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Nonstationary Quantum Mechanics. IV. Nonadiabatic Properties of the Schrödinger Equation in Adiabatic Processes

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It is shown that the nonstationary Schrödinger equation does not satisfy a well-known adiabatical principle in thermodynamics. A "renormalization procedure" based on the possible existence of a time-irreversible basic evolution equation is proposed with the help of which one comes to agreement in a variety of specific cases of an adiabatic inclusion of a perturbing potential. The ideology of the present article IV rests essentially on the ideology of the preceding articles, in particular article I.

1. INTRODUCTION

In (T1)[1] we demonstrated a difficulty of logic in the application of the Schrödinger equation (SE) to the nonstationary case. No difficulty of this type exists in the stationary case. This fact, combined with the well-known efficiency of the SE in the stationary case from the point of view of experiment, shows that one has to consider the following alternative: The fundamental evolution equation of a microsystem is time-irreversible (T1). In the stationary case it coincides with the stationary SE, the role of the corresponding irreversible additional term gradually increasing (starting from zero) with the "increase of nonstationarity" of the system. In essentially nonstationary cases this term may play an important role and lead to clear-cut disagreement with experiment, a verification of which seems to already exist [cf. the discussion of some experimental results in (T1)]. The

[1] By (T1), (T2), (T3), and (T5) we denote, correspondingly, articles parts I, II, III, and V of our series "Nonstationary Quantum Mechanics" (Todorov, 1980a–d).

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considerations in (T3) showed the presence of disagreement between classical mechanics and the nonstatic SE in the case of potentials rapidly varying with time exactly in the regions of space in which the classical approximation should hold best. This phenomenon is evidence of the nonphysical character of the SE in the nonstationary case and it encourages further investigations in the field of time-dependent potentials.

It is natural to turn now to slowly varying potentials with time and see whether the SE has nonphysical peculiarities in this case too. It was said already that the magnitude of the additional irreversible terms must decrease with the decrease of the speed of inclusion of the nonstationary perturbation. But if we examine time intervals which are large enough, the insignificant difference between the SE and the hypothetical basic evolution equation may lead to noticeable effects due to some kind of slow accumulation. We certainly do not know yet the exact form of the basic equation and cannot compare its solution with the solution of the SE for such cases. But practice has taught us what one should expect in adiabatic (in the present work we use this word as a synonym for very slow) processes and one must check whether the SE gives the expected result and whether some known peculiarities of the hypothetical equation (T1) can be employed for the removal of eventual nonphysical terms in the solutions of the SE. This is precisely what will be done in what follows.

2. DISAGREEMENT BETWEEN THE SE AND AN ADIABATICAL PRINCIPLE IN THERMODYNAMICS

A well-known principle in thermodynamics says that in an adiabatic process the system of interest will pass through a well-defined series of intermediate states (between the initial and final ones), any one state being uniquely determined in any moment t by the values of the thermodynamical parameters in this t. In other words, our system is practically in equilibrium at any moment t and this state of equilibrium corresponds to the values of the thermodynamical parameters (volume, pressure, external fields) at t.

It would be impossible to construct a coherent picture of thermodynamics without this fundamental principle. Its full agreement with experiment is not, and cannot be, doubted.

An important feature of the above principle is the fact that no definite law of the variation of the thermodynamical parameters is fixed. They can vary arbitrarily with time, as long as this variation is slow enough (adiabatic). Concretely, the system may come in different ways to some fixed final values of its parameters and its final state is always uniquely determined by these parameters and not by the way in which they are reached if the variation of the parameters is adiabatic.

In the case when the system of interest does not exchange heat with other bodies the above may be simply illustrated with the consideration by Landau and Lifschitz (1964) of the variation of the entropy $S(R)$ in the presence of a slowly varying parameter $R(t)$. Indeed, $dS/dt = (dS/dR)(dR/dt)$ can be represented as a series $a_1 dR/dt + a_2 (dR)^2/dt^2 + \ldots$, a_i being constants and dR/dt the corresponding small quantity. We have always $dS/dt \geqslant 0$, so that $a_1 = 0$ since the first-order term changes its sign together with dR/dt. This immediately shows that $dS/dR = 0$ in such processes—a result which will be shown to be completely out of reach of the SE, the solution of which is strongly influenced by the specific dependence of R on t.

It is a truism that the solution of the SE cannot be given in a simple analytical form in the general case. For that reason we shall employ the theory of nonstationary perturbations (TNSP) in its ordinary form to the case of a system with a discrete energy spectrum considering that the perturbation included is small. It will be shown that the SE agrees with the said principle only in the first-order approximation of the TNSP generally, marked disagreement appearing in the higher-order approximations. In cases when the adiabatic perturbation is not small (after its full inclusion) this will, evidently, mean that the SE is in complete disagreement with the adiabatic principle since the order of magnitude of the corrections is the same as that of the nonperturbed solutions then.

For the sake of simplicity we shall examine real-valued complete orthonormal sets of eigenfunctions of the initial nonperturbed Hamiltonian $H_0 = H_i$. An additional assumption will be the coincidence of the initial state ψ_i of our system with the nondegenerated ground state $\psi_1^{(0)}$ of H_0 (the cases of one-dimensional motion of a single particle, e.g., satisfy the above requirements). The former restriction, being by no means substantial, leads to a considerable economy of effort. The assumption $\psi_i = \psi_1^{(0)}$ corresponds to a temperature $T_i = 0$ of the many-body system. We choose such a ψ_i since in a number of cases (inherent semiconductors, dielectrics, superconductors) the energy of the electronic ground state $\psi_1^{(0)}$ is separated from the first excited level by a finite energy gap so that one can be sure that, at least in this case, the application of perturbation theory to a many-body system is lawful (no zeros in the denominators).

As we pointed out, the SE will give different final states ψ_f after an adiabatic inclusion of an arbitrary weak perturbation $V(x) = RW(x)$ ($R \ll 1$ being the small parameter and x denoting all the degrees of freedom), depending on the way in which $V(x)$ is included and not coinciding, generally, with the corresponding ground state ψ_1 of the final Hamiltonian

$H_f = H_i + V$. Thus the natural requirement that a ground state of $H_i = H_0$ be transformed into a ground state of $H_f = H_0 + V$ in an adiabatic process irrespective of the specific way in which V is included is not satisfied by the SE.

