orientation with respect to this plane defines an "up" and a "down" direction.: the nitrogen atom can be either "above" the plane or "below" it, or in a linear superposition of the two.

The benzene molecule



The benzene ring must include both single and double (covalent) bonds between the carbon atoms. There are two possible arrangements of these kinds of bonds (described either by an arbitrary labelling of the carbon atoms or by physically labelling them in some way). Can there be linear superpositions of the electronic states of the valence electrons?

Neutral K meson oscillations



Mesons are made of a quark and an anti-quark. Uncharged strange mesons are called K_0 mesons. Since the strange quark (s) has charge $-1/3$, the same as a down quark (d), there are two possible kinds of K_0— either one with a strange anti-quark and a down quark ($d\bar{s}$, called the K_0) or one with a strange quark and a down anti-quark ($\bar{d}s$, called the $\bar{K}_0$). Are linear superpositions of these two states allowed?

Outline

The Hilbert space

In all the examples above, we have started with two quantum states (call them $|1\rangle$ and $|2\rangle$) which are orthogonal, and we have claimed that quantum states which are arbitrary superpositions of these two can exist.

It is useful to keep in mind a concrete representation of the two states

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Since an overall phase is immaterial to all that follows, we could also have chosen, for example,

$$|1\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1+2i \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |2\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 \\ 1+2i \end{pmatrix}.$$

In quantum mechanics, these two choices are indistinguishable.

Hermitean operators for two-state systems

Take the most general 2×2 complex matrix

$$A = \begin{pmatrix} z_1 & z_2 \\ z_3 & z_4 \end{pmatrix}.$$

If $A^+ = A$ then z_1 and z_4 are real and $z_2 = z_3^*$. So, the most general Hermitean matrix, is specified by four real parameters:

$$\begin{aligned} H &= \begin{pmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{pmatrix} \\ &= a_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + a_3 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= a_0 \mathbf{1} + a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3, \end{aligned}$$

where the three Hermitean matrices σ_1, σ_2 and σ_3 are called the Pauli matrices.

Algebra of Pauli Matrices

- The Pauli matrices are square roots of unity: $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1$.
- Since the Pauli matrices have vanishing trace and their squares are identity, the eigenvalues of each of them must be $+1$ and -1 (the eigenvalues are square roots of unity).
- The Pauli matrices do not commute with each other—

$$[\sigma_1, \sigma_2] = 2i\sigma_3, \quad [\sigma_2, \sigma_3] = 2i\sigma_1, \quad [\sigma_3, \sigma_1] = 2i\sigma_2.$$

  In terms of the completely anti-symmetric symbol (the Levi-Civita symbol) we can write $[\sigma_j, \sigma_k] = 2i\epsilon_{jkl}\sigma_l$. Here we have chosen the convention that $\epsilon_{123} = 1$.
- The Pauli matrices anti-commute with each other: $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$.
- Using the notation $\sigma_0 = 1$, any Hermitean matrix can be written in the form $H = a_i\sigma_i$. There are no restrictions on the real numbers a_i, and there are no relations between them.

Eigenvectors of Pauli matrices

- The states $|1\rangle$ and $|2\rangle$ are eigenvectors of σ_3 with eigenvalues 1 and -1 respectively.
- Since none of the Pauli matrices commute with each other, they cannot be simultaneously diagonalized.
- The eigenvectors of σ_1 are $|+\rangle$ and $|-\rangle$, where $|\pm\rangle = (|1\rangle \pm |2\rangle)/\sqrt{2}$. Hence the unitary transformation that rotates the eigenbasis of σ_3 into that of σ_1 is

$$U_{31} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}.$$

  Check that this indeed diagonalizes σ_1. What does it do to the other Pauli matrices?
- What are the eigenvectors of σ_2? Construct the unitary transformation which diagonalizes σ_2, and check what it does to the other Pauli matrices.

Functions of matrices

- If A is a diagonal matrix, and $B = f(A)$, then B is diagonal and $B_{ii} = f(A_{ii})$.
- If A can be diagonalized, then $f(A)$ can be found by first diagonalizing $A \to UAU^\dagger$, then constructing $B = f(UAU^\dagger)$ in this basis, and finally transforming back, $B \to U^\dagger BU = U^\dagger f(UAU^\dagger)U$.
- The exponentials of Pauli matrices can easily be found in this way. For example,

$$\exp(a\sigma_3) = \begin{pmatrix} e^a & 0 \\ 0 & e^{-a} \end{pmatrix}.$$

  All other Pauli matrices look the same in their eigenbasis. (Exponentiate the other Pauli matrices)
- The eigenvalues of unitary matrices are complex numbers of unit modulus. Every unitary matrix, U, can be written as $\exp(iH)$ where H is a Hermitean matrix.

