The physics of 2-state systems

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Symmetric 2-state Hamiltonian

Whenever the two possible basis states of the quantum system cannot be distinguished from each other, the Hamiltonian must be symmetric under their exchange. Since $\sigma_1 |1\rangle = |2\rangle$, we find

$$\langle 2| H |2\rangle = \langle 1| H |1\rangle = \langle 2| \sigma_1^\dagger H \sigma_1 |2\rangle .$$

since the two states cannot be distinguished. Also, in that case, we must have

$$\langle 2| H |1\rangle = \langle 1| H |2\rangle = \langle 2| \sigma_1^\dagger H \sigma_1 |1\rangle .$$

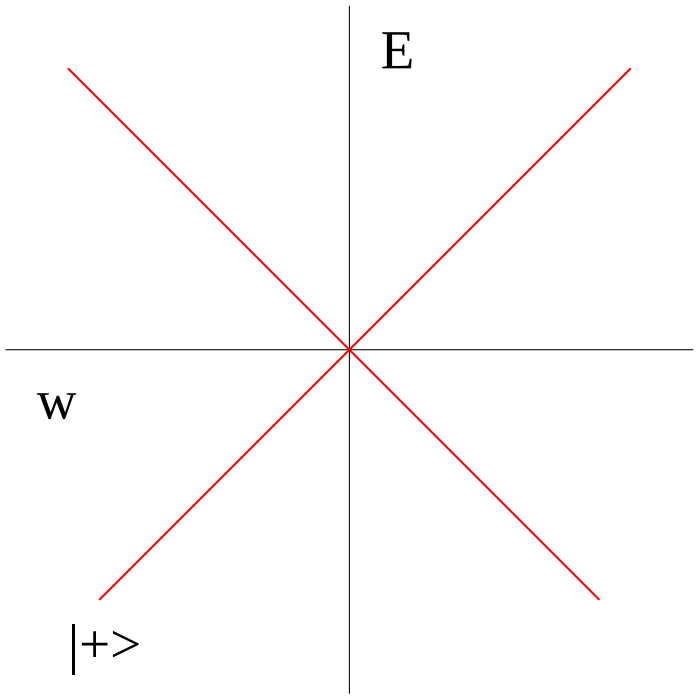
In other words, we have

$$H = \sigma_1^\dagger H \sigma_1, \quad i.e., \quad [H, \sigma_1] = 0.$$

The only Pauli matrices which commute with σ_1 are identity and itself. Hence, the symmetry above requires that $H = E_0 + w\sigma_1$. E_0 is called the unperturbed energy (or zeroth order energy), and w is called the mixing parameter.

Resonant stabilization

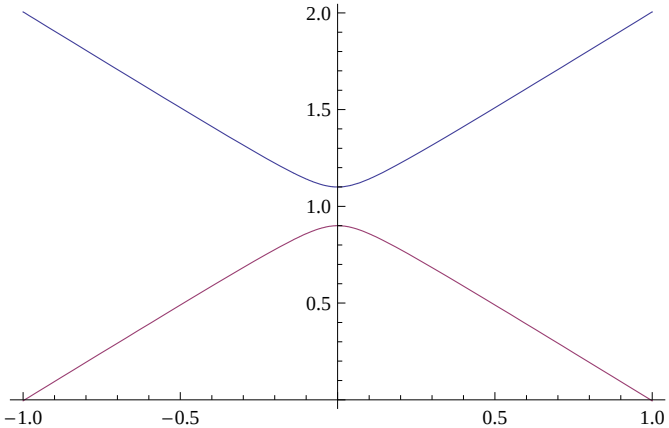
For any value of w, including zero, we can label their simultaneous eigenstates by the eigenvalues of $\mathbf{1}$ (which are the degenerate pair 1), and those of σ_0. In other words, we have $|+\rangle = |1, 1\rangle$ and $|-\rangle = |1, -1\rangle$. As a result, the eigenvalues of $H = E_0 + w\sigma_1$ are $E_\pm = E_0 \pm w$. There is a level crossing, *i.e.*, degeneracy, at $w = 0$.



Actually we can always choose $w < 0$, the lowest energy state is $|+\rangle$. The energy of this state is lower than that of $|1\rangle$ and $|2\rangle$. This is true of of H_2^+ and benzene. This general feature of symmetric states is called resonant stabilization.

