STATIONARY AND NONSTATIONARY PROBLEMS IN QUANTUM MECHANICS THAT CAN BE SOLVED BY MEANS OF CONTOUR INTEGRATION

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It is shown that if the energy operator consists of a time-independent part H_0 and a perturbation which depends linearly on time and is a projection operator onto a state $|\varphi\rangle$, the exact solution of the Schrödinger equation can be expressed as a contour integral. The S-matrix for such a problem possesses the triangular property and decomposes into elementary Landau-Zener factors, each of which mixes only a pair of states. Similar results are derived for the corresponding stationary problem. Some generalizations are considered, as well as examples, and the connection with previous solutions of the problem of electron detachment and of ionization in atomic and ionic collisions.

1. INTRODUCTION

FEW quantum-mechanical problems are known for which the Schrödinger equation can be solved exactly. This is particularly true for nonstationary problems, in which the energy operator depends on the time explicitly. Nevertheless the analysis and solution of such problems is extremely important in the most varied fields of physics. One of the most natural examples is the collision of atoms or ions, when the motion of the heavy nuclei can be treated classically and the various inelastic processes can be investigated by solving nonstationary Schrödinger equations for the electrons.

It is well known that for slow collisions (weak time dependence of the energy operator) the adiabatic approximation, first introduced by Born and Fock[1,2], is applicable. Here transitions are practically possible only if the eigenvalues of the instantaneous energy operator are almost degenerate.

In the case in which one can neglect the transitions between all states with the exception of two, and restricts oneself to the so-called two-level approximation, the problem can be reduced to solving a system of two coupled differential equations of the first order. In the simplest case we obtain the so-called Landau-Zener formula[3,4]. The two-level approximation has been further analyzed, the Landau-Zener formula has been made more precise, and its domain of applicability was investigated in many papers[5,6].

However the two-level (or several-level) approximation turns out to be unsatisfactory in a series of cases, and it becomes necessary to study the interaction of a large number (or even an infinite number) of states, in particular in the case where we deal with an electron transition into the continuous spectrum (ionization, recombination, free-free transitions). In the latter case we have to deal with an infinite system of equations, or a partial differential equation, even after the problem has been schematized to the utmost.

Here in real situations there naturally arises the case in which a system of parallel terms (eigenvalues of the energy operator for which the differences are independent of the time) is present, and in addition one term of a different nature, which in the zeroth approximation intersects all these terms. When the interaction is taken into account there occurs a "quasi-intersection," such that the picture is approximately as illustrated in Fig. 1.

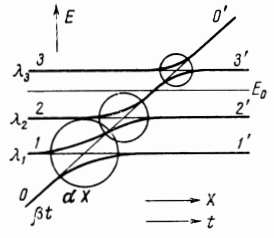

FIG 1.

In the case when the level splitting at each quasi-intersection point is small compared with the distance to the other levels, we can carry through the computation by considering separately each such region, and multiplying the transition probabilities obtained in this manner. In the opposite situation this cannot be done, in general.

We shall show, however, that the above-mentioned limitation can be lifted under certain conditions; this justifies using the Landau-Zener formula far beyond its formal limits of applicability, and leads to very simple and intuitive conclusions on the structure of the S-matrix for problems of this kind.

Problems of this kind were initially considered for concrete processes (electron detachment or ionization in slow atomic and ionic collisions, electronic transitions in crystals[7-12]. The method expounded in the present paper allows to consider all these problems in a unified manner, and in addition opens up possibilities for new applications in all those cases when one deals with the interaction of one state of the system with a group of states of a different nature (preionization, free-free transitions in collisions, analogous processes in solids, etc.).

