ADIABATIC PERTURBATION OF DISCRETE SPECTRUM STATES

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The probabilities for quantum transitions between the states of a discrete spectrum are calculated for a system in adiabatic conditions, no assumptions being made regarding the form of the Hamiltonian. The calculations are performed with an accuracy to a pre-exponential factor of the order of unity.

THE author has calculated previously [1] for a one-dimensional linear oscillator the probabilities of quantum transitions under the influence of an adiabatic change in the frequency. In the present communication we calculate the transition probabilities in an arbitrary quantum system which is under adiabatic external conditions. Such a system is described by a Hamiltonian that varies "slowly" with the time. We assume that the time dependence of the Hamiltonian is analytic. We are interested in transitions between discrete spectrum states. Accordingly, we seek a solution of the Schrödinger equation in the form

$$\psi(x, t) = \sum_n a_n(t)\psi_n(x, t)\exp\left\{-i\int^t E_n(t')\,dt'\right\}. \quad (1)$$

Here $\psi_n(x,t)$ satisfies an equation with a Hamiltonian that has a parametric time dependence

$$H(t)\psi_n(x, t) = E_n(t)\psi_n(x, t), \quad (2)$$

and x denotes the set of all the coordinates.

Since we intend to continue the solutions of (2) into the region of complex t, we subject the functions $\psi_n(x,t)$ to analytic orthonormalization conditions (without complex conjugation)

$$\int\psi_n(x, t)\psi_m(x, t)\,dx = \delta_{mn}. \quad (3)$$

Substituting (1) into the temporal Schrödinger equation and using (2), we obtain

$$\dot{a}_n + \sum_{m\neq n} c_{mn}a_m\exp\left\{i\int^t \omega_{nm}(t')\,dt'\right\} = 0,$$

$$c_{mn} = \int\dot{\psi}_m(x, t)\psi_n(x, t)\,dx,$$

$$\omega_{mn}(t) = E_n(t) - E_m(t), \qquad \hbar = 1. \quad (4)$$

These equations must be solved subject to initial conditions*

$$a_n(t) \to \delta_{nk} \text{ as } t \to -\infty. \quad (5)$$

The adiabaticity condition $\omega T \gg 1$ (ω is the characteristic frequency $E_n - E_m$ of the Hamiltonian $H(t)$ and T is the characteristic time of its variation) implies smallness of c_{nm}/ω. This enables us to solve (4) by successive approximation.

In the first approximation we have

$$a_n(+\infty) = \int_{-\infty}^{\infty} c_{nk}\exp\left\{i\int^t \omega_{nk}(t')\,dt'\right\}dt. \quad (6)$$

The integral in (6) is calculated by the steepest descent method, and we obtain the well known result that the transition probabilities are exponentially small if the different terms n and k do not cross. If any two terms cross, then, as can be readily shown, the corresponding matrix element c_{nk} vanishes and there are no transitions between such states in the first approximation. As can be seen from (6), the probabilities are maximal for transitions to "neighboring" levels, such as are of interest to us.

It is easy to show (see, for example, [1]) that (6) yields the correct order of magnitude of the result (correct order of the exponential function), but an incorrect factor preceding the exponential function.

To obtain the correct pre-exponential factor it would be necessary to take into account the next orders of perturbation theory, all of which give results of the same order of magnitude. In practice, naturally, this is not feasible. However, if we consider the system (4) with t complex, we can readily show that a contribution to the transition probability is made only by the neighborhoods of the singular points of the Hamiltonian.

In fact, this property is possessed by all the terms of the perturbation-theory series. We can therefore solve the system (4) in the neighborhoods of the singular points of the Hamiltonian

*It is assumed that H(t) tends to constant values $H_\pm$ as $t \to \pm\infty$.

and then "join" the resultant solutions with the constant amplitudes a_n for $t \to \pm\infty$. It is obvious that the singularities of the Hamiltonian can be due only to crossing of the terms (for a complex value of the time t), or to splitting of the discrete term from the continuous spectrum. We consider the case when the singularities of the former type are significant.

If the Hamiltonian H has no special form then, generally speaking, only two terms can cross at a given point t_0.* To calculate the greatest transition probability within neighboring levels it is necessary to take into account only the point of intersection of these terms, i.e., to retain in the system (4) only the matrix elements c_{mn} corresponding to two levels. The system (4) is then transformed into two equations:

$$\dot{a}_1 + c_{12}\exp\left\{i\int^t \omega(t')\,dt'\right\}a_2 = 0,$$
$$\dot{a}_2 + c_{21}\exp\left\{-i\int^t \omega(t')\,dt'\right\}a_1 = 0. \qquad (7)$$

As can be seen from (5) and (3), $c_{21} = -c_{12}$. Thus, Eq. (7) contains two functions $\omega(t)$ and $c(t) \equiv c_{12}(t)$. To solve the system we must investigate the behavior of these functions near the point t_0 where the terms cross.

Solving the stationary solution for the two terms in the vicinity of the intersection point, we can obtain a relation between the transition frequency at the instant t and the frequency at the instant t_1 (see [2]):

$$\omega_{12}(t) = \{[\omega_{12}(t_1) + v_{11}(t_1, t) - v_{22}(t_1, t)]^2 + 4v_{12}^2(t_1, t)\}^{1/2}; \qquad (8)$$

here

$$v_{ik} = \int \psi_i(x, t_1)\,[H(t) - H(t_1)]\,\psi_k(x, t_1)\,dx.$$

It is natural to assume that the radicand in (8) has a simple zero when $t = t_0$; thus, $\omega(t)$ behaves like $(t - t_0)^{1/2}$ near the point of intersection of the terms.

