QUANTUM TRANSITIONS IN THE ADIABATIC APPROXIMATION

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Submitted to JETP editor August 24, 1959

J. Exptl. Theoret. Phys. (U.S.S.R.) **38**, 570-578 (February, 1960)

The probabilities of quantum transitions in the discrete spectrum have been found in the adiabatic approximation assuming a very simple time dependence of the Hamiltonian. The time behavior of the adiabatic invariants has been examined on the example of the classical linear oscillator.

1. ACCURACY OF THE ADIABATIC INVARIANTS

IN certain physical problems we encounter quantities which change very little for slow variations of the external conditions. Such quantities are called adiabatic invariants. Examples of adiabatic invariants are the ratio of the energy over the frequency of the harmonic oscillator or the magnetic moment of a particle in a space or time dependent magnetic field. The adiabatic invariants of quantum mechanics are the quantum numbers, as was first noted by Einstein.[1] It is clear that the adiabatic invariants are not exact integrals of motion. The problem of the accuracy with which the adiabatic invariants are conserved has been discussed in a number of papers.[2-5]

Let α be a small parameter which characterizes the "slowness" of the change in the external conditions as compared to the characteristic period of the motion of the system. For example, in the case of a particle moving in a magnetic field which varies slowly in space or time, we have the parameters $r_L H^{-1}\nabla H$ and $\omega_L^{-1} H^{-1} dH/dt$, respectively, where H is the magnetic field, and r_L and ω_L are the Larmour radius and frequency. In the case of the oscillator this parameter is the ratio $\omega^{-2} d\omega/dt$.

Alfvén[2] has shown that the magnetic moment of a particle in a magnetic field is conserved with an accuracy up to first order in the small parameter. It was then found by Helwig[3] that the invariants are conserved with an accuracy up to the next order of smallness. Later it was shown by Kruskal for the motion of a particle in a magnetic field, and by Kulsrud[4] for the classical harmonic oscillator, that the adiabatic invariants are conserved with an accuracy including all powers of the small parameter. Finally, Lenard[5] proved the same for the nonlinear one-dimensional oscillator

The following derivation refers to the case in which the variation of the external conditions can be described by an analytic function of the time. It will be shown that in this case the variation of the adiabatic invariant of the classical oscillator is exponentially small. The calculation of this variation will be carried out.* Let us assume that the oscillator frequency $\omega(t)$ takes the constant values $\omega_\pm$ as $t \to \pm\infty$. The asymptotic values of the action $J = E/\omega$ for $t \to \pm\infty$ are equal to $J_\pm$. We seek the variation $\Delta J = J_+ - J_-$.

The real solution of the oscillator equation

$$\ddot{x} + \omega^2(t)\, x = 0 \qquad (1.1)$$

has the asymptotic form

$$x_\pm = \tfrac{1}{2}(c_\pm e^{i\omega_\pm t} + c_\pm^* e^{-i\omega_\pm t}). \qquad (1.2)$$

It is known, on the other hand, that there exists a complex solution of the equation of the type (1.1) which has the asymptotic form

$$y_- = e^{i\omega_- t} + Re^{-i\omega_- t}, \quad y_+ = De^{i\omega_+ t}, \qquad (1.3)$$

where R and D are the amplitudes of the reflected and transmitted waves. Taking the real part of (1.3) and comparing with (1.2), we find

$$c_- = 1 + R^*, \; c_+ = D. \qquad (1.4)$$

From the conservation law for the number of particles we obtain the following relation between R and D:

$$\omega_-(1 - |R|^2) = \omega_+ |D|^2. \qquad (1.5)$$

For the action of the oscillator we find from (1.2)

$$J_\pm = \tfrac{1}{2}\,\omega_\pm c_\pm c_\pm^*. \qquad (1.6)$$

Using (1.4) and (1.5) we can write the equation (1.6) in the form

*The idea of this derivation is due to L. P. Pitaevskiĭ.

$$J_- = \tfrac{1}{2}\omega_- |1+R|^2, \quad J_+ = \tfrac{1}{2}\omega_-(1-|R|^2). \quad (1.7)$$

We have thus

$$J_- - J_+ = \omega_-(|R|^2 + \operatorname{Re} R). \quad (1.8)$$

We emphasize that this expression is exact.

