ON THE THEORY OF UNSTABLE STATES

YA. B. ZEL'DOVICH

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A perturbation theory is developed and an expression is given for the amplitude (corresponding to a given initial state) of a state that decays exponentially with time. A final expression is obtained which plays the role of the norm of such a state.

An exponentially decaying state that describes, for example, the phenomenon of α decay, is characterized by a complex value of the energy, the imaginary part of the energy giving the decay probability. The wave function of this state increases exponentially in absolute value at large distances, and therefore the usual methods of normalization, of perturbation theory, and of expansion in terms of eigenfunctions do not apply to this state. We develop here a perturbation theory which gives an expression in terms of a quadrature for the changes of the mean energy and of the decay probability corresponding to an arbitrarily small change of the potential.

If the state is initially described by a certain wave function, then for a long time interval thereafter the wave function is close to an exponentially decaying function with a definite amplitude. This amplitude is also calculated in terms of quadratures.

The solutions of both problems—that of the energy and that of the amplitude of the exponentially decaying state—involve a quantity that plays the role of the norm of this state:

$$\lim_{\alpha \to 0} \int_0^\infty \chi^2 \exp(-\alpha r^2) r^2 dr.$$

For the calculation of this quantity we shall give a direct method which enables us to avoid the limiting process $\alpha \to 0$.

1. Let us consider a particle moving in a spherical potential with a barrier, i.e., moving like the α particle in the Gamow theory of α decay.

Let the corresponding Schrödinger equation have the formal solution

$$\psi(r, t) = e^{-iE't}\chi(r)$$

with the complex value $E' = E_0 - i\gamma$. The discrete value E' is obtained from the condition that at large distances $\chi(r)$ contains only an outgoing wave:

$$\chi(r) \approx Cr^{-1}e^{ikr}, \qquad r \to \infty,$$

$$k = +\sqrt{2E'}, \qquad \hbar = m = 1.$$

This solution is of interest not only as a description of an unstable state; the corresponding eigenvalue is a singular point—a pole—(in the complex plane) of the matrix for the scattering of a particle by the potential.

As is well known, $|\chi(r)|$ increases exponentially for $r \to \infty$; the function χ cannot be normalized, and in particular cannot be regarded as a wave function in the usual sense: it does not belong to the complete system of eigenfunctions ψ_n of the Hamiltonian operator. We cannot apply to χ the usual formulas of perturbation theory, for example

$$\delta E_n = \int \psi^* \delta H \cdot \psi_n d\tau \Big/ \int \psi_n^* \psi_n d\tau,$$

and the expansion of the function of an arbitrary state in terms of eigenfunctions:

$$\varphi(r) = A_n\psi_n, \qquad A_n = \int \psi_n^* \varphi \, d\tau \Big/ \int \psi_n^* \psi_n d\tau.$$

We shall find the expressions that replace these well known formulas in the case of the function χ.

Let us begin with the perturbation theory. In the simplest case of an S wave and a potential such that $V(r) = 0$ for $r > R$, by using the methods developed in references 1 and 2 we get without difficulty the expression

$$\delta E' = \int \chi^2(r)\, \delta V(r)\, d\tau \Big/ \left\{ \int [\chi^2(r) - (Cr^{-1}e^{ikr})^2]\, d\tau - C^2/2ik \right\}, \tag{1}$$

where C is the coefficient in the asymptotic formula for the unperturbed solution χ: $\chi(r) \approx Cr^{-1}e^{ikr}$ as $r \to \infty$. The two integrals—in the numerator and in the denominator—can be thought of as taken over all space: in the numerator the region of integration is fixed by the region of the perturbation $\delta V(r)$, and in the denominator the integrand is zero for $r > R$.

We note that the integrands do not contain the square of the absolute value, but the complex quantity χ^2, and therefore $\delta E'$ is complex. The expression (1) gives not only the change of the energy E_0, but also the change of the decay probability $w = 2\gamma$.

To derive Eq. (1) we introduce the variable

$$y = d\ln\chi/dr; \qquad \chi(r) = \exp\left\{\int_0^r y(q)\,dq\right\}. \tag{2}$$

Schrödinger's equation then takes the form

$$dy/dr = -y^2 - 2[E' - V(r)], \tag{3}$$

and the equation for the perturbation of y is

$$d\,\delta y/dr = -2y\,\delta y + 2[\delta E' - \delta V(r)]. \tag{4}$$

The condition of regularity of χ at $r = 0$ uniquely determines $y(0)$, so that $\delta y(0) = 0$, and from this we have

$$\delta y(r) = \exp\left\{-2\int_0^r y\,dr\right\}\int_0^r [\delta V(q) - \delta E']\exp\left\{2\int_0^q y\,dq\right\}dq$$

$$= \frac{2}{\chi^2(r)}\int_0^r [\delta V(q) - \delta E']\,\chi^2(q)\,dq. \tag{5}$$

The boundary condition for the perturbed problem for $r > R$ is

$$d\ln\chi'/dr = y + \delta y = i\sqrt{2(E' + \delta E')}$$

$$= i\sqrt{2E'} + i\delta E'/2E',$$

$$\delta y = i\delta E'/\sqrt{2E'} = i\delta E'/k. \tag{6}$$

Comparing Eqs. (6) and (5), we now get Eq. (1) by an elementary calculation.

