QUANTUM TRANSITIONS TO A CONTINUOUS SPECTRUM INDUCED BY AN ADIABATIC PERTURBATION. II

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Adiabatic perturbation of the states of a particle in a spherically symmetric field is investigated for arbitrary values of the angular momentum. The dependence of the transition probability to a continuous spectrum on the energy and adiabaticity parameter is determined. A system model with an infinite number of discrete levels that condense towards the continuum boundary is considered.

1. In the first part of this paper (see [1]) we investigated the adiabatic perturbation of the s-state of a particle in a spherically-symmetrical potential, and obtained the transition amplitude and the continuous spectrum, apart from a universal numerical factor. The case $l = 0$ in a centrally-symmetrical field is exceptional, owing to the absence of a centrifugal barrier. It is of interest to consider the same problem for arbitrary values of the angular momentum. It turns out that the corresponding analysis must be radically modified, and the final result is no longer as universal as when $l = 0$.

We assume as before that the number of the discrete levels is finite, and that the dependence of the Hamiltonian on the time does not violate spherical symmetry. The main contribution to the transition probability is given by the vicinity of the point t_0 of the complex plane t, in which the quantity $E_0(t)$ (the discrete level occupied by the system as $t \to -\infty$) vanishes. In the transition region, the inequalities $ka \ll 1$ and $k_0 \ll 1$ are satisfied (see [1] for notation). It is necessary to ascertain the behavior of the instantaneous eigenfunctions of the continuous and discrete spectra in the indicated region of energy values.

Let us consider first the potential $U(r) = U_0 f(r/a)$, which vanishes for $r > a$. In the internal region we can neglect the energy in the radial Schrodinger equation, incurring thereby a relative error of the order of $(k_0 a)^2$. The solution of the equation

$$\chi'' - \left[2U_0 f\left(\frac{r}{a}\right) + \frac{l(l+1)}{r^2}\right]\chi = 0, \qquad (1)$$

which vanishes when $r = 0$, will be denoted by $A\varphi_l(r/a; \lambda)$, where $\lambda^2 \equiv 2U_0 a^2$, with A constant. We shall assume that $\varphi_l(r/a; \lambda)$ is normalized by the condition $\varphi_l(1; \lambda) = 1$. For $r > a$ the solution of Eq. (1), corresponding to the discrete level $E_0 \equiv -k_0^2/2$, is of the form

$$\chi_0(r > a) = A\,[\sqrt{k_0 a} K_{l+1/2}(k_0 a)]^{-1} \sqrt{k_0 r} K_{l+1/2}(k_0 r). \qquad (2)$$

Here K—Macdonald function. The constant factor in (2) is chosen such as to satisfy the condition of continuity at $r = a$. Equating the logarithmic derivatives of the solution in the internal and external regions, we obtain an equation for the energy eigenvalues:

$$\frac{a^{-1}\varphi_l'(1; \lambda)}{\varphi_l(1; \lambda)}\,[1 + O((k_0 a)^2)] \equiv a^{-1} F_l(\lambda)\,[1 + O((k_0 a)^2)]$$

$$= \frac{d}{dr} \ln \left\{(k_0 r)^{-l} \sum_0^\infty c_n (k_0 r)^{2n} + (k_0 r)^{l+1} \sum_0^\infty b_n (k_0 r)^{2n}\right\}_{r=a} \qquad (3)$$

The Macdonald function is represented in the form of a power series. We transform (3), retaining only the principal terms in $k_0 a$:

$$F_l(\lambda)\,[1 + O((k_0 a)^2)]$$

$$= -l + 2\frac{c_1}{c_0}(k_0 a)^2 + \ldots + (2l+1)\frac{b_0}{c_0}(k_0 a)^{2l+1} + \ldots \qquad (4)$$

Equation (4) has a root $k_0 = 0$ if λ satisfies the relation $F_l(\lambda) + l = 0$. Let the corresponding value of λ be λ_0. For λ close to λ_0 (which corresponds to t close to t_0) we obtain

$$\lambda - \lambda_0 \sim (k_0 a)^2 + \ldots + \text{const} \cdot (k_0 a)^{2l+1} + \ldots \qquad (5)$$