We shall need the corrections to the eigenfunctions and eigenvalues of H_i in the presence of $V(x)$ as provided by the theory of stationary perturbations (TSP) in our discussion. The TSP will be employed in the form given in most of the textbooks of quantum mechanics (cf., e.g., Davidov, 1963). We are interested here in the correction to $\psi_1^{(0)}$ due to $V(x)$ ($\{\psi_n^{(0)}\}$ and $E_n^{(0)}$, $n=1,2,\ldots$ denoting, correspondingly, the sets of eigenfunctions and eigenvalues of H_i), so we start from

$$(H_i + V)\psi_1 = E_1\psi_1 \tag{1}$$

where ψ_1 (the ground state of H_f) is given by

$$\psi_1 = \sum_m c_m \psi_m^{(0)}, \qquad c_m = c_m^{(0)} = c_m^{(1)} + c_m^{(2)} + \cdots \tag{2}$$

$c_m^{(\alpha)}$ being the correction of an order of magnitude α in respect to $R(c_m^{(0)} = \delta_{1m})$, and

$$E_1 = E_1^{(0)} + E_1^{(1)} + \cdots, \tag{3}$$

$E_1^{(\alpha)}$ being the correction to $E_1^{(0)}$ of an order of magnitude R^α. Proceeding as usually and having in mind that because of our assumption $\psi_k^{(0)*} = \psi_k^{(0)}, k=1,2,\ldots$ we have $\langle m|V|n\rangle = V_{mn} = \langle n|V|m\rangle = V_{nm}, n, m = 1,2,\ldots$ ($|l\rangle = \psi_l^{(0)}$) one comes to the following expressions for the first four corrections to $c_m^{(0)}$ and $E_1^{(0)}$:

$$c_1^{(1)} = 0 \tag{4}$$

$$c_k^{(1)} = \frac{V_{k1}}{\hbar\omega_{1k}} \qquad (k \neq 1) \tag{4'}$$

$$c_1^{(2)} = -\frac{1}{2}\sum_k{}' \frac{V_{k1}}{\hbar^2\omega_{1k}^2} \tag{5}$$

$$c_k^{(2)} = \sum_m{}' \frac{V_{km}V_{m1}}{\hbar^2\omega_{1m}\omega_{1k}} - \frac{V_{k1}V_{11}}{\hbar^2\omega_{1k}^2} \qquad (k \neq 1) \tag{5'}$$

$$c_1^{(3)} = -\sum_k{}'\sum_m{}' \frac{V_{1k}V_{km}V_{m1}}{\hbar^2\omega_{1k}^2\omega_{1m}} + \sum_k{}' \frac{V_{11}V_{k1}^2}{\hbar^3\omega_{1k}^3} \tag{6}$$

$$c_k^{(3)} = -\frac{V_{11}}{\hbar^3\omega_{1k}^2}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}} + \frac{V_{11}^2V_{k1}}{\hbar^3\omega_{1k}^3}$$

$$-\frac{V_{k1}}{\hbar^3\omega_{1k}^2}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}} + \sum_m{}'\sum_n{}'\frac{V_{km}V_{mn}V_{n1}}{\hbar^3\omega_{1m}\omega_{1n}\omega_{1k}}$$

$$-\frac{V_{11}}{\hbar^3\omega_{1k}}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^2} - \frac{V_{k1}}{2\hbar^3\omega_{1k}}\sum_m{}'\frac{V_{m1}^2}{\omega_{1m}^2} \qquad (k=1) \qquad (6')$$

$$c_1^{(4)} = \frac{2V_{11}}{\hbar^4}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^3\omega_{1m}} - \frac{3}{2}\frac{V_{11}^2}{\hbar^4}\sum_k{}'\frac{V_{k1}^2}{\omega_{1k}^4} + \frac{1}{\hbar^4}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\sum_k{}'\frac{V_{k1}^2}{\omega_{1k}^3}$$

$$-\frac{1}{\hbar^4}\sum_k{}'\sum_m{}'\sum_n{}'\frac{V_{1k}V_{km}V_{mn}V_{n1}}{\omega_{1k}^2\omega_{1m}\omega_{1n}} - \frac{1}{2\hbar^4}\sum_k{}'\sum_m{}'\sum_n{}'\frac{V_{km}V_{kn}V_{m1}V_{n1}}{\omega_{1k}^2\omega_{1m}\omega_{1n}}$$

$$+\frac{V_{11}}{\hbar^4}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}^2} + \frac{3}{8\hbar^4}\sum_m{}'\frac{V_{m1}^2}{\omega_{1m}^2}\sum_k{}'\frac{V_{k1}^2}{\omega_{1k}^2} \qquad (7)$$

$$c_k^{(4)} = \frac{1}{\hbar^4}\Bigg[\frac{V_{11}^2}{\omega_{1k}^3}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}} - \frac{V_{11}^3V_{k1}}{\omega_{1k}^4} + \frac{2V_{11}V_{k1}}{\omega_{1k}^3}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}$$

$$-\frac{V_{11}}{\omega_{1k}^2}\sum_k{}'\sum_m{}'\frac{V_{km}V_{mn}V_{n1}}{\omega_{1m}\omega_{1n}} + \frac{V_{11}^2}{\omega_{1k}^2}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^2} + \frac{3}{2}\frac{V_{11}V_{k1}}{\omega_{1k}^2}\sum_m{}'\frac{V_{m1}^2}{\omega_{1m}^2}$$

$$-\frac{1}{\omega_{1k}^2}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}} - \frac{V_{k1}}{\omega_{1k}^2}\sum_m{}'\sum_n{}'\frac{V_{1m}V_{mn}V_{n1}}{\omega_{1m}\omega_{1n}}$$

$$-\frac{V_{11}}{\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{km}V_{mn}V_{n1}}{\omega_{1m}^2\omega_{1n}} + \frac{V_{11}^2}{\omega_{1k}}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^3}$$

$$-\frac{1}{\omega_{1k}}\sum_n{}'\frac{V_{1n}^2}{\omega_{1n}}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^2} + \frac{1}{\omega_{1k}}\sum_m{}'\sum_n{}'\sum_p{}'\frac{V_{km}V_{mn}V_{np}V_{p1}}{\omega_{1m}\omega_{1n}\omega_{1p}}$$

$$-\frac{V_{11}}{\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{km}V_{mn}V_{n1}}{\omega_{1m}\omega_{1n}^2} - \frac{1}{2\omega_{1k}}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}}\sum_n{}'\frac{V_{n1}^2}{\omega_{1n}^2}$$

$$-\frac{V_{k1}}{\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{1m}V_{mn}V_{n1}}{\omega_{1m}^2\omega_{1n}} + \frac{V_{11}V_{k1}}{\omega_{1k}}\sum_m{}'\frac{V_{m1}^2}{\omega_{1m}^3}\Bigg] \qquad (k\neq 1) \qquad (7')$$

$$E_1^{(1)} = V_{11} \tag{8}$$

$$E_1^{(2)} = \frac{1}{\hbar} \sum_m{}' \frac{V_{1m}^2}{\omega_{1m}} \tag{9}$$

$$E_1^{(3)} = \frac{1}{\hbar^2} \left[\sum_k{}' \sum_m{}' \frac{V_{1k} V_{km} V_{m1}}{\omega_{1k} \omega_{1m}} - V_{11} \sum_k{}' \frac{V_{1k}}{\omega_{1k}^2} \right] \tag{10}$$

$$E^{(4)} = \frac{1}{\hbar^3} \left[\sum_k{}' \sum_m{}' \sum_n{}' \frac{V_{1k} V_{km} V_{mn} V_{n1}}{\omega_{1k} \omega_{1m} \omega_{1m}} - 2V_{11} \sum_k{}' \sum_m{}' \frac{V_{1k} V_{km} V_{m1}}{\omega_{1k} \omega_{1m}^2} \right.$$
$$\left. + V_{11}^2 \sum_k{}' \frac{V_{1k}^2}{\omega_{1k}^3} - \sum_m{}' \frac{V_{1m}^2}{\omega_{1m}} \sum_k{}' \frac{V_{1k}^2}{\omega_{1k}^2} \right] \tag{11}$$

In the above notations $\omega_{jk} = -\omega_{kj} = (E_j^{(0)} - E_k^{(0)})/\hbar$, and $\Sigma'_q \ldots$ means summation over all possible integers q with the exception of $q = 1$. Let us recall that $c_1^{(\alpha)}$ is obtained by using the requirement that the wave function be normalized to unity in the αth approximation of the TSP.

