Singular behavior at avoided crossings in an iterative perturbation

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The topological space of a bound conservative quantum system is studied in reference to the corresponding integrable one with the concept of parallel transport. A scheme of iterative perturbation is proposed. The destruction of invariant subspaces due to the singular behavior at avoided crossings is carefully investigated. It is shown that before the first avoided crossing the invariant subspaces are merely distorted, and after the first avoided crossing the invariant subspaces begin to be destroyed.

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I. INTRODUCTION

Quantum chaos is currently one of the most intriguing problems in physics [1–4], but unfortunately even the concept of quantum chaos has not yet been precisely defined. In view of the quantum-classical correspondence, it is natural to seek first a theorem for quantum systems parallel to the Kolmogorov-Arnold-Moser (KAM) theorem for classical systems [5]. This is not an easy task due to the uncertainty principle of quantum systems. Zhang *et al.* [6] have recently presented the definition of the quantum phase space, but only the algorithm for seeking the manifestation of quantum chaos via the classical analogy is provided. However, as for classical systems a sufficiently complex topological structure of the configuration manifold of a natural system is an obstruction to its complete integrability [5]; we can alternatively study the property of the topological spaces of quantum systems. Inspired by the works on Berry's phase [7], we have studied the problem of quantum integrability and nonintegrability with the help of the concept of parallel transport [8]. It has been pointed out that there exist singularities in the parameter space. In the presence of the singularity, we can no longer connect the eigenstates of the studied system with those of the integrable reference system by a continuous unitary transformation. An additional permutation should be supplemented to the continuous unitary transformation. Thus the derivatives of eigenfunctions and eigenenergies are discontinuous at the resulting avoided crossing. We have pointed out that the invariant subspaces begin to be destroyed at the first avoided crossing, and furthermore global destruction may result through successive overlapped avoided crossings. The conclusion reached for quantum systems is parallel to that of the KAM theorem for classical systems. However, the way to obtain the conclusion is quite different. Therefore in this article we try to use alternatively the iterative perturbation for obtaining the same conclusion. Special attention is paid to singular behavior at avoided crossings in iterative perturbation.

II. TOPOLOGICAL STUDY WITH THE METHOD OF ITERATIVE PERTURBATION

For brevity, the quantum system H studied here is assumed to be a bound conservative one. Any state of the system evolves in the Hilbert space determined by the dynamic group G of the system. This space can be described with all possible eigenstates of a complete set of commuting observables $I_\alpha^{(0)}$ $(\alpha=1,2,\ldots,n)$ corresponding to a certain subgroup chain of the dynamic group,

$$[I_\alpha^{(0)},I_\beta^{(0)}]=0,\quad \alpha,\beta=1,2,\ldots,n\ , \tag{1}$$

$$I_\alpha^{(0)}|\mathbf{m}\rangle e^{i\delta_\mathbf{m}}=\mathcal{I}_\alpha(\mathbf{m})|\mathbf{m}\rangle e^{i\delta_\mathbf{m}},\quad \alpha=1,2,\ldots,n\ , \tag{2}$$

where the arbitrary phase $\delta_\mathbf{m}$ is explicitly given. This space corresponds to the classical phase space and is the basis for the kinematic description of quantum states. A state of the system at any instant can be expressed as a varying superposition of the states $|\mathbf{m}\rangle e^{i\delta_\mathbf{m}}$.

The Hamiltonian $H(0)$ of an integrable system with the same dynamic group commutes with all the commuting observables $I_\alpha^{(0)}$ $(\alpha=1,2,\ldots,n)$ and has simultaneous eigenstates with them

$$[H(0),I_\alpha^{(0)}]=0,\quad \alpha=1,2,\ldots,n\ , \tag{3}$$

$$H(0)|\mathbf{m}\rangle e^{i\delta_\mathbf{m}}=E_\mathbf{m}^{(0)}|\mathbf{m}\rangle e^{i\delta_\mathbf{m}}\ . \tag{4}$$

All states constructed from basic vectors $|\mathbf{m}\rangle e^{i\delta_\mathbf{m}}$ with eigenenergies $E_\mathbf{m}^{(0)}$ lying inside an interval

$E_0-\frac{1}{2}\Delta E<E_{\mathbf{m}}^{(0)}<E_0+\frac{1}{2}\Delta E$ constitute an energy shell. The energy shell can be further subdivided according to the remaining $(n-1)$ commuting observables into invariant subspaces. Then, a wave packet with energy spread ΔE initially determined by the remaining $(n-1)$ commuting observables will evolve all the time in the corresponding invariant subspace.