Outline

Time evolution

- Planck's hypothesis, when extended to all quantum states, contains the rule for time evolution of quantum states. All waves evolve through the phase factor $\exp(-i\omega t)$. Since $E = \hbar\omega$, a quantum state of definite energy evolves as $\exp(-iEt/\hbar)$.
- The time evolution of an arbitrary superposition of states must, therefore, be given by $|\psi(t)\rangle = U(t - t_0)\,|\psi(t_0)\rangle$, where $U(t) = \exp\left(-iHt/\hbar\right)$, and H is the Hamiltonian operator. The evolution operator is unitary since H is Hermitean.
- Using the definition of matrix exponentials, one sees that the time derivative of $U(t)$ is $-iHU(t)/\hbar$. This gives us Schrödinger's equation

$$i\hbar\frac{d}{dt}\,|\psi\rangle = H\,|\psi\rangle\,.$$

The complete solution needs one initial condition, *i.e.*, $|\psi(t_0)\rangle$.

The general evolution operator

The most general 2×2 Hermitean matrix is the most general Hamiltonian for a 2-level system. So, the most general evolution operator is $U = \exp(-it \sum_i a_i \sigma_i/\hbar)$. Write $\mathbf{a} = (a_1, a_2, a_3) = |a|\hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is a real unit 3-vector. The matrix $s = \hat{\mathbf{n}} \cdot \sigma$ has eigenvalues ± 1 since $s^2 = 1$. (Prove this)
Then the energy eigenvalues are $E_\pm = a_0 \pm |a|$, and

$$U = V^\dagger \begin{pmatrix} \exp(-iE_+ t/\hbar) & 0 \\ 0 & \exp(-iE_- t/\hbar) \end{pmatrix} V,$$

where V is the unitary matrix which diagonalizes s. Writing $\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, one finds that

$$s = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & \cos\theta \end{pmatrix}, \qquad V = \begin{pmatrix} \cos(\theta/2)e^{i\phi} & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2)e^{-i\phi} \end{pmatrix}.$$

(Show this. What is the corresponding expression for U?)

Time evolution

If an initial quantum state is

$$|\psi(t_0)\rangle = \cos\alpha\,|E_+\rangle + \sin\alpha e^{i\beta}\,|E_-\rangle\,,$$

where the two basis states on the right are eigenstates of the Hamiltonian, then, after time evolution one has

$$|\psi(t)\rangle = \cos\alpha e^{-iE_+t/\hbar}\,|E_+\rangle + \sin\alpha e^{i(\beta - E_-t/\hbar)}\,|E_-\rangle\,.$$

Amplitudes such as

$$\langle\psi(t_0)|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(\cos^2\alpha e^{-iE_+t/\hbar} + \sin^2\alpha e^{-iE_-t/\hbar)}\right),$$

are oscillatory.

How do you apply this argument to the double slit experiment?

Problem 4.1

The most general 2×2 unitary matrix is

$$U = \begin{pmatrix} z_1 & w_1 \\ z_2 & w_2 \end{pmatrix}, \quad \text{with} \quad U^\dagger U = 1 = U U^\dagger.$$

Choosing $z_1 = \cos\theta \exp(i\phi)$, $z_2 = \sin\theta \exp(i\phi')$, $w_1 = \cos\psi \exp(i\alpha)$, $w_2 = \sin\psi \exp(i\alpha')$ satisfies the normalization constraints from $U^\dagger U$. The normalization constraints from $UU^\dagger$ further imply that $\cos^2\phi = \sin^2\theta$.

1. Complete the evaluation using the normalization constraints. What is the determinant of U?
2. Note that any overall phase of wavefunctions does not matter. Can this be used to restrict the class of unitary transformations required in quantum mechanics? (For example by putting a condition on the determinant of U)
3. Compare this parametrization with the unitary evolution operator and find when the two are the same.

Outline

Keywords and References

Keywords

Double-slit experiment, H_2^+, NH_3, benzene, K_0-$\overline{K}_0$ oscillations, 2-state systems, Pauli matrices, exponentials of matrices, Planck's hypothesis, evolution operator, Schrödinger's equation.

References

The Feynman Lectures in Physics (Vol 3), by R. P. Feynman *et al*: chapters 9, 10 and 11.
Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz: chapter 8.
Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë: chapter 3.
Mathematical Methods for Physicists, by G. Arfken.