In order to go over to the adiabatic approximation, we must substitute in (1.8) the reflection amplitude R as calculated in the quasi-classical approximation. This calculation was done by Pokrovskiĭ et al.[6] If $\omega^2(t)$ is an analytic function without zeroes on the real axis and a simple root at the point t_0 of the complex plane, we have thus

$$R = -i \exp\left\{2i \int^{t_0} \omega(t)\,dt\right\}. \quad (1.9)$$

Substituting (1.9) in (1.8), we obtain

$$J_- - J_+ = \omega_-(e^{-4\sigma} + \sin 2\rho e^{-2\sigma}), \quad \rho + i\sigma = \int^{t_0} \omega(t)\,dt, \quad (1.10)$$

where ρ and σ are real numbers.

We see that the variation of the adiabatic invariant is an exponentially small quantity. Besides this, the variation depends on the "initial" phase, owing to the presence of the term Re R in (1.8). It is easily shown that, if the k-th derivative of the function $\omega(t)$ has a finite discontinuity on the real axis, the variation of the adiabatic invariant is proportional to the k-th power of the small parameter.

2. QUANTUM TRANSITIONS IN THE DISCRETE SPECTRUM

As is known,[7] the adiabatic invariants of quantum mechanics are the quantum numbers and the distribution over the stationary states of the system. The problem of the variation of the adiabatic invariants with time is, therefore, essentially the problem of calculating the transition probabilities between the stationary states. This problem of quantum mechanics can be solved only by a few methods, in particular, that of perturbation theory. Below we shall develop a method which permits the computation of transition probabilities in a special case in which perturbation theory is not applicable.

Let us assume that the Hamiltonian of the system with a discrete spectrum depends on some parameter $\lambda(t)$ which is a slowly varying function of time. The parameter $\lambda(t)$ goes asymptotically to $\lambda_\pm$ for $t \to \pm\infty$. For $t \to \pm\infty$ the system then has stationary states. We emphasize that the difference between the asymptotic values of the energy at $t \to \pm\infty$ is not assumed to be small, but can have any arbitrary value. The small parameter used in the solution is the ratio

$$\omega_{mn}^{-1}\, d\ln\lambda / dt = \alpha, \quad (2.1)$$

where ω_{mn} is the transition frequency of the Hamiltonian $H(\lambda)$.

Our procedure is the following: let us assume that for $t \to -\infty$ the system was in the n-th stationary state of the Hamiltonian H (the value of the Hamiltonian H for $\lambda(t) = \lambda_-$). The wave function of the system was then ψ_{n-}. For $t \to +\infty$ the wave function can be expanded in terms of the eigenfunctions of the Hamiltonian H_+ $(\lambda = \lambda_+)$:

$$\psi = \sum_k a_{nk}\psi_{k+}. \quad (2.2)$$

The problem consists in finding the transition amplitudes a_{nk}. We note that it is meaningless to ask for the transition amplitudes at intermediate times, since the Hamiltonian depends on the time and stationary states can be defined only with an accuracy given by $\omega_{mn}^{-1}\partial H/\partial t$.

The solution of the proposed problem will be discussed first on the example of the harmonic oscillator.

3. THE QUANTUM OSCILLATOR IN THE ADIABATIC APPROXIMATION

The problem consists in solving the Schrödinger equation

$$i\partial\psi / \partial t = H\psi \quad (3.1)$$

with the Hamiltonian

$$H = -\tfrac{1}{2}\partial^2/\partial x^2 + \tfrac{1}{2}\omega^2(t)\,x^2. \quad (3.2)$$

Here and in the following we set $\mu = \hbar = 1$. Let us assume that for $t = t_0 \to -\infty$ there exists a solution of the stationary equation

$$H(t_0)\,\psi(t_0) = E(t_0)\,\psi(t_0). \quad (3.3)$$

As is well known (see, for example, reference 8), the solution of (3.1), $\psi(t)$, can then be expressed through $\psi(t_0)$,

$$\psi(t) = S(t_0, t)\,\psi(t_0), \quad (3.4)$$

with the help of the S matrix, which satisfies the equation

$$i\partial S / \partial t = HS. \quad (3.5)$$

Using (3.4), we can rewrite (3.3) in the form of an equation for $\psi(t)$:

$$H(t_0, t)\,\psi(t) = E(t_0)\,\psi(t), \quad (3.6)$$

where

$$H(t_0, t) = S^{-1}(t_0, t)\,H(t_0)\,S(t_0, t)$$

is the usual oscillator Hamiltonian made up of the operators $\hat{p}(t_0, t)$ and $\hat{x}(t_0, t)$. These latter can be determined from the equation of motion

$$\ddot{\hat{x}} + \omega^2(t)\,\hat{x} = 0. \qquad (3.7)$$

By virtue of its linearity we can solve this equation assuming that $\hat{x}$ is a c number. The solution for $t \to \pm\infty$ is asymptotically

$$\hat{x}_\pm = \hat{c}_\pm e^{i\omega_\pm(t-t_0)} + \hat{c}_\pm^+ e^{-i\omega_\pm(t-t_0)},$$
$$\hat{p}_\pm = i\omega_\pm\,[\hat{c}_\pm e^{i\omega_\pm(t-t_0)} + \hat{c}_\pm^+ e^{-i\omega_\pm(t-t_0)}]. \qquad (3.8)$$

From the definition of the operators in the Heisenberg representation we have for $t_0 = t$

$$\hat{x}\,(t,\,t) = \hat{x},\ \hat{p}\,(t,t) = \hat{p}. \qquad (3.9)$$

From this we find easily

$$\hat{c}_+ = \tfrac{1}{2}\,(\hat{x} - i\omega_+^{-1}\hat{p}). \qquad (3.10)$$

The connection between $\hat{c}_+$ and $\hat{c}_-$ is readily obtained by a method analogous to that described in Sec. 1 for the classical oscillator. The result is

$$\hat{c}_- = (1 - |R|^2)^{-1} D^*\,(\hat{c}_+ - R\hat{c}_+^+). \qquad (3.11)$$

Here R and D are the reflection and transmission amplitudes in the corresponding scattering problem.

Using (3.8), we find

$$\hat{c}_- = \frac{D^*}{2(1-|R|^2)}\left[(1-R)\,\hat{x} + \frac{\hat{p}}{i\omega_+}(1+R)\right]. \qquad (3.12)$$

Substituting (3.8) in the Hamiltonian

$$H_- = \omega_-^2\,(\hat{c}_-\hat{c}_-^+ + \hat{c}_-^+\hat{c}_-)$$

and using the law of conservation of the number of particles, we obtain

$$H\,(t_0, t) = \frac{\omega_+\omega_-}{2(1-|R|^2)}\Big\{|1-R|^2\hat{x}^2 + \frac{\hat{p}^2}{\omega_+^2}|1+R|^2$$
$$+ \frac{1}{\omega_+}\,\mathrm{Im}\,[(1+R)\,(1-R^*)]\,(\hat{p}\hat{x} + \hat{x}\hat{p})\Big\}. \qquad (3.13)$$

As can be readily verified, the normalized solution of equation (3.6) with the Hamiltonian (3:13) has now the form

$$\psi_n(t) = \left(\frac{\omega_+}{\pi}\,\mathrm{Re}\,\frac{1-R}{1+R}\right)^{1/4}(2^n n!)^{-1/2}\exp\left\{-\frac{\omega_+ x^2}{2}\,\frac{1-R}{1+R}\right\}$$
$$+ H_n\left[\left(\omega_+\,\mathrm{Re}\,\frac{1-R}{1+R}\right)^{1/2} x\right], \qquad (3.14)$$

where the H_n are Hermite polynomials. For the computation of the transition amplitudes we must expand this function in terms of the eigenfunctions ψ_{k^+} of the Hamiltonian H_+,

$$\psi_{k+} = (\omega_+/\pi)^{1/4}(2^k k!)^{-1/2}\exp\{-\omega_+ x^2/2\}\,H_k(\omega_+^{1/2}x). \qquad (3.15)$$

The amplitudes are equal to

$$a_{nk} = \int_{-\infty}^{\infty}\psi_n(t)\,\psi_{k+}^*\,dx. \qquad (3.16)$$

If we assume that $R \ll 1$, the main part of the transition amplitude can be calculated from the leading term in the integral defining a_{nk}:

$$I_{nk} = \int_{-\infty}^{\infty}\exp(-\xi^2)\exp(R\xi^2)\,H_n[(1-\mathrm{Re}\,R)\,\xi]\,H_k(\xi)\,d\xi$$
$$\xi = \sqrt{\omega_+}\,x. \qquad (3.17)$$

