Generalized Adiabatic Invariance*

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In this paper we find the quantities that are adiabatic invariants of any desired order for a general slowly time-dependent Hamiltonian. In a preceding paper, we chose a quantity that was initially an adiabatic invariant to first order, and sought the conditions to be imposed upon the Hamiltonian so that the quantum mechanical adiabatic theorem would be valid to mth order. [We found that this occurs when the first $(m - 1)$ time derivatives of the Hamiltonian at the initial and final time instants are equal to zero.] Here we look for a quantity that is an adiabatic invariant to mth order for any Hamiltonian that changes slowly in time, and that does not fulfill any special condition (its first time derivatives are not zero initially and finally).

I. INTRODUCTION

In many cases it is possible to obtain an asymptotic solution of the equations of motion by perturbation theory. For many problems of quantum mechanics, it is too much to require the convergence in the mathematical sense of the formal series of perturbation method. In all practical problems, only the first several terms are calculated and the whole series may ultimately be divergent. Thus we are led to regard them as asymptotic rather than power series. The range of applicability of perturbation methods is much extended by this new interpretation.

Kato[1] shows also that the perturbation method gives asymptotic series which are correct so far as the coefficients can be calculated by means of operators within the Hilbert space. It is important to note that this was established independently of the convergence or divergence of the formal series. In fact it is rather usual that the series has only a finite number of significant terms.

The significance of the adiabatic theory can only be appreciated by noting that the adiabatic expansion in the appropriate expansion parameter is asymptotic rather than convergent. Thus, the higher-order adiabatic theory may give very great accuracy when the first term is already quite good, but it usually makes matters worse when the first term is mediocre.[2]

Therefore, in many cases it is possible to obtain an asymptotic solution of the equations of motion by perturbation theory. We are going to show in this paper how we can construct an asymptotic integral of equations of motion of a quantum mechanical system which is constant to any desired order.

The adiabatic theorem is divided into two parts. In the first place it states the existence of a virtual change in the system which may be called adiabatic transformation. Secondly, it asserts that the dynamical transformation defined by the Schrödinger equation goes over to the adiabatic transformation in the limit when the time dependence of the Hamiltonian is infinitely slow. Therefore, first we have to find the unitary operator representing the adiabatic transformation.

The construction of this adiabatic transformation constitutes the main part of the present note. Our proof is rather formal and not faultless from the point of view of mathematical rigor.

Kruskal[3] has studied the gyration of a charged particle in a magnetic field when the magnetic field at the position of the particle changes only a little during one gyration period. The guiding center approximation is then formulated by considering the ratio $\epsilon = e/m$ to be numerically small, where m is the mass of the particle and e its charge. An asymptotic analysis is called for in Kruskal's work. Once having completed the expansion of the equations of motion, he claims that there is an adiabatic invariant which is constant to all orders, an invariant that is given by the magnetic moment to lowest order. Of course this result is only asymptotic, i.e., the constancy to all orders does not mean

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[3] M. Kruskal, U. S. Atomic Energy Commission, Rept. NYO 7903 (1958).

exact constancy, but merely that the deviation from constancy goes to zero faster than any power of ϵ.

Kruskal's argument is valid quite generally for any classical system describable by a Hamiltonian, of which the particle moving in a given electromagnetic field constitutes a particular example.[4,5]

Berkowitz and Gardner[6] have shown that, in effect, the expression presented by Kruskal in Ref. 1 is indeed an asymptotic representation of the exact solution of the initial-value problem, valid as $\epsilon \to 0$. These authors have given, therefore, mathematical rigor to Kruskal's deductions.

In this paper we fix our attention on the quantum mechanical domain. We introduce the idea of generalized adiabatic invariants, which are the operators that are adiabatic invariants to any desired order in the parameter that measures the slow time variation of any explicitly time-dependent Hamiltonian. Let us observe that the generalized adiabatic invariants to mth order are not equivalent to the adiabatic invariants to mth order that were studied in a preceding paper[7] in which we gave the conditions that make the quantum mechanical adiabatic theorem valid to mth order. In Ref. 7 we chose a quantity that initially was an adiabatic invariant to first order, and sought the conditions to be imposed upon the Hamiltonian so that the quantum mechanical adiabatic theorem would be valid to mth order. [We found out that this occurs when the first $(m - 1)$ time derivatives of the Hamiltonian at the initial and final time instants are equal to zero.] Here we look for a quantity that is an adiabatic invariant to mth order for any Hamiltonian that changes slowly in time and that does not fulfill any special condition (its first time derivatives are not zero initially and finally). The new results of this paper are essentially contained in Secs. 3, 4, and 6.

In Sec. 5 we show how the generalized adiabatic invariant to mth order becomes the adiabatic invariant to mth order when the appropriate conditions are imposed upon the Hamiltonian, i.e., when we demand that the first $m - 1$ time derivatives of the Hamiltonian be zero initially and finally.

The research presented in this paper is carried on for a quantum mechanical system. However, following the operational techniques developed elsewhere[8-11] for classical mechanics, quite similar theorems can be proved for the classical domain; some clarifications may be needed, however.