Instead of the Schrödinger equation, we can take the Neumann equation

$$i\hbar\frac{\partial\rho}{\partial t}=H\rho-\rho H \tag{5}$$

together with the condition

$$\rho^2=\rho \tag{6}$$

as the dynamic equation of the state. Though the Wigner transform of the density matrix

$$\rho_w(\boldsymbol{\theta},\mathbf{m};t)=\sum_{\mathbf{x}}\langle\mathbf{m}-\mathbf{x}/2|\rho|\mathbf{m}+\mathbf{x}/2\rangle e^{i\mathbf{x}\cdot\boldsymbol{\theta}} \tag{7}$$

is not positive definite, its average value $\bar{\rho}_w(\boldsymbol{\theta},\mathbf{m};t)$ over a certain region conforming to the uncertainty principle is positive definite and can be approximately regarded as a regular function continuously varying with $\boldsymbol{\theta},\mathbf{m}$ in the classical limit in the case of regular motion. Moreover, the Neumann equation and the condition (6) become [9,10]

$$\frac{\partial\bar{\rho}(\boldsymbol{\theta},\mathbf{I};t)}{\partial t}=\left[\frac{\partial H}{\partial\boldsymbol{\theta}}\cdot\frac{\partial}{\partial\mathbf{I}}-\frac{\partial H}{\partial\mathbf{I}}\cdot\frac{\partial}{\partial\boldsymbol{\theta}}\right]\bar{\rho}(\boldsymbol{\theta},\mathbf{I};t) \tag{8}$$

and

$$\bar{\rho}(\boldsymbol{\theta},\mathbf{I};t)\bar{\rho}(\boldsymbol{\theta},\mathbf{I};t)=\bar{\rho}(\boldsymbol{\theta},\mathbf{I};t) \tag{9}$$

in the classical limit. The condition (9) can only be satisfied by the special δ function

$$\rho(\boldsymbol{\theta},\mathbf{I};t)=\delta(\boldsymbol{\theta}-\boldsymbol{\theta}(t))\delta(\mathbf{I}-\mathbf{I}(t)) , \tag{10}$$

and correspondingly the Liouville equation (8) reduces to the Hamilton equations of motion for $\theta(t)$ and $I(t)$. Therefore a wave packet of energy spread ΔE moving in a definite invariant subspace of the energy shell corresponds to a phase point moving in a definite invariant torus of the energy surface. Based on the quantum-classical analogy, the existence of invariant subspaces in an energy shell is taken as the characteristic topological property of an integrable quantum system.

In order to ascertain whether a quantum system H with the same dynamic group G as $H(0)$ has the above topological property, we must first establish the one-to-one correspondence between eigenstates of H and $H(0)$. It is assumed that the eigenenergies $E_{\mathbf{m}}^{(0)}$ are nondegenerate or can be made nondegenerate with infinitesimally small perturbing terms. An auxiliary Hamiltonian of the following form is introduced:

$$H(\lambda)=H(0)+\lambda V , \tag{11}$$

in which $H(0)$ and V are chosen as the diagonal and off-diagonal parts of the Hamiltonian matrix in the $|\mathbf{m}\rangle$ representation,

$$H(0)=\sum_{\mathbf{m}}|\mathbf{m}\rangle\langle\mathbf{m}|H|\mathbf{m}\rangle\langle\mathbf{m}| , \tag{12}$$

$$V=\sum_{\mathbf{m}\neq\mathbf{n}}|\mathbf{m}\rangle\langle\mathbf{m}|H|\mathbf{n}\rangle\langle\mathbf{n}| \tag{13}$$

and represent the integrable Hamiltonian and perturbing term, respectively. No part of V is commutable with $I_\alpha^{(0)}$. As $H(\lambda)$ varies continuously with λ from $H(0)$ to H, we can have eigenenergies of $H(\lambda)$

$$H(\lambda)|\psi_s(\lambda)\rangle=E_s(\lambda)|\psi_s(\lambda)\rangle \tag{14}$$

also varying continuously with λ if there is no singular point in the interval. At the same time, we fix the phase relationship of the eigenstates $|\psi_s(\lambda)\rangle$ with the condition

$$\langle\psi_s(\lambda)|\psi_s(\lambda+\epsilon)\rangle=1+O(\epsilon^2) \tag{15}$$

for parallel transport. In such a way, the one-to-one correspondence between the eigenstates in energy shells of H and $H(0)$ has been precisely established.