The integral (3.17) is calculated in the Appendix. The result is

$$a_{nk} = \left(\frac{k!}{n!}\right)^{1/2} 2^{(n-k)/2}\left[\left(\frac{k-n}{2}\right)!\right]^{-1} R^{(k-n)/2}$$
$$+ O\,(R^{(k-n)/2+1})\ \text{for}\ k > n,$$
$$a_{nk} = \left(\frac{n!}{k!}\right)^{1/2} 2^{(k-n)/2}\left[\left(\frac{n-k}{2}\right)!\right]^{-1}(-R^*)^{(n-k)/2}$$
$$+ O\,(R^{(n-k)/2+1})\ \text{for}\ k < n, \qquad (3.18)$$

in particular

$$a_{nn} = 1 + O\,(R). \qquad (3.19)$$

We see in this way that the main part of the transition amplitude is a universal matrix multiplied by some power of the reflection amplitude.

Since $\omega(t)$ is assumed to be a slowly varying function of time, we must find the reflection amplitude R in the quasi-classical approximation. We quote here the corresponding results from the paper of Pokrovskiĭ, Savvinykh, and Ulinich,[6] where this computation was carried out.

If $\omega^2(t)$ is an analytic function without zeroes on the real axis and a simple root at the point t_0 of the complex plane, the reflection amplitude is equal to

$$R = F\,(\mu/\alpha)\exp\left\{2i\int^{t_0}\omega\,(t)\,dt\right\},$$
$$F\,(x) = \frac{2\pi i\exp\{ix\ln(x/2e) - \pi x/2\}}{\Gamma(ix/2)\,\Gamma(1+ix/2)}. \qquad (3.20)$$

Here μ is a parameter of the order of the quantity $(\omega_+ - \omega_-)/(\omega_+ + \omega_-)$ (not necessarily small), and α is a small parameter of the order of the quantity ω'/ω^2 (for the exact definition of these parameters see reference 6).

If $x = \mu/\alpha \to 0$, $|F(x)| \approx \pi x$, which corresponds to the case where perturbation theory is valid. For $x \to \infty$, $F(x) \approx -i$. Then

$$a_{nk} = \begin{cases} \left(\frac{k!}{n!}\right)^{1/2} 2^{(n-k)/2}\left[\left(\frac{k-n}{2}\right)!\right]^{-1}\exp\left\{i(k-n)\int^{t_0}\omega\,(t)\,dt\right\} & (k>n) \\ \left(\frac{n!}{k!}\right)^{1/2} 2^{(k-n)/2}\left[\left(\frac{n-k}{2}\right)!\right]^{-1}\exp\left\{i(n-k)\int^{t_0^*}\omega\,(t)\,dt\right\} & (k<n). \end{cases} \qquad (3.21)$$

We see that the transition amplitude is exponentially small and the transition probability does not depend on the "initial" phase.

By taking the classical limit of (3.18) we readily obtain the variation of the adiabatic invariant for the classical oscillator. We shall present here the corresponding calculation with an accuracy up to the first order in the reflection coefficient R. To obtain the quasi-classical wave function, we must take a wide selection of states in the region of large quantum numbers.

Let this wave function be

$$\Phi_\pm = \sum \gamma_n^\pm \psi_n^\pm \text{ for } t \to \pm\infty. \quad (3.22)$$

We note here that the $\gamma_n^\pm$ must satisfy the following condition in order that the function $\Phi_\pm$ describe a classical particle on a trajectory:

$$(1/\gamma_n^\pm)\, d\gamma_n^\pm / dn \ll 1. \quad (3.23)$$

The average value of the action $J_\pm$ is determined by

$$J_\pm = \sum_n |\gamma_n^\pm|^2 \left(n + \tfrac{1}{2}\right). \quad (3.24)$$

We have the following relation between γ_n^+ and γ_n^- with an accuracy up to order R:

$$\gamma_n^+ = \gamma_n^- a_{nn} + \gamma_{n-2}^- a_{n-2,\,n} + \gamma_{n+2}^- a_{n+2,\,n}. \quad (3.25)$$