As $t \to t_0$, the left side of (5), being a regular function of the time, vanishes in general linearly. When $l = 0$, the principal contribution of the right side of (5) is made by the term proportional to $(k_0 a)^{2l+1} = k_0 a$. As $t \to t_0$, consequently, $k_0(t)$ vanishes linearly and $E_0(t)$ vanishes quadratically,

as has been indeed assumed in [1]. For all the other values of l we obtain $E_0(t \to t_0) \sim t - t_0$. This circumstance changes somewhat the estimates of the quantities of interest, compared with the data of [1]. The dimension of the transition region is estimated with the aid of the relation

$$\int_{t_0}^{t} E_0(t)\,dt = \int_{t_0}^{t} \dot{E}_0(t_0)\,(t-t_0)\,dt \sim 1. \qquad (6)$$

Hence

$$t - t_0 \sim [\dot{E}_0(t_0)]^{-1/2} \sim (U_0/T)^{-1/2} = \sqrt{aT}.$$

The quantity $E_0(t)$ has in the region of the transition an order of magnitude $\sqrt{\alpha}\,U_0$. The essential energy region in the continuous spectrum corresponds, as before, to $E \sim \alpha U_0 \ll E_0(t)$ [1)].

Let us clarify now the question of the relative role of the internal and external regions in the calculation of the matrix elements $(\partial/\partial t)_{0E}$ and $(\partial/\partial t)_{E\epsilon}$. We write the normalization condition for the discrete-spectrum function:

$$A^2 \int_0^a \left[\varphi_l\left(\frac{r}{a};\lambda\right)\right]^2 dr + A^2\,[k_0 a K_{l+1/2}^2(k_0 a)]^{-1} \int_a^\infty k_0 r K_{l+1/2}^2(k_0 r)\,dr = 1. \qquad (7)$$

Introducing

$$s_l(\lambda) \equiv \int_0^1 \varphi_l^2(z;\lambda)\,dz$$

[$s(\lambda)$ is of the order of unity], we obtain from (7), in the principal order with respect to $k_0 a$

$$A^2 a s(\lambda) + A^2 (2k_0 a)^{2l} \int_a^\infty \exp(-2k_0 r) \times \left[\sum_{n=0}^{l} \frac{(l+n)!\,l!}{n!\,(l-n)!\,(2l)!}(2k_0 r)^{-n}\right]^2 dr = 1. \qquad (8)$$

When $l \neq 0$ the integral in the left side of (8) is equal to $(1/2k_0) \times [1 + O(k_0 a)]$, and the second term is much larger than the first. Therefore only the asymptotic region is of importance in the wave functions. On the other hand, if $l \neq 0$, then by virtue of the condition $k_0 a \ll 1$ the integral in (a) is taken essentially at the lower limit, so that we obtain

$$A^2 \left\{a s(\lambda) + \frac{a}{2l-1}[1 + O(k_0 a)]\right\} = 1. \qquad (9)$$

Thus, the internal and the external regions give contributions of equal order of magnitude to the normalization. Owing to the centrifugal barrier, the particle spends approximately an equal fraction of the time outside and inside the potential well, although its deBroglie wavelength is much larger than the dimension of the potential. We see therefore that the result of our problem should depend on the details of the potential, unlike the case $l = 0$ (compare with [1]).