The wave functions of the stationary states in the vicinity of the point of intersection of the terms are connected with the functions at the instant t_1 by the equations

$$\psi_1(t) = [(1 + k)^{1/2}\psi_1(t_1) - (1 - k)^{1/2}\psi_2(t_1)]/\sqrt{2},$$
$$\psi_2(t) = [(1 - k)^{1/2}\psi_1(t_1) + (1 + k)^{1/2}\psi_2(t_1)]/\sqrt{2}. \quad (9)$$

Here

$$k(t_1, t) = [\omega(t_1) + v_{11}(t_1, t) - v_{22}(t_1, t)]/\omega(t). \qquad (10)$$

Taking into account the fact that the wave functions at the instant t_1 are orthonormalized, we can readily obtain from (9)

$$c(t) = \int \dot{\psi}_2(x, t)\,\psi_1(x, t)\,dt = -\dot{k}/2\,(1 - k^2)^{1/2}. \qquad (11)$$

Using (10) and noting that as $t \to t_0$ the numerator in (10) tends to a constant value, we can easily obtain

$$c(t) = \dot{\omega}/2i\omega. \qquad (12)$$

In the vicinity of the term crossing point the system (7) has the form

$$\dot{a}_1 + \frac{\dot{\omega}}{2i\omega}a_2 \exp\left\{i\int^t \omega(t')\,dt'\right\} = 0,$$
$$\dot{a}_2 - \frac{\dot{\omega}}{2i\omega}a_1 \exp\left\{-i\int^t \omega(t')\,dt'\right\} = 0. \qquad (13)$$

These equations are conveniently solved with initial conditions

$$a_2 \to 0, \qquad a_1 \to 1 \text{ as } t \to -\infty. \qquad (14)$$

We introduce a new unknown function y(t) with the aid of the equality

$$y(t) = \frac{a_1}{\sqrt{\omega}}\exp\left\{-\frac{i}{2}\int^t \omega(t')\,dt'\right\} + \frac{ia_2}{\sqrt{\omega}}\exp\left\{\frac{i}{2}\int^t \omega(t')\,dt'\right\}. \qquad (15)$$

It is easy to verify that y(t) satisfies the equation

$$\ddot{y} + (\omega(t)/2)^2\,y = 0. \qquad (16)$$

From (14) and (15) follows an initial condition for

$$y \sim \exp\left\{-\frac{i}{2}\int^t \omega(t')\,dt'\right\} \text{ as } t \to -\infty. \qquad (17)$$

As $t \to +\infty$ we obtain

$$y \to A\exp\left\{-\frac{i}{2}\int^t \omega(t')\,dt'\right\} + R\exp\left\{\frac{i}{2}\int^t \omega(t')\,dt'\right\}. \qquad (18)$$

The value of R was calculated by Pokrovskii and Khalatnikov, who investigated the above-barrier reflection of a quasi-classical particle. Its value is

$$R = i\exp\left\{i\int^{t_0} \omega(t)\,dt\right\}. \qquad (19)$$

Comparing (18) and (15), we obtain the transition amplitude

$$a_2(+\infty) = \exp\left\{i\int^{t_0} \omega(t)\,dt\right\}. \qquad (20)$$

We see that the absolute value of the factor in front of the exponential function in the expression for the transition amplitude is unity. Expression (20) actually contains an arbitrary phase (since the lower limit of integration has not been defined). The phase of the transition amplitude can be determined accurate to π. Assume that when $t \to -\infty$ the wave function is

*The linear oscillator is in a class by itself, for all terms cross when $\omega = 0$.

$$\psi(t) \rightarrow \psi_1(x, -\infty) \exp[-iE_1(-\infty)t]. \qquad (21)$$

By virtue of conditions (3), the wave function $\psi_1(x, t)$ is defined apart from the sign. As $t \rightarrow +\infty$

$$\psi(t) \rightarrow a_1(+\infty)\psi_1(x, +\infty)\exp[-iE_1(+\infty)t] + a_2(+\infty)\psi_2(x, +\infty)\exp[-iE_2(+\infty)t]. \qquad (22)$$

Comparing (1) with (21) and (22) we can readily determine the phase of the transition amplitude, i.e., establish the lower limit of the integral in (19). Elementary calculations yield for $a_2(+\infty)$ the final expression

$$a_2(+\infty) = \exp\left\{ i \int_{-\infty}^{t_0} [E_1(t) - E_1(-\infty)]\,dt - i \int_{+\infty}^{t_0} [E_2(t) - E_2(+\infty)]\,dt + i\,[E_1(-\infty) - E_2(+\infty)]\,t_0 \right\}. \qquad (23)$$

The transition probability is

$$w_{12} = \exp\left\{ i \int_{t_0^*}^{t_0} \omega(t)\,dt \right\}. \qquad (24)$$

The formulas obtained determine completely the probability of transition of the quantum system to a "neighboring" level, with a maximum order of magnitude. As for transitions to farther levels, transitions through a virtual level can compete here with the above-considered process of "direct" transition. This question needs, however, additional investigation.

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