The one-to-one correspondent states $|\psi_s(\lambda)\rangle$ and $|\psi_s(0)\rangle$ can always be connected by a unitary transformation,

$$|\psi_s(\lambda)\rangle=U(\lambda,0)|\psi_s(0)\rangle . \tag{16}$$

However, the unitary transformations in general can be classified into the following two categories: (i) proper unitary transformation [denoted as $R(\lambda,0)$ afterwards], i.e., continuous unitary transformation without discrete permutation,

$$\lim_{\lambda\to 0}R(\lambda,0)=1 ; \tag{17}$$

(ii) improper unitary transformation [denoted still as $U(\lambda,0)$ afterwards], there exist discrete permutations in addition to the continuous unitary transformation,

$$\lim_{\lambda\to 0}U(\lambda,0)\neq 1 . \tag{18}$$

With the proper unitary transformation $R(\lambda,0)$,

$$|\psi_s(\lambda)\rangle=R(\lambda,0)|\psi_s(0)\rangle \tag{19}$$

the energy shells of H and $H(0)$ are in homeomorphism [11]. Moreover, we have

$$I_\alpha(\lambda)|\psi_s(\lambda)\rangle=\mathcal{I}_{\alpha,s}|\psi_s(\lambda)\rangle , \tag{20}$$

where

$$I_\alpha(\lambda)=R(\lambda,0)I_\alpha^{(0)}R^\dagger(\lambda,0) \tag{21}$$

are renormalized conserved quantities. As $I_\alpha(\lambda)$ constitutes a complete set of commutable quantities, $H(\lambda)$ must be a function of $I_\alpha(\lambda)$. The states $|\psi_s(\lambda)\rangle$ are still characterized by the same set of quantum numbers and subdivided into invariant subspaces in the same way as $|\psi_s(0)\rangle$. These invariant subspaces are merely distorted. The energy shells of H have the same topological structure as those of $H(0)$.

It is radically different in the case of improper unitary transformations. The energy shells of H and $H(0)$ are not in homeomorphism. The above discussion can no longer be valid.

The topological study is therefore concentrated to the point whether or not $|\psi_s(\lambda)\rangle$ can be connected to $|\psi_s(0)\rangle$ by a proper unitary transformation. This problem can be most directly studied with the method of iterative perturbation.

In this article, a scheme of iterative perturbation is formulated so as to push the solution as forward as possible. Provided we make no condition on the normalization of the eigenstate $|\psi_s(\lambda)\rangle$, we may always split it into two parts

$$|\psi_s(\lambda)\rangle=|\psi_s(0)\rangle+|f(\lambda)\rangle\ , \tag{22}$$

where the change due to the perturbation is orthogonal to the unperturbed state $|\psi_s(0)\rangle$, i.e.,

$$\langle\psi_s(0)|f(\lambda)\rangle=0\ . \tag{23}$$

Introducing the projection operators

$$P=|\psi_s(0)\rangle\langle\psi_s(0)|,\quad Q=1-P \tag{24}$$

and applying Q to Eq. (14), we readily obtain

$$[E_s(\lambda)-H(0)]|f(\lambda)\rangle=Q\lambda V|\psi_s(\lambda)\rangle\ . \tag{25}$$

Substituting the formal solution of (25) into (22), we obtain

$$|\psi_s(\lambda)\rangle=|\psi_s(0)\rangle+\frac{1}{E_s(\lambda)-H(0)}Q\lambda V|\psi_s(\lambda)\rangle\ , \tag{26}$$

Eq. (26) is an inhomogeneous integral equation for which the iteration method is particularly suitable. Therefore we solve the problem with iteration by taking $E(\lambda)$ as a function of $|\psi_s(\lambda)\rangle$,

$$E_s(\lambda)=\frac{\langle\psi_s(\lambda)|H(\lambda)|\psi_s(\lambda)\rangle}{\langle\psi_s(\lambda)|\psi_s(\lambda)\rangle} \tag{27}$$

instead of

$$E_s(\lambda)=E_0+\langle\psi_s(0)|(\lambda V)|\psi_s(\lambda)\rangle \tag{28}$$

as in the Brillouin-Wigner perturbation expansion [12].