Now, what one lawfully expects is that the TNSP must ensure corrections to $\psi_1^{(0)}$ which are essentially small (i.e., of the order of magnitude of R, R^2, and so on). Because we examine adiabatic processes, the duration $T = t_f - t_i$ of the process of inclusion of $V(x)$ will be very great ($T \to \infty$), and inessential divergent terms of an order of magnitude T, T^2, and so on may appear owing to a possible appearing of a constant factor $\exp[i\beta T]$ in the wave function; the real quantity β here depends on R, $W(x)$, and the way in which $V = RW$ is included, as we shall see. The final state satisfies this requirement (though, as was already said, it does not satisfy the adiabatic principle).

According to our natural requirement the wave function

$$\psi_1(t) = \sum_{m=1}^{\infty} d_m(t) \psi_m^{(0)}(x) \tag{12}$$

must be of the following form in moment $t = t_f$:

$$\psi_1(t_f) = e^{i\beta T} \sum_{m=1}^{\infty} (c_m + \text{vanishing terms}) \psi_m^{(0)} \tag{13}$$

c_m being the same as in equations (2) and the vanishing terms tending to zero when $T \to \infty$. In this way we require that one must come essentially to the ground eigenstate of $H_f = H_i + V$ with the improving of the adiabaticity of the process. Let us see now what actually happens in a number of specific cases.

Defining $a_k(t)$ with the help of

$$d_k(t) = a_k(t)\exp\left[-iE_k^{(0)}t/\hbar\right] \tag{14}$$

one comes to the following equation for $a_k(t)$:

$$a_k(t) = a_k(t_i) + \frac{1}{i\hbar}\sum_n \int_{t_i}^{t} V_{kn}(t')e^{i\omega_{kn}t'}a_n(t')\,dt' \tag{15}$$

In our case $(\psi_i = \psi_1^{(0)})\, a_k(t_i) = \delta_{1k}$, so that

$$a_k(t) = \delta_{1k} + a_k^{(1)}(t) + a_k^{(2)}(t) + \cdots \tag{16}$$

where $a_k^{(\alpha)}(t)$ is the αth-order correction to a_k $(\sim R^\alpha)$ when $\psi_i(t_i) = \psi_1^{(0)}$. The term $a_k^{(\alpha)}(t)$ is obtained from

$$\begin{aligned} a_k^{(\alpha)}(t) &= \frac{1}{i\hbar}\sum_n \int_{t_i}^{t} V_{kn}(t')e^{i\omega_{kn}t'}a_n^{(\alpha-1)}(t')\,dt' \\ &= \frac{1}{i\hbar}\sum_n{}' \int_{t_i}^{t} V_{kn}(t')e^{i\omega_{kn}t'}a_n^{(\alpha-1)}(t')\,dt' \\ &\quad + \frac{1}{i\hbar}\int_{t_i}^{t} V_{k1}(t')e^{i\omega_{k1}t'}a_1^{(\alpha-1)}(t')\,dt' \end{aligned} \tag{17}$$

[the separation of the term containing $a_1^{(\alpha-1)}(t)$ is made for the sake of convenience in the calculations since this term is of a different type compared to the rest].

The first specific case which will be examined is

$$\begin{aligned} &V(x,t) = 0, \qquad -\infty < t \leqslant 0, \qquad V(x,t) = (t/T)V(x), \qquad 0 \leqslant t \leqslant T, \\ &V(x,t) = V(x), \qquad t \geqslant T \end{aligned} \tag{18}$$

which corresponds to $t_i = 0$, $t_f = T$, T being assumed to be very large (we shall let T tend to ∞ in the end in accord with the above said). We must stress here that T^{-1} is not an additional small parameter in the problem of the same type as R since what we have in fact is the combination t/T which is ~ 1, generally. T^{-1} characterizes only the adiabaticity of inclusion of V, the only small parameter in the TNSP series being R.

From equations (15)–(17) it follows that we have in the case (18)

$$a_1^{(1)}(t)=\frac{t^2V_{11}}{2i\hbar T} \tag{19}$$

$$a_k^{(1)}(t)=\frac{1}{\hbar T}\left[\left(\frac{tV_{k1}}{\omega_{1k}}-\frac{iV_{k1}}{\omega_{1k}^2}\right)e^{i\omega_{k1}t}+\frac{iV_{k1}}{\omega_{1k}^2}\right] \qquad (k\neq 1) \tag{20}$$

for $0\leqslant t\leqslant T$; V_{km}, obviously, denotes $\langle k|V(x)|m\rangle$ and does not depend on t.

Thus the coefficients $d_m(T)$ [equation (14)] have an expected form in moment $t=T$ with a precision including first-order terms:

$$d_m(T)=\exp\left[\frac{T}{i\hbar}\left(\frac{V_{11}}{2}+\cdots\right)\right](b_m^{(0)}+b_m^{(1)})\exp\left(\frac{-iE^{(0)}T}{\hbar}\right) \tag{21}$$

where

$$b_m^{(0)}=\delta_{1m}, \qquad b_1^{(1)}=c_1^{(1)}=0, \qquad b_k^{(1)}=c_k^{(1)}-\frac{iV_{k1}}{\hbar T}\left(\frac{1}{\omega_{1k}^2}-\frac{e^{i\omega_{k1}T}}{\omega_{1k}^2}\right)$$

$(k\neq 1)$, the last two terms tending to 0 when $T\to\infty$, the term $V_{11}T/2i\hbar$ being treated as a result of the decomposition of $\exp[(TV_{11}/2i\hbar)+\cdots]=1+TV_{11}/2i\hbar+\cdots$. The inessential exponential factor $\exp[T(V_{11}/2+\cdots)/i\hbar]\exp[-iE_1^{(0)}T/\hbar]$ is common for all terms.

Having in mind the values (19) and (20) of $a_m^{(1)}(t)$, one obtains in the second order of the TNSP

$$a_k^{(1)}(t)=\frac{1}{\hbar^2T^2}\left(\frac{t^2}{\omega_{1k}}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}}-\frac{3t^2V_{11}V_{k1}}{2\omega_{1k}^2}-\frac{it^3V_{11}V_{k1}}{2\omega_{1k}}\right)e^{i\omega_{k1}t}$$

$$+O(T)+O(T^{-2}) \qquad (k\neq 1) \tag{22}$$

where $O(T^{-n})$ is a term $\sim T^{-n}$ at a moment $t=T$, i.e., $O(T^{-n})$ are infinitesimal terms in any moment t.

