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NANOSCALE SCIENCE & TECHNOLOGY

V

Two-Level Quantum Systems
(Qubits)

Lecture notes
2005

5.1 Qubit description

Quantum bit (qubit) is an elementary unit of a quantum computer. Similar to classical computers, qubits in a quantum computer are connected in a network so that one qubit can affect the state of the others; the state of each qubit is controlled by external "knob", and also the qubits interconnections are controllable. Similar to classical bits which can switch between the two states, "on" and "off", quantum bits have only two energy levels; such systems are known in quantum mechanics as two-level systems.

Two-level systems are the simplest quantum mechanical systems. Spin 1/2 is a natural two-level quantum system. Other quantum systems, e.g. solid state devices, contain many energy levels. Nevertheless, such multilevel systems could be employed for qubit operation if there is the possibility to selectively manipulate only two (usually lowest) energy levels. This implies that while performing a task required by quantum algorithm, the system stays within the two selected levels, and the transitions to the other levels are forbidden or at least efficiently suppressed. Such a constraint is the first basic criterium for choosing a solid stated system as a qubit.

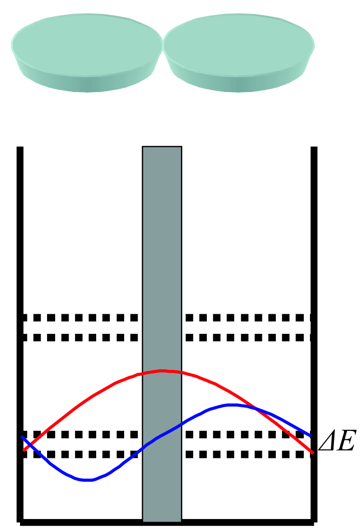

Figure 1: Coupled quantum dots and energy diagram; electronic levels in a closed dot are more distant compared to the level splitting due to tunneling between the dots; two lowest split levels can serve as a qubit.

A qubit system different from spin 1/2 can be illustrated with a double quantum dot structure. The energy diagram of this system is sketched on Fig. 1: the two quantum boxes connected via opaque tunnel barrier. If the boxes are identical, and the barrier is completely non-transparent, the energy spectrum consists of doubly degenerate levels, E_n. If the tunnel probability T is not equal to zero, the degeneracy is removed, and levels form a set of tight pairs whose splitting, $\Delta E_n \sim T(E_n - E_{n-1})$, is much smaller than the distance between the level pairs, $E_n - E_{n-1}$. The lowest level pair then is well separated from the other levels and can be considered for qubit applications.

In this Note we describe how two-level quantum systems are generally described, how they evolve in time, and how they are operated.

Two-level quantum system is characterized by the (normalized) state vector

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\phi}|1\rangle, \tag{5.1}$$

which belongs to a Hilbert space formed by the two basis vectors $|0\rangle$, and $|1\rangle$, also called the computational basis. The basis vectors can be presented as eigenvectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{5.2}$$

of the Pauli matrix σ_z,

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.3}$$

The state (5.1) is characterized with the two angles, θ and ϕ, and thus can be viewed as a point on a 3d unit sphere (the Bloch sphere) or, equivalently, as a unit 3d vector (the Bloch vector), see Fig. 2. The north pole represents the state $|0\rangle$, while the south pole corresponds to the state $|1\rangle$; the equatorial states describe equally weighted superpositions of the basis states, known as the "cat states". Within such a mapping, an arbitrary state of a two-level system can be described as a rotation from the north pole of the $|0\rangle$ state,

$$|\psi\rangle = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{5.4}$$

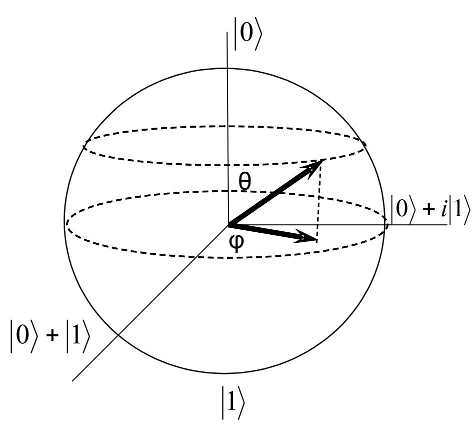

Figure 2: The Bloch sphere. Points on the sphere correspond to the quantum states $|\psi\rangle$; in particular, the north and south poles correspond to the computational basis states $|0\rangle$ and $|1\rangle$; superposition cat-states $|\psi\rangle = |0\rangle + e^{i\phi}|1\rangle$ are situated on the equator.

