NONSTATIONARY PROBLEMS OF QUANTUM MECHANICS AND THE LAPLACE TRANSFORM

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NONSTATIONARY PROBLEMS OF QUANTUM MECHANICS AND THE LAPLACE TRANSFORM

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Very few cases are known in which the nonstationary Schrödinger equation

$$H(t)\psi = [H_0 + V(t)]\psi = i\,\partial\psi/\partial t \tag{1}$$

with a time-dependent energy operator H can be solved exactly, or reduced to the solution of a stationary problem with a time-independent operator H_0. We shall show that for a special, but nevertheless fairly broad, class of operators $V(t)$ of the form

$$V = |\varphi\rangle\beta t\langle\varphi| \tag{2}$$

the problem can be solved exactly in the form of a contour integral (below we shall use Dirac notation). Thus, the operator V must depend linearly on time and be a projection operator onto some vector $|\varphi\rangle$ in the space of functions $|\psi\rangle$. We shall show below that in this case the properties of the energy operator H (in particular, the behavior of its eigenvalues with time) are such that, for various concrete problems, for example in collision theory, the real energy operator can be approximately replaced by an operator of this type. We shall seek a solution of equation (1) in the form

$$|\psi\rangle = \int_C e^{-iEt}F(E)(H_0 - E)^{-1}|\varphi\rangle\,dE. \tag{3}$$

Substituting (3) into (1), taking (2) into account, integrating by parts, and equating the integrand to zero, we obtain the equation for $F(E)$

$$(d/dE)\,[F(E)\langle\varphi|(H_0 - E)^{-1}|\varphi\rangle] = -(i/\beta)F(E). \tag{4}$$

Hence we obtain explicitly the solution of equation (1)

$$|\psi\rangle = N\int_C \frac{(H_0-E)^{-1}|\varphi\rangle}{\langle\varphi|(H_0-E)^{-1}|\varphi\rangle}\exp\left[-\frac{i}{\beta}\int^E \frac{dE'}{\langle\varphi|(H_0-E')^{-1}|\varphi\rangle} - iEt\right] dE. \tag{5}$$

From the assumption that the nonintegral term in integration by parts must vanish, there follows the condition on the contour C

$$\exp\left[-\frac{i}{\beta}\int^E \frac{dE'}{\langle\varphi|(H_0-E')^{-1}|\varphi\rangle} - iEt\right]\Bigg|_C = 0. \tag{6}$$

Let us now prove that the saddle points of the exponential function coincide with the instantaneous eigenvalues of the energy operator H. Indeed, the condition determining the saddle points has the form

$$\langle\varphi|(H_0-E)^{-1}|\varphi\rangle = -(\beta t)^{-1}. \tag{7}$$

Multiplying the equation for the eigenfunctions

$$[H_0 - E + |\varphi\rangle\beta t\langle\varphi|]|\psi\rangle = 0 \tag{8}$$

on the left by $\langle\varphi|(H_0-E)^{-1}$, we likewise arrive at equation (7).

It should be noted that, in the presence of a continuous spectrum of the operator H_0, the operator $(H_0-E)^{-1}$ has a cut along the region of the continuous spectrum. Then equation (7) may have solutions on the "unphysical" sheet, correspond-

corresponding to quasistationary or virtual states of the system, and transitions of the roots from the physical sheet to the "nonphysical" one are possible as t changes (see (1)).

As $t \to \pm\infty$, the eigenvalues of H tend to limiting values, which are determined by the equation

$$\langle\varphi|(H_0-E)^{-1}|\varphi\rangle = 0. \tag{9}$$

For $t=0$ the saddle points evidently coincide with the eigenvalues of H_0.

Let us choose a representation in which the operator V is diagonal. Then the matrix H has, in this representation, the form

$$\begin{pmatrix} H_{00}+\beta t & H_{01} & H_{02}\dots \\ H_{10} & H_{11} & H_{12}\dots \\ H_{20} & H_{21} & H_{22}\dots \\ \dots & \dots & \dots \end{pmatrix}. \tag{10}$$