2. NONSTATIONARY PROBLEMS

We consider a nonstationary problem with the energy operator H(t) consisting of a time-independent operator H_0 and a perturbation V(t), where V(t) has a linear time-

dependence and is a projection operator onto some state $|\varphi\rangle$[13]. We search for a solution of the Schrödinger equation

$$(H_0+|\varphi\rangle\,\beta t\,\langle\varphi|)\,|\psi\rangle = i\,\frac{\partial}{\partial t}|\psi\rangle \quad (\beta>0) \tag{1}$$

in the form of a contour integral

$$|\psi\rangle = \int_C G(E)\,|\varphi\rangle\,F(E)\,e^{-iEt}dE, \tag{2}$$

where $G(E) = (H_0 - E)^{-1}$ is the resolvent operator, the kernel of which is the Green's function of the operator H_0. Substituting (2) into (1), integrating by parts under the assumption that the integrated term vanishes, and equating the integrands, we derive an equation for the function F(E):

$$F(E) = i\beta\,\frac{d}{dE}\,[F(E)\langle\varphi|G(E)\,|\varphi\rangle], \tag{3}$$

and thus, obtain a solution of (1) in the form

$$|\psi\rangle = N\int_C \frac{G(E)\,|\varphi\rangle}{\langle\varphi|G(E)\,|\varphi\rangle}\exp\Big(-\frac{i}{\beta}\int^E \frac{dE'}{\langle\varphi|G(E')\,|\varphi\rangle} - iEt\Big)\,dE. \tag{4}$$

Thus, if we know the Green's function of the operator H_0 (i.e., if we have a complete solution of the stationary problem) we can obtain the solution to a whole series of nonstationary problems of the type (1), with arbitrary state $|\varphi\rangle$, in the form of a contour integral. Here we have made no assumptions whatsoever about the number of degrees of freedom and about the character of the spectrum of the operator H_0.

The integrated term in the integration by parts must vanish. This yields the following condition to be imposed on the contour C:

$$\exp\Big[-\frac{i}{\beta}\int^E \frac{dE'}{\langle\varphi|G(E')\,|\varphi\rangle} - iEt\Big]\Big|_C = 0. \tag{5}$$

We now show that the saddle points of the exponential function in (4) and (5) coincide with the instantaneous eigenvalues of the energy operator H. Indeed, the condition determining the saddle points has the form

$$\langle\varphi|G(E)\,|\varphi\rangle = -(\beta t)^{-1}. \tag{6}$$

Multiplying the eigenvalue equation

$$[(H_0 - E) + |\varphi\rangle\beta t\langle\varphi|]\,|\psi\rangle = 0 \tag{7}$$

by $\langle\varphi|(H_0 - E)^{-1}$ from the left, we are led to Eq. (6) also.

It should be remarked that if the operator H_0 has a continuous spectrum, the operator G(E) will have a cut along the region occupied by the continuous spectrum. Then Eq. (6) has solutions on the "unphysical sheet," corresponding to quasistationary or virtual states of the system, and it is possible that as t varies, the roots go over from the physical sheet into the unphysical sheet.[14]

For $t \to \pm\infty$ the eigenvalues of H converge to the limiting values determined from the equation

$$\langle\varphi|G(E)\,|\varphi\rangle = 0. \tag{8}$$

for t = 0 the saddle points obviously coincide with the eigenvalues of H_0.

We now consider the case when the operator H_0 has only discrete eigenvalues. We select a basis such that the zeroth row and column corresponds to the state $|\varphi\rangle$. Then the operator H will have the matrix representation

$$H = \begin{pmatrix} h_{00}+\beta t, & h_{01}, & h_{02}\ldots \\ h_{10}, & h_{11}, & h_{12}\ldots \\ \ldots & \ldots & \ldots \end{pmatrix}. \tag{9}$$

Selecting further the origin of time in such a manner that $h_{00} = 0$, and diagonalizing the submatrix

$$\begin{pmatrix} h_{11}, & h_{12}\ldots \\ h_{21}, & h_{22}\ldots \\ \ldots & \ldots \end{pmatrix},$$

we obtain the representation which is most suitable for the case at hand[7]

$$H = \begin{pmatrix} \beta t, & h_1, & h_2\ldots \\ h_1, & \lambda_1, & 0\ldots \\ h_2, & 0, & \lambda_2\ldots \\ \ldots & \ldots & \ldots \end{pmatrix}. \tag{10}$$

By a suitable choice of phase factors one can always make the constants h_1, h_2, ... real and positive. It is easy to see that if βt is large compared to h_i and λ_i, then the eigenvalues of H are close to βt and λ_i, so that the λ_i are the asymptotic eigenvalues of H and solutions of Eq. (7). It should be stressed that the eigenvalues λ_i and the eigenvalues of H_0 are respectively the poles and zeros of the function $\langle\varphi|G(E)|\varphi\rangle$, therefore they never coincide and will alternate with each other.