Lack of symmetry: avoided crossings

Take an unperturbed Hamiltonian $H_0 = E_0 + \Delta\sigma_3$. The original energies are $E_1 = E_0 + \Delta$ and $E_2 = E_0 - \Delta$. The eigenstates $|1\rangle$ and $|2\rangle$ can be distinguished, since they have different energies.



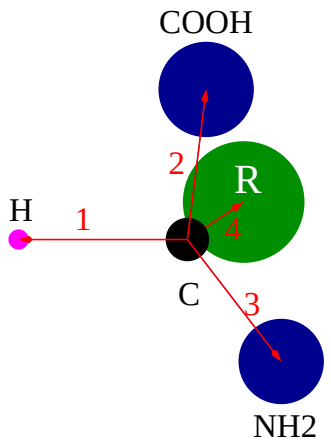
The permutation generator, $S = w\sigma_1 + w'\sigma_2$, does not commute with H_0. If $H = H_0 + S$, then the energy levels are $E_\pm = E_0 \pm \sqrt{\Delta^2 + |W|^2}$, where $W = w + iw'$. In general the energy splitting is quadratic in $|W|$; although, for $\Delta \ll |W|$, it is nearly linear, as in the earlier example.

For $\Delta \gg |W|$ it may seem that the energy levels might cross, but any $|W|$, no matter how small, causes avoided level crossings.

Level crossing implies symmetry

1. The only case in which level crossing occurs is the special Hamiltonian $H_0 = E_0$. In this special case the Hamiltonian commutes with any fixed linear combination, $S = w\sigma_1 + w'\sigma_2$, *i.e.*, $[H_0, S] = 0$. The vanishing of the commutator means a symmetry under permutations: *i.e.*, the Hamiltonian cannot distinguish the two states.
2. Since H_0 and S are simultaneously diagonalizable, the effect of the perturbation is linear in $W = w + iw'$. The states are degenerate when $W = 0$.
3. The permutation symmetry is broken for all other H_0, *i.e.*, $[H_0, S] \neq 0$ in general. In such cases the two states do not have equal energies even in the absence of a perturbation by S.
4. In general, the degeneracy of energy levels is a signal for a symmetry of the Hamiltonian.

Symmetry breaking



Amino acids come in two configurations. The plane Π_{23} is defined by the vectors $\mathbf{r}_2$ and $\mathbf{r}_3$. Reflect $\mathbf{r}_1$ and $\mathbf{r}_4$ in an imaginary mirror in the plane Π_{23}. This reflected molecule cannot be rotated into the original molecule. These are said to be two different chiralities.

Since there is no resonant stabilization of these two conformations of molecules, there must be breaking of the symmetry between them. Stereochemistry is the result of broken symmetry.

Raising and lowering operators

- The lowering and raising operators are

$$a = \frac{1}{2}(\sigma_1 - i\sigma_2) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad a^\dagger = \frac{1}{2}(\sigma_1 + i\sigma_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

  They are Hermitean conjugates of each other.
- They have the action $a|1\rangle = |2\rangle$ and $a|2\rangle = 0$, $a^\dagger|2\rangle = |1\rangle$ and $a^\dagger|1\rangle = 0$. Clearly $a^2 = (a^\dagger)^2 = 0$.
- Compute $[a^\dagger, a]$ and $\{a^\dagger, a\}$?
- Note that a and $a^\dagger$ cannot be diagonalized.
- Every matrix function of a and $a^\dagger$ contains only two terms in its Taylor expansion. For example, $\exp(ax) = 1 + ax$ for any scalar x. Note that $\sqrt{2}|+\rangle = \exp(a)|1\rangle = \exp(a^\dagger)|2\rangle$.
- The state vector $\exp(az)|1\rangle$ (for any complex z) is proportional to the most general (normalized) state vector for a two-state system. (Does each z correspond to an unique normalized state? Is this related to the Bloch sphere?)

An oscillation experiment

A typical oscillation experiment consists of the following steps:

1. Prepare the system in a fixed state, say $|1\rangle$.
2. Let the state then evolve freely, under a Hamiltonian H, for some time, t.
3. Find the probability, $P(t)$, that the state is $|1\rangle$.

Clearly, if $|1\rangle$ was an eigenstate of H, then $P(t) = 1$, and there are no oscillations. Also, if the two states are degenerate, then every state, including $|1\rangle$, is an eigenstate of H. As a result there are no oscillations.

If H has non-degenerate eigenstates, neither of which is $|1\rangle$, then there will be oscillations.