Let us proceed to find the wave function χ_k in the energy region of significance. Accurate to quantities of order $(ka)^2$, the function χ_k coincides when $r < a$ with the solution $\varphi_l(r/a;\lambda)$ introduced above for Eq. (1). In the external region (normalization to an energy δ-function) we have

$$\chi_k(r > a) = \sqrt{r}[\sin\delta J_{-l-1/2}(kr) + (-)^l \cos\delta J_{l+1/2}(kr)]. \qquad (10)$$

By choosing the correct constant in front of $\varphi_l(r/a;\lambda)$ we obtain for $r < a$

$$\chi_k(r < a) = \sqrt{a}[\sin\delta J_{-l-1/2}(ka) + (-)^l \cos\delta J_{l+1/2}(ka)]\varphi_l(r/a;\lambda). \qquad (11)$$

In formulas (10) and (11) J denotes the Bessel function, and δ the scattering phase in the field $U(r)$. It is simplest to determine δ from the requirement that χ_0 and χ_k be orthogonal:

$$\int_0^a A\sqrt{a}\,[\sin\delta J_{-l-1/2}(ka) + (-)^l \cos\delta J_{l+1/2}(ka)]\,\varphi_l^2\left(\frac{r}{a};\lambda\right)dr + \int_a^\infty A\,[\sqrt{k_0 a}K_{l+1/2}(k_0 a)]^{-1}\sqrt{k_0 r}K_{l+1/2}(k_0 r) \times \sqrt{r}\,[\sin\delta J_{-l-1/2}(kr) + (-)^l \cos\delta J_{l+1/2}(kr)]\,dr = 0. \qquad (12)$$

The calculations yield in the principal order in ka

$$\tan\delta = -[(2l-1)!!]^{-2}\left[s(\lambda) + \frac{1}{2l-1}\right]^{-1} \frac{(ka)^{2l+1}}{(ka)^2 + (k_0 a)^2}. \qquad (13)$$

Formulas (2), (9)—(10), and (13) enable us to calculate the quantities

$$\int_0^\infty \dot{\chi}_0 \chi_k\,dr, \qquad \int_0^\infty \dot{\chi}_k \chi_{k'}\,dr$$

[1)] The estimates given pertain to values of l of the order of unity, so that the characteristic E_0 is of the order of U_0, and Im t_0 is of the order of T. With increasing l, the energy of the bound state decreases (in absolute value), and a situation can arise when the adiabaticity condition is violated for real t. This case calls for a separate analysis (two close points where adiabaticity is violated). Here, on the other hand, l is assumed such as to satisfy the inequality

$$\left|\int_{t_0^*}^{t_0} E_0(t)\,dt\right| \gg 1.$$

in the transition region. Only δ must be differentiated with respect to the time, since a and λ change little in the selected vicinity of the point t_0. The subsequent manipulation is perfectly analogous to that contained in [1]. Changing variables and the unknown function, we exclude the dimensional parameters from Eq. (3) of the first part of this paper (see [1]). The dependence on the details of the potential remains only in the form of $s(\lambda)$.

We obtain for the amplitude of transition into the state with energy E

$$a(E) = g_l(\lambda)\frac{(ka)^{l+1/2}}{[\dot{E}_0(t_0)]^{1/2}\,a}\exp\left[iEt_0 - i\int^{t_0} E_0 dt\right]. \quad (14)$$

The factor $g_l(\lambda)$ is not universal. Its value, however, is determined only by the value $s(\lambda)$ of the integral of the square of the wave function over the region inside the well. The energy distribution in the continuous spectrum is of the form

$$dn(E)/dE \equiv |a(E)|^2 \sim E^{l+1/2}e^{-\sigma E}, \qquad \sigma \equiv 2|\operatorname{Im} t_0| \quad (15)$$

(we have written out only the energy-dependent factors). The total "ionization" probability P depends on the adiabaticity parameter via the formula

$$P \sim \alpha^{l+1/2}\exp(-B_l/\alpha), \quad (16)$$

B_l does not depend on α.

In the case of smooth potentials, formulas (15) and (16) remain in force. Indeed, we then have for $\tan\delta$ a formula analogous to (13):

$$\tan\delta = -bk^{2l+1}/(E - E_0), \quad (17)$$

where b is a positive constant (see [2]). This leads to the same energy dependence of dn/dE and α—dependence of P. However, the coefficients in the corresponding formulas depend essentially on the form of the potential.