The transition amplitudes a_{mn} for large m and n can be written asymptotically

$$a_{nn} = 1 + i \operatorname{Im} R\left(n + \tfrac{1}{2}\right), \qquad a_{n+2,\,n} = \tfrac{1}{2}\left(n - \tfrac{1}{2}\right) R,$$

$$a_{n-2,\,n} = -\tfrac{1}{2}\left(n + \tfrac{3}{2}\right) R^*. \quad (3.26)$$

Substituting (3.26) in (3.25) and using (3.23), we readily obtain

$$|\gamma_n^+|^2 = |\gamma_n^-|^2 (1 - 2 \operatorname{Re} R). \quad (3.27)$$

As can be seen from (3.24), we have then

$$(J_+ - J_-)/J_+ = -2 \operatorname{Re} R.$$

This result agrees with an accuracy up to order R with the variation of the action of the classical oscillator as found in Sec. 1 [cf. Eq. (1.8)].

4. TRANSITION PROBABILITIES FOR POTENTIALS OF THE FORM λ(t) V(x)

Let us now consider the problem of calculating the transition amplitudes for a potential of the type λ(t) V(x) with a discrete spectrum. We determine the eigenfunctions and the eigenvalues of the time dependent Hamiltonian from the equation

$$H(x|t)\psi_n(x|t) = E_n(t)\psi_n(x|t) \quad (4.1)$$

and expand the wave function in terms of these functions. For the expansion coefficients we obtain a system of equations which is usually taken as the basis of adiabatic perturbation theory (see, for example, reference 8):

$$a_n = \sum_{k \neq n} \omega_{nk}^{-1} a_k (\partial H/\partial t)_{nk} \exp\left\{i \int^t \omega_{nk}(t)\, dt\right\}. \quad (4.2)$$

If $a_k \to \delta_{km}$ for $t \to -\infty$, we conclude from (4.2)

$$a_n(t) = \delta_{mn} + \sum_{k \neq n} \int_{-\infty}^{t} \omega_{nk}^{-1} a_k(t') (\partial H/\partial t')_{nk} \times \exp\left\{i \int^{t'} \omega_{nk}(t'')\, dt''\right\} dt'. \quad (4.3)$$

We apply the iteration method to equation (4.3), taking $\omega_{mn}^{-1}\partial H/\partial t$ as a small quantity. Assuming that $\omega_{nk} \neq 0$ on the real axis, we can close the contour of integration either in the upper or in the lower half plane. Therefore only the poles of the expression under the integral (4.3) will play a role in the iteration series. It is natural to assume that the poles of the expression under the integral (4.3) will coincide with the zeroes and poles of the function λ(t).

Let us consider the behavior of the integrand near a zero of the function λ(t). (The analytic continuation of the solutions of the stationary equation (4.1) into the complex plane will be taken along the line Im λ = 0.) Let us assume that the asymptotes of V(x) follow a power law, which for simplicity we take to be the same in both cases:

$$V(x) \approx A|x|^{2l} \qquad (l > 0) \text{ for } x \to \pm\infty. \quad (4.4)$$

We write V(x) in the form

$$V(x) = A|x|^{2l} + U(x). \quad (4.5)$$

Let us introduce the new variable

$$\xi = \lambda^{1/2(l+1)} x.$$

In this case equation (4.1) takes the form

$$d^2\psi_n/d\xi^2 + [E_n \lambda^{1/(l+1)} + A|\xi|^{2l} + \lambda^{l/(l+1)} U(\xi\lambda^{-1/2(l+1)})]\psi_n = 0. \quad (4.6)$$

It is seen from (4.4) that the inequality

$$A|\xi|^{2l} \gg \lambda^{l/(l+1)} U(\xi\lambda^{-1/2(l+1)}) \quad (4.7)$$

is valid everywhere except in a small region of order $\lambda^{1/2(l+1)}$ near $\xi = 0$. For the solution of equation (4.1) near a zero of λ(t) we can therefore replace the potential in (4.1) by its asymptotic value. It is then readily verified that (4.3) can be rewritten in the form

$$a_n(t) = \delta_{mn} + \sum_{k \neq n} \int_{-\infty}^{t} c_{nk} a_k \lambda' \lambda^{-1} \exp\left\{i \int^{t'} \omega_{nk}\, dt''\right\} dt', \quad (4.8)$$

where c_{nk} is a matrix which depends only on the asymptotic form of V(x) and not on the form of the function λ(t).