In contrast with the conventional use of the operator calculus in quantum mechanics, it is generally not appropriate to apply that method to classical mechanics unless considerable care is taken. The Hilbert space upon which a quantum mechanical Hamiltonian operator is defined is simple, and is assumed not to change its properties in a time flight, or according to other changes of parameters implicitly included in the system, such as constants of motion, initial conditions and so on. The Hilbert space for classical mechanics[12,13] is, however, not so simple. It is impossible to know its Hermitian character when the energy surfaces of $(2n - 1)$ dimensions, defined by the equation $H = E$ in $2n$-dimensional phase space, are not closed. But we should mention that the formal developments of classical and quantum mechanics in Hilbert space can be rigorously used in classical mechanics if we restrict the classical system to a multiperiodic system.

Our paper starts now with a short exposition of the quantum mechanical adiabatic theorem, presented for the sake of completeness and in order to fix the notation. We generalize the method inmediately, and define the generalized adiabatic invariants to mth order. The paper ends by showing how the first part of Ref. 7 can be deduced from the present theorem by simply imposing the appropriate restrictions to the Hamiltonian.

2. QUANTUM MECHANICAL ADIABATIC THEOREM

Let us suppose that the Hamiltonian $H(t)$ of the system changes continuously from $H_0 = H(t_0)$ at the instant $t = t_0$, to $H_1 = H(t_1)$ corresponding to $t = t_1$.

We call $T = t_1 - t_0$ the time interval during which the evolution of the system takes place. We introduce the fictitious time τ that results when we measure the physical time t with the parameter T as unity. The Hamiltonian of the system at the instant $t = t_0 + \tau T$ is $H(\tau)$, an operator that is a given continuous function of τ,

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and such that

$$H(0) = H_0, \qquad H(1) = H_1.$$

We are going to study the case when T is large and the evolution of the system takes place while the fictitious time changes from $\tau = 0$ to $\tau = 1$.

Let us call $U_T(\tau)$ the evolution operator where τ is the fictitious time that, together with T, was defined above.

$$i\hbar(d/d\tau)U_T(\tau) = TH(\tau)U_T(\tau), \qquad (1)$$

where $H(\tau)$ is the slowly time-dependent Hamiltonian, given by the expression

$$H(\tau) = \sum_j E_j^{(1)}(\tau)P_j^{(1)}(\tau), \qquad (2)$$

where $P_j^{(1)}(\tau)$ are the projection operators of the stationary states, states that we suppose discrete and nondegenerate.

Let us call $R^{(1)}(\tau)$ a unitary operator such that

$$P_j^{(1)}(\tau) = R^{(1)}(\tau)P_j^{(1)}(0)R^{(1)\dagger}(\tau). \qquad (3)$$

It is completely defined by the initial condition $R^{(1)}(0) = I$ and the differential equation

$$i\hbar(d/d\tau)R^{(1)}(\tau) = K^{(1)}(\tau)R^{(1)}(\tau). \qquad (4)$$

The operator $K^{(1)}(\tau)$ obeys the following commutation relations:

$$[K^{(1)}(\tau), P_j^{(1)}(\tau)] = i\hbar(d/d\tau)P_j^{(1)}(\tau), \qquad (j = 1, 2, 3, \cdots), \qquad (5)$$

and is determined without ambiguity if we add the following supplementary condition:

$$P_j^{(1)}(\tau)K^{(1)}(\tau)P_j^{(1)}(\tau) = 0, \quad (j = 1, 2, 3, \cdots), \qquad (6)$$

equations that yield the following expression for $K^{(1)}(\tau)$:

$$K^{(1)}(\tau) = i\hbar \sum_j [(d/d\tau)P_j^{(1)}(\tau)]P_j^{(1)}(\tau). \qquad (7)$$

The unitary transformation $R^{(1)\dagger}(\tau)$, applied to the operators and vectors of Schrödinger's picture, produces a new picture: the picture of the rotating axis,

$$H^{(1)}(\tau) = R^{(1)\dagger}(\tau)H(\tau)R^{(1)}(\tau) = \sum_j E_j^{(1)}(\tau)P_j^{(1)}(0), \qquad (8)$$

$$K_1^{(1)}(\tau) = R^{(1)\dagger}(\tau)K^{(1)}(\tau)R^{(1)}(\tau). \qquad (9)$$

The evolution operator $U^{(1)}(\tau) \equiv R^{(1)}(\tau)U_T(\tau)$ in the new picture is defined by the initial condition $U^{(1)}(0) = I$ and the equation

$$i\hbar(d/d\tau)U^{(1)}(\tau) = [TH^{(1)}(\tau) - K_1^{(1)}(\tau)]U^{(1)}(\tau), \qquad (10)$$

an equation that, in the demonstration of the adiabatic theorem in quantum mechanics, is treated by the method of perturbations considering $K_1^{(1)}(\tau)$ as the perturbation of $TH^{(1)}(\tau)$.