For the case when only four levels are present, the general picture of the terms is represented in Fig. 1. If the h_i are small compared to the difference $|\lambda_{i+1} - \lambda_i|$ then the level splitting at the quasiintersection points $\beta t_i = \lambda_i$ will be small and equal to $2h_i$. In the two-level approximation the Landau-Zener formula shows that the probability for a nonadiabatic transition (i.e., the probability for the system to "move along" the unperturbed term) will be $p_i = \exp(-2\pi h_i^2/\beta)$. The probability for adiabatic behavior, i.e., that the system will move along the real term line is $q_i = 1 - p_i$.

Let us write Eq. (4) in this representation. The equation determining the eigenvalues of H_0 is of the form

$$|H_0 - E| = -\prod_i(\lambda_i - E)\Big[E + \sum_j h_j^2(\lambda_j - E)^{-1}\Big] = 0. \tag{11}$$

It is easy to compute the inverse matrix $(H_0 - E)^{-1}$ and the quantities $\langle\varphi|G(E)|\varphi\rangle$, $G|\varphi\rangle$. We obtain

$$\langle\varphi|\psi\rangle = \langle 0|\psi\rangle = N\int_C L(E)\,dE, \quad \langle n|\psi\rangle = Nh_n\int_C (\lambda_n - E)^{-1}L(E)\,dE,$$

$$L(E) = \prod_m(\lambda_m - E)^{-ih_m^2/\beta}\exp(iE^2/2\beta - iEt). \tag{12}$$

We see that the asymptotic eigenvalues λ_m are poles and branch points of the integrand. For large values of t the saddle points are situated close to the λ_i, and as t varies from $-\infty$ to $+\infty$ they move over from λ_i to λ_{i+1}. The first saddle point at $t \to -\infty$ is close to βt, and as $t \to +\infty$ it is close to λ_i; the last (if it exists) is for $t \to -\infty$ close to the largest λ_N, and for $t \to +\infty$ it is close to βt.

We now wish to determine the integration path. If at $t \to -\infty$ the system was in the state $|\varphi\rangle$, the contour is required only to pass through the saddle point $E \approx \beta t$. The exponential in the integrand vanishes at the end points of the integration path, if the latter go to infinity via the first and third quadrants of the complex plane. The general form of the integration contour is illustrated in Fig. 2a. If one assumes $|\beta t| \gg |\lambda_m|$, then in the

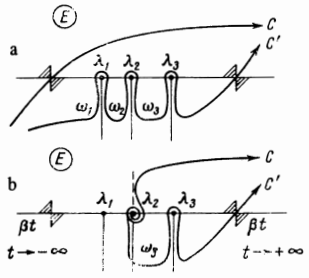

FIG. 2.

vicinity of $E = \beta t$ the factors $(\lambda_m - E)^{-ih_m^2/\beta}$ have their absolute values close to unity, and computing the integral by the saddle-point method, we obtain

$$\left| \int_C L(E)\,dE \right| \to (2\pi\beta)^{1/2}, \tag{13}$$

consequently the normalization constant N equals $(2\pi\beta)^{-1/2}$. Obviously, all other components vanish at $t \to -\infty$, on account of the factors $(\lambda_m - E)^{-1}$.