Equation (14) can be written explicitly as

$$|\psi_k(\lambda)\rangle=|\psi_k(0)\rangle+\sum_{j(\neq k)}x_j(\lambda)|\psi_j(0)\rangle\ . \tag{22'}$$

Then we have correspondingly

$$x_i(\lambda)=\frac{1}{E_k(\lambda)-H(0)_{ii}}\left[\sum_{j(\neq i,k)}H(\lambda)_{ij}x_j(\lambda)+H(\lambda)_{ik}\right],\quad i=1,\ldots,k-1,k+1,\ldots,n\ , \tag{26'}$$

$$E_k(\lambda)=\left[1+\sum_{j(\neq k)}x_j(\lambda)^2\right]^{-1}\times\left[H(\lambda)_{kk}+2\sum_{j(\neq k)}H(\lambda)_{jk}x_j(\lambda)+\sum_{i,j(\neq k)}H(\lambda)_{ij}x_i(\lambda)x_j(\lambda)\right]. \tag{27'}$$

The result of iteration depends strongly on the initial point taken. In order to study the eigenstates $|\psi_k(\lambda)\rangle$ topologically, we take the initial point as

$$[|\psi_k(\lambda)\rangle]_{\text{initial}}=|\psi_k(0)\rangle \tag{29}$$

or

$$[x_j(\lambda)]_{\text{initial}}=0,\quad j=1,\ldots,k-1,k+1,\ldots,n\ . \tag{29'}$$

The functional iteration is very involved. However, we know in general that the iteration can only succeed for cases in which the obtained $|\psi_s(\lambda)\rangle$ still retains the main feature of $|\psi_s(0)\rangle$. This is possible only for small λ. As the interaction between every two neighboring states results in a repulsive effect when λ increases, the interaction of a certain kth state with all states above (or below) may make the eigenenergy of this state closer to that of the $(k-1)$th [or $(k+1)$th] state. This effect results in a rather small denominator $E_k(\lambda)-E_{k-1}(0)$ [or $E_{k+1}(0)-E_k(\lambda)$] and considerably strong mixing with the neighboring $(k-1)$th [or $(k+1)$th] state. When λ increases further to a critical value λ_1, the mixing becomes so strong that $|\psi_k(\lambda)\rangle$ ceases to keep the main feature of $|\psi_k(0)\rangle$, and the iterative perturbation begins to fail for this state. Thus λ_1 is the first singular point in the λ space. Therefore we have the following conclusions.

(i) In case all the states $|\psi_s(\lambda)\rangle$ can be obtained from $|\psi_s(0)\rangle$ with iterative perturbation, $|\psi_s(\lambda)\rangle$ and $|\psi_s(0)\rangle$ can be connected with a proper unitary transformation $R(\lambda,0)$. Then the system has renormalized conserved quantities $I_\alpha(\lambda)$ corresponding to $I_\alpha^{(0)}$, and $R(\lambda,0)$ is the corresponding renormalization transformation. States $|\psi_s(\lambda)\rangle$ can be characterized by the same set of quantum numbers and subdivided in the same way into invariant subspaces as for $|\psi_s(0)\rangle$. These invariant subspaces are merely distorted. The system has the same topological structure as before and is said to be completely integrable.

(ii) In case the iterative perturbation begins to fail at two neighboring states, not all the states $|\psi_s(\lambda)\rangle$ can be connected to $|\psi_s(0)\rangle$ with a proper unitary transformation. [It is impossible that the iterative perturbation begins to fail for one state alone. If $(n-1)$ states have been obtained by iteration, the last one is already determined due to completeness and orthogonality conditions.] The invariant subspaces involving those states begin to be destroyed.

The problem can also be viewed from the opposite direction by taking Eqs. (26), (27), and (29) as a mapping $R(\lambda,0)$ for obtaining $|\psi_s(\lambda)\rangle$ from $|\psi_s(0)\rangle$. From (25) we have

$$Q[E_s(\lambda)-H(0)-\lambda V]|\psi_s(\lambda)\rangle=Q[E_s(\lambda)-H(\lambda)]|\psi_s(\lambda)\rangle=0 \tag{30}$$

and from (27) we have

$$\langle\psi_s(\lambda)|(P+Q)[E_s(\lambda)-H(\lambda)]|\psi_s(\lambda)\rangle=\langle\psi_s(\lambda)|P[E_s(\lambda)-H(\lambda)]|\psi_s(\lambda)\rangle=0\ . \tag{31}$$

Combining these equations we have

$$[E_s(\lambda)-H(\lambda)]|\psi_s(\lambda)\rangle=0\ . \tag{14'}$$

$|\psi_s(\lambda)\rangle$ obtained from such mapping are just eigenstates of $H(\lambda)$ satisfying the condition (15), provided the mapping is well defined. The topological structure of $H(0)$ remains unchanged; on the other hand, if the mapping is not well defined, the topological structure of $H(0)$ is no longer preserved.

The iterative perturbation represents precisely the homeomorphic mapping in topological studies of quantum systems. It is somewhat different from the conventional mapping [13] in which the form of mapping is not derived from the definite physical problem, and the initial point of iteration is not specified as required in topological studies.