5.2 Qubit dynamics

Time evolution of a two-level system is governed by the Schrödinger equation,

$$i\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle, \tag{5.5}$$

with the Hamiltonian presented by a 2×2 matrix,

$$\hat{H} = -\frac{1}{2}\begin{pmatrix} \epsilon & \Delta \\ \Delta & -\epsilon \end{pmatrix}, \tag{5.6}$$

which can be equivalently expressed through the Pauli matrices, σ_x and σ_z,

$$\hat{H} = -\frac{1}{2}(\epsilon\,\sigma_z + \Delta\,\sigma_x). \tag{5.7}$$

This Hamiltonian can be interpreted as a result of interaction, with strength Δ, of the levels $\pm\epsilon$ corresponding to the computational basis.

It is useful to know the eigenenergies and eigenstates of the Hamiltonian (5.6), which are derived from the stationary Schródinger equation,

$$\hat{H}|\psi\rangle = E|\psi\rangle. \tag{5.8}$$

Denoting the components of the eigenstates as a_1, a_2, we get

$$(\hat{H} - E)|\psi\rangle = -\frac{1}{2}\begin{pmatrix} \epsilon + 2E & \Delta \\ \Delta & -\epsilon + 2E \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0. \tag{5.9}$$

The eigenvalues are determined by

$$det(\hat{H} - E) = E^2 - \frac{1}{4}(\epsilon^2 + \Delta^2) = 0, \tag{5.10}$$

with the result

$$E_{1,2} = \pm\frac{1}{2}\sqrt{\epsilon^2 + \Delta^2}. \tag{5.11}$$

The eigenvectors are given by:

$$a_2 = -a_1\frac{\Delta}{\epsilon + 2E}. \tag{5.12}$$

After normalization

$$a_1 = 1/\sqrt{1 + \left(\frac{\Delta}{\epsilon + 2E}\right)^2} = \frac{1}{\sqrt{2}}\sqrt{1 \pm \frac{\epsilon}{|2E|}} \tag{5.13}$$

$$a_2 = \pm\sqrt{1 - a_1^2} = \pm\frac{1}{\sqrt{2}}\sqrt{1 \mp \frac{\epsilon}{|2E|}} \tag{5.14}$$

We finally simplify the notation by fixing the signs of the amplitudes,

$$a_1 = \frac{1}{\sqrt{2}}\sqrt{1 + \frac{\epsilon}{|2E|}}\ ;\ a_2 = \frac{1}{\sqrt{2}}\sqrt{1 - \frac{\epsilon}{|2E|}}\ ; \tag{5.15}$$

and explicitly writing down all the energy eigenstates,

$$|E_1\rangle = a_1|0\rangle + a_2|1\rangle \tag{5.16}$$
$$|E_2\rangle = a_2|0\rangle - a_1|1\rangle \tag{5.17}$$

where

$$E_1 = -\frac{1}{2}\sqrt{\epsilon_1^2 + \Delta_1^2}\ ;\ E_2 = +\frac{1}{2}\sqrt{\epsilon_1^2 + \Delta_1^2} \tag{5.18}$$

At the degeneracy point $\epsilon_1 = 0$ where $|a_1| = |a_2| = 1/\sqrt{2}$, we have,

$$|E_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{5.19}$$
$$|E_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \tag{5.20}$$

5.3 The state evolution on the Bloch sphere

To study the time-evolution of a general state, a convenient way is to expand in the basis of energy eigenstates,

$$|\psi(t)\rangle = c_1|E_1\rangle e^{-iE_1t/\hbar} + c_2|E_2\rangle e^{-iE_2t/\hbar} \tag{5.21}$$

The coefficients c_1, c_2 here fix the initial state at $t = 0$. The angle parametrization is again possible, $c_1 = \cos\theta',\ c_2 = \sin\theta' e^{i\phi'}$, the primed angles referring to a new coordinate system: the poles onf the Bloch sphere are now associated with the Hamiltonian eigenbasis $|E_1\rangle$, $|E_2\rangle$, which is obtained by rotation from the earlier introduced computational basis, Eq. (5.1).