If we further diagonalize the submatrix

$$\begin{pmatrix} H_{11} & H_{12}\dots \\ H_{21} & H_{22}\dots \\ \dots & \dots \end{pmatrix} \to \begin{pmatrix} \lambda_1 & 0\dots \\ 0 & \lambda_2\dots \\ \dots & \dots \end{pmatrix}; \qquad \lambda_1 < \lambda_2 < \dots, \tag{11}$$

then the matrix H will be reduced to the form

$$\begin{pmatrix} H_{00}+\beta t & H'_{01} & H'_{02}\dots \\ H'_{10} & \lambda_1 & 0\dots \\ H'_{20} & 0 & \lambda_2\dots \\ \dots & \dots & \dots \end{pmatrix}. \tag{12}$$

If $|\beta t| \gg |H'_{0n}|$, $n = 0, 1, 2, \dots$, then the eigenvalues of the matrix will be close to $\lambda_1, \lambda_2, \dots$, and, consequently, $\lambda_1, \lambda_2, \dots$ are limiting eigenvalues of the operator H and roots of equation (9). In addition to these eigenvalues, the operator H will have one more, close to βt for large $|t|$. The projection operator $|\varphi\rangle\langle\varphi|$ is nonnegative; therefore, as βt increases, all eigenvalues λ_n also increase monotonically. At the same time, since the matrix (12) is obtained from (11) by "bordering" (see (2)), the eigenvalues (11) and (12) separate one another on the real axis E, so that when t varies from $-\infty$ to $+\infty$ the level βt passes into λ_1, λ_1 into λ_2, and so on.

The spectrum of the operator H as a function of t (the terms) is shown in Fig. 1 for the case when H_0 has only three levels. In doing so we can always exclude from consideration those levels whose eigenfunctions are orthogonal to $|\varphi\rangle$ and, consequently, do not interact with the perturbation V.

Thus, at the points $\lambda_1, \lambda_2, \dots$ the function $\langle\varphi|(H_0 - E)^{-1}|\varphi\rangle^{-1}$ has simple poles with real residues $r_1, r_2, \dots$. Consequently, the integrand in formula (5) behaves at the points λ_n as $(E-\lambda_n)^{-1-ir_n/\beta}$ and, on encircling λ_n, acquires the additional factor $e^{2\pi r_n/\beta}$, so that the λ_n are branch points.

If we suppose that as $t \to -\infty$ the system was in the state λ_n, then we must choose the contour so that as $t \to -\infty$ it passes only through the given saddle point: both branches of the contour should be directed into regions in which the exponential (6) tends to zero. As t changes from $-\infty$ to $+\infty$, the contour must be deformed, and it will pass through many saddle points; moreover, the "heights" of these saddles will, in the limit $t \to \infty$, differ by time-independent factors of the type $e^{-\pi r_n/\beta}$. In this way one can obtain all transition probabilities, the S-matrix, etc.

By the same method one can solve quantum problems in which an external parameter (for example, the distance between nuclei in the collision of ato-

variables), which explicitly depended on time in the class of problems considered above, is replaced by the quantum degree of freedom X, corresponding to free

Fig. 1

Figure 1: Fig. 1

Fig. 2

Figure 2: Fig. 2

motion with effective mass M. Then the energy is an integral of the motion, and we arrive at the equation

$$\left(-\frac{1}{2M}\frac{\partial^2}{\partial X^2}+H_0+|\varphi\rangle\alpha X\langle\varphi|\right)|\psi\rangle=E_0|\psi\rangle. \tag{13}$$

In an analogous way we obtain the solution

$$|\psi\rangle=N\int_C(2E)^{-1/2}\langle\varphi|(H_0-E_0+E)^{-1}|\varphi\rangle^{-1}(H_0-E_0+E)^{-1}|\varphi\rangle\times$$

$$\times\exp\left[(iM/\alpha)\int^E(2E')^{-1/2}\langle\varphi|(H_0-E_0+E')^{-1}|\varphi\rangle dE'+i(2E)^{1/2}X\right]dE. \tag{14}$$

For large M and not too small E_0 one can trace the transition to the classical treatment of the coordinate X, when it changes uniformly with time, and we return to equations (1), (2).