III. ILLUSTRATION WITH A THREE-LEVEL LIPKIN MODEL

We consider the following three-level Lipkin model [14] as an illustration. Suppose there are three single particle levels with the same parity and spin, their degeneracies are $\Omega=2j+1$. The model Hamiltonian is composed of the collective operators,

$$K_{ij}=\sum_{\alpha=1}^{\Omega} a_{i\alpha}^{\dagger}a_{i\alpha},\quad i,j=0,1,2\ . \tag{32}$$

Both the total number of the particles $\sum_i K_{ii}$ and the degeneracy Ω are assumed to be equal to 4,

$$\begin{aligned}H=&\epsilon_1K_{11}+\epsilon_2K_{22}-\kappa_2(K_{20}K_{20}+K_{02}K_{02})\\&-\kappa_1(K_{10}K_{10}+K_{01}K_{01})+\mu_1(K_{21}K_{20}+K_{02}K_{12})\\&+\mu_2(K_{12}K_{10}+K_{01}K_{21})\ ,\\ \epsilon_1=&1.1,\quad \epsilon_2=1.6,\quad \kappa_1=0.43\ ,\\ \kappa_2=&0.71,\quad \mu_1=0.73,\quad \mu_2=0.683\ .\end{aligned} \tag{33}$$

The first line represents the integrable $H(0)$, while the next two lines represent the perturbing term V. Only the off-diagonal matrix elements of $H(\lambda)=H(0)+\lambda V$ are λ dependent. As $H(\lambda)$ is invariant to time reversal, we consider in the following the orthogonal transformation instead of the general unitary one.

(i) When λ is small, the iterative perturbation for all the states converges quickly. Correspondingly,

$$\langle\psi_{s'}(0)|\psi_{s''}(\lambda)\rangle=\langle\psi_{s'}(0)|R(\lambda,0)|\psi_{s''}(0)\rangle \tag{34}$$

is the matrix representation of the renormalization transformation. The states $|\psi_s(\lambda)\rangle$ can be characterized by the same quantum numbers as for $|\psi_s(0)\rangle$.

(ii) When λ increases, the iteration for the ninth and tenth states converges slower than the others.

When λ increases to the value $\lambda=0.223-\epsilon$, the iteration for states other than the ninth and tenth ones converges. But the results for the ninth and tenth states after thousands of iterations shows only a sign of approaching the final result.

(iii) When λ increases to a value beyond 0.223, the results for the ninth and tenth states after thousands iterations show no definite sign of convergence.

The overlaps $\langle\psi_k^{(r)}(\lambda)|\psi_k^{(r+1)}(\lambda)\rangle$ at different stages r of iteration are shown in Fig. 1 for two values of λ. The overlap approaches the value unity in case the iterative perturbation converges. But if the iterative perturbation fails, the overlap remains to be approximately one-half after thousands of iterations, while $|\psi_k^{(r)}(\lambda)\rangle$ changes violently at different stages of iteration.

The topological properties of the system $H(\lambda)$ are not influenced by any proper unitary transformation. This very important property enables one to study the topological structure with the transformed Hamiltonian matrix $\overline{H(\lambda)}_{ij}$ in which the influence on the ninth and tenth states from the others has been explicitly expressed in the transformed 2×2 submatrix and no more coupling between the two states and others needs to be considered. At the same time, the initial point of iteration is transformed to $\bar{x}_j=0$ $(j=1,\ldots,k-1,k+1,\ldots,n)$. The problem of convergence of iteration for these two states can then be shown clearly.