3. GENERALIZATION OF THE PROCEDURE

To generalize the preceding procedure we have to treat (10) as we have treated (1), i.e., as if it were the initial Schrödinger equation. We have to find the fictitious time-dependent projection operators corresponding to the Hamiltonian $H_1^{(1)}(\tau) \equiv H^{(1)}(\tau) - (1/T)K_1^{(1)}(\tau)$, operators that we will call $P_j^{(2)}(\tau)$. The subspace subtended by $P_j^{(2)}(\tau)$, according to the theorems of T. Kato, should have the same number of dimensions that the subspace projected by $P_j^{(1)}(\tau)$, i.e., the instantaneous eigenstates of $H_1^{(1)}(\tau)$ should not be degenerate. Indeed, Kato[1] says that the Hamiltonian operator $H_\lambda = H_0 + \lambda H_1$ that is a function of the real parameter λ, is a regular function of λ if the propagator $G_\lambda(z) = -[1/(H_\lambda - z)]$ is regular in the proximity of $\lambda = 0$, for some fixed z; then it is shown that the same is true for every z not belonging to the spectrum of H_0. In this paper we assume that $H_1^{(1)}(\tau)$, and all the Hamiltonians whose eigenstates and projection operators will be used, are regular in the real parameter $1/T$. When these conditions are satisfied, T. Kato shows that the multiplicity of the eigenvalues is independent of λ, or, in our case, of $1/T$. Correspondingly, all along the present paper we suppose that the successive series of instantaneous eigenvalues that will be defined are not degenerate. Perhaps this condition is much too restrictive and, as a consequence, we may leave out some cases for which the concept of generalized adiabatic invariance could still be valid. We should like to remark that it is not our intention to present here the most general case; we rather intend to introduce the generalized adiabatic invariants, taking as a model the steps developed in Sec. 1, which constitute the usual demonstration of the adiabatic theorem. Other conditions require different procedure, as can be seen in another paper of T. Kato.[14]

Following the theory of perturbations in quantum mechanics, we can write the projection operators $P_j^{(2)}(\tau)$ as a function of the projection operators of $H^{(1)}(\tau)$ and of the perturbation $(1/T)K_1^{(1)}(\tau)$. And, because the projection operators of $H^{(1)}(\tau)$ are independent of τ as can be seen from (8), we have

$$P_j^{(2)}(\tau) = P_j^{(1)}(0) + (1/T)F_j^{(1)}(\tau), \qquad (j = 1, 2, 3, \cdots), \qquad (11)$$

where $F_j^{(1)}(\tau)$ contains only powers of $1/T$.

[14] T. Kato, J. Phys. Soc. Japan 5, 435 (1950).

We try now to establish a second rotating-axis picture for the operators $P_j^{(2)}(\tau)$ as follows:

$$P_j^{(2)}(\tau) = R^{(2)}(\tau)P_j^{(2)}(0)R^{(2)\dagger}(\tau), \qquad (j = 1, 2, 3, \cdots), \tag{12}$$

where the unitary operator $R^{(2)}(\tau)$ is defined by the condition $R^{(2)}(0) = I$, and the differential equation

$$i\hbar(d/d\tau)R^{(2)}(\tau) = K^{(2)}(\tau)R^{(2)}(\tau), \tag{13}$$

in which the operator $K^{(2)}(\tau)$ obeys, similarly to $K^{(1)}(\tau)$, the commutation relations

$$[K^{(2)}(\tau), P_j^{(2)}(\tau)] = i\hbar(d/d\tau)P_j^{(2)}(\tau), \qquad (j = 1, 2, 3, \cdots), \tag{14}$$

and complementary conditions

$$P_j^{(2)}(\tau)K^{(2)}(\tau)P_j^{(2)}(\tau) = 0, \quad (j = 1, 2, 3, \cdots). \tag{15}$$

Therefore, such an operator has the form

$$K^{(2)}(\tau) = i\hbar \sum_j [(d/d\tau)P_j^{(2)}(\tau)]P_j^{(2)}(\tau). \tag{16}$$

In the new picture, we define

$$H^{(2)}(\tau) \equiv R^{(2)\dagger}(\tau)H_1^{(1)}(\tau)R^{(2)}(\tau) = \sum_j E_j^{(2)}(\tau)P_j^{(2)}(0), \tag{17}$$

where $E_j^{(2)}(\tau)$ are the instantaneous eigenvalues of $H_1^{(1)}(\tau)$, and $P_j^{(2)}(0)$ are its initial projectors.

The new evolution operator

$$U^{(2)}(\tau) \equiv R^{(2)\dagger}(\tau)U^{(1)}(\tau)$$

obeys the equation

$$i\hbar(d/d\tau)U^{(2)}(\tau) = [TH^{(2)}(\tau) - K_2^{(2)}(\tau)]U^{(2)}(\tau), \tag{18}$$

when

$$K_2^{(2)}(\tau) \equiv R^{(2)\dagger}(\tau)K^{(2)}(\tau)R^{(2)}(\tau). \tag{19}$$

Evidently, the original evolution operator in relation to the new one is given by the expression

$$U_T(\tau) = R^{(1)}(\tau)R^{(2)}(\tau)U^{(2)}(\tau). \tag{20}$$

This process can be repeated indefinitely, and so we get the procedure to arrive at the generalized adiabatic invariance.