It is easy to see that the state time evolution is represented on the Bloch sphere by rotation of the Bloch vector with constant angular speed $(E_1 - E_2)/\hbar$ around the direction defined by the energy eigenbasis. Indeed, according to Eq. (5.21), in the primed coordinate system, the polar angle remains constant, $\theta' = \text{const}$, while the azimuthal angle grows, $\phi'(t) = \phi'(0) + (E_1 - E_2)t/\hbar$.

The dynamics on the Bloch sphere is conveniently described in terms of the density matrix for a pure quantum state,

$$\hat{\rho} = |\psi\rangle\langle\psi|. \tag{5.22}$$

This is a 2×2 Hermitian matrix whose diagonal elements ρ_1 and ρ_2 define occupation probabilities of the basis states, hence satisfying the normalization condition $\rho_1 + \rho_2 = 1$, while the off-diagonal elements give information about the quantum phase. For example, the density matrix of the state (5.21) has the form,

$$\hat{\rho} = \begin{pmatrix} |c_1|^2 & c_1c_2^* e^{i(E_1-E_2)t/\hbar} \\ c_1^*c_2 e^{-i(E_1-E_2)t/\hbar} & |c_2|^2 \end{pmatrix}. \tag{5.23}$$

The density matrix can be mapped on a real 3-vector by means of the standard expansion in terms of the Pauli σ-matrices,

$$\hat{\rho} = \frac{1}{2}(1 + \rho_x\sigma_x + \rho_y\sigma_y + \rho_z\sigma_z). \tag{5.24}$$

Direct calculation of the density matrix Eq. (5.22) using Eq. (5.1) and comparing with Eq. (5.24) shows that the vector $\boldsymbol{\rho} = (\rho_x, \rho_y, \rho_z)$ coincides with the Bloch vector,

$$\boldsymbol{\rho} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta) \tag{5.25}$$

introduced in Fig. 2 and also shown in Fig. 3. In the same σ-matrix basis, the two-level Hamiltonian (5.7) is represented with a 3-vector,

$$\boldsymbol{H} = (-\Delta/2,\ 0,\ -\epsilon/2). \tag{5.26}$$

shown in Fig. 3.

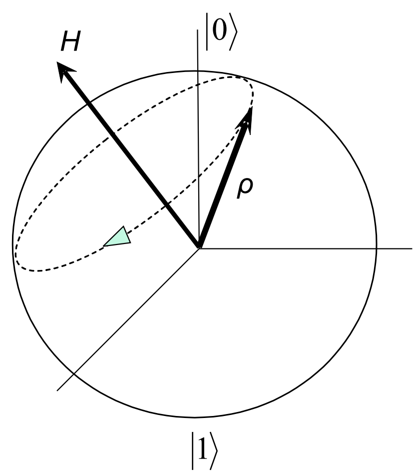

Figure 3: The Bloch sphere: the Bloch vector ρ represents the state of the two-level system (same as in Fig. 2); the vector H represents the two-level Hamiltonian.

The time evolution of the density matrix is given by the Liouville equation,

$$i\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}]. \tag{5.27}$$

The vector form of the Liouville equation is readily derived by inserting Eqs. (5.24), (5.7) into Eq. (5.27) and using the commutation relations for the Pauli matrices,

$$\partial_t\boldsymbol{\rho} = \frac{1}{\hbar}[\,\boldsymbol{H}\,\times\,\boldsymbol{\rho}\,]. \tag{5.28}$$

This equation coincides with the Bloch equation for a magnetic moment evolving in a magnetic field, the role of the magnetic moment being played by the Bloch vector $\boldsymbol{\rho}$ which rotates around the effective "magnetic field" **H** associated with the Hamiltonian of the qubit (plus any driving fields) (Fig. 3).

5.4 Control of the qubit state

To perform any algorithm, one should be able to prepare the qubit in arbitrary quantum state. This means that there must be ways to access any point on the Bloch sphere. As it was mentioned, free evolution of a two-level system consists of a rotation around the Hamiltonian vector direction with angular velocity $E_1 - E_2$ (this motion is called precession using the magnetic moment analogy). In other words, the free precession gives access to all states with the same initial polar angle θ'. To change the polar angle, one method is to apply rectangular pulses which suddenly change the Hamiltonian and, consequently, the axis of the Bloch vector rotation. Sudden pulse switching means that the time-dependent Hamiltonian is changed so fast on the time scale of the free precession that the state vector can be treated as time-independent - frozen - during the switching time interval. It is clear that the possibility to change direction of the Hamiltonian vector to any given value provides the means to access any point on the Bloch sphere.