If we prescribe $\delta V = \epsilon =$ const in the entire infinite volume, we must obviously get $\delta E' = \epsilon$; Therefore the finite expression in the denominator of Eq. (1) can be regarded as the definition of the diverging integral $\int\chi^2 dr$. This latter integral does have any unambiguous meaning because of the fact that

$$|\chi| \sim \exp(\gamma r/\sqrt{2E_0}) \to \infty \quad \text{for } r \to \infty$$

and does not become convergent if we multiply the integrand by $e^{-\alpha r}$ and subsequently take the limit $\alpha \to 0$. Convergence can be achieved by multiplication by $e^{-\alpha r^2}$:

$$\int\chi^2\,d\tau \equiv \lim_{\alpha\to 0}\int\chi^2 e^{-\alpha r^2}\,d\tau = J$$

$$= \int[\chi^2 - (Cr^{-1}e^{ikr})^2]\,d\tau - C^2/2ik. \tag{7}$$

Equation (1) can then be written in the form

$$\delta E' = \int\chi^2\delta V\,d\tau \Big/ \int\chi^2\,d\tau. \tag{1a}$$

2. Let us now consider the nonstationary problem. Suppose that at the initial time the wave function

$$\psi(r, t = 0) = \varphi(r)$$

is prescribed. It is well known that the asymptotic form of the solution is

$$\psi(r, t) = Ae^{-iE't}\chi(r) + O(r, t), \tag{8}$$

where $O(r, t)$ falls off like $t^{-3/2}$ for small r [for further details about $O(r, t)$ see the paper of Khalfin[3]].

Despite the fact that the first term decreases exponentially as $e^{-\gamma t}$ and the second only by a power law, the separation of the first term is justified over a wide range of values of t for $\gamma \ll E_0$. Drukarev[4] has shown that the approach of $\psi(r, t)$ to the asymptotic expression (8) occurs nonuniformly at small r ($r < vt$, where v is the speed of the particle corresponding to the energy E_0). As has been shown by Fok and Krylov,[5] the coefficient A in the first term of Eq. (8) is proportional to the residue (at the pole $E = E'$) of the spectral density of the initial state $\varphi(r)$ when it is expanded in terms of the continuous-spectrum eigenfunctions $\psi(E, r)$ that correspond to real values of E.

The coefficient A can be expressed in terms of $\varphi(r)$ and $\chi(r)$ by a simple quadrature:

$$A = \int\varphi\chi\,d\tau \Big/ \int\chi^2\,d\tau, \tag{9}$$

where $\int\chi^2 d\tau$ is defined by Eq. (7).

To verify this we introduce, following N. A. Dmitriev, a function $\psi(r, s)$ defined by the formula

$$\psi(r, s) = -i\int_0^\infty \psi(r, t)\,e^{ist}\,dt, \tag{10}$$

for those values of s for which the integral converges. In the region where the integral diverges, we define $\psi(r, s)$ as the analytic continuation of the function defined by the integral (10).

The Schrödinger equation gives

$$-s\psi(r, s) - \tfrac{1}{2}\Delta\psi(r, s) + V(r)\psi(r, s) = -\varphi(r). \tag{11}$$

In the region $r > R$, where $V(r) = 0$ and $\varphi(r) = 0$, the solution is of the form

$$\psi(r, s) = [f(s)\exp(ir\sqrt{2s}) + f_1(s)\exp(ir\sqrt{2s})]\,r^{-1}, \tag{12}$$

where f and f_1 are arbitrary functions.

Considering the region $\operatorname{Im} s > 0$, where $\psi(r, s)$ is given by a convergent integral, we convince ourselves that $f_1(r, s) \equiv 0$, since $|\psi(r, s)|$ cannot increase for $r \to \infty$. The condition that $\psi(r, s)$ is a diverging wave for large r is extended by the analytic continuation to arbitrary values of s.

The function $\chi(r)$ that describes the decaying state satisfies the same condition for $r \to \infty$ and an equation analogous to Eq. (11) but without the right member:

$$-E'\chi(r) - \tfrac{1}{2}\Delta\chi(r) + V(r)\chi(r) = 0 \qquad (13)$$

It follows from this that the solution of the equation (11) with the right member has a pole at $s = E'$ (with $\operatorname{Im} s = -\gamma < 0$):

$$\psi(r, s) = a\chi(r)/(s - E') + \psi_1(r, s), \qquad (14)$$

where $\psi_1(r, E')$ is regular.