Let us observe that $K_2^{(2)}(\tau)$ is of the order of magnitude of $1/T$. Indeed, combining (16) with (11) we find

$$K^{(2)}(\tau) = i\hbar \sum_j [(d/d\tau)F_j^{(1)}(\tau)]P_j^{(2)}(\tau), \tag{21}$$

and $K_2^{(2)}(\tau)$ is of the same order of magnitude of $K^{(2)}(\tau)$. Therefore, in the Hamiltonian

$$H_2^{(2)}(\tau) \equiv H^{(2)}(\tau) - (1/T)K_2^{(2)}(\tau), \tag{22}$$

the term $-(1/T)K_2^{(2)}(\tau)$ is, at least, proportional to $1/T^2$. We said before that $F_j^{(1)}(\tau)$ contains only powers of $1/T$; if the first terms of the expansion of $F_j^{(1)}(\tau)$ in powers of $1/T$ do not depend on τ, expression (21) tells us that $K^{(2)}(\tau)$ is proportional to even higher powers of $1/T$ than the second.

The equation for $U^{(2)}(\tau)$ could be integrated without difficulty if we could neglect $K_2^{(2)}(\tau)$ in comparison with $TH^{(2)}(\tau)$. The solution of the Schrödinger equation that appears when we do so,

$$i\hbar(d/d\tau)\phi^{(2)}(\tau) = TH^{(2)}(\tau)\phi^{(2)}(\tau), \tag{23}$$

may be written, with the initial condition $\phi^{(2)}(0) = I$,

$$\phi^{(2)}(\tau) = \sum_j \exp(-iT\varphi_j^{(2)}(\tau)\hbar^{-1})P_j^{(2)}(0), \tag{24}$$

where

$$\varphi_j^{(2)}(\tau) = \int_0^\tau E_j^{(2)}(\tau')\,d\tau'. \tag{25}$$

If, as we will see immediately, $U^{(2)}(\tau)$ tends toward $\phi^{(2)}(\tau)$ for large T, we will have approximately

$$U_T(\tau) \simeq R^{(1)}(\tau)R^{(2)}(\tau)\phi^{(2)}(\tau). \tag{26}$$

We are now going to show that, indeed, (26) is a good approximation for $U_T(\tau)$ for large T. The complete solution of (18) can be written by means of the formula for time-dependent perturbations as follows:

$$U^{(2)}(\tau) = \phi^{(2)}(\tau)U_2^{(2)}[\tau], \tag{27}$$

where the equation satisfied by $U_2^{(2)}[\tau]$ is

$$U_2^{(2)}[\tau] = 1 + \frac{i}{\hbar}\int_0^\tau K_2^{(2)}[\tau']U_2^{(2)}[\tau']\,d\tau', \tag{28}$$

with

$$K_2^{(2)}[\tau] \equiv \phi^{(2)\dagger}(\tau)K_2^{(2)}(\tau)\phi^{(2)}(\tau).$$

We plan to show now that the kernel $K_2^{(2)}[\tau']$ is a sum of oscillating functions whose frequencies increase with T, and that therefore the integral in the second member of the Volterra equation (28) goes to zero when $T \to \infty$.

Any operator $\mathfrak{L}$ admits the following decomposition

$$\mathfrak{L} = \sum_{j,k} \mathfrak{L}_{jk}, \tag{29}$$

where we use the following notation:

$$\mathfrak{L}_{jk} = P_j^{(2)}(0)\mathfrak{L}P_k^{(2)}(0). \tag{30}$$

We shall use this decomposition for the kernel of the integral equation (28),

$$K_2^{(2)}[\tau] = \sum_{j,k} (\exp \{(iT/\hbar)[\varphi_j^{(2)}(\tau) - \varphi_k(\tau)]\} P_j^{(2)}(0) K_2^{(2)}(\tau) P_k^{(2)}(0)) = \sum_{\substack{j,k \\ j \neq k}} (\exp \{(iT/\hbar)[\varphi_j^{(2)}(\tau) - \varphi_k^{(2)}(\tau)]\} K_2^{(2)}(\tau)_{jk}), \quad (31)$$

an expression in which we have introduced the condition $j \neq k$ because, from (15), we deduce

$$K_2^{(2)}(\tau)_{jj} = 0 \qquad (j = 1, 2, 3, \cdots). \quad (32)$$

The frequency of the oscillations can be obtained by calculating the derivative of the phase of the exponentials with respect to τ. And so we see that the frequency is never zero because the system is not degenerate, and that it is proportional to T.