Representing the second term in the brackets as

$$-t^2V_{11}V_{k1}/\hbar^2T^2\omega_{1k}^2-t^2V_{11}V_{k1}/2\hbar^2T^2\omega_{1k}^2$$

we see that

$$d_k(T)=\exp\left[\frac{T}{i\hbar}\left(\frac{V_{11}}{2}+\cdots\right)\right]\exp\left(-\frac{iE_1^{(0)}T}{\hbar}\right)$$

$$\times\left[c_k^{(0)}+c_k^{(1)}+c_k^{(2)}-\frac{iV_{k1}}{\hbar T\omega_{1k}^2}(1-e^{i\omega_{k1}T})\right]$$

$$-\frac{V_{11}V_{k1}e^{-iE_k^{(0)}T/\hbar}}{2\hbar^2\omega_{1k}^2}+O(T^{-1})+O(T^{-2}) \qquad (k\neq 1) \quad (23)$$

with a precision including second-order terms in R. Let us point out that the "infinitesimal terms" (as we shall call from now on the terms proportional to $T^{-n}, n=1,2,\ldots$ at $t=T$) are essential in the second-order calculations since, e.g., .

$$\frac{-iV_{k1}}{\hbar T\omega_{1k}^2}\frac{TV_{11}}{2i\hbar}=-\frac{V_{11}V_{k1}}{2\hbar^2\omega_{1k}^2}$$

is a finite term for all possible values of T. In such a way $\psi_f(T)$ is different from the ground eigenstate ψ_1 of H_f in the second order of the TNSP since the term $-V_{11}V_{k1}\exp[-iE_k^{(0)}t/\hbar]/2\hbar^2\omega_{1k}^2$ in equation (23) is of the same order of magnitude as $c_k^{(2)}$ and breaks the postulated natural picture. The magnitude of this term does not depend on T, so it is impossible to remove it by letting $T\to\infty$.

What mechanism creates the said inconvenient term in $d_k(T)$? The answer of this question may not only help in understanding the phenomenon, but it can imply the creation of some simple "renormalization procedure" for the removal of such terms.

It is easy to see that the presence of the above term in $d_k(T)$ is due to the presence of the constant last term in the right-hand side of (20). The latter term will give a contribution equal to $iV_{k1}\exp[-iE_k^{(0)}t/\hbar]/\hbar T\omega_{1k}^2$ in $d_k^{(1)}(t)(0<t<T)$. Terms that depend on t only through the factor $\exp(-iE_k^{(0)}t/\hbar)$ will appear in $d_k^{(q)}(t), q\geq 2$, too—this will be seen in our subsequent discussion. In such a way we shall have in the end

$$d_1(t)=f_1(t)+K_1\exp\left[-iE_1^{(0)}t/\hbar\right] \qquad (24)$$

where K_1 are some constants. Equation (12) will thus give

$$\psi_1(t)=\psi_1'(t)+\psi_1''(t) \qquad (25)$$

where

$$\psi_1'(t)=\sum_m f_m(t)\psi_m^{(0)} \quad \text{and} \quad \psi_1''(t)=\sum_m K_m \exp\left(-\frac{iE_m^{(0)}t}{\hbar}\right)\psi_m^{(0)}$$

$\psi_1''(t)$ is, obviously, a solution of the nonperturbed SE $i\hbar\partial\psi_1''/\partial t=H_i\psi_1''$. The decomposition (25) of $\psi_1(t)$ is an expression of a simple fact discussed in any book on differential equations. Namely, the general solution of the linear differential equation $Lu=w$, L being a linear operator, is given by $u=u_0+u'$, where u_0 is the general solution of the homogeneous linear equation $Lu_0=0$ and u' is a solution of the inhomogeneous equation $Lu'=w$. If one has found u', then the concrete choice of specific constants in u_0 is made in accord with the requirement of definite (e.g., initial) conditions for u. In our case $L=-i\hbar\partial/\partial t-H_0$, $w=V(x,t)\psi_1(x,t)$. The TNSP gives a solution $\psi_1'(t)=\Sigma_m f_m(t)\psi_m^{(0)}$ of the corresponding inhomogeneous equation which is combined with $\psi_1''(t)$ in such a way (see above) that the initial condition $\psi_i(t_i)=\psi_1^{(0)}$ is fulfilled. The initial value of ψ_1'' is, evidently,

$$\psi_1''(t_i)=\psi_1^{(0)}+O(T^{-1})+\cdots+O(T^{-n})+\cdots \tag{26}$$

According to the discussion in (T1) the general evolution equation is not the SE but

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi+\hat{\Gamma}\psi \tag{27}$$

where the last term $\hat{\Gamma}\psi$ creates time-irreversibility. Some additional information (hidden variables) may be necessary for the solution of (27), but in the case $H=H_0=H_i$, $\psi_i(t_i)\approx$the right-hand side of (26), the result of (27) should be equal practically with certainty to

$$\psi(t)=\sum_{m=1}^{\infty} e_m(t)\psi_m^{(0)}(t)\to\psi_1^{(0)}, \qquad t\to\infty \tag{28}$$

if $e_m(t_i)$ are of the same order of magnitude as K_m because $\psi_i(t_i)$ almost coincides with $\psi_1^{(0)}$ in this case. The time dependence of $|e_m(t)|_{m>2}$ will be of the form $\exp[-|(E_m^{(0)}-E_1^{(0)})t/\hbar|]$. [This property of $e_m(t)$ is discussed in (T1), where it is shown that in the case $H=H_0$ the initial wave packet must relax to some eigenstate $\psi_m^{(0)}$ of H_0 automatically, without any measurement process.]

Certainly, one cannot assert a priori that equation (27) is a linear equation. But one can well argue as follows: The terms $K_m\exp[-iE_m^{(0)}t/\hbar]$,

K_m being infinitesimal, appear due to the weak nonadiabaticity in the first and (or) next time derivatives of $V(x, t)$ in moment $t = t_i$. These terms play an exaggerated role in the TNSP due to the concept that the homogeneous time-reversible equation $i\hbar\partial\psi/\partial t = H_0\psi$ describes the free evolution of a system. According to another concept this is not the necessary equation and the role of possible terms of the same order of magnitude (due to the weak initial nonadiabaticity in the time-derivatives of V) in $d_m(t)$ is expected to be negligible. This is supported by the fact that in the homogeneous equation of the type (27) small deviations from $\psi_i^{(0)}$ of the above-said order of magnitude should disappear in an exponential fashion with time while in the SE they are "immortal." And it is worth stressing that for a fixed t and $T \to \infty$ equation (27) is practically homogeneous in the above sense.

It is logical then to try the simplest possibility in the search for a prescription giving the necessary result $d_m^{(\alpha)}(T) = K(c_m^{(\alpha)} + \text{infinitesimal terms})$, $|K| = 1$, K being the same for $m, \alpha = 1, 2, \ldots$. It consists in the striking out of all constant terms $K_m^{(\alpha)}$ in $a_m^{(\alpha)}(t)$, $m = 2, 3, \ldots, \alpha = 1, 2, \ldots$ (giving the "free" terms $K_m^{(\alpha)} \exp[-iE_m^{(0)}t/\hbar]$ in $d_m^{(\alpha)}$) and applying then equation (17) for the calculation of $a_m^{(\alpha+1)}(t)$ with a subsequent striking out of all constant terms which will appear in this way of action in $a_m^{(\alpha+1)}(t)$. This prescription, implied by equation (27), turns out to be remarkably efficient: Applying it in any specific case we come to the expected form of $d_m^{(\alpha)}(t)$, $\alpha = 1, 2, \ldots$. We are not able to give a general mathematical proof of this, but we shall show that it is true for a number of cases in which one can come to comparatively large α ($\alpha = 3, 4$) without disproportionate efforts. The efficiency of the prescription in all these cases leaves little doubt about its general applicability [all possible $V(x, t)$ and $\alpha = 1, 2, \ldots$]. It is worth emphasizing that the prescription is highly unequivocal: All the constant terms are clearly discernible from the rest in any order of magnitude and no grounds for speculation exist.