For $t \to +\infty$ the factor e^{-iEt} vanishes rapidly in the lower half-plane and the saddle point $E \approx \beta t$ is to the right of the branch points λ_n. In order to determine the asymptotic behavior it is necessary to deform the contour C, representing it as a sum of loops ω_n which go around the points λ_n as illustrated in Fig. 2a (the curve C'). Only the loop ω_n yields a finite contribution to the component $\langle n|\psi\rangle$ as $t \to \infty$, and only that part of the contour is essential for which the absolute squares of the factors $(\lambda_m - E)^{-ih_m^2/\beta}$ are close to one, for $m > n$, and close to p_n for $m < n$.

We then obtain for the transition probabilities

$$|S_{0n}|^2 = \lim_{t\to\infty} |\langle n|\psi\rangle|^2 = h_n^2(2\pi\beta)^{-1}p_1p_2\ldots p_n \times \left| \int_{C'} (\lambda_n - E)^{-1-ih_n^2/\beta} e^{iEt}\,dE \right|^2$$

$$= h_n^2(2\pi\beta)^{-1}p_1p_2\ldots p_{n-1}p_n^{1/2}|2\pi/\Gamma(1 + ih_n^2/\beta)|^2 = p_1\ldots p_{n-1}q_n, \tag{14}$$

$$|S_{00}|^2 = \lim_{t\to\infty} |\langle 0|\psi\rangle|^2 = p_1p_2\ldots p_N. \tag{15}$$

In the case in which the initial state for $t \to -\infty$ is n ($n \neq 0$), a contour which passes only through one saddle point is represented in Fig. 2b (the curve C). Near the point λ_n the contour has a shape reminiscent of a logarithmic spiral, i.e. to the curve of steepest descent for the function $(\lambda_n - E)^{-1} - ih_n^2/\beta$. Making use of the formula

$$\int_\sigma e^t t^{-z}\,dt = -2\pi i[\Gamma(z)(1 - e^{2\pi iz})]^{-1} \qquad (\mathrm{Im}\, z > 0), \tag{16}$$

where the contour σ has the form of a spiral near the origin and goes to infinity along the upper side of the left hand cut, it is easy to derive the normalization factor for this case:

$$N = (2\pi\beta p_1p_2\ldots p_{n-1})^{-1/2}(1 - p_n)^{1/2}. \tag{17}$$

For $t \to +\infty$ the contour should be deformed in the manner illustrated in Fig. 2b (the curve C').

We obtain the following expressions for the transition probabilities:

$$|S_{nm}|^2 = 0, \quad 0 < m < n,$$
$$|S_{nn}|^2 = p_n,$$
$$|S_{nm}|^2 = (1 - p_n)p_{n+1}\ldots p_{m-1}(1 - p_m), \quad m > n,$$
$$|S_{n0}|^2 = (1 - p_n)p_{n+1}\ldots p_N. \tag{18}$$

We see that for $m < n$ the transition probability is zero, since the contour misses the corresponding saddle points. This means that as t goes from $t \to -\infty$ to $t \to +\infty$ the energy of the system cannot decrease—a property which may be called the triangular character of the S-matrix[15]. (This terminology is somewhat misleading since there are matrix elements S_{n0} which are not zero.) Since the operator V increases monotonically, it is obvious that the average energy of any state must increase also. The assertion we have derived is much stronger. Detailed balance and time reversal invariance are violated by the zero-state $|\varphi\rangle$, which has different energies at $t \to -\infty$ and $t \to +\infty$.

It can also be seen from Eqs. (14), (15), and (18) that all transition probabilities can be computed as successive products of the probabilities p_n and q_n of the elementary transitions between the states 0 and n in each quasi-intersection point (cf. Fig. 1). In other words, the S-matrix can be decomposed into a product of simple factors, each of which affects only a pair of "intersecting" states according to the Landau-Zener formula. Denoting each such S-matrix by S_{0n} we obtain

$$S = S_{01}S_{02}\ldots S_{0N}. \tag{19}$$

This result automatically implies the triangular property.