Let us now consider the operator

$$F(\tau) = \int_0^\tau K_2^{(2)}[\sigma]\, d\sigma, \quad (33)$$

whose diagonal elements are all zero while their nondiagonal elements are

$$F_{j,k} = \int_0^\tau \exp\left[\frac{iT}{\hbar}(\varphi_j^{(2)}(\sigma) - \varphi_k^{(2)}(\sigma))\right] \times K_2^{(2)}(\sigma)_{jk}\, d\sigma \qquad (j \neq k), \quad (34)$$

where $K_2^{(2)}(\sigma)$ only contains negative powers of T and is, at least, proportional to $1/T$. Integrating by parts it is easy to see that $F_{jk}(\tau)$ goes as $1/T^2$. With this result we can deduce immediately, also integrating by parts, that

$$U_2^{(2)}[\tau] = 1 + O(1/T^2). \quad (35)$$

With this conclusion we arrive at the following expression for $U_T(\tau)$:

$$U_T(\tau) = R^{(1)}(\tau)R^{(2)}(\tau)\phi^{(2)}(\tau)[1 + O(1/T^2)] \qquad (T \to \infty). \quad (36)$$

4. GENERALIZED ADIABATIC INVARIANTS

If we perform only the first transformation $R^{(1)}(\tau)$, the result admits a simple physical interpretation: a system that initially is in the state selected by $P_j^{(1)}(0)$, will end up in the state selected by $P_j^{(1)}(1)$. This is the statement of the well-known theorem.

To state the generalized adiabatic theorem, we have to perform successively more than one transformations from a rotating axis picture to another rotating axis picture. Then, after the lth transformation, we have the following approximation for the evolution operator of the system:

$$U_T(\tau) = R^{(1)}(\tau)R^{(2)}(\tau) \cdots R^{(l)}(\tau)\phi^{(l)}(\tau) \times [1 + O(1/T^l)] \qquad (T \to \infty). \quad (37)$$

Let us remark now that this expression is an excellent approximation for the evolution operator of a system with any Hamiltonian that has a slow time dependence. No further requirement is imposed upon the Hamiltonian so far as its time dependence is concerned, and we can approximate its evolution operator to any desired power of $1/T$.

We may now present another consequence of the result (37), a consequence which is deduced by evaluating the following product:

$$\begin{aligned} U_T(\tau)P_j^{(l)}(0) &\simeq R^{(1)}(\tau)R^{(2)}(\tau) \cdots \times R^{(l)}(\tau)P_j^{(l)}(0)R^{(l)\dagger}(\tau)R^{(l)}(\tau)\phi^{(l)}(\tau) \\ &= R^{(1)}(\tau)R^{(2)}(\tau) \cdots \times R^{(l-1)}(\tau)P_j^{(l)}(\tau)R^{(l)}(\tau)\phi^{(l)}(\tau) \\ &= R^{(1)}(\tau)R^{(2)}(\tau) \cdots R^{(l-1)}(\tau)P_j^{(l)}(\tau)R^{(l-1)\dagger}(\tau) \cdots \times R^{(2)\dagger}(\tau)R^{(1)\dagger}(\tau)U_T(\tau). \end{aligned} \quad (38)$$

Due to the above relation, we may now state the generalized adiabatic theorem in the following manner. A system whose state is initially a vector $|l\rangle$ whose projector is $P_j^{(l)}(0)$ will end up its evolution in a state that is a vector of the Hilbert subspace projected by the following projection operator:

$$S_j^{(l)}(1) = R^{(1)}(1)R^{(2)}(1) \cdots \times R^{(l-1)}(1)P_j^{(l-1)\dagger}(1)R^{(l-1)\dagger}(1) \cdots R^{(2)\dagger}(1)R^{(1)\dagger}(1), \quad (39)$$

with an approximation of the order of $1/T^l$.

Let us now find out the observables that are generalized adiabatic invariants. Suppose that we have performed l transformations. We get the following evolution operator in the resulting picture:

$$U^{(l)}(\tau) = \phi^{(l)}(\tau)U_l^{(l)}[\tau]. \quad (40)$$

With a procedure similar to that presented before, this will show that

$$U_l^{(l)}[\tau] = 1 + O(1/T^l). \quad (41)$$

Therefore an observable $\mathcal{L}^{(l)}$ which is a constant of the motion generated by the unitary operator $\phi^{(l)}(\tau)$ in this picture will become

$$\mathcal{L}^{(l)}(\tau) = U^{(l)\dagger}(\tau)\mathcal{L}^{(l)}U^{(l)}(\tau) = U_l^{(l)\dagger}[\tau]\mathcal{L}^{(l)}U_l^{(l)}[\tau] = \mathcal{L}^{(l)} + O(1/T^l), \quad (42)$$

where $\mathcal{L}^{(l)} = \mathcal{L}^{(l)}(0)$. Therefore the observables that commute with $H^{(l)}(\tau)$, i.e., those that commute with $H^{(l)}(0)$, are adiabatic invariants of lth order in the lth rotating-axis picture. Throughout this paper we suppose that the projection operators $P_j^{(l)}(0)$ (for all j and any l) form a complete and orthonormal set.