The removal of the constant terms in $a_m^{(\alpha)}(t)$ has two effects on $\psi(t)$. One of them consists in a "renormalization" of the initial conditions with some infinitemisal terms (we shall have now $\psi(t_i) = \psi_1^{(0)} + O(T^{-1}) + \cdots$; this affects the normalization of $\psi(t)$ as well:

$$\int |\psi(t)|^2\, dx = \int |\psi(t_i)|^2\, dx = 1 + O(T^{-1}) + \ldots)$$

This effect is insignificant since it is most probably simply an expression of the fact that in this way we cut off some transitory processes having a characteristic relaxation time $\tau \sim \hbar/(E_2^{(0)} - E_1^{(0)})$ in which time infinitesimal terms of the order of magnitude of K_m, $m \geq 2$, have not yet died away. So this infinitesimal breaking of the initial conditions and the normalization of $\psi(t)$ need not be taken seriously.

The second effect is much more interesting. The SE for $a_m^{(2)}(t)$ is

$$i\hbar \frac{da_m^{(2)}}{dt} = \sum_k \langle m|V(t)|k\rangle e^{i\omega_{mk}t} a_k^{(1)}(t) \tag{29}$$

from which it follows that the cutting off of the constant terms in $a_k^{(1)}(t)$, having an order of magnitude $O(T^{-1})$ in the case (18), modifies the SE with terms $O(T^{-1})$ in the second order of the TNSP, and, in spite of the infinitesimal character of these additional quantities, the accumulation of their influence for large T turns out to be important in the said order. In such a way we come to a property which was discussed in the beginning: The equation(s) satisfied by a_m after the application of our prescription tend to the SE with the improving of the adiabaticity of the process ($T \to \infty$) giving, nevertheless, essentially different results when $t_f - t_i \sim T \to \infty$. This may serve as an illustrative example to the discussion of the possible role of symmetry-breaking terms in the quantum Liouville equation in the end of (T2).

We can check now directly the efficiency of our prescription in several specific cases.

3. APPLICATION OF THE PRESCRIPTION TO SPECIFIC CASES

We shall denote now by $a_m^{(\alpha)'}(t)$ the expressions obtained from equation (17) with a subsequent cutting off of the infinitesimal constant terms in $a_m^{(\alpha)}(t)$. Returning to our case (18) we obtain now

$$a_1^{(1)'}(t) = \frac{t^2}{T} \frac{V_{11}}{2i\hbar}$$

$$a_k^{(1)'}(t) = \frac{V_{k1}}{\hbar T \omega_{1k}} \left(t - \frac{i}{\omega_{1k}} \right) e^{i\omega_{k1}t} \qquad (k \neq 1) \tag{30}$$

for $0 < t < T$. Using these expressions for the calculation of $a_m^{(2)'}(t)$, $m > 2$ (no such terms appear in $a_1^{(\alpha)'}(t)$, $\alpha = 1, 2, \ldots$) resulting from equation (17) we obtain

$$a_1^{(2)'}(t)=\frac{1}{\hbar^2T^2}\left(\frac{t^3}{3i}\sum_n{}'\frac{V_{1n}^2}{\omega_{1n}}-\frac{t^2}{2}\sum_n{}'\frac{V_{1n}^2}{\omega_{1n}^2}-\frac{V_{11}^2t^4}{8}\right) \tag{31}$$

$$a_k^{(2)'}(t)=\frac{1}{\hbar^2T^2}\left[\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}}\left(\frac{t^2}{\omega_{1k}}+\frac{2t}{i\omega_{1k}^2}-\frac{2}{\omega_{1k}^3}\right)-\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}^2}\left(\frac{it}{\omega_{1k}}+\frac{1}{\omega_{1k}^2}\right)\right.$$
$$\left.+V_{11}V_{k1}\left(-\frac{it^3}{2\omega_{1k}}-\frac{3t^2}{2\omega_{1k}^2}+\frac{3it}{\omega_{1k}^3}+\frac{3}{\omega_{1k}^4}\right)\right]e^{i\omega_{k1}t}\quad(k\neq1) \tag{32}$$

The coefficients $b_m^{(\alpha)'}$ can be defined with the help of equation (21) by replacing there $d_m(T)$ and $b_m^{(\alpha)}$ by $d_m'(T)$ and $b_m^{(\alpha)'}$. Having in mind the initial conditions and substituting $t=T$ in (30), we obtain

$$b_1^{(0)'}=1=c_1^{(0)},\qquad b_k^{(0)'}=0=c_k^{(0)}\qquad(k\neq1) \tag{33}$$

$$b_1^{(1)'}=0=c_1^{(1)} \tag{34}$$

$$b_k^{(1)'}=c_k^{(1)}-\frac{iV_{k1}}{\hbar T\omega_{1k}^2}=c_k^{(1)}+\text{infinitesimal term} \tag{35}$$

The expressions (8)–(11) about $E_1^{(\alpha)}$ show that the "divergent" terms in $a_1^{(2)'}(T)(T\to\infty)$ can be attributed to the fact that the left exponential factor in the right-hand side of (21) is actually

$$L=\exp\left[\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{2}+\frac{E_1^{(2)}}{3}+\cdots\right)\right] \tag{36}$$

Subtracting from $d_m^{(2)'}(T)$ the second-order terms, arising from the multiplication of $b_m^{(0)'}+b_m^{(1)'}$ by $L\exp[-iE_1^{(0)}T/\hbar]$, we come to

$$b_1^{(2)'}=c_1^{(2)} \tag{37}$$

$$b_k^{(2)'}=\frac{1}{\hbar^2}\left\{\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}}\left[\frac{1}{\omega_{1k}}-\frac{2}{T\omega_{1k}^2}\left(i+\frac{1}{\omega_{1k}}\right)\right]\right.$$
$$\left.-\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^2}\left(\frac{i}{T\omega_{1k}}+\frac{1}{T^2\omega_{1k}^2}\right)+\frac{V_{11}V_{k1}}{\omega_{1k}^2}\left(-1+\frac{3i}{T\omega_{1k}}+\frac{3}{T^2\omega_{1k}^2}\right)\right\}$$
$$=c_k^{(2)}+\text{infinitesimal terms}\qquad(k\neq1) \tag{38}$$

In such a way we have the expected picture for $d_m^{(\alpha)'}(T)$ in the second order.

