QUANTUM TRANSITIONS TO A CONTINUOUS SPECTRUM, DUE TO ADIABATIC PERTURBATIONS

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Submitted to JETP editor May 7, 1963

J. Exptl. Theoret. Phys. (U.S.S.R.) 45, 1518-1522 (November, 1963)

The probabilities for transition from the states of a discrete spectrum to a continuous spectrum under the action of an adiabatic perturbation are computed. The calculations are performed accurate to a numerical coefficient.

QUANTUM transitions between discrete-spectrum states were investigated in the adiabatic approximation by Dykhne[1,2]. It was made clear that the main feature of the problem is that all the terms of the adiabatic perturbation theory series are equal in magnitude, and that the entire series must be summed to obtain the correct result. This difficulty is overcome by considering the Schrödinger equation with complex values of the time. It is then sufficient to solve the equation in the vicinity of some points of the complex t plane, in which the adiabaticity conditions $\omega T \gg 1$ are violated (ω — natural frequency of the system and T — characteristic time of variation of the external conditions). Violation of adiabaticity can be connected either with singularities of the parameters of the Hamiltonian as functions of the time, with term crossing, or finally with transition from the discrete to the continuous spectrum. In the present paper we consider precisely the last type of singularity. The characteristic difficulty of this problem lies in the fact that for the continuous spectrum the adiabaticity condition $\omega T \gg 1$ is violated for all instants of time, and not only in the vicinity of the critical points ($\omega = 0$ for the continuous spectrum).

We shall assume that the potential decreases sufficiently rapidly with distance, so that the number of negative-energy levels is finite. The case when terms condense towards the boundary of the continuous spectrum calls for a separate analysis. The small parameter of the problem is the quantity $\alpha \equiv (\omega T)^{-1} \ll 1$. The meanings of ω and T are the same as before; ω obviously coincides in order of magnitude with the distance from the last discrete level to the boundary of the continuous spectrum $E = 0$.

The problem is formulated as follows: let the system be described by a Hamiltonian that depends parametrically on the time, and is in some state E_0 of the discrete spectrum as $t \to -\infty$. It is required to find the probability a(E) of observing the system in a state with energy $E > 0$ as $t \to +\infty$. This problem retains the main qualitative singularities of the ordinary adiabatic situation, such as the like contribution of all orders of perturbation theory.

There are, however, some essential differences. It becomes necessary to take into account the virtual transitions between the states of the continuum (see [2]). For transition to a state with any energy E, the critical point is the root of the equation $E_0(t) = 0$ and not $E_0(t) = E$ as in the case of the crossing of terms. Finally, the transition probability contains in the pre-exponential factor a power-law smallness in the adiabaticity parameter.

1. Let a particle with $l = 0$ be in a spherically symmetrical potential U(r), where the time variation of the parameters of the potential does not violate the symmetry. We also assume that the boundary of the continuous spectrum does not shift, i.e., $U(r \to \infty) = 0$ for all t.

We write down the Born-Fock system of equations[3], separating explicity the integrations over the continuous spectrum ($\hbar = m = 1$):

$$\dot{a}_n = \sum_{m \neq n} K_{nm}(t)\, a_m(t) + \int_0^\infty K_{n\varepsilon}(t)\, a(\varepsilon, t)\, d\varepsilon,$$

$$\dot{a}(E) = \sum_m K_{Em}(t)\, a_m(t) + \int_0^\infty K_{E\varepsilon}(t)\, a(\varepsilon, t)\, d\varepsilon,$$

$$K_{nm} = \int \dot{\psi}_n^* \psi_m dq \exp\left[i \int^t (E_n - E_m)\, dt' \right],$$

$$K_{Em} = \int \dot{\psi}_E^* \psi_m dq \exp\left[iEt - i \int^t E_m dt' \right],$$

$$K_{E\varepsilon} = \int \dot{\psi}_E^* \psi_\varepsilon\, dq \exp\left[i (E - \varepsilon) t \right], \qquad (1)$$

where ψ_E, ψ_n — instantaneous wave functions, satisfying the equations

$$H\psi_n^{(t)} = E_n(t)\psi_n(t), \qquad H\psi_E(t) = E\psi_E(t). \tag{2}$$

The wave functions of the continuous spectrum are assumed normalized to an energy δ-function.

Equations (1) must be solved in the vicinity of the point t_0, where any one of the discrete levels vanishes. The distance from this level to the other negative-energy levels remains of the same order of magnitude as that away from t_0 (the terms do not condense!). Consequently, in system (1) we can retain only those terms, which pertain to this discrete level E_0. As $T \to -\infty$ we should have $a_0 = 1$ and $a(E) \equiv 0$.