Now, the evolution operator of the system is (37). Therefore the quantity

$$I^{(l)}(\tau) = R^{(1)}(\tau)R^{(2)}(\tau)\cdots \times R^{(l)}(\tau)\mathcal{L}^{(l)}R^{(l)\dagger}(\tau)\cdots R^{(2)\dagger}(\tau)R^{(1)\dagger}(\tau) \qquad (43)$$

is the generalized adiabatic invariant of lth order. It depends explicitly on time but its expected value is constant during the evolution of the system with an approximation of the order $1/T^l$. In general, therefore, the generalized adiabatic invariants depend explicitly on time; later we shall study the case when such an explicit dependence does not appear.

5. COMPARATION WITH THE ADIABATIC THEOREM OF lTH ORDER

In a preceding paper[7] we have shown that a system that initially is in a state belonging to the subspace projected by $P_j^{(1)}(0)$ will end up in the state belonging to the subspace projected by $P_j^{(1)}(1)$ with an error of the order $(1/T^l)$ when its $(l-1)$ first time derivatives of $H(\tau)$ are zero initially and finally. This is the statement of the adiabatic theorem of lth order. We now want to compare this result with the present generalized adiabatic invariance of lth order.

The comparison will be reduced to showing that we obtain the adiabatic theorem of lth order from the generalized adiabatic theorem of the same order when we add to the second theorem the extra conditions that the first $(l-1)$ time derivatives of the Hamiltonian $H(\tau)$ are zero initially and finally.

To achieve our aim, we have to show, at first, two properties of the operators that generate the successive changes of pictures, which are directly due to the fact that the first $(l-1)$ time derivatives of the Hamiltonian are zero at certain time instants.

The first one is concerned with the behavior of the unitary operators $R^{(1)}(\tau)$, $R^{(2)}(\tau)$, $\cdots$, $R^{(l)}(\tau)$ and of their first time derivatives for a certain τ at which the first $(l-1)$ time derivatives of $H(\tau)$ are zero. Indeed in Ref. 7 we have shown that when the first $(l-1)$ time derivatives of $H(\tau)$ are zero, $K^{(1)}(\tau)$ and its first $(l-2)$ time derivatives are zero. From (9) we immediately deduce that $K_1^{(1)}(\tau)$ and its $(l-2)$ time derivatives are also zero for the same values of τ.

The unitary operator $R^{(1)}(\tau)$ satisfies the differential equation (4), from whose successive differentiation with respect to the parameter τ we find that the unitary operator $R^{(1)}(\tau)$ has its $(l-1)$ time derivatives equal to zero for the values of τ for which the first $(l-1)$ time derivatives of $H(\tau)$ are equal to zero. This result, together with the fact that the Hamiltonian $H_1^{(1)}(\tau)$ was defined by means of the relation

$$\begin{aligned} H_1^{(1)}(\tau) &= H^{(1)}(\tau) - (1/T)K_1^{(1)}(\tau) \\ &= R^{(1)\dagger}(\tau)H(\tau)R^{(1)}(\tau) - (1/T)K_1^{(1)}(\tau), \end{aligned} \qquad (44)$$

allow us to show that, for the above-mentioned values of τ, the $(l-2)$ first time derivatives of $H_1^{(1)}(\tau)$ are zero while the $(l-1)$st time derivative of the same operator is

$$\frac{d^{l-1}}{d\tau^{l-1}} H_1^{(1)}(\tau) = -\frac{1}{T}\frac{d^{l-1}}{d\tau^{l-1}} K_1^{(1)}(\tau). \qquad (45)$$

The results of Ref. 7 and the above properties of the operators $K_1^{(1)}(\tau)$, $R^{(1)}(\tau)$, and $H_1^{(1)}(\tau)$ can be extended further by the same procedure to all the series of similar operators that we have introduced in Sec. 3. And so we arrive at the first statement that we needed, i.e., to the fact that, for the values of τ for which the first $(l-1)$ time derivatives of $H(\tau)$ are zero, $K_1^{(1)}(\tau)$ and its first $(l-2)$ time derivatives, the first $(l-1)$ time derivatives of $R^{(1)}(\tau)$, and the first $(l-2)$ time derivatives of $H_1^{(1)}(\tau)$ are zero; $K_2^{(2)}(\tau)$ and its first $(l-3)$ time derivatives, the first $(l-2)$ time derivatives of $R^{(2)}(\tau)$, and the first $(l-3)$ time derivatives of $H_2^{(2)}(\tau)$ are zero; and so on.