Using (31) and (32) one obtains

$$a_1^{(3)'}(t) = \frac{1}{\hbar^3 T^3}\left(\frac{t^4}{4i}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}\omega_{1m}} - t^3\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}}\right.$$
$$-\frac{t^2}{i}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^3\omega_{1m}} - \frac{t^2}{2i}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}^2}$$
$$-\frac{V_{11}t^5}{6}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}} - \frac{V_{11}t^4}{2i}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}} + V_{11}t^3\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^3}$$
$$\left.+\frac{3V_{11}t^2}{2i}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^4} - \frac{V_{11}^3t^6}{48i}\right) \tag{39}$$

We shall bring our calculations as far as the fourth order in R. For that reason we shall not fill pages with the entire kilometrical expression for $a_k^{(3)'}(t), k\neq 1$, necessary for the higher-order calculations but shall adduce only those terms that are essential for the fourth-order approximation in R (i.e., which do not give factors of the type $T^{-n}, n=1,2,\ldots,$ in $a_m^{(4)}(T), m=1,2,\ldots$). This approximate expression $a_k^{(3)'}(t)$ obtained with the help of our prescription is equal to

$$a_k^{(3)'}(t) \approx \frac{1}{\hbar^2 T^3}\left\{\frac{t^3}{\omega_{1k}}\sum_n{}'\sum_m{}'\frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}\omega_{1m}} - \frac{V_{11}t^3}{\omega_{1k}}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}}\left(\frac{it}{2}+\frac{2}{\omega_{1k}}\right)\right.$$
$$-\frac{3V_{11}t^3}{2\omega_{1k}}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}^2} - \frac{V_{k1}t^3}{3\omega_{1k}}\sum_n{}'\frac{V_{1n}^2}{\omega_{1n}}\left(it+\frac{4}{\omega_{1k}}\right)$$
$$\left.-\frac{V_{k1}t^3}{2\omega_{1k}}\sum_n{}'\frac{V_{1n}^2}{\omega_{1n}^2} - \frac{V_{k1}V_{11}^2t^5}{8\omega_{1k}} - \frac{5V_{k1}V_{11}^2t^4}{8i\omega_{1k}^2} + \frac{5V_{k1}V_{11}^2t^3}{2\omega_{1k}^3}\right\}e^{i\omega_{k1}t}$$
$$+\left[\frac{3t^2}{i\omega_{1k}^2}\sum_n{}'\sum_m{}'\frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}\omega_{1m}} - \frac{2it^2}{\omega_{1k}}\sum_n{}'\sum_m{}'\frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}^2\omega_{1m}}\right.$$
$$-\frac{it^2}{\omega_{1k}}\sum_n{}'\sum_m{}'\frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}\omega_{1m}^2} + \frac{6it^2V_{11}}{\omega_{1k}^3}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}} - \frac{9V_{11}t^2}{2i\omega_{1k}^2}$$

$$\times \sum_n{}' \frac{V_{kn}V_{n1}}{\omega_{1n}^2} + \frac{3iV_{11}t^2}{\omega_{1k}} \sum_n{}' \frac{V_{kn}V_{n1}}{\omega_{1n}^3} + \frac{4iV_{k1}t^2}{\omega_{1k}^3} \sum_n{}' \frac{V_{1n}^2}{\omega_{1n}}$$

$$- \frac{3V_{k1}t^2}{2i\omega_{1k}^2} \sum_n{}' \frac{V_{1n}^2}{\omega_{1n}} + \frac{15V_{k1}V_{11}^2t^2}{2i\omega_{ik}^4} \Bigg] \frac{e^{i\omega_{k1}t}}{\hbar^3 T^3} \qquad (k \neq 1) \tag{40}$$

where the term in the square brackets can be neglected in the calculation of $a_k^{(4)\prime}(t)$, $k \neq 1$, but cannot be neglected in the calculation of $a_1^{(4)\prime}(t)$.

From equation (39) it follows that we have in fact

$$L = \exp\left[\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{2} + \frac{E_1^{(2)}}{3} + \frac{E_1^{(3)}}{4} + \cdots\right)\right] \tag{41}$$

Our further way of action is practically identical to the one which led to the calculation of $b_m^{(2)\prime}$, $m = 1,2,\ldots$: We subtract from $d_m^{(3)\prime}(T)$, $m = 1,2,\ldots$, the third-order expression (in R) resulting from the multiplication of $b_m^{(0)\prime} + b_m^{(1)\prime} + b_m^{(2)\prime}$ by $L\exp[-iE_1^{(0)}T/\hbar]$, which gives

$$b_1^{(3)\prime} = \frac{1}{\hbar^3}\left(- \sum_k{}' \sum_m{}' \frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}} + V_{11} \sum_k{}' \frac{V_{1k}^2}{\omega_{1k}^3} - \frac{1}{iT} \sum_k{}' \sum_m{}' \frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^3\omega_{1m}} \right.$$

$$\left. - \frac{1}{2iT} \sum_k{}' \sum_m{}' \frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}^2} + \frac{3V_{11}}{2iT} \sum_k{}' \frac{V_{1k}^2}{\omega_{1k}^4} \right)$$

$$= c_1^{(3)} + \text{infinitesimal terms} \tag{42}$$

$$b_k^{(3)\prime} = c_k^{(3)} + \frac{1}{\hbar^3 T}\left(\frac{3}{i\omega_{1k}^2} \sum_n{}' \sum_m{}' \frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}\omega_{1m}} - \frac{2i}{\omega_{1k}} \sum_n{}' \sum_m{}' \frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}^2\omega_{1m}} \right.$$

$$- \frac{i}{\omega_{1k}} \sum_n{}' \sum_m{}' \frac{V_{kn}V_{nm}V_{m1}}{\omega_{1n}\omega_{1m}^2} + \frac{5iV_{11}}{\omega_{1k}^3} \sum_m{}' \frac{V_{km}V_{m1}}{\omega_{1m}}$$

$$- \frac{4V_{11}}{i\omega_{1k}^2} \sum_m{}' \frac{V_{km}V_{m1}}{\omega_{1m}^2} + \frac{3iV_{11}}{\omega_{1k}} \sum_m{}' \frac{V_{km}V_{m1}}{\omega_{1m}^3}$$

$$\left. + \frac{4iV_{k1}}{\omega_{ik}^3} \sum_m{}' \frac{V_{1m}^2}{\omega_{1m}} - \frac{3V_{k1}}{2i\omega_{1k}^2} \sum_m{}' \frac{V_{1m}^2}{\omega_{1m}^2} + \frac{6V_{k1}V_{11}^2}{i\omega_{1k}^4} \right) + O(T^{-2}) + O(T^{-3})$$

$$= c_k^{(3)} + \text{infinitesimal terms} \qquad (k \neq 1) \tag{43}$$

the terms $O(T^{-2})$ and $O(T^{-3})$ being, obviously, inessential for the calculation of $b_k^{(4)'}$. This means that our prescription gives an "actual adiabatic result" in the third order too. The same applies to the fourth order in R, in which we adduce only those terms in $a_m^{(4)'}(t), m=1,2,\ldots,$ which do not contain negative degrees of T at $t=T$:

$$L=\exp\left[\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{2}+\frac{E_1^{(2)}}{3}+\frac{E_1^{(3)}}{4}+\frac{E_1^{(4)}}{5}+\cdots\right)\right] \tag{44}$$