In the case when the quantities h_n are comparable to the distance between parallel terms, i.e., to $|\lambda_n - \lambda_{n+1}|$ and $|\lambda_n - \lambda_{n-1}|$, they are no longer determined directly in terms of the distance between the levels at the quasi-intersection points. It can be seen from Eq. (10) that

$$h_n = \langle n|H|0\rangle. \tag{20}$$

The assumption that these matrix elements do not depend on t for sufficiently large time intervals is one of the fundamental conditions for the applicability of the method.

It can also be seen from Eqs. (14) and (15) that the simplest expression results for the probability w(E) for the transition of the system from the state $|\varphi\rangle$ into any state with an energy larger than E:

$$w(E) = \prod_{\lambda_n < E} p_n = \exp\Big(-2\pi\beta^{-1}\sum_{\lambda_n<E} h_n^2\Big). \tag{21}$$

It is now easy to discuss the situation when H_0 has also a portion of continuous spectrum. Then, if we increase, for example, the portion of space through which the particle moves, the eigenvalues λ_n will become denser in that part of the energy interval, and the matrix elements h_n will converge to zero. In the limit the function $\langle\varphi|G(E)|\varphi\rangle^{-1}$ will have a cut along the real axis, with the discontinuity $\Delta(E)$ of the imaginary part equal to

$$\Delta(E) = 2\pi\left(\frac{dn}{dE}h_n^2\right)_{\lambda_n = E}. \tag{22}$$

Thus if the operator H_0 has only a continuous spectrum, the probability w(E) becomes

$$w(E) = \exp\Big[-\beta^{-1}\int_{\mathscr{E}}^{E}\Delta(E')\,dE'\Big], \tag{23}$$

where $\mathscr{E}$ is the lower limit of the continuous spectrum of H_0.

If the initial state n is situated in the continuous spectrum, then the passage to the limit requires a change of normalization of the initial state, since a normalized wave function would vanish everywhere. Using a delta-function normalization in the energy, we obtain

$$\psi_E = (dn/dE)^{1/2}\psi_n$$

and in view of the fact that h_n^2 as well as q_n converge to zero, we obtain for the transition probability from a state of energy E_0 into a state with energy larger than E, the expression

$$w(E_0, E) = \lim_{\Delta\lambda_n\to 0}\Big(\frac{dn}{dE}\frac{2\pi}{\beta}h_n^2\Big)_{\lambda_n=E_0}$$
$$\times\exp\Big(-\beta^{-1}\int_{E_0}^{E}\frac{dn}{dE'}h_n^2\,dE'\Big) = \beta^{-1}\Delta(E_0)\exp\Big(-\beta^{-1}\int_{E_0}^{E}\Delta(E')\,dE'\Big). \tag{24}$$

The transition probability into all states with energy smaller than E_0 is zero.

3. STATIONARY PROBLEMS

Until now we have considered an energy operator H which was explicitly dependent on time. In other words, the system had an external parameter with an a priori given time dependence. In ionic or atomic collisions such a parameter is the distance between the nuclei. If the energy of the motion of the nuclei is small and comparable to the energy of the electronic transitions, this parameter should also be included into the quantum-dynamical discussion. We assume that to this additional degree of freedom, to be denoted by X, corresponds an effective mass M, and we retain all the assumptions already made about the operator H in Sec. 2. We are then led to the stationary quantum-mechanical problem (cf.[8,13,16,17]):

$$\Big[-\frac{1}{2M}\frac{\partial^2}{\partial X^2} + H_0 + |\varphi\rangle\,\alpha X\,\langle\varphi|\Big]\,|\psi\rangle = E_0|\psi\rangle, \tag{25}$$

where E_0 is the total energy, H_0 does not depend on X, $\alpha > 0$. In this case, for large positive or negative X, the wave function will have the form of plane waves, multiplied by the wave functions of the asymptotic states, $|n\rangle$, defined in Sec. 2. Each state will have two reaction channels, corresponding to reflection or transmission of the wave. We denote these channels by n ($X \to -\infty$) and n′ ($X \to +\infty$). All channels for which the energy λ_n is larger than E_0 will be closed. Figure 1 illustrates the case when channels 0, 1, 1′, 2, and 2′ are open, and 3, 3′, and 0′ are closed. The channel 0′ is always closed: for "motion" along a slanted term there is always reflection, if X is sufficiently large.