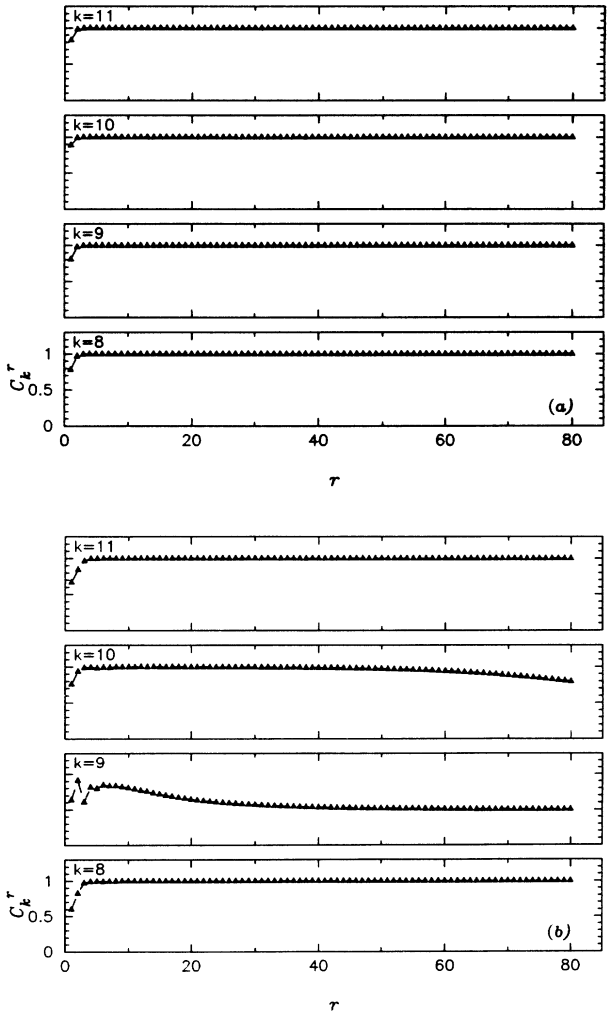

FIG. 1. Variation of $C_k^{(r)}=\langle\psi_k^{(r)}(\lambda)|\psi_k^{(r+1)}(\lambda)\rangle$ with λ for $k=8,9,10,11$ when (a) $\lambda=0.18$, (b) $\lambda=0.30$.

With that transformation, the states $|\psi_s(0)\rangle$ $(s=1,\ldots,8,11,\ldots,15)$ are required to be directly transformed to $|\psi_s(\lambda)\rangle$ $(s=1,\ldots,8,11,\ldots,15)$ without any rotation in the two-dimensional subspace complementary to the subspace spanned by $|\psi_s(\lambda)\rangle$ $(s=1,\ldots,8,11,\ldots,15)$. This is just an element of SO(15)/SO(2) and can be uniquely determined with the states $|\psi_s(\lambda)\rangle$ $(s=1,\ldots,8,11,\ldots,15)$ already obtained from iteration. Writing the matrix elements explicitly, we have

$$R_c(\lambda)_{j,s}=\langle\psi_j(0)|\psi_s(\lambda)\rangle\ ,\quad s=1,\ldots,8,11,\ldots,15\ , \tag{35}$$

$$R_c(\lambda)_{j,t}=\langle\psi_j(0)|\psi'_t(\lambda)\rangle,\quad t=9,10\ ,$$

where $|\psi'_t(\lambda)\rangle$ $(t=9,10)$ are normalized orthogonal states obtained directly from $|\psi_t(0)\rangle$ $(t=9,10)$ and can be determined as follows:

$$|\psi'_9(\lambda)\rangle=\frac{|\xi_9(\lambda)\rangle+|\xi_{10}(\lambda)\rangle}{2[1+\langle\xi_9(\lambda)|\xi_{10}(\lambda)\rangle]^{1/2}}+\frac{|\xi_9(\lambda)\rangle-|\xi_{10}(\lambda)\rangle}{2[1-\langle\xi_9(\lambda)|\xi_{10}(\lambda)\rangle]^{1/2}}\ ,$$

$$|\psi'_{10}(\lambda)\rangle=\frac{|\xi_9(\lambda)\rangle+|\xi_{10}(\lambda)\rangle}{2[1+\langle\xi_9(\lambda)|\xi_{10}(\lambda)\rangle]^{1/2}}-\frac{|\xi_9(\lambda)\rangle-|\xi_{10}(\lambda)\rangle}{2[1-\langle\xi_9(\lambda)|\xi_{10}(\lambda)\rangle]^{1/2}}\ , \tag{36a}$$

$$|\xi_t(\lambda)\rangle=\frac{(1-\sum'_{i(\neq 9,10)}|\psi_i(\lambda)\rangle\langle\psi_i(\lambda)|)|\psi_t(0)\rangle}{\left[1-\sum'_{i(\neq 9,10)}\langle\psi_t(0)|\psi_i(\lambda)\rangle\langle\psi_i(\lambda)|\psi_t(0)\rangle\right]^{1/2}}\quad(t=9,10)\ . \tag{36b}$$

The transformed Hamiltonian matrix now becomes

$$\overline{H(\lambda)}_{ij}=[R_c(\lambda)^{\dagger}H(\lambda)R_c(\lambda)]_{ij}$$

$$=\begin{bmatrix}\overline{H(\lambda)}_{11} & & & & & & & \\ & \overline{H(\lambda)}_{22} & & & & 0 & & \\ & & \ddots & & & & & \\ & & & \overline{H(\lambda)}_{9,9} & \overline{H(\lambda)}_{9,10} & & & \\ & & & \overline{H(\lambda)}_{9,10} & \overline{H(\lambda)}_{10,10} & & & \\ & 0 & & & & \ddots & & \\ & & & & & & \overline{H(\lambda)}_{15,15} & \end{bmatrix} \tag{37}$$

such that $\overline{H(\lambda)}_{ss}=E_s(\lambda)$ $(s=1,\ldots,8,11,\ldots,15)$ as shown in Fig. 2 and $\overline{H(\lambda)}_{99}$ and $\overline{H(\lambda)}_{10,10}$ become λ dependent and intersect at $\lambda=\lambda_1=0.223$ as shown in the inset of Fig. 2.

Owing to the particular form of $\overline{H(\lambda)}$, the further iterative perturbation can in fact be performed in the two-dimensional subspace by taking the diagonal part as $\underline{H(0)}$ and off-diagonal part as V. As $\overline{H(\lambda)}_{99}$ and $\overline{H(\lambda)}_{10,10}$ intersect at λ_1, the results of iterative perturbation on the two sides of the singular point λ_1 become

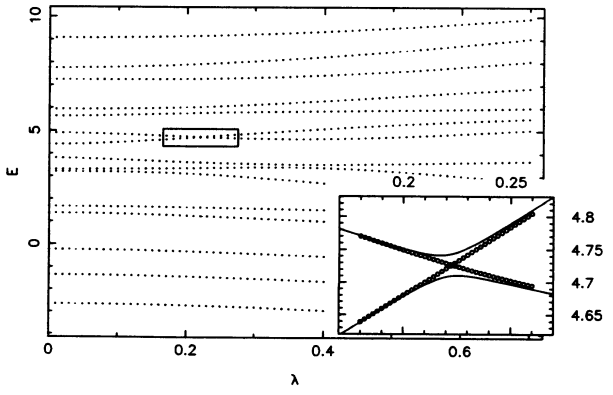

FIG. 2. Variation of eigenenergies $\underline{E}(\lambda)$ (dotted line) and transformed diagonal matrix elements $\overline{H(\lambda)}_{99}$ and $\overline{H(\lambda)}_{10,10}$ (see inset) with λ.

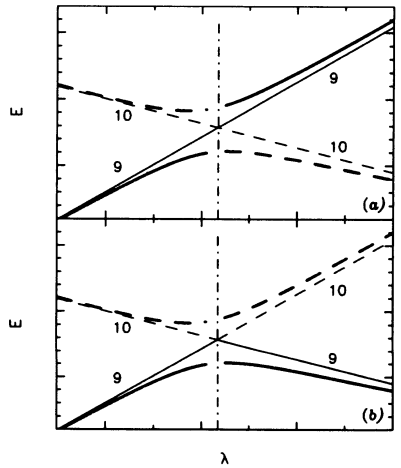

FIG. 3. Iterative perturbation for the ninth and tenth states in the neighborhood of the first singular point $\lambda=\lambda_1=0.223$ for (a) without any permutation, (b) after a permutation.

discontinuous as shown in Fig. 3(a). Only if a permutation is performed to make $H(\lambda)_{99} < H(\lambda)_{10,10}$ beyond the singular point λ_1, the results of iterative perturbation can then conform to condition (15) and appear as an avoided crossing as shown in Fig. 3(b). This explains why λ_1 is the singular point and the iterative perturbation fails at that point. Therefore we have up to this first singular point,

$$R(\lambda_1-\epsilon,0)=R_l(\lambda_1-\epsilon,0)R_c(\lambda_1-\epsilon,0)\ , \tag{38}$$

$$R_l(\lambda_1-\epsilon,0)=R_c(\lambda_1-\epsilon,0)R_l'(\lambda_1-\epsilon,0) \times R_c^{-1}(\lambda_1-\epsilon,0)\ , \tag{39}$$

and

$$R_l'(\lambda_1-\epsilon,0)=\begin{pmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & \cos\left(\frac{\pi}{4}-\epsilon\right) & \pm\sin\left(\frac{\pi}{4}-\epsilon\right) & & & \\ & & & \mp\sin\left(\frac{\pi}{4}-\epsilon\right) & \cos\left(\frac{\pi}{4}-\epsilon\right) & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{pmatrix} \tag{40}$$

is a $\pm\pi/4$ rotation localized in the two-dimensional subspace relating to the ninth and tenth states.

The iterative perturbation after the first singular point λ_1 can be performed as before up to the second singular point λ_2 by taking $|\psi_s(\lambda_1+\epsilon_1)\rangle$ as initial points, where $|\psi_s(\lambda_1+\epsilon_1)\rangle$ is obtained from $|\psi_s(\lambda_1-\epsilon_1)\rangle$ with the condition (15) for parallel transport,

$$\lim_{\epsilon\to 0}|\psi_s(\lambda_1+\epsilon)\rangle=\lim_{\epsilon\to 0}|\psi_s(\lambda_1-\epsilon)\rangle\ . \tag{41}$$

Then we have

$$U(\lambda_2-\epsilon_2,0)=\lim_{\epsilon_1\to 0}[R_l(\lambda_2-\epsilon_2,\lambda_1+\epsilon_1) \times R_c(\lambda_2-\epsilon_2,\lambda_1+\epsilon_1)] \times[R_l(\lambda_1-\epsilon_1,0)R_c(\lambda_1-\epsilon_1,0)]\ , \tag{42}$$

where $[R_l(\lambda_2-\epsilon_2,\lambda_1+\epsilon_1)R_c(\lambda_2-\epsilon_2,\lambda_1+\epsilon_1)]$ in the $|\psi_s(\lambda_1+\epsilon_1)\rangle$ representation is similar in form to $R_l(\lambda_1-\epsilon_1,0)R_c(\lambda_1-\epsilon_1,0)$ in the $|\psi_s(0)\rangle$ representation. Here $U(\lambda_2-\epsilon_2,0)$ is a piecewise-continuous orthogonal transformation.

If there exist r successive singular points in the interval $\lambda=0$ to 1, we have in general

$$U(1,0)=\lim_{\epsilon_1,\ldots,\epsilon_2\to 0}R(1,\lambda_r+\epsilon_r)[R_l(\lambda_r-\epsilon_r,\lambda_{r-1}+\epsilon_{r-1}) \times R_c(\lambda_r-\epsilon_r,\lambda_{r-1}+\epsilon_{r-1})]\cdots[R_l(\lambda_2-\epsilon_2,\lambda_1+\epsilon_1)R_c(\lambda_2-\epsilon_2,\lambda_1+\epsilon_1)] \times[R_l(\lambda_1-\epsilon_1,0)R_c(\lambda_1-\epsilon_1,0)]\ . \tag{43}$$

$U(1,0)$ can be written in an abbreviated form as

$$U(1,0)=R(1,\lambda_r)[R_l(\lambda_r,\lambda_{r-1})R_c(\lambda_r,\lambda_{r-1})]\cdots[R_l(\lambda_2,\lambda_1)R_c(\lambda_2,\lambda_1)][R_l(\lambda_1,0)R_c(\lambda_1,0)] \tag{43'}$$

with the limiting process understood.

The above discussion on the singular behavior at avoided crossings in iterative perturbation can be generalized to N-dimensional cases and can be utilized as the key point in discussing the partial integrability or nonintegrability of quantum systems. Detailed discussions are planned to be published in separate papers [8].

IV. SUMMARY

In this article, the integrability or the loss of integrability of quantum systems is studied from a topological approach as follows.

(1) Any state of the quantum system H evolves in the Hilbert space determined by the dynamic group G of the system.

(2) Eigenstates of the quantum system H with eigenenergies lying within an interval $E_0-\frac{1}{2}\Delta E<E_s<E_0+\frac{1}{2}\Delta E$ are used as basic vectors of an energy shell. A collection of these energy shells constitutes the Hilbert space. They form a topological space.

(3) If the one-to-one correspondent eigenstates of H and $H(0)$, established with the help of parallel transport,

can be obtained with the method of iterative perturbation, the topological spaces of H and $H(0)$ are in homeomorphism.

(4) As the topological property of an integrable system, that the energy shell can be further subdivided into invariant subspaces is invariant to homeomorphic mapping. The quantum system H is integrable provided its topological space is in homeomorphism with that of the integrable system $H(0)$.

(5) On the other hand, if the iterative perturbation for the auxiliary Hamiltonian $H(\lambda)$ ($\lambda=0$ to 1) first fails at a certain singular point λ_1 due to strong mixing of two neighboring states, the invariant subspaces of the energy shell involving these two states begin to be destroyed.

(6) After the first singular point λ_1 the iterative perturbation can be performed as before by taking $|\psi_s(\lambda_1+\epsilon)\rangle$, a parallel transport of $|\psi_s(\lambda_1-\epsilon)\rangle$, as the initial point. Such a piecewise-continuous orthogonal transformation results in an avoided crossing of the energy levels.

(7) The following conclusion is then reached. Before the first avoided crossing, the invariant subspaces of energy shells of $H(\lambda)$ are merely distorted, and after the first avoided crossing, the invariant subspaces of the energy shell involving the avoided crossing begin to be destroyed. This conclusion is the key point in discussing the partial integrability or nonintegrability of quantum systems.

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