Fig. 1

Fig. 2

Finally, one can write the solution in explicit form for equations (1) or (13), when the multiplier at the projection operator is a linear-fractional function of t (or X). We shall write the solution only for the case

$$V=|\varphi\rangle(\gamma t)^{-1}\langle\varphi|. \tag{15}$$

Then as $t\to\pm\infty$ the operators H and H_0 coincide; however, at $t=0$ a singularity appears to which it is difficult to assign any physical meaning. The general behavior of the terms for the case when H_0 has only three levels is shown in Fig. 2. The solution of equation (1) is obtained in the form

$$|\psi\rangle=N\int_C(H_0-E)^{-1}|\varphi\rangle\exp\left[-\frac{i}{\gamma}\int^E\langle\varphi|(H_0-E')^{-1}|\varphi\rangle dE'-iEt\right]dE. \tag{16}$$

The use of the general formulas given here in solving concrete problems is connected above all with the possibility of calculating the function $(H_0 - E)^{-1}|\varphi\rangle$. It is easy to represent it in the form of an integral if the resolvent operator for H_0 is known, whose kernel is the Green' s function. The Green' s function is known for many one-dimensional problems and for some many-dimensional ones (free particle, oscillator, hydrogen atom, short-range potential, etc.). Examples of concrete problems solved by the method considered here can be found in papers (^{3}) (H_0 is a free particle, φ is a δ-function) and (^{4}) (H_0 is a free particle in a half-space, φ is a δ-function). The simplest example is also the Landau-Zener approximation (^{5}) ($H_0 = a\sigma_x$, where σ_x is the Pauli matrix, $\psi(\sigma)$ is a two-component function, $\varphi = \delta_{1\sigma}$). A quantum treatment of the Landau-Zener approximation corresponding to formulas (13), (14) was carried out ···

but in the paper^6. Obviously, in collisions of atoms and ions the transition from equation (1) to (13) is necessary when the energy of the colliding particles is comparable with the change in energy in the given inelastic process.

It is seen from Fig. 1 that our approximation is convenient to use when one considers transitions between a group of terms running parallel (or a continuum) and a single term which, in the absence of perturbation, intersects the remaining terms at a certain angle. Such a picture often occurs approximately in collisions of atoms and molecules, when ionization or excitation of vibrational or rotational levels of molecules takes place. Apparently, other applications are also possible.

In conclusion, for greater concreteness, we give the explicit form of the formulas obtained for the case when V is a short-range potential, i.e., φ is a δ-function in the coordinate representation. In the one-dimensional case the Schrödinger equation has the form

$$[-\tfrac{1}{2}\partial^2/\partial x^2 + V_0(x)]\psi = i\,\partial\psi/\partial t. \tag{17}$$

The operator V, different from zero only at the point x_0, may be replaced by the boundary condition

$$(\partial\psi/\partial x)\big|_{x_0-0}^{x_0+0} = 2\beta t\psi(x_0, t). \tag{18}$$

Then the solution may be represented in the form

$$\psi = N\int_C^t \frac{G(x_0, x, E)}{G(x_0, x_0, E)} \exp\left[-\frac{i}{\beta}\int^E \frac{dE'}{G(x_0, x_0, E')} - iEt\right], \tag{19}$$

where G is the Green' s function for the operator H_0. In this case, as $t \to \pm\infty$, there is an impenetrable barrier at the point x_0; the limiting eigenvalues of the operator H correspond to energy levels in the right and left parts of the potential well V_0, separated by this barrier. Thus, here we have two systems, independent as $t \to \pm\infty$ and interacting at finite t, which is formally similar to problems of collision theory. In the three-dimensional case a short-range potential may be replaced by the boundary condition(^{2},^{3})

$$\psi = A(t)\left[|r - r_0|^{-1} + \beta t\right] + O(|r - r_0|). \tag{20}$$

As $t \to \pm\infty$ this potential ceases to affect H, so that $H \to H_0$, and no separation of the system into two parts occurs. The solution in this case may be written in the form

$$\psi = N \int_C G(r, r_0, E) \exp\left[\frac{i}{\beta}\int^E G_{\text{reg}}(r_0, r_0, E')\, dE' - iEt\right] dE, \tag{21}$$

where G_{reg} is the Green' s function with the singular part subtracted. It is precisely to these formulas that the problems solved in(^{2},^{3}) reduce.

It is easy to see that the derivation of all the formulas given is entirely analogous to the Laplace method for solving ordinary linear differential equations with coefficients depending linearly on the argument(^{7}), so that in fact these formulas are a generalization of the Laplace method to the case where the coefficients in the equation are not numbers, but operators.

In the problems considered, the time-dependent perturbation may be regarded as small as $t \to \pm\infty$. However, for finite t it is by no means small, and the problem is solved exactly, without expansion in a perturbation-theory series. From this point of view, the formulas obtained are also of interest.

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Note: Figure translations are in progress. See original paper for figures.

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