In concluding this section, we note the following. If in addition to the level E_0 there exist also quasidiscrete levels due to the centrifugal barrier, then a different "ionization" mechanism is possible along with the direct transition to the continuous spectrum. The system can effect a non-adiabatic transition to a quasidiscrete level and then decay. In this case the energy distribution in the continuous spectrum should have maxima at $E = \operatorname{Re}E_n$, where E_n—complex values of the energy of the quasi stationary states. The critical points for this type of transitions are the points of intersection t_n of the corresponding pairs of terms, i.e., the roots of the equations $E_0(t) = E_n(t)$. The foregoing analysis presupposes that the main contribution is that of the point t_0, i.e., $\operatorname{Im} t_0 < \operatorname{Im} t_n$.

Of greatest interest from the point of view of applications is the case of a potential that decreases at infinity like 1/r. The discrete spectrum contains an infinite number of levels which condense towards the boundary of the continuum E = 0. It is easy to see that if the problem reduces to one-dimensional (i.e., the variables in the stationary Schrödinger equation can be separated), then all the terms cross at one point. Indeed, satisfaction of the equation $E_n(t) = E_n(t)$ for any pair of terms is impossible, for this would mean the occurrence of degenerate states in the one-dimensional problem. To the contrary, the terms can cross at the zeroes or the poles of the parameters of the potential, regarded as functions of the time, but the crossing condition is then satisfied for all the E_n at the same time.

For example, in potentials of the form $U(r) = B(t)f(r)$ all the terms cross at $t = t_0$, where the function $B(t)$ vanishes [$E_n(t_0) = 0$ for any n]. The method developed in the preceding article[1] is applicable also to such a situation. The critical point is obviously the common zero of the functions $E_n(t)$, where the discrete spectrum vanishes [2].

Let us consider the s-state of the particle in a spherically symmetrical potential $B(t)f(r)$ with asymptotic behavior $U(r \to \infty) \sim -B(t)/r$. In the region $r \gtrsim L$, where $U(r)$ can be replaced by an asymptotic value, the wave functions $\chi = r\psi(r)$ of the continuous and of the discrete spectra satisfy respectively the equations

$$\chi'' + (k^2 + B/r)\chi = 0, \quad (18)$$

$$\chi_n'' + (-k_n^2 + B/r)\chi_n = 0, \quad k_n^2 = -2E_n. \quad (19)$$

The solution of (18), normalized to an energy δ-function, is of the form

$$\chi_E = \frac{e^{-\pi B/2k}}{[2\pi k]^{1/2}}\left[e^{-i\delta(k)}W_{-iB/k,1/2}(2ikr) - e^{i\delta(k)}W_{iB/k,1/2}(-2ikr)\right], \quad (20)$$

W—Whittaker function[4]. The meaning of the quantity $\delta(k)$ is clear from the asymptotic behavior of χ_E:

[2] Of course, such a problem is highly idealized and can at best be regarded only as a model of the system with condensing terms. In real physical systems (for example, in collisions between heavy atoms), multiple pairwise term crossings apparently take place. During a single collision the system passes many times near the critical points, and the transition to the continuous spectrum is realized via successive transitions (diffusion) over the excited states of the discrete spectrum.

$$\chi_E(r\to\infty)\sim\left[\frac{2}{\pi k}\right]^{1/2}\sin\left(kr+\frac{B}{k}\ln 2kr+\delta(k)\right). \quad (21)$$

The wave function of the discrete spectrum pertaining to the level E_n is a solution of (19), decreasing at infinity:

$$\chi_n = C_n W_{B/k_n,\,1/2}(2k_n r), \quad (22)$$

C_n—normalization factor.