The problem consists in determining the transition probabilities between the open channels. By the same method as in Sec. 2, it is easy to obtain the solution in the form of an integral:

$$|\psi\rangle = N\int_C G(E)\,|\varphi\rangle\Phi(E)\exp\Big(i\alpha^{-1}\int^{E}\Phi(E')\,dE' + iPX\Big)\,dE, \tag{26}$$
$$P = [2M(E_0 - E)]^{1/2}, \quad \Phi(E) = \langle\varphi|G(E)\,|\varphi\rangle^{-1}\frac{dP}{dE}.$$

The transition to the classical limit for the motion along X, for $E_0 \gg E$, can be obtained by setting $X = v_0 t$, $p \approx (2ME_0)^{1/2} - Ev_0^{-1}$, $E_0 = Mv_0^2/2$, $dP/dE \approx -v_0^{-1}$, $\beta = \alpha v_0$. Then (26) goes over into (4). The function $\Phi(E)$ occurring in the integral has poles at the same points λ_i, but in addition it has a branch point $E = E_0$, corresponding to reflection for motion along the zero term.

The selection of the integration contour and analysis of the asymptotic properties of the function $|\psi\rangle$ can be carried out by the same method as for the nonstationary problem. The residues of the function $\Phi(E)$ at the poles λ_n, quantities which determine the probabilities of elementary transitions, are

$$h_n^2(dP/dE)_{\lambda_n} = h_n^2/v_n,\ v_n = [2(E_0 - \lambda_n)/M]^{-1/2}.$$

Denoting

$$p_n = \exp(-2\pi h_n^2 v_n^{-1}\alpha_n^{-1}), \tag{27}$$

we obtain for the transition probabilities of the open channels n and m′ the same equations, (14) and (18), as before. In place of the formula (15) we have $S_{00'}^2 = 0$, and for transition probabilities involving reflections we obtain

$$\begin{aligned} &|S_{nm}|^2 = q_n p_{n+1}\ \ldots\ p_{n_0}p_{n_0}p_{n_0-1}\ \ldots\ p_{m+1}q_m,\\ &|S_{00}|^2 = p_1\ \ldots\ p_{n_0}p_{n_0}\ \ldots\ p_1,\quad \lambda_{n_0} < E_0 < \lambda_{n_0+1},\\ &|S_{n'm'}|^2 = 0. \end{aligned} \tag{28}$$

Time reversal symmetry is here, obviously, verified, so that, e.g., $S_{nm'} = S_{m'n'}$, etc.

Thus: a) transitions from the left to the right with decrease of energy, and transitions from the right to the left with increase of energy, are forbidden; b) there is no reflection for motion from the right to the left along an arbitrary term. The formula giving the decomposition of the S-matrix taking into account reflection at E_0 has the form

$$S = S_1S_2\ \ldots\ S_{n_0}S_{n_0}S_{n_0-1}\ \ldots\ S_1. \tag{29}$$

Consequently, the properties considered in Sec. 2 are preserved in this case too. We must only take into account the presence of the turning point, and the fact that at the points of intersection of the unperturbed terms, the velocities v_n have different values. If $E_0 \gg E$, all $v_n \approx v_0$; then, if we neglect the product $p_1p_2\ \ldots\ p_{n_0}$ and take into account the fact that $\beta = \alpha v_0$, we arrive at the previous formulas (14), (15), and (18). It is also easy to generalize these formulas to the case when H_0 has a continuous spectrum.