Given this first statement, and remembering that $(1/T)K_1^{(1)}(\tau)$ is the perturbation that, by the methods of time-independent perturbations, yields $P_j^{(2)}(\tau)$ from $P_j^{(1)}(0)$, in agreement with (11) and that similarly $P_j^{(3)}(\tau)$ is deduced from $P_j^{(2)}(0)$ by a perturbation proportional to $K_2^{(2)}(\tau)$, we deduce that

$$\begin{aligned} P_j^{(1)}(0) &= P_j^{(2)}(\tau) = P_j^{(3)}(\tau) = \cdots \\ &= P_j^{(l-1)}(\tau) = P_j^{(l)}(\tau), \end{aligned} \qquad (46)$$

for the values of τ for which the $(l-1)$ time derivatives of $H(\tau)$ are zero; the operators $K_1^{(1)}(\tau)$; $K_2^{(2)}(\tau)$; $\cdots$; $K_{l-1}^{(l-1)}(\tau)$ will be zero for the same values of τ, where $K_{l-1}^{(l-1)}(\tau)$ characterizes the change of rotating-axis picture.

The second property we must show regarding the unitary operators $R^{(2)}(\tau)$, $R^{(3)}(\tau)$, $\cdots$, $R^{(l)}(\tau)$ is that, for the values of τ for which the first $(l-1)$ time derivatives of $H(\tau)$ are zero, the unitary operators $R^{(2)}(\tau)$, $R^{(3)}(\tau)$, $\cdots$, $R^{(l)}(\tau)$ [$R^{(1)}(\tau)$ is not included] commute with any of the projectors $P_j^{(1)}(0)$. Indeed, to show this theorem it is sufficient to apply (46) to the relations like (3), (12), and so on, successively. Therefore, from (12) and (46) we have

$$P_i^{(2)}(\tau) = P_i^{(1)}(0) = R^{(2)}(\tau)P_i^{(2)}(0)R^{(2)\dagger}(\tau), \quad (47)$$

which is equivalent to

$$[R^{(2)}(\tau), P_i^{(1)}(0)] = 0 \qquad (j = 1, 2, 3, \cdots), \quad (48)$$

and similarly for the other unitary operators $R^{(3)}(\tau)$, $R^{(4)}(\tau), \cdots, R^{(l)}(\tau)$. However, we cannot deduce that, for these values of τ, $R^{(1)}(\tau)$ also commutes with any $P_i^{(1)}(0)$. If the projection operators $P_i^{(1)}(0)$ for all j constitute a complete set, relation (48) implies that the unitary operators $R^{(2)}(\tau)$, which satisfy the same, are unity. Therefore, if the $(l-1)$ first time derivatives of $H(\tau)$ are zero at the initial and final instants, the unitary operators $R^{(2)}(\tau)$, $R^{(3)}(\tau), \cdots, R^{(l)}(\tau)$ will commute with all $P_i^{(1)}(0)$, and then we will deduce that the system that initially was at a state whose projector is $P_i^{(1)}(0)$ will end up at a state whose projector is $P_i^{(1)}(1)$, with an error smaller that $1/T^l$. This is so because at the final instant, in this case, the projector $S_i^{(1)}(1)$ of (39) becomes

$$\begin{aligned} R^{(1)}(1)R^{(2)}(1) \cdots R^{(l-1)}(1)P_i^{(1)}(0) \\ \times R^{(l-1)\dagger}(1) \cdots R^{(2)\dagger}(1)R^{(1)\dagger}(1) \\ = R^{(1)}(1)P_i^{(1)}(0)R^{(1)\dagger}(1) = P_i^{(1)}(1). \quad (49)\end{aligned}$$

This concludes our comparison of the generalized adiabatic invariance with the adiabatic invariance of order l. Let us study now the relations between the corresponding adiabatic invariants in both cases. Indeed, because in this case $K_{l-1}^{(l-1)}(\tau), \cdots, K_2^{(2)}(\tau)$, $K_1^{(1)}(\tau)$ are zero for the values of τ when the first $(l-1)$ time derivatives of $H(\tau)$ are zero, we deduce, for those values of τ,

$$\begin{aligned} H_1^{(1)}(\tau) = H^{(1)}(\tau), \qquad H_2^{(2)}(\tau) = H^{(2)}(\tau), \cdots \\ H_{l-1}^{(l-1)}(\tau) = H^{(l-1)}(\tau), \\ E_i^{(2)}(\tau) = E_i^{(1)}(\tau), \qquad E_i^{(3)}(\tau) = E_i^{(2)}(\tau), \cdots \\ E_i^{(l)}(\tau) = E_i^{(l-1)}(\tau), \quad (50)\end{aligned}$$

and from relations like (8), (17), and so on, we get

$$\begin{aligned} H^{(2)}(\tau) &\equiv R^{(2)\dagger}(\tau)H_1^{(1)}(\tau)R^{(2)}(\tau) \\ &= R^{(2)\dagger}(\tau)H^{(1)}(\tau)R^{(2)}(\tau) \\ &= \sum_i E_i^{(1)}(\tau)R^{(2)\dagger}(\tau)P_i^{(1)}(0)R^{(2)}(\tau) = H^{(1)}(\tau), \quad (51)\end{aligned}$$

given (48) and similar relations. Continuing the same procedure, we deduce, for these particular values of τ,

$$H^{(1)}(\tau) = H^{(2)}(\tau) = \cdots = H^{(l-1)}(\tau) = H^{(l)}(\tau), \quad (52)$$

which are $(l-1)$ equations.