Solving these equations with respect to $a(E,t)$, we get

$$\dot{a}(E,t) = K_{E0}\Big[1 + \int_{-\infty}^{t} d\tau \int_0^\infty K_{0\varepsilon} a(\varepsilon,\tau)\, d\varepsilon\Big] + \int_0^\infty K_{E\varepsilon} a(\varepsilon,t)\, d\varepsilon. \tag{3}$$

2. Let us clarify the behavior of the matrix elements K_{0E} and $K_{E\epsilon}$ in the region of t close to t_0 of interest to us. The wave function of the state E_0 behaves asymptotically like $Cr^{-1}\exp(-k_0 r)$, where C is a normalization factor and $-k_0^2(t)/2 \equiv E_0(t)$. As $k_0(t) \to 0$, the normalization integral diverges at large r, so that we can calculate C from the asymptotic expression for $\psi_0(r)$. We get

$$\psi_0(r) = \sqrt{2k_0}\, e^{-k_0 r}/r. \tag{4}$$

In the region inside the potential well we can neglect $k_0^2(t)$ as $t \to t_0$. The Schrödinger equation assumes the form

$$\chi_0'' - 2U(r)\chi_0 = 0, \qquad \chi_0(r) = \psi_0(r)/r. \tag{5}$$

The potential $U(r)$ can be written in the form $U_0 f(r/L)$, where U_0 and L are the characteristic depth and width of the well, and the function $f(x)$ is of the order of unity in the interval $x \equiv r/L \sim 1$. By finding for (5) a solution that vanishes at $x = 0$, and calculating the logarithmic derivative χ_0 for $x \sim 1$, we obtain a certain function F of a single parameter U_0L^2.

The eigenvalue k_0 is determined from the equation

$$-k_0 L = F(U_0 L^2). \tag{6}$$

The zeroes of the function F determine the critical values of the parameter E_0L^2, for which the discrete levels vanish from the well. We assume these zeroes to be simple, inasmuch as this is justified in all the known cases that admit of an exact solution of the Schrödinger equation. Obviously, the zeroes of $k_0(t)$ will also be simple, since the critical values of the parameter U_0L^2 are attained at the regular points $U_0(t)$ and $L(t)$ as functions of the time.

The zeroes of $k_0(t)$ are located in complex-conjugate points of the plane, since k_0 is real on the real axis. We consider first the simplest case, when the region of the transition is much smaller than the distance between the zeroes. The following representation then holds true for $k_0(t)$:

$$k_0(t) = \dot{k}_0(t_0)\,(t - t_0). \tag{7}$$

The dimension of the transition region is determined by the condition

$$\int_{t_0}^{t} \Big(\frac{k_0^2(\tau)}{2} + E\Big)\, d\tau = \frac{\dot{k}_0^2 (t-t_0)^3}{6} + E(t-t_0) \sim 1. \tag{8}$$

There are two possibilities: either the term in (8) is much larger than or of the same order as the second, and then the transition region is $t - t_0 \sim k_0^{-2/3} \sim \alpha^{1/3} T$ and does not depend on E, or else the second term is much larger than the first. It is easy to see, however, that we can confine ourselves only to the first case. In fact, this means that we are considering energies satisfying the condition $E \lesssim U_0\alpha^{2/3}$. On the other hand, it follows from (3) that the amplitude of the probability of transition into the state E is essentially proportional to $\exp(iEt_0) \sim \exp(-ET) \sim \exp(E/\alpha U_0)$. Thus, the main contribution is made by states with $E \sim \alpha U_0$, and we can confine ourselves to a solution of Eq. (3) for $E \ll U_0\alpha^{2/3}$.

In the transition region $E_0(t)$ is of the order of $U_0\alpha^{2/3}$. It follows therefore that in the calculation of the matrix elements K_{0E} and $K_{E\epsilon}$ the main contribution to the integrals will be made by the regions of values of r which are much smaller than the dimensions of the well. We assume that the number of discrete levels is of the order of unity, i.e., $U_0L^2 \sim 1$. This means that $1/k_0 \sim U_0^{-1/2}\alpha^{-1/3} \gg L$ and $1/k \equiv 1/\sqrt{2E} \gg U_0^{1/2}\alpha^{-1/3} \gg L$. We must therefore replace the wave functions ψ_0 and ψ_E by their asymptotic expressions. For ψ_0 the asymptotic expression is given by (4), and for ψ_E by

$$\psi_E = (2/\pi k)^{1/2} r^{-1} \sin[kr + \delta(k)]. \tag{9}$$

It remains to determine the phase $\delta(k)$. We see that the inequalities obtained above, $k_0L \ll 1$ and $kL \ll 1$, are the conditions for the applicability of the resonant-scattering theory. In this case, as is well known (see [4]), the phase in the asymptotic expression for the wave function of the continuous spectrum is given by

$$\tan\delta(k) = -k/k_0(t). \qquad (10)$$

We are now in a position, using (4), (9), and (10), to calculate the coefficients K_{E0} and $K_{E\epsilon}$ of (3). As a result we get

$$K_{E0} = \frac{2}{\sqrt{\pi}} \frac{\dot{k}_0 \sqrt{k_0}\,(2E)^{1/4}}{(k_0^2+2E)^{3/2}} \exp\left[iEt + \frac{i}{2}\int_*^t k_0^2(\tau)\,d\tau\right],$$

$$K_{E\varepsilon} = \frac{1}{\pi} \frac{\dot{k}_0\,(2E\cdot 2\varepsilon)^{1/4}}{(k_0^2+2E)^{1/2}\,(k_0^2+2\varepsilon)^{1/2}} \mathrm{P}\frac{1}{E-\varepsilon} e^{i(E-\varepsilon)t}, \qquad (11)$$

where P is the symbol for the principal value.