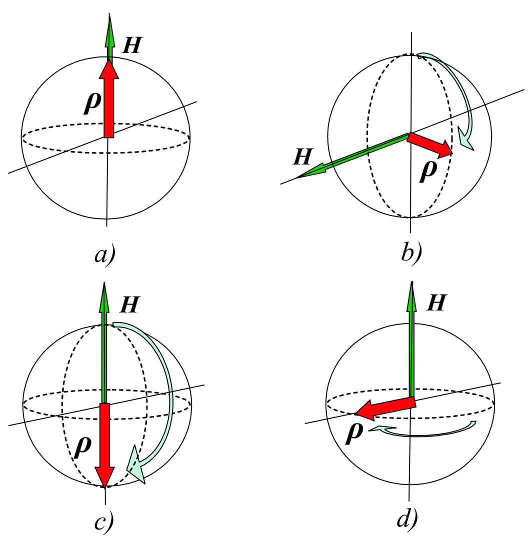

Figure 4: Qubit operations with dc-pulses: the vector H represents the qubit Hamiltonian, and the vector ρ represents the qubit state. a) The qubit is initialized to the ground state; b) the Hamiltonian vector H is suddenly rotated towards x-axis, and the qubit state vector ρ starts to precess around H; c) when qubit vector reaches the south pole of the Bloch sphere, the Hamiltonian vector H is switched back to the initial position; the vector ρ remains at the south pole, indicating complete inversion of the level population (π-pulse); d) if the Hamiltonian vector H is switched back when the qubit vector reaches the equator of the Bloch sphere ($\pi/2$-pulse), then the ρ vector remains precessing at the equator, representing equal-weighted superposition of the qubit states (cat states) $|\psi\rangle = |0\rangle + e^{i\phi}|1\rangle$; this operation is the basis for the Hadamard gate.

Let us consider, for example, the diagonal qubit Hamiltonian, $\Delta = 0$, and apply a pulse $\delta\epsilon$ during a time τ. This operation will change the precession speed and thus add a shift to the phases of the qubit eigenstates, $\pm\delta\epsilon\tau/2\hbar$. If the applied pulse is such that $\epsilon + \delta\epsilon$ becomes zero, and instead, the σ_x component, Δ, is switched on, as illustrated in Fig 4, then the state vector will rotate around the x-axis, and after the time $\Delta\tau/2\hbar = \pi$ (π-pulse) the ground state, $|0\rangle$, will flip and become, $|1\rangle$. This "spin flip" manipulation corresponds to the quantum NOT operation. Furthermore, if the pulse duration is twice smaller ($\pi/2$-pulse), then the ground state vector will approach the equator of the Bloch sphere and precess along it after the end of the operation. This manipulation, known as the Hadamard gate, is the way of preparing the cat states.

5.5 Harmonic perturbation and Rabi oscillation

Another way to manipulate the Bloch vector is to apply harmonic perturbation with small amplitude λ and resonant frequency $\hbar\omega = E_2 - E_1$. this method is an analogue to the NMR technique for true spin systems.

Let us consider the situation when the harmonic perturbation is added to the z-component of the Hamiltonian corresponding to a modulation of the computational basis levels with a microwave field. In the energy eigenbasis, $|E_1\rangle$, $|E_2\rangle$, the Hamiltonian will take the form,

$$\hat{H} = E_1\sigma_z + (\lambda_z\,\sigma_z + \lambda_x\,\sigma_x)\cos\omega t, \tag{5.29}$$

$$\lambda_z = \lambda\frac{\epsilon}{E_2}, \quad \lambda_x = \lambda\frac{\Delta}{E_2}. \tag{5.30}$$

The first perturbative term determines small periodic oscillations of the qubit energy splitting, while the second term will induce interlevel transitions. It is easy to establish that despite the amplitude of the perturbation is small, $\lambda/E_2 \ll 1$, the system will be driven far away from the initial state because of the resonance.