Therefore, the constants of the motion $\mathfrak{L}^{(l)}$ of $H^{(l)}(\tau)$, are also, in this case, the constants of the motion of $H^{(1)}(\tau)$, constants which, since $P_i^{(1)}(0)$ in (8) are a complete set of projectors, are also the constants of the motion of $H^{(1)}(0)$,

$$\mathfrak{L}^{(l)} = \mathfrak{L}^{(1)}. \quad (53)$$

But we have shown before that $R^{(2)}(\tau), R^{(3)}(\tau), \cdots$, $R^{(l)}(\tau)$, for these particular values of τ, are unity. Therefore, in this case, (43) becomes

$$I^{(1)}(\tau) = R^{(1)}(\tau)\mathfrak{L}^{(1)}R^{(1)\dagger}(\tau), \quad (54)$$

a quantity that now is the generalized adiabatic invariant of lth order.

There remains to identify

$$I^{(1)}(\tau) = R^{(1)}(\tau)\mathfrak{L}^{(1)}R^{(1)\dagger}(\tau),$$

where $\mathfrak{L}^{(1)}$ are the constants of the motion of $H^{(1)}(\tau)$ with the constants of the motion of $H(\tau)$. But from (8) we have that the commutator $[H^{(1)}(\tau), I^{(1)}(\tau)]=0$ implies

$$\begin{aligned} [H(\tau), R^{(1)}(\tau)\mathfrak{L}^{(1)}R^{(1)\dagger}(\tau)] \\ = [H(\tau), I^{(1)}(\tau)] = 0, \quad (55)\end{aligned}$$

and therefore for these values of τ which make zero the first $(l-1)$ time derivatives of $H(\tau)$, the instantaneous constants of the motion of $H(\tau)$ are adiabatic invariants of lth order. This is the meaning of the adiabatic theorem of lth order.

6. GENERAL CASE

The most general case is that situation in which we study the generalized adiabatic invariance of order l when the first $(l'-1)$ time derivatives of $H(\tau)$ are zero initially and finally. We can study two alternatives: either $l > l'$ or $l < l'$. The results for the third alternative $l = l'$ were studied in the preceding section.

Let's begin with the case $l > l'$. We deduce, as before, that for the values of τ for which the first $(l'-1)$ time derivatives of $H(\tau)$ are zero, $K_1^{(1)}(\tau)$ and its first $(l'-2)$ time derivatives, the first $(l'-1)$ time derivatives of $R^{(1)}(\tau)$, and the first $(l'-2)$ time derivatives of $H_1^{(1)}(\tau)$, are zero; $K_2^{(2)}(\tau)$ and its first $(l'-3)$ time derivatives, the first $(l'-2)$ time derivatives of $R^{(2)}(\tau)$, and the first $(l'-3)$ time derivatives of $H_2^{(2)}(\tau)$ are zero, and so on.

We will deduce that, as in (46),

$$P_i^{(1)}(0) = P_i^{(2)}(\tau) = \cdots = P_i^{(l')}(\tau), \quad (56)$$

and since the $P_i^{(1)}(0)$ form a complete set, we will deduce that

$$R^{(2)}(\tau) = R^{(3)}(\tau) = \cdots = R^{(l')}(\tau) = I \qquad (57)$$

for these particular values of τ. Nothing can be said about $R^{(1)}(\tau)$ and about $R^{(h)}(\tau)$, where $h > l'$. Therefore in this case the adiabatic theorem may be stated as follows; a system whose state is initially a vector $|l_i\rangle$ whose projector is $P_i^{(l)}(0)$ will end up its evolution in a state that is a vector of the Hilbert space whose projector is

$$\begin{aligned} S_i^{(l)}(1) = R^{(1)}(1)R^{(l'+1)}(1) \cdots \\ \times R^{(l-1)}(1)P_i^{(l)}(1)R^{(l-1)\dagger}(1) \cdots \\ \times R^{(l'+1)\dagger}(1)R^{(1)\dagger}(d), \end{aligned} \qquad (58)$$

with an approximation of the order $1/T^l$. Similarly, we will obtain an expression for the adiabatic invariant in this case.

The last case to study corresponds to $l < l'$. Relation (57) is also valid now initially and finally, and here the generalized adiabatic theorem of order l is completely equivalent to the adiabatic theorem of l'th order.

7. CONCLUSION

We would like to remark that even better approximation for the generalized adiabatic invariance can be obtained in the case when the expansion in powers of $1/T$ of $F_i^{(1)}(\tau)$ will make that the first term of this expansion independent of the fictitious time τ, because then relations like (16) would give a $K_2^{(2)}(\tau)$ that will be smaller than the one used in our exposition. Besides this point, there remain others whose study may be of some profit. We mention, for instance, the combination of the generalized adiabatic invariance with the extended adiabatic invariance which, following the paper of S. Tamor,[15] will be published by us soon.[16] The reader may like to compare the present new concept of generalized adiabatic invariance with some relevant previous work on adiabatic invariants of any order.[4, 17, 18]

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