The calculation of $K_{E\epsilon}$ shows that the integral in the last term of (3) must be taken in the sense of the principal value. This question does not arise with respect to the first term, since the integrand is continuous.

3. Using (7) and (11), and introducing new variables W and τ as well as a new unknown function $C(W, \tau)$ by means of the formulas

$$W = E\,[\dot{k}_0(t_0)]^{-2/3}, \qquad \tau = (t-t_0)\,[\dot{k}_0(t_0)]^{2/3},$$

$$a(E,t) = \frac{E^{1/4}}{\sqrt{\dot{k}_0(t_0)}} \exp\left(iEt_0 + \frac{i}{2}\int_*^{t_0} k_0^2(t)\,dt\right) C(W,\tau), \qquad (12)$$

we obtain the following equation for $C(W, \tau)$

$$\frac{\partial C(W,\tau)}{\partial\tau} = \frac{2^{5/4}}{\sqrt{\pi}} \frac{\sqrt{\tau}}{(\tau^2+2W)^{3/2}} \exp\left(iW\tau + \frac{i}{3}\tau^3\right)$$
$$\times\left\{1 + \frac{2^{5/4}}{\sqrt{\pi}} \int_{-\infty}^{\tau} \sqrt{\tau'}\,d\tau' \int_0^{\infty} \sqrt{\frac{W'}{(2W'+\tau'^2)^3}}\right.$$
$$\left.\times \exp\left(-iW'\tau' - \frac{i}{3}\tau'^3\right) C(W',\tau')\,dW'\right\} + \frac{\sqrt{2}}{\pi} \frac{e^{iW\tau}}{\sqrt{2W+\tau^2}}$$
$$\times \mathrm{P}\int \sqrt{\frac{W'}{2W'+\tau^2}} \frac{e^{-iW'\tau}}{W-W'} C(W',\tau)\,dW'. \qquad (13)$$

We were unable to find a solution of Eq. (13). It is easy to note, however, that this equation does not contain the parameters of the problem at all. In addition, we are interested only in the region $W \ll 1$, which corresponds to the inequality presented above $E \ll U_0\alpha^{2/3}$. We can verify by direct substitution that for fixed τ and as $W \to 0$ the function $C(W, \tau)$ tends to a constant. The magnitude of this constant is determined by the behavior of $C(W, \tau)$ in the region $W \sim 1$, so that we cannot seek $C(W \to 0, \tau)$ by putting formally $W = 0$ in (13).

Thus, the probability of transition to the continuous spectrum is obtained accurate to the numerical factor

$$g \equiv C(W \to 0,\ \tau \to +\infty), \qquad (14)$$

and we arrive at the following result:

$$a(E, t \to +\infty) = g\frac{E^{1/4}}{(\dot{k}_0)^{1/2}} \exp\left(iEt_0 + \frac{i}{2}\int_*^{t_0} k_0^2(t)\,dt\right). \qquad (15)$$

The energy distribution in the continuous spectrum is of the form

$$\frac{dn(E)}{dE} = \frac{|g|^2}{|\dot{k}_0|} \exp\left\{\frac{i}{2}\int_{t_0^*}^{t_0} k_0^2(t)\,dt\right\} \sqrt{E}\,e^{-E\sigma},$$
$$\sigma \equiv 2|\operatorname{Im} t_0|. \qquad (16)$$

The total probability of "ionization" P is equal to

$$P = \frac{\sqrt{\pi}}{2}|g|^2 \exp\left\{\frac{i}{2}\int_{t_0^*}^{t_0} k_0^2(t)\,dt\right\} \Big/ |\dot{k}_0|\,\sigma^{3/2} \sim \sqrt{\alpha}\,e^{-A/\alpha},$$
$$A \sim 1. \qquad (17)$$

If we are dealing with atomic collisions [1)], then the role of the time is assumed by the quantity $\int dR/v(R)$, where R and v are the relative coordinate and the velocity of the nuclei. For the ionization probability as a function of the velocity of the colliding atoms we obtain the expression

$$P(v) \sim \sqrt{v/v_0}\,e^{-v_0/v}, \qquad (18)$$

where v_0 is a quantity on the order of the orbital electron velocity.

The author is grateful to A. M. Dykhne and V. L. Pokrovskiĭ for valuable remarks and for a discussion of the work.

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[2] A. M. Dykhne, JETP **41**, 1324 (1961), Soviet Phys. JETP **14**, 941 (1962).

[3] L. Schiff, Quantum Mechanics, McGraw-Hill, New York, 1949.

[4] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Pergamon, 1958.

Translated by J. G. Adashko
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[1)] For example, the decay of negative ions in slow collisions. The number of discrete levels of the "extra" electron is finite, corresponding to the situation considered above.