5.5.1 Perturbative analysis

To convince ourselves that it is so, we consider a more general case of a multilevel electronic system, e.g. a quantum dot, subject to a weak electromagnetic radiation or time-oscillation of the gate potential. This field will induce interlevel transitions with small amplitudes proportional to the small magnitude of the applied field, hence the perturbation theory seems to apply. Let the Hamiltonian of the unperturbed dot to be $\hat{H}$, and the nonstationary potential to have the form $\hat{V}\cos\omega t$. Then the wave function obeys nonstationary Schrödinger equation,

$$i\dot{\psi}(t) = (\hat{H} + \hat{V}\cos\omega t)\psi(t). \tag{5.31}$$

In this section, we choose for simplicity the units where $\hbar = 1$. Let $\{\varphi_n\}$ to be a complete set of eigenstates of the Hamiltonian $\hat{H}$, $\hat{H}\varphi_n = E_n\varphi_n$. Let us assume that in the absence of external field, the system is in the ground state φ_1. Then in the presence of the field, the wave function will assume the form

$$\psi(t) = \varphi_0 e^{-iE_0 t} + \sum_{n>1} a_n(t)\varphi_n e^{-iE_n t}, \quad a_n \ll 1. \tag{5.32}$$

In the first order perturbation expansion, the coefficients a_n in Eq. (5.32) obey the following equations,

$$i\dot{a}_n = V_{1n} \cos\omega t e^{i(E_n - E_1)t}. \tag{5.33}$$

In this equation, V_{1n} is the transition matrix element, $V_{1n} = (\varphi_n, \hat{V}\varphi_1)$. The solution reads

$$a_n = -\frac{V_{1n}}{2}\left(\frac{e^{i(E_n-E_1+\omega)t}}{E_n - E_1 + \omega} + \frac{e^{i(E_n-E_1-\omega)t}}{E_n - E_1 - \omega}\right). \tag{5.34}$$

It is clear from this equation that the transition amplitudes are indeed small when $V_{1n}/(E_n - E_1 - \omega) \ll 1$ for all n. However, if the resonance condition, $E_n - E_1 - \omega = 0$ is fulfilled for some level n, then the perturbation procedure fails, and the transition amplitude to the resonant level becomes large. The resonance condition allows selective efficient coupling of the level pairs, which is the basis for defining the qubit.

Note that the non-equidistant property of the spectrum is essential for resonant selection, otherwise, more than two levels will be coupled (see Fig. 5). For this reason the system such as linear oscillator, whose energy spectrum is known to be equidistant, is not suitable for qubit operation; certain amount of non-linearity is required for a quantum system to serve as a qubit.

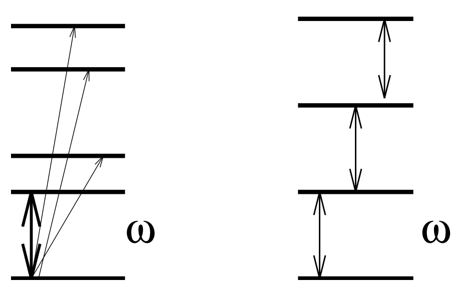

Figure 5: Resonant transition in non-equidistant spectrum involves two levels (left), while in an equidistant spectrum of linear oscillator many levels are coupled (right

5.5.2 Resonant approximation

Let us return to the two-level system, Eq. (5.29), and consider the resonant dynamics under the condition, $E_2 - E_1 - \hbar\omega = 0$. In this case, as we have established, the probability amplitudes of both eigenstates are not small, and the qubit wave function acquires the form,

$$|\psi\rangle = a(t)e^{-iE_1 t/\hbar}|E_1\rangle + b(t)e^{-iE_2 t/\hbar}|E_2\rangle. \tag{5.35}$$

Substituting this ansatz into the Schrödinger equation,

$$i\hbar|\dot{\psi}\rangle = \hat{H}(t)\,|\psi\rangle, \tag{5.36}$$

we get the following equations for the coefficients,

$$
\begin{aligned}
i\hbar\dot{a} &= \lambda_x \cos\omega t \, e^{i(E_1-E_2)t/\hbar} \, b, \\
i\hbar\dot{b} &= \lambda_x \cos\omega t \, e^{i(E_2-E_1)t/\hbar} \, a.
\end{aligned} \tag{5.37}
$$

(Here we have neglected a small diagonal perturbation, λ_z.)