$$\begin{aligned}
a_1^{(4)'}(t)=\frac{1}{\hbar^4T^4}\Bigg(&\frac{t^5}{5i}\sum_k{}'\sum_n{}'\sum_m{}'\frac{V_{1k}V_{kn}V_{nm}V_{m1}}{\omega_{1k}\omega_{1m}\omega_{1n}}-\frac{3V_{11}t^6}{24}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}\omega_{1m}}\\
&-\frac{9V_{11}t^5}{10i}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}}-\frac{t^6}{18}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\\
&-\frac{11t^5}{30i}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^2}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}-\frac{V_{11}^2t^7}{24i}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}}+\frac{3V_{11}^2t^6}{16}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^2}\\
&+\frac{7V_{11}^2t^5}{10i}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^3}\\
&-t^4\sum_k{}'\sum_n{}'\sum_m{}'\frac{V_{1k}V_{kn}V_{nm}V_{m1}}{\omega_{1k}^2\omega_{1m}\omega_{1n}}-\frac{t^4}{2}\sum_k{}'\sum_n{}'\sum_m{}'\frac{V_{1k}V_{kn}V_{nm}V_{m1}}{\omega_{1k}\omega_{1n}^2\omega_{1m}}\\
&+\frac{5V_{11}t^4}{2}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^3\omega_{1m}}\\
&+\frac{5V_{11}t^4}{4}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}^2\omega_{1m}^2}+t^4\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^3}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\\
&+\frac{3t^4}{8}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^2}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}^2}-\frac{9V_{11}^2t^4}{4}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^4}+\frac{V_{11}^2t^8}{384}\Bigg)
\end{aligned} \tag{45}$$

$$\begin{aligned}
a_k^{(4)'}(t)\approx\frac{1}{\hbar^4T^4}\Bigg[&\frac{t^4}{\omega_{1k}}\sum_m{}'\sum_n{}'\sum_p{}'\frac{V_{km}V_{mn}V_{np}V_{p1}}{\omega_{1m}\omega_{1n}\omega_{1p}}-\left(it+\frac{5}{\omega_{1k}}\right)\\
&\times\frac{V_{11}t^4}{2\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{km}V_{mn}V_{n1}}{\omega_{1m}\omega_{1n}}-\frac{2V_{11}t^4}{\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{km}V_{mn}V_{n1}}{\omega_{1m}^2\omega_{1n}}
\end{aligned}$$

$$-\frac{3V_{11}t^4}{2\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{km}V_{mn}V_{n1}}{\omega_{1m}\omega_{1n}^2}-\frac{t^4}{3\omega_{1k}}(it+5)\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}}$$

$$-\frac{4t^4}{3\omega_{1k}}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}^2}-\frac{t^4}{2\omega_{1k}}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}^2}\sum_n{}'\frac{V_{kn}V_{n1}}{\omega_{1n}}$$

$$-\frac{V_{11}^2t^4}{4\omega_{1k}}\left(\frac{t^2}{2}+\frac{3t}{i\omega_{1k}}-\frac{15}{4\omega_{1k}^2}\right)\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}}+\frac{5V_{11}^2t^4}{8\omega_{1k}}\left(it+\frac{5}{\omega_{1k}}\right)$$

$$\times\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^2}+\frac{5V_{11}^2t^4}{2\omega_{1k}}\sum_m{}'\frac{V_{km}V_{m1}}{\omega_{1m}^3}-\frac{V_{k1}t^4}{4\omega_{1k}}\left(it+\frac{5}{\omega_{1k}}\right)$$

$$\times\sum_m{}'\sum_n{}'\frac{V_{1m}V_{mn}V_{n1}}{\omega_{1m}\omega_{1n}}-\frac{V_{k1}t^4}{\omega_{1k}}\sum_m{}'\sum_n{}'\frac{V_{1m}V_{mn}V_{n1}}{\omega_{1m}^2\omega_{1n}}-\frac{V_{11}V_{k1}t^4}{\omega_{1k}}$$

$$\left(\frac{t^2}{6}+\frac{t}{i\omega_{1k}}-\frac{5}{\omega_{1k}^2}\right)\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}+\frac{V_{11}V_{k1}t^4}{2\omega_{1k}}\left(it+\frac{5}{\omega_{1k}}\right)\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}^2}$$

$$+\frac{V_{11}V_{k1}t^4}{\omega_{1k}}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}^3}+\frac{iV_{11}^3V_{k1}t^7}{48\omega_{1k}}+\frac{7V_{11}^3V_{k1}t^6}{48\omega_{1k}^2}$$

$$\left.-\frac{7iV_{11}^3V_{k1}t^5}{8\omega_{1k}^3}-\frac{105V_{11}^3V_{k1}t^4}{24\omega_{1k}^4}\right]e^{i\omega_{k1}t}\qquad(k\neq 1) \tag{46}$$

Equations (44)–(46) and the above straightforward procedure give

$$b_m^{(4)\prime}=c_m^{(4)}+\text{infinitesimal terms},\qquad m=1,2,\ldots \tag{47}$$

in moment $t=T$.

As we have mentioned above, the expressions for $b_m^{(\alpha)\prime}$, $m=1,2,\ldots,\alpha=1,2,\ldots$ are obtained with the help of the decomposition

$$\exp[A]=1+\frac{A}{1!}+\frac{A^2}{2!}+\cdots$$

in which

$$A=\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{2}+\frac{E_1^{(2)}}{3}+\frac{E_1^{(3)}}{4}+\frac{E_1^{(4)}}{5}+\cdots\right)$$

(it is evident that the nth term inside the brackets will be equal to $E_1^{(n)}/(n+1)$ for $n \geqslant 5$). As long as our calculations involve terms $\sim R^\alpha, \alpha \leqslant 4$, we need only those terms of the above decomposition in which $\alpha \leqslant 4$. It is worth writing them down:

$$
\begin{aligned}
&\exp\left[\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{2}+\frac{E_1^{(2)}}{3}+\frac{E_1^{(3)}}{4}+\frac{E_1^{(4)}}{5}+\cdots\right)\right] \\
&\approx 1+T\left(\frac{V_{11}}{2i\hbar}+\frac{1}{3i\hbar^2}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}+\frac{1}{4i\hbar^3}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}\omega_{1m}}-\frac{V_{11}}{4i\hbar^3}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^2}\right. \\
&\quad+\frac{1}{5i\hbar^4}\sum_k{}'\sum_m{}'\sum_n{}'\frac{V_{1k}V_{km}V_{mn}V_{n1}}{\omega_{1k}\omega_{1m}\omega_{1n}}-\frac{2V_{11}}{5i\hbar^4}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}\omega_{1m}^2} \\
&\quad\left.+\frac{V_{11}^2}{5i\hbar^4}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^3}-\frac{1}{5i\hbar^4}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^2}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\right) \\
&\quad+T^2\left(-\frac{V_{11}^2}{8\hbar^2}-\frac{V_{11}}{6\hbar^3}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}}-\frac{V_{11}}{8\hbar^4}\sum_k{}'\sum_m{}'\frac{V_{1k}V_{km}V_{m1}}{\omega_{1k}\omega_{1m}}\right. \\
&\quad\left.+\frac{V_{11}^2}{8\hbar^4}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}^2}-\frac{1}{18\hbar^4}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}}\sum_m{}'\frac{V_{1m}^2}{\omega_{1m}}\right) \\
&\quad+\frac{iV_{11}^3T^3}{48\hbar^3}+\frac{iV_{11}^2T^3}{24\hbar^4}\sum_k{}'\frac{V_{1k}^2}{\omega_{1k}}+\frac{V_{11}^4T^4}{384\hbar^4}
\end{aligned}
\tag{48}
$$