4. POSSIBLE GENERALIZATIONS AND EXAMPLES

In addition to the case where V has a linear time-dependence, the problem can also be easily solved for any linear fractional function of time, and in particular, if V is inversely proportional to the time. Then the equation

$$[H_0 + |\varphi\rangle\gamma t^{-1}\langle\varphi|]|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle \tag{30}$$

has the solution

$$|\psi\rangle = N\int_C G(E)\,|\psi\rangle\exp\Big(i\int^{E}\langle\varphi|G(E')\,|\varphi\rangle\,dE' - iEt\Big)\,dE, \tag{31}$$

which has a form even simpler than (4). Unfortunately, the perturbation becomes infinite at t = 0, which makes this model more complicated in practical cases. The

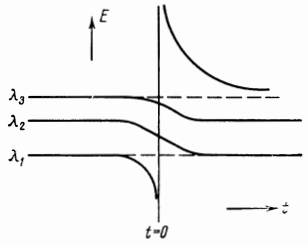

FIG. 3

general shape of the terms for the case of three discrete states is represented in Fig. 3. In some cases, when terms that go off to infinity may be neglected, one can still utilize this model. In particular, for the nonstationary problem

$$(H_0 e^{\alpha t} + |\psi\rangle\, b\, \langle\varphi|)\,|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle, \tag{32}$$

i.e., for exponentially diverging terms interacting with one horizontal term, the substitution $e^{\alpha t} = s$ reduces the problem (32) to (30) and thus, the problem is also rigorously solvable. For a system with two states this problem has been treated by Nikitin[5], and also in [9], and was used for a discussion of the problem of nonresonant charge exchange, and for a computation of transitions among fine structure components in alkali metals in collisions.

It is also easy to write down the solution of the corresponding quantum problem.

If the operator V depends quadratically on time, we are led to a second order equation for F(E), and the problem reduces to an investigation of this equation, and a discussion of the solution in the vicinity of the points λ_i. The quadratic time-dependence allows us to introduce time-reversal invariance explicitly, and thus facilitates the utilization of the model in concrete cases. We finally remark that the equation

$$(H_0 + |\varphi\rangle\, e^{\alpha t}\, \langle\varphi|)\,|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle \tag{33}$$

leads to a functional equation for the function F(E), equation which relates the values F(E) and F(E + α), and in some cases this equation is easily solved or analyzed. In the two-level approximation elementary transformations transform (33) into (32).

The simplest problem referring to the class discussed in Sec. 2 is the Landau-Zener model itself. In this case the vector $|\psi\rangle$ has two components and the operator H is of the form

$$H = \begin{pmatrix} \beta t & h \\ h & \lambda \end{pmatrix}, \tag{34}$$

leading to the well-known solution. Another example is the case of one degree of freedom x, and $|\varphi\rangle = \delta(x - x_0)$. Then $\langle\varphi|G(E)|\varphi\rangle = G(x_0, x_0, E)$ and the solution of Eq. (1) has the form

$$|\psi\rangle = N\int_C \frac{G(x_0, x, E)}{G(x_0, x_0, E)} \exp\left(-\frac{i}{\beta}\int^E \frac{dE'}{G(x_0, x_0, E')} - iEt\right) dE. \tag{35}$$

For this example it is easy to clarify the meaning of the asymptotic states $|n\rangle$ and of the eigenvalues λ_n. Indeed, if H_0 is the energy operator for a particle in a potential well,

$$G(x_0, x_0, E) = \psi_1(x_0, E)\psi_2(x_0, E),$$

where ψ_1 and ψ_2 are the solutions of the Schrödinger equation satisfying the boundary conditions for $x \to -\infty$ and $x \to +\infty$, respectively. It can be seen from here that the equation $G(x_0, x_0, E) = 0$ has as its roots the energy levels in the right and left parts of the potential well, if the well is separated by an impenetrable barrier, and in addition there is one level localized near the point x_0. Thus, in this case there are two independent energy level systems before the interaction, for the two parts of the potential well separated by the impenetrable barrier, and in addition there is one level localized in the vicinity of x_0. As t varies from $-\infty$ to 0, the barrier gradually disappears, and the levels get "mixed up." As t approaches $+\infty$ the barrier appears again, but this time without the state localized at x_0. This method allows one to determine the transition probability between all the levels of such a problem.