As in the case with a finite number of levels of negative energy, an important role is played only by a small vicinity of the point t_0, where $B(t)$ vanishes. It is obvious that all the $k_n(t)$ vanish simultaneously with $B(t)$, i.e., the discrete spectrum vanishes. Near t_0, the state of the system is such that the particle spends a greater part of the time in the region $r \gtrsim L$. Therefore in calculating the matrix elements $\partial/\partial t$ we can replace the exact wave functions by expressions (20) and (22). In addition, we can state that the spectrum at $t \to t_0$ should be reminiscent of a hydrogen spectrum, since the situation in question is analogous to the hydrogen-like states of complex atoms (see [2], Sec. 68). The deviation from a Coulomb potential at small distances is taken into account formally as a change in the boundary condition for $r = 0$, imposed on the wave function. For the energy levels we obtain in this case the expression $k_n(t) = B(t)(n+\Delta)^{-1}$. In any case, it is obvious that as $t \to t_0$ the ratio $k_n(t)/B(t)$ tends to a constant (which of course depends on n). It is precisely this circumstance which will be used in what follows.

We shall assume that $B(t)$ has a simple zero at $t = t_0$. Carrying out the same analysis as in [1], we can check on the correctness of the following relations in the transition region:

$$k_i(t) \sim B(t) \sim B_0\alpha^{1/3}, \qquad k \sim (T)^{-1/2} \sim B_0\alpha^{1/2}. \quad (23)$$

Here B_0—characteristic value of the function $B(t)$, and the index i designates the discrete level which the system occupied at $t \to -\infty$. The adiabatic parameter is in this case $\alpha \equiv (B_0^2 T)^{-1}$. Thus, the essential energy region corresponds to $k \ll B(t)$.

We now clarify the behavior of the phase $\delta(k)$ in the parameter-value region of interest to us. As is well known, the scattering phase $\delta(k)$ is the limit of $\delta(k; r)$ as $r \to \infty$, determined in the following manner. The solution of the Schrödinger equation

$$\chi'' + [k^2 - 2U(r)]\chi = 0 \quad (24)$$

is sought in the form

$$\chi = A(r)\sin[kr + \delta(k; r)] \quad (25)$$

under the supplementary condition

$$d\chi/dr = kA(r)\cos[kr + \delta(k; r)]. \quad (26)$$

From (24)—(26) we obtain an equation for δ:

$$d\delta/d\rho = -2k^{-2}U(\rho)\sin^2[\rho + \delta(\rho)], \qquad \rho \equiv k(r). \quad (27)$$

When $r = 0$ we should have $\chi(0) = 0$. However $A(r = 0)$ cannot vanish by virtue of condition (26), for otherwise Eq. (24) would have only a zero solution. Consequently $\delta(r = 0) = 0$ and we obtain from (27)

$$\delta(\rho) = -\frac{2}{k^2}\int_0^\rho U(\rho')\sin^2[\rho' + \delta(\rho')]\,d\rho'. \quad (28)$$

As $\rho \to \infty$ the integral diverges logarithmically ($u(\rho \to \infty) \sim 1/\rho$). The phase $\delta(k)$ contained in (20) is obviously equal to $\delta(\rho \to \infty)$ after subtracting the logarithmic term.

Let us estimate the contribution of the region $r \leq L$, which corresponds to $\rho \lesssim kL$. In the case in question the condition $kL \ll 1$ is satisfied, so that it follows from (27) (we assume that $U(0)$ is finite) that $\delta(\rho \to 0) \sim \rho^3$. The integral (28) over the interval $[0; \rho \sim kL \ll 1]$ has an order of magnitude $k^{-2}U(0)(kL)^3 = U(0)L^2kL$. We assume that $U(0)L^2 \sim 1$, which corresponds to the number of levels in a "cut-off" well of order of unity. Under this assumption, the influence of the region $r \lesssim L$ is negligibly small [$U(0)L^2kL \ll 1$]. The slow decrease of the potential at infinity causes the main contribution to the scattering phase at low energies to be given by large values of r. However, at large $r (r \gg L)$ we can replace $U(r)$ by its asymptotic value, and the condition $B/k \gg 1$ is precisely a criterion for the Coulomb field to be quasiclassical (see [2]). Calculating $\delta(k)$ with the quasiclassical approximation formulas, we obtain

$$\delta(k) = -\frac{B}{k}\ln\frac{B}{k} + \frac{B}{k} - \frac{\pi}{4} + O\left(\frac{k}{B}\right). \quad (29)$$

Formulas (20), (22), and (29) enable us to find the quantities

$$\int \dot{\chi}_E\chi_n\,dr, \qquad \int \dot{\chi}_E\chi_\varepsilon\,dr.$$

The integrals of the products of Whittaker functions are calculated by a formula derived by Erdelyi [3]. In this case they are expressed in terms of the Appel hypergeometric function of two variables. The resultant expressions are too cumbersome and are therefore not written out here.

