Semiclassical level curvatures and quantum transport phenomena

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The semiclassical expression of level curvature for quantized chaotic systems with periodic lattice symmetry is derived. From this expression, the transport property of such systems is investigated via the Thouless formula. The relation between the Thouless formula and the Kubo formula is studied in an unusual way. It is revealed that Akkermans's result on the relation between them from random matrix theory, which is for the metallic regime, corresponds to the universality of the underlying classical chaotic dynamics. The test of the expression obtained here is done for the quantized kicked rotator system. [S1063-651X(96)11810-9]

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I. INTRODUCTION

In this paper, motivated by recent extensive studies on quantum chaology, mesoscopic systems, and foundation of statistical mechanics, we discuss the transport phenomena in quantized chaotic systems. In order to characterize the transport property of mesoscopic systems, one uses several formulas, i.e., Kubo formula [1,2], Thouless formula [3,4], Landauer formula [5,6], and Byers-Yang formula [7]. Among them, the Kubo formula is derived from the microscopic dynamics with the assumption of ergodicity and the adiabatic switching of external field. In this sense, the Kubo formula is the most fundamental and reliable among the above formulas, because the others are hypothetical and only for the specific systems.

Recent studies on mesoscopic systems examine the parametric dependence of the energy levels from several view points, i.e., usual and field theoretical random matrix theory [8,9] and semiclassical theory [10,11]. Their interest is focused at the two-point correlation of energy levels, namely, $\langle d(E,\lambda)d(E+\Delta E,\lambda+d\lambda)\rangle$, where E is energy, λ is the system parameter, and $d(E,\lambda)$ is the density of states. If the parametric dependence is due to symmetry of systems (e.g., periodicity), we can consider the transport property by using the Thouless formula or Byers-Yang formula. In such a study, the Thouless formula particularly plays an essential role. The sensitivity of the energy level to the change of the boundary condition provides us with the conductance of a given system via the Thouless formula:

$$g=\frac{1}{\Delta}\left\langle \left|\frac{\partial^2 E_n}{\partial \phi^2}\right|_{\phi=0}\right\rangle, \tag{1}$$

where ϕ is the Bloch parameter and the bracket means the average over the whole energy levels. The first derivative $\partial E/\partial\phi$ and second derivative $\partial^2 E/\partial\phi^2$ are called the level velocity and level curvature, respectively. However, the derivation of the Thouless formula is hypothetical as shown later in Sec. II. It is natural to ask about the theoretical foundation of the Thouless formula. Therefore, the main