If one assumes that $H_0 = -\frac{1}{2}\partial/\partial x^2$ is the operator of a free particle, we obtain directly

$$G(x, E) = (-2E)^{-1/2}\exp\left(-\sqrt{-2E}\,|x|\right), \quad G(x_0, x_0, E) = (-2E)^{-1/2}, \tag{36}$$

$$\Delta(E) \sim E^{1/2}, \quad -\ln w(E) \sim E^{3/2} \tag{37}$$

—a result derived in[10], i.e., we obtain the spectrum of emitted particles when a bound state is expelled from a well of small radius into the continuous spectrum.

Another example of application of this method can be obtained by considering a three-dimensional potential well of small diameter and variable depth—a model which was used in[10,11]. If the nonstationary boundary condition at the point $\mathbf{r}_0$, where the well is, is written in the form

$$|\psi\rangle = A(t)\left(\frac{1}{|\mathbf{r} - \mathbf{r}_0|} + \beta t\right) + O(|\mathbf{r} - \mathbf{r}_0|), \tag{38}$$

the problem is also exactly solvable.

In distinction from the one-dimensional case the well disappears for $t \to +\infty$, and $H \to H_0$. At $t \to -\infty$ one may also consider $H \to H_0$, since the well becomes very deep, the energy of the bound state inside $E \approx -\beta v^2/2$ becomes very large, and it has no influence on the other states. There is no division of the system into two parts at $t \to \pm\infty$, and in this respect too the three-dimensional problem is simpler than its one-dimensional counterpart.

The solution of the nonstationary Schrödinger equation

$$(-\tfrac{1}{2}\nabla^2 + U_0(\mathbf{r}))\,|\psi\rangle = H_0|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle \tag{39}$$

with the boundary condition (38) can be written in the form

$$|\psi\rangle = N\int_C G(\mathbf{r}, \mathbf{r}_0, E)\exp\left(\frac{i}{\beta}\int^E G_{reg}(\mathbf{r}_0, \mathbf{r}_0, E')\,dE' - iEt\right) dE, \tag{40}$$

where G_{reg} is the Green's function from which the singular part has been subtracted, and is determined by the formula

$$G(\mathbf{r}, \mathbf{r}', E) = \frac{1}{2\pi}\left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} + G_{reg}(\mathbf{r}, \mathbf{r}', E)\right). \tag{41}$$

Thus the problem is reduced to the determination of the residues of the function $G_{reg}(E)$ at the poles, i.e., at the points corresponding to the discrete eigenvalues of H_0, and to the determination of the discontinuity of $G_{reg}(E)$

across the cut, where H_0 has its continuous spectrum.

If $U_0 = 0$, $G(r, E) = (2\pi r)^{-1}\exp(-(-2Er)^{1/2})$, $G_{reg}(E) = -(-2E)^{1/2}$, and it is easy to derive the same result (37) as in the one-dimensional case. If one considers that $U_0 = 0$, but the particle moves in a half-space with the boundary condition $|\psi\rangle = 0$ (antisymmetric case) or $\partial|\psi\rangle/\partial n = 0$ (symmetric case) on the boundary surface, then the Green's function is easily obtained by the method of images, and we arrive at the model used in[11] for the description of the process of electron detachment in collisions of negative ions with an atom. The case of a potential U_0 which has Coulomb behavior for large r, has been used in[12] for the description of ionization on slow atomic collisions.

An example of a stationary problem discussed by this method is the Landau-Zener problem with one horizontal term, solved in[16]. This was the example where the triangular property of the S-matrix was noted.

We remark in conclusion that usually those quantum mechanics problems which can be exactly solved involve only few (one, two) nontrivial parameters, which restricts their applicability. In the class of problems considered here there is an infinite number of such parameters (e.g. h_n, λ_n), it is possible to consider discrete, continuous and mixed zonal (periodic fields) spectra for the operator H_0. Therefore it can be expected that this mathematical method will be useful for the description of the most varied physical objects.

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