{$b_m^{(\alpha)'}$ is obtained after the subtraction from $d_m^{(\alpha)'}(T)$ of those terms in $(b_m^{(0)'}+b_m^{(1)'}+\cdots+b_m^{(\alpha-1)'})\exp(-iE_1^{(0)}T/\hbar)\times$[right-hand side of equation (48)] which contain R^α}. In such a way the simple prescription formulated above gives the necessary result in the specific case (18): In the approximation of fourth (and, little doubt, any) order of magnitude in R we have

$$
\begin{aligned}
d_m'(T)=&\exp\left[\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{2}+\cdots+\frac{E_1^{(4)}}{5}+\cdots\right)\right] \\
&\times\left(c_m^{(0)}+c_m^{(1)}+c_m^{(2)}+\cdots+\text{infinitesimal terms}\right)\exp\left[-iE_1^{(0)}T/\hbar\right], \\
&m=1,2,\ldots
\end{aligned}
\tag{49}
$$

Acting analogically, one obtains that our prescription "works" in other specific cases too, eliminating the corresponding nonadiabatical terms. Thus, for instance, in the case

$$V(x,t)=0, \qquad t\leqslant 0,$$

$$V(x,t)=\frac{t^2}{T^2}V(x),\, 0\leqslant t\leqslant T,\, V(x,t)=V(x), \qquad t\geqslant T \tag{50}$$

we have

$$d'_m(T)=\exp\left[\frac{T}{i\hbar}\left(\frac{E_1^{(1)}}{3}+\frac{E_1^{(2)}}{5}+\frac{E_1^{(3)}}{7}+\ldots\right)\right]$$
$$\times\left(c_m^{(0)}+c_m^{(1)}+c_m^{(2)}+c_m^{(3)}+\cdots+\text{infinitesimal terms}\right)\exp\left[-iE_1^{(0)}T/\hbar\right],$$
$$m=1,2,\ldots \tag{51}$$

(the calculation being carried out by us as far as third-order terms in R; the nth term, $n>3$, in the exponential sum, no doubt, is equal to $E_1^{(n)}/2n+1$).

In the case

$$V(x,t)=0, \qquad t\leqslant T=-\pi/2\omega,$$

$$V(x,t)=V(x)\cos\omega t=V(x)\frac{e^{i\omega t}+e^{-i\omega t}}{2}, \qquad T\leqslant t\leqslant 0,$$

$$V(x,t)=V(x), \qquad t\geqslant 0 \tag{52}$$

our prescription gives

$$d'_m(T)=\exp\left[\frac{1}{i\hbar\omega}\left(E_1^{(1)}+\frac{\pi}{4}E_1^{(2)}+\frac{2}{3}E_1^{(3)}+\ldots\right)\right]$$
$$\times\left(c_m^{(0)}+c_m^{(1)}+c_m^{(2)}+c_m^{(3)}+\text{infinitesimal terms}\right)\exp\left[-iE_1^{(0)}T/\hbar\right] \tag{53}$$

[the calculation being carried out again as far as third-order terms; the initial condition, as always, if $\psi_i(t_i)=\psi_1^{(0)}$].

The expressions (49), (51), and (53) show that the quantity β in $\exp[i\beta T]$ [see equation (13)] depends on $R, W(x)$ (through $E_1^{(\alpha)}$, $\alpha=1,2,\ldots$), and the way in which $V(x,t)$ is included (different types of series $\Sigma_{\alpha=1}^{\infty}h_\alpha E_1^{(\alpha)}$ in the exponents, h_α being the corresponding coefficients). It can be easily seen, besides, that constant terms will appear in any $a_m^{(\alpha)}(t)$ for arbitrary

$\alpha=1,2,\ldots, m=2,3,\ldots$ (through a straightforward solution of the SE using the TNSP). The role of these terms is determined by the specific dependence of $V(x,t)$ on t. For instance, in the case (50) the finite "nonphysical" terms in the TNSP solution will appear for the first time in the terms containing R^3. Analogically, it is fairly obvious that in the case $V(x,t)=t^nT^{-n}V(x), n=3,4,\ldots,$ such terms will appear in order $n+1$ of the TNSP because of the proportionality of the constant terms in $a_k^{(1)}(t), k\neq 1$, to T^{-n}. In such a way one comes to the conclusion that the SE will not produce nonadiabatic terms only in cases when all the time derivatives of $V(x,t)$ are equal to zero in moment t_i and vary adiabatically with time for $t\geqslant t_i$. This can be easily checked in the case

$$V(x)e^{\varepsilon t}=V(x,t), \qquad -\infty<t\leqslant 0, \qquad V(x,t)=V(x), \qquad t\geqslant 0 \quad (54)$$

where ε is a small positive constant ($\varepsilon\to+0$). But one must be careful in cases of this type ($t_f-t_i=T=\infty$) since the TNSP can turn out to be inapplicable in some of them. This is so, e.g., in the case $V(x,t)=V(x)e^{\varepsilon t}\cos\omega t$, $-\infty<t\leqslant 0$, $V(x,t)=V(x)$, $t\geqslant 0$, $\varepsilon\to+0$, $\omega\to+0$, $\omega/\varepsilon\to\infty$. The reason for this lies in the fact that, because of the infinite number of oscillations of $\cos\omega t$ in t_f-t_i, one can no longer assert that the final result must differ slightly from ψ_i (with terms $\sim\varepsilon$, ε^2, etc.).

Up to here we considered only the discrete spectrum case. In the next article (T5) of the present series we shall examine the continuous spectrum case.

4. CONCLUSION

We shall summarize first briefly the results of the preceding discussion.

It was shown in Section 2 that the SE does not satisfy the adiabatic principle formulated there. This result is rigorous and is easily obtained from the TNSP. The prescription for the removal of the corresponding "nonadiabatic" terms was developed on purely intuitive grounds. Namely, it was assumed that in adiabatic processes the perturbation procedure for the unknown irreversible equation is built in a similar fashion to the one of the SE. In this procedure we omit only such infinitesimal terms as are due to the concept that the corresponding homogeneous equation is the time-reversible SE and which cannot play a noticeable role in a time-irreversible equation of the type (27). This is not what one would call a mathematically rigorous way of proceeding. Still, it is really surprising that an expected property of the said equation [the existence of which is motivated in (T1)] helps to obtain a desirable result in the specific cases examined.

It is worth recalling here that according to the arguments in (T1) and (T2) the inherent physical properties of a given system the evolution of which is described by a relevant time-irreversible equation are sufficient for the description of all the characteristic features of the system (including the thermodynamical properties of a pure quantum state). The SE is too sensitive to any nonadiabaticity, even when it is very slight and appears in higher-order time derivatives of the perturbation (cf. the discussion at the end of Section 3), to be the correct equation in nonstationary situations. A correct equation must be insensitive to small nonadiabatic effects. This was illustrated in the beginning of Section 2.

There exists an interesting similarity between our way of action and the prescriptions of quantum field theory for the removal of ultraviolet divergences appearing in the perturbation series. Namely, the nonvanishing nonphysical terms which are infinite in field theory and finite in our case appear in the second and higher nonvanishing orders of magnitude of perturbation theory. A part of such terms in any order of the theory higher than (and in our case equal to) 2 is compensated by the (in our case infinitesimal) counter terms of the prescription for the lower orders, but any new order of magnitude inevitably contains some (in our case infinitesimal) terms which have to be cut off on the spot in order to avoid trouble in higher orders. More important than these formal similarities is the fact that our discussion here is in accord with the point of view that a physical approach to the problem of the existence of undesirable terms may not only formulate some prescription for their removal but explain them as well.

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