Let us now focus on the slow evolution of the coefficients on the time scale of qubit precession, and average Eqs. (5.37) over the period of the precession. This approximation is known in the theory of two-level systems as the "rotating wave approximation". Then, taking into account the resonance condition, we get the simple equations,

$$
i\hbar\dot{a} = \frac{\lambda_x}{2}\, b, \quad i\hbar\dot{b}\frac{\lambda_x}{2}\, a, \tag{5.38}
$$

whose solutions read,

$$
\begin{aligned}
a^{(1)}(t) &= \quad b^{(1)}(t) = e^{-i\lambda_x t/2\hbar}, \\
a^{(2)}(t) &= - \quad b^{(2)}(t) = e^{i\lambda_x t/2\hbar}.
\end{aligned} \tag{5.39}
$$

Thus, the dynamics of a resonantly driven qubit is characterized by a linear combination of the two wave functions,

$$
\begin{aligned}
|\psi^{(1)}\rangle &= \frac{1}{\sqrt{2}} e^{-i\lambda_x t/2\hbar} \left(e^{-iE_1 t/\hbar}|E_1\rangle + e^{-iE_2 t/\hbar}|E_2\rangle \right), \\
|\psi^{(2)}\rangle &= \frac{1}{\sqrt{2}} e^{i\lambda_x t/2\hbar} \left(e^{-iE_1 t/\hbar}|E_1\rangle - e^{-iE_2 t/\hbar}|E_2\rangle \right).
\end{aligned} \tag{5.40}
$$

Let us assume that the qubit was initially in the ground state, $|E_1\rangle$, and that the

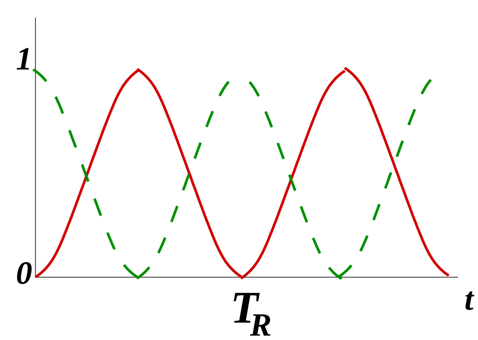

Figure 6: Rabi oscillation of populations of lower level (full line) and upper level (dashed line) at exact resonance (zero detuning). $T_R = 2\pi/\Omega_R$ is the period of Rabi oscillations.

perturbation was switched on instantly. Then the wave function of the driven qubit will take the form,

$$
|\psi\rangle = \cos\frac{\lambda_x t}{2\hbar}\, e^{-iE_1 t/\hbar}|E_1\rangle + i\sin\frac{\lambda_x t}{2\hbar}\, e^{-iE_2 t/\hbar}|E_2\rangle. \tag{5.41}
$$

Correspondingly, the probabilities of the level occupations,

$$
\begin{aligned}
P_1 &= \cos^2 \frac{\lambda_x t}{2\hbar} = \frac{1}{2}\left(1 + \cos \frac{\lambda_x t}{\hbar}\right), \\
P_2 &= \sin^2 \frac{\lambda_x t}{2\hbar} = \frac{1}{2}\left(1 - \cos \frac{\lambda_x t}{\hbar}\right),
\end{aligned} \tag{5.42}
$$

will oscillate in time with small frequency $\Omega_R = \lambda_x/\hbar \ll \omega$.

In other words, the resonant dynamics of a two-level quantum system consists of periodic inversion of the level populations as illustrated in Fig. 6. Such a dynamic behavior is known as Rabi oscillation. The characteristic feature of this dynamics is that the frequency of Rabi oscillation is proportional to a small *amplitude* of the applied perturbation. Using the magnetic moment analogy, the phenomenon is associated with a magnetic resonance (e.g., nuclear magnetic resonance, NMR), when small transverse magnetic field oscillating with frequency equal to the frequency of the free precession produces large effect - slow full-scale rotation of the magnetic moment around a horizontal axis (magnetic moment nutation).

5.5.3 Home problem

Derive equations for time-dependent level populations in more general, non-resonant case, $E_2 - E_1 - \hbar\omega \neq 0$, assuming however, that deviation from resonance is small compared to $\hbar\omega$.