We proceed to the initial system of equations (see [1], formula (1)) and to new unknown functions $C_n(\tau)$ and $C(W, \tau)$ as well as to new variables

W and τ, with the aid of the relations

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

$$a_n(t) = C_n(\tau)\exp\left[-\frac{i}{2}\int^{t_0}(k_n^2 - k_i^2)\,dt\right],$$

$$a(E, t) = C(W, \tau)[B(t_0)]^{-1/3}\exp\left[iEt_0 + \frac{i}{2}\int^{t_0} k_i^2(t)\,dt\right]. \quad (30)$$

The resultant system of equations with respect to $C_n(\tau)$ and $C(W, \tau)$ does not contain the parameters of the problem. The condition $k \ll B(t)$ corresponds in the new variables to the inequality $W \ll 1$. For the transition amplitudes we obtain

$$a_n = g_n\exp\left[i\int^{t_0}(E_n - E_i)\,dt\right], \quad (31)$$

$$a(E) = g'[B(t_0)]^{-1/3}\exp\left[iEt_0 - i\int^{t_0} E_i(t)\,dt\right], \quad (32)$$

where g_n and g' are numerical coefficients.

A striking fact is the difference between (32) and the corresponding result for a potential that decreases rapidly with the distance [see [1], formula (15)]. The transition probability $|a(E)|^2$ does not tend to zero as $E \to 0$ if $U(r)$ behaves like $1/r$ as $r \to \infty$. This may be connected with the fact that in a Coulomb field there exists a zero-energy wave function which does not vanish identically (see [2]). Owing to the slowness in the decrease of $U(r)$ at infinity, the state with $E = 0$ turns out, as it were, to be more attainable than in rapidly decreasing potentials.

The energy distribution in the continuous spectrum is of the form

$$\frac{dn(E)}{dE} = |g'|^2|B(t_0)|^{-2/3}\exp\left(-i\int_{t_0^*}^{t_0} E_i\,dt\right)e^{-\sigma E},$$

$$\sigma \equiv 2|\operatorname{Im} t_0|. \quad (33)$$

The total ionization probability again contains a power-law smallness in the pre-exponential factor:

$$P = |g'|^2|\dot{B}(t_0)|^{-2/3}\sigma^{-1}\exp\left(-i\int_{t_0^*}^{t_0} E_i\,dt\right) \sim \alpha^{1/3}e^{-A_i/\alpha}. \quad (34)$$

Here A_i does not depend on α and decreases with increasing i.[3)]

The results obtained cannot be applied directly to calculations of atomic collisions, for in this case the assumption above concerning the spherical symmetry of the perturbation is not satisfied. There exists a more realistic model of ionization at slow atomic collisions. The influence of the ion and the atom on the electron can be described at large distances by the action of the field of a Coulomb center with constant charge and a dipole with variable moment (the dipole moment depends on the internuclear distance). In this case the variables in the Schrödinger equation separate and the problem becomes analogous to the preceding ones. The next communication will be devoted to this topic.

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[3)] The integral in (33) and (34) is taken over an interval much larger than the dimension of the transition region, whereas the entire analysis given above pertains only to a small vicinity of the point t_0. This, however, is not contradictory. The exponential in (33) and (34) is merely

$$\left|\exp\left(-i\int_{\bar{t}}^{t_0} E_i(t)\,dt\right)\right|^2,$$

where $\bar{t}$ – arbitrary real point. This follows from the reality of $E_i(t)$ on the real axis: $E_i(t^*) = [E_i(t)]^*$. A similar remark holds for the analogous formulas of the preceding article[1].