To determine a we multiply Eq. (11) by $\chi(r)$ and Eq. (13) by $\psi(r, s)$ and subtract one equation from the other. We then integrate over the volume $0 < r < R$ and substitute the expression for $\psi(r, s)$ in the form (14). Then finally for $s \to E'$ we get an expression for a that coincides with the expression (9) for A.

Inverting the relation (1), we find that the pole term in Eq. (14) gives the exponential term in Eq. (8) with $A = a$, and this completes the derivation of (9).

3. The formulas are easily extended to the case of states with $l \neq 0$. In this case all formulas contain instead of χ^2 the product $\chi(\mathbf{r})\tilde{\chi}^*(\mathbf{r})$, where $\tilde{\chi}(\mathbf{r})$ is the solution of the adjoint equation (cf. reference 6). In the present case, since the operator H is Hermitian, the taking of the adjoint reduces to changing the sign of i in the boundary condition

$$\partial \ln r\chi/\partial r = +i\sqrt{2E'}, \qquad \partial \ln r\tilde{\chi}/\partial r = -i\sqrt{2E'^*}$$
$$(r \to \infty).$$

After separating off the angular factor in $\chi(\mathbf{r}) = P(\theta, \varphi)z(r)$, we get

$$\tilde{\chi} = \tilde{P}\tilde{z}, \qquad \tilde{P} = P, \qquad \tilde{z} = z^*,$$

so that finally

$$\delta E' = \int \tilde{\chi}^* \chi \delta V \, d\tau \Big/ \int \tilde{\chi}^* \chi \, d\tau, \qquad (15)$$

$$\psi(\mathbf{r}, t) = Ae^{-iE't}\chi(\mathbf{r}) + O(r, t), \qquad (16)$$

$$A = \int \tilde{\chi}^*(\mathbf{r})\varphi(\mathbf{r})\, d\tau \Big/ \int \tilde{\chi}^*(\mathbf{r})\chi(\mathbf{r})\, d\tau. \qquad (17)$$

In the equation for the radial function z(r) the effective potential U(r) includes the centrifugal potential:

$$U(r) = V(r) + r^{-2} l(l+1),$$

and therefore in the region $r > R$, where $V(r) = 0$, the function z(r) can be expressed in terms of a Hankel function of half-integral order of the complex argument kr (k is complex when E′ is complex).

For $r \to \infty$ we also have $|\chi| \to \infty$, and therefore to give a definite meaning to the integral that plays the role of the normalization we must again either multiply the integrand by $e^{-\alpha r^2}$ and then let $\alpha \to 0$ or else use a finite expression of the type of (1), which does not require the passage to the limit:

$$\int_0^\infty z^2 r^2 dr = \int_0^r z^2 r^2 dr + r^2 z^2 \frac{\partial^2}{\partial E' \partial r} \ln(rz). \qquad (18)$$

For $r > R$ we get into the region where z(r) can be expressed in terms of a Hankel function, and the derivatives in the second term can be taken in an elementary way. Furthermore, it is easily verified that in virtue of the equation satisfied by z(r) the right member of (18) does not depend on r. The problem is solved in a similar way for the Coulomb potential, the only difference being that for $r > R$ the quantity z is expressed by a hypergeometric function.

Finally, in the case of a V(r) that contains, besides the Coulomb and centrifugal potentials, another part that is everywhere different from zero but that decreases sufficiently rapidly (exponentially), we must bring into the treatment, along with the solution z(r) of the complete equation, another function $z_1(r)$ that is a solution of the equation with $V(r) = 0$ and coincides with z(r) in the limit $r \to \infty$ $[z(\infty) = z_1(\infty)]$. The function z_1 can be expressed in terms of known (Hankel and hypergeometric) functions:

$$\int_0^\infty z^2 r^2 dr = \int_0^\rho z^2 r^2 dr + \int_0^\infty (z^2 - z_1^2) r^2 dr + z_1^2 \frac{\partial^2}{\partial E' \partial r} \ln(rz_1)\Big|_{r=\rho}. \qquad (19)$$

For $l \neq 0$ we must treat separately a neighborhood of the origin, $0 < r < \rho$, because of the fact that the Hankel function has a nonintegrable singularity at zero. It is assumed that after we have separated out from V(r) the terms of orders $1/r$ and $1/r^2$, V(r) falls off in such a way that $z^2 - z_1^2$ is a function that is integrable for $r \to \infty$.

In the case of a potential of complicated form, for which the integrals can only be calculated numerically, the advantage of the expression (19) as compared with (18) is that in Eq. (19) one takes the derivative of known functions.

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