Rabi formula

The most general time dependent state in a two-state system is

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

Inverting our earlier solution for the energy eigenstates in terms of the basis states, we find (using the overall phase freedom)

$$|1\rangle = \cos\frac{\theta}{2}\,|E_+\rangle + \sin\frac{\theta}{2}\mathrm{e}^{-i\phi}\,|E_-\rangle\,.$$

If we start the system off in the state $|1\rangle$ at time $t = 0$, then $\alpha = \theta/2$ and $\beta = -\phi$. The probability that at any time the system can again be found in the state $|1\rangle$ is given by the Rabi formula

$$P(t) = \left|\langle 1|\psi(t)\rangle\right|^2 = 1 - \frac{|W|^2}{\Delta^2+|W|^2}\sin^2\left(\frac{t\sqrt{\Delta^2+|W|^2}}{\hbar}\right),$$

since $\tan\theta = |W|/\Delta$. This formula describes oscillations in K_0-$\overline{K}_0$, and ν_e-ν_μ, *etc.*.

Observational considerations

The dimensions of W and Δ are that of E. It is useful to return to the parametrization $|W| = \Delta \tan\theta$, and write

$$P(t) = 1 - \sin^2\theta \ \sin^2\left(\frac{t\Delta}{\hbar\cos\theta}\right).$$

For fixed Δ, as $|W|$ becomes large, $\theta \to \pi/2$, and as $|W|$ becomes small $\theta \to 0$. So for $|W| \gg \Delta$, the contrast between minimum and maximum values of $P(t)$ becomes largest. In this limit, the spacing between minima (or maxima) goes as $\pi\hbar/|W|$.

With decreasing $|W|$, the contrast decreases and the spacing between minima (or maxima) of $P(t)$ goes to $\pi\hbar/\Delta$, *i.e.*, becomes constant. There are no oscillations when there is exact degeneracy.

Quantum Zeno Effect

Zeno's Paradox: An arrow cannot move, Achilles cannot win a race against a tortoise. False, because an accurate measurement of position does not mean that the velocity is zero. The meaning of derivatives not properly understood until Newton and his contemporaries.

Quantum Zeno effect: Repeated measurements can prevent change of state. Prepare a 2-state system in a state $|1\rangle$. After time t its state changes to something else, the probability of finding it again in state t is given by $P(t)$. Perform the measurement, and then wait for another interval of time t. Now the probability of finding system in $|1\rangle$ is again $P(t)$. However, if the state was not measured at time t, then the probability is $P(2t) \neq P(t)$ in general.

Classical Larmor precession

Consider a system with a magnetic moment $\mathbf{m}$. This system possesses an angular momentum $\mathbf{j}$, such that $\mathbf{m} = \gamma \mathbf{j}$, where the scalar γ is called the gyromagnetic ratio. If this system is placed within an uniform magnetic field, $\mathbf{B}$, then the Hamiltonian is $H = -\gamma \mathbf{j} \cdot \mathbf{B}$.

The equation of motion is

$$\dot{\mathbf{m}} = \mathbf{m} \times \mathbf{B}.$$

Taking dot products with $\mathbf{m}$ and $\mathbf{B}$, we see that both $\mathbf{m} \cdot \mathbf{m}$, and $\mathbf{m} \cdot \mathbf{B}$ are conserved.

In other words, the motion consists of a vector of constant magnitude, $\mathbf{m}$, rotating around $\mathbf{B}$ making a constant angle with it. This motion is called Larmor precession.

Quantum Larmor precession

The quantum mechanics of any 2-state system can always be written in the form $H = -\gamma\hbar\sigma \cdot \mathbf{B}/2$. The energy eigenvalues are $\pm\gamma\hbar|B|/2$. We can choose $\mathbf{B}$ to lie in the z-direction. Then the eigenvectors are $|1\rangle$ and $|2\rangle$.

As before, a generic state of the system is

$$|\psi(t)\rangle = \cos\frac{\theta}{2}\,|1\rangle + \sin\frac{\theta}{2}\mathrm{e}^{-i(\phi-\omega_L t)}\,|2\rangle\,.$$

where $\omega_L = \gamma|B|$. Setting $\mathbf{m} = \gamma\hbar\sigma/2$, we can check that

$$\langle\psi(t)|\mathbf{m}|\psi(t)\rangle = \frac{1}{2}\gamma\hbar(\sin\theta\cos\{\phi-\omega_L t\}, \sin\theta\sin\{\phi-\omega_L t\}, \cos\theta).$$

This shows that we have a quantum description of Larmor precession with $|\mathbf{m}| = \gamma\hbar/2$. So the 2-state system formally resembles a classical system with $|\mathbf{j}| = \hbar/2$.

Density matrices: general considerations

1. A density matrix, ρ, describes an ensemble of quantum systems. The expectation value of a measurement, A, over the ensemble is $\langle A \rangle = \mathrm{Tr}\, A\rho$.
2. Since the overlap of any state with itself is unity, $\mathrm{Tr}\, \rho = 1$.
3. The density matrix for a pure state, $|\psi\rangle$ is $\rho = |\psi\rangle \langle\psi|$. In this case $\mathrm{Tr}\, \rho = 1$ and $\mathrm{Tr}\, \rho^2 = 1$.
4. In terms of a complete set of states, $|i\rangle$, one can write
$$\rho = \sum_{ij} \rho_{ij} |i\rangle \langle j| .$$
5. Since $|j(t)\rangle = U(t)|j\rangle$, $\rho(t)$ is obtained by the adjoint action— $U(t)\rho(0)U^\dagger(t)$. As a result,
$$i\hbar \frac{d}{dt}\rho(t) = [H, \rho(t)].$$
This is called von Neumann's equation.

Density matrix for 2-state systems

The density matrix for a 2-state system is $\rho = 1/2 + \mathbf{m}\cdot\sigma$. As a result, the expectation values $\langle\sigma_i\rangle = \mathrm{Tr}\,\sigma_i\rho = m_i$. The eigenvalues are $1/2 \pm |\mathbf{m}|$; these need not be positive.

Take the Hamiltonian to be $H = -\hbar\mathbf{B}\cdot\sigma/2$. Then

$$[H,\rho] = -\frac{\hbar}{2}\sum_{jk=1}^{3} B_j m_k [\sigma_j,\sigma_k] = -i\hbar\sum_{jkl=1}^{3}\epsilon_{jkl}B_j m_k \sigma_l.$$

This can be reduced by multiplying both sides by σ_k and taking a trace, to give

$$\dot{\mathbf{m}} = \mathbf{m}\times\mathbf{B}.$$

This looks like the classical equation for a spin precessing in an effective magnetic field which can be constructed from the Hamiltonian.

Pure states: the Bloch sphere

For the pure state ensemble built from the generic quantum state

$$|\psi\rangle = \cos\frac{\theta}{2}|E_+\rangle + \sin\frac{\theta}{2}e^{-i\phi}|E_-\rangle\,,$$

one has $\mathbf{m} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. We have chosen the eigenstates of the Hamiltonian as the basis states. Pure state ensembles correspond to points on a sphere (called the Bloch sphere).

The time evolution of this state adds a phase ωt to ϕ (where $\omega = (E_- - E_+)/\hbar$. This is an example of the general evolution of the density matrix: the vector $\mathbf{m}$ precesses around a certain direction.

What happens to pure state ensembles of the eigenvectors of the Hamiltonian?.

The canonical ensemble: a mixed state

The canonical ensemble describes a 2-state system evolving through a Hamiltonian H but which is also allowed to exchange energy with the environment (called a heat bath). In equilibrium one has $[H, \rho] = 0$, and the allowed density matrices are $f(H)$. The canonical ensemble has $\rho = \exp(-H/T)/Z$ where $Z = \mathrm{Tr}\, \exp(-H/T)$. For the 2-state system, we can write $H = -\gamma\hbar B\sigma_3/2$. Hence $Z = 2\cosh(\gamma\hbar B/2T)$, and

$$\rho(B,T) = \frac{1}{2\cosh(\gamma\hbar B/2T)} \begin{pmatrix} \exp(-\gamma\hbar B/2T) & 0 \\ 0 & \exp(\gamma\hbar B/2T) \end{pmatrix}.$$

This gives $\langle J_x\rangle = \langle J_y\rangle = 0$ and $\langle J_z\rangle = -(\hbar/2)\tanh(\gamma\hbar B/2T)$. This is the Curie-Weiss law.

Note the resemblance between this ρ and the unitary evolution operator!

Keywords and References

Keywords

Unperturbed energy, mixing parameter, resonant stabilization, avoided level crossings, Rabi formula, gyromagnetic ratio, Larmor precession, Bloch sphere, canonical ensemble, heat bath, Curie-Weiss law.

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