From (4.8) we obtain for the transition amplitude in first approximation

$$a_{nm} = B'_{nm} \exp \left\{ i \int^{t_0} \omega_{mn} \, dt \right\}. \quad (4.9)$$

Here B'_{nm} is a matrix which is completely determined by the first term in the asymptotic expansion of the potential. Since the same zero or pole which determines the first term in the iteration series used for the calculation of the integrals will play an analogous role in all succeeding terms, it is clear that all terms of this series will be proportional to the same exponential $\exp\{i\int^{t_0} \omega_{mn}\, dt\}$ and therefore have the same order of smallness. It is easily shown that the convergence of this series is guaranteed by the fast decrease of the factors multiplying the exponentials. By summing up the whole series we obtain the expression

$$a_{nm} = B_{mn} \exp \left\{ i \int^{t_0} \omega_{mn} \, dt \right\}. \quad (4.10)$$

Since the matrix B_{nm} is a universal quantity, it can be obtained from the solution of the Schrödinger equation with an arbitrary potential possessing the given asymptotic values. For example, if the potential has the asymptotic behavior Ax^2, we find for the transition amplitude, using the results of Sec. 3,

$$a_{nm} = \begin{cases} \left(\frac{m!}{n!}\right) 2^{(n-m)/2} \left[\left(\frac{m-n}{2}\right)!\right]^{-1} \exp\left\{ i \int^{t_0} \omega_{mn}\, dt \right\} & (m > n) \\ \left(\frac{n!}{m!}\right)^{1/2} 2^{(m-n)/2} \left[\left(\frac{n-m}{2}\right)!\right]^{-1} \exp\left\{ i \int^{t_0} \omega_{nm}\, dt \right\} & (m < n). \end{cases} \quad (4.11)$$

I take this opportunity to express my sincere gratitude to Yu. B. Rumer and V. L. Pokrovskiĭ for suggesting this problem and for many valuable comments concerning this work.

APPENDIX

We present here the approximate evaluation of the integral (3.17). We expand the function under the integral into a series in powers of R and Re R. The general term of this series is evidently equal to

$$\frac{R^p(-\operatorname{Re} R)^q}{p!\; q!} \int_{-\infty}^{\infty} \exp(-\xi^2)\, \xi^{2p+q} H_n^{(q)}(\xi) H_k(\xi)\, d\xi. \quad (A.1)$$

This matrix element is different from zero only if

$$2p + q \geqslant |n - k - q|. \quad (A.2)$$

It is seen from (A.1) that for given n and k the term with the lowest value of $p+q$ has the largest value. We must therefore look for the minimum of the expression $p+q$ under the subsidiary condition (A.2).

We discuss the cases $n < k$ and $n > k$ separately. In the first case formula (A.2) becomes $2p \geq k-n$. The minimum of $p+q$ occurs at $q = 0$, $p = (k-n)/2$. We therefore have

$$I_{nk} = \frac{R^p}{p!} (\xi^{k-n})_{nk} = R^{(k-n)/2} \left[\left(\frac{k-n}{2}\right)!\right]^{-1} \left(\frac{k!}{n!}\right)^{1/2} \times 2^{(n-k)/2} + O(R^{(k-n)/2+1}). \quad (A.3)$$

If $n > k$, (A.2) gives

$$p + q \geqslant (n-k)/2. \quad (A.4)$$

In this case we must sum over all terms of the series which satisfy the condition $p+q = (n-k)/2$. As can be readily seen, this sum is equal to

$$\sum_{p,q} \frac{R^p(-\operatorname{Re} R)^q 2^q}{p!\; q!} (\xi^{n-k})_{nk} = \left(-R^*\right)^{(n-k)/2} \times \left[\left(\frac{n-k}{2}\right)!\right]^{-1} \left(\frac{n!}{k!}\right)^{1/2} 2^{(k-n)/2} + O\left(R^{(n-k)/2+1}\right). \quad (A.5)$$

Formulas (A.3) and (A.5) lead to (3.18).

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Translated by R. Lipperheide
111