Two-state systems

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Outline

The Hilbert space of two state systems

For all two state systems, we have an orthogonal basis, which we have represented by the vectors

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

In this basis the three Pauli matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Also, $H = \sum_{j=0}^{3} a_j \sigma_j$ is Hermitean if a_j are real (σ_0 is the identity matrix).
The matrix $\exp(ixH)$ is unitary if H is Hermitean and x is real.
We have also introduced a rotated basis

$$|+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), \quad \text{and} \quad |-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle).$$

In this basis σ_1 is diagonal.

Resonant stabilization

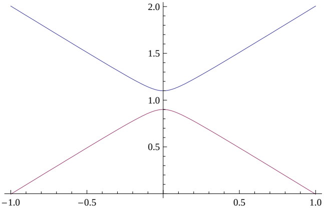
Whenever the two possible basis states of the quantum system cannot be distinguished from each other, the Hamiltonian must be symmetric under their exchange. Since σ_1 exchanges the two quantum states $|1\rangle$ and $|2\rangle$, we have

$$H = \sigma_1 H \sigma_1^{-1}, \quad i.e., \quad [H, \sigma_1] = 0.$$

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**.

By the arguments given previously, the eigenvalues of this Hamiltonian are $E_\pm = E_0 \pm w$, and the eigenvectors are $|+\rangle$ and $|-\rangle$. If $w < 0$, then the lowest energy state is $|+\rangle$. The energy of the superposition state is lower than that of the original states. This is true of of H_2^+, benzene and ammonia. This general feature of symmetric states is called **resonant stabilization**.

Avoided crossings



Consider the unperturbed Hamiltonian $H_0 = E_0 + \Delta\sigma_3$, so that the original energies are $E_1 = E_0 + \Delta$ and $E_2 = E_0 - \Delta$. If the full Hamiltonian is $H = H_0 + w\sigma_1 + w'\sigma_2$, then the energy levels of the system are $E_\pm = E_0 \pm \sqrt{\Delta^2 + |W|^2}$, where $W = w + iw'$. For general values of Δ, the energy splitting is quadratic in the mixing parameter, $|W|$. However, for $\Delta \ll |W|$, the splitting is linear in $|W|$, as was worked out in the earlier example.

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

Level crossing: an extra symmetry

1. The only case in which level crossing occurs is the special Hamiltonian $H = E_0$. In this special case the Hamiltonian commutes with all three Pauli matrices, *i.e.*, $[H, \sigma_i] = 0$. Since the vanishing of the commutator implies a symmetry, this means that the symmetry is enlarged from permutation symmetry of the two basis states to something larger.
2. The simplest symmetry of the system, *i.e.*, the symmetry under interchange of the two basis states, predicted an avoided level crossing. An enlarged symmetry is needed for levels to cross. At the point where the two levels become degenerate, there is an enhanced symmetry.
3. In general, unexpected degeneracy of energy levels is a signal for an unexpected enlargement of the symmetry of the problem.

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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 the neutral Kaon system, oscillations of (solar) neutrinos between ν_e and ν_μ, *etc.*

Classical Larmor precession

Consider a system with a magnetic moment $\mathbf{m}$. This system must possess 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

$$\frac{d}{dt}\mathbf{m} = \mathbf{m} \times \mathbf{B}.$$

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 rotating around $\mathbf{B}$ making a constant angle with it. This motion is called **Larmor precession**.

Quantum Larmor precession

The quantum mechanics of a system of spin 1/2 moving in a constant magnetic field is obtained by taking $H = -\frac{\gamma}{2}\sigma\cdot\mathbf{B}$ (the angular momentum is replaced by the operator $\hbar\sigma/2$). If the direction of $\mathbf{B}$ is the z-direction, then the energies are $\pm\gamma\hbar|B|/2$, and the eigenvectors are $|1\rangle$ and $|2\rangle$. If the initial quantum state is

$$|\psi(0)\rangle = \cos\frac{\theta}{2}|1\rangle + \sin\frac{\theta}{2}\mathrm{e}^{-i\phi}|2\rangle,$$

then, at any time t the quantum state is

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

where $\omega_L = \gamma|B|$. The expectation values

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

show that we have a quantum description of Larmor precession.

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Density matrices

The density matrix appropriate to a two-state system is $\rho = 1/2 + \mathbf{s} \cdot \sigma$. As a result, the expectation values $\langle \sigma_i \rangle = \mathrm{Tr}\, \sigma_i \rho = s_i$.
Take the Hamiltonian of the system to be $H = h_0 + \mathbf{h} \cdot \sigma$. Then

$$[H, \rho] = \sum_{jk=1}^{3} h_j s_k [\sigma_j, \sigma_k] = 2i \sum_{jkl=1}^{3} \epsilon_{jkl} h_j s_k \sigma_l.$$

The von Neumann equation (*i.e.*, the evolution equation for the density matrix) can be reduced by multiplying both sides by σ_k and taking a trace. This gives the equation

$$\hbar \frac{d\mathbf{s}}{dt} = 2\mathbf{h} \times \mathbf{s}.$$

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

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

one has $\mathbf{s} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. 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 $\mathbf{s}$ precesses around a certain direction.

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

The canonical ensemble: a mixed state

A thermal ensemble of two state systems is the **canonical ensemble**. In this ensemble we are concerned with the physics of a two state system whose time evolution is governed by a Hamiltonian H but which is also allowed to exchange energy with the environment (called a **heat bath**). In equilibrium such a density matrix does not evolve. Hence $[H, \rho] = 0$, and the only allowed density matrices are $f(H)$.

The canonical ensemble is described by the density matrix $\rho = \exp(-H/T)/Z$ where $Z = \mathrm{Tr}\,\exp(-H/T)$. For a spin-1/2 system immersed in a magnetic field of strength B, pointing in the z direction, $H = -\gamma\hbar B\sigma_3/2$. 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!

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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 $a^2 = (a^\dagger)^2 = 0$.
- **What are $[a^\dagger, a]$ 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?**)

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References

1. The Feynman Lectures in Physics (Vol 3), by R. P. Feynman *et al*. Examples pf two-state systems are discussed in detail in chapters 9, 10 and 11 of this book.
2. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material on Pauli matrices can be found in chapter 8 of this book. There are also a couple of useful problems regarding the manipulation of the Pauli matrices.
3. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 3 of this book discusses several two-state systems in the kind of detail that is the hallmark of this book.
4. There is a nice article about solar neutrino observations in the web page `http://nobelprize.org/nobel_prizes/physics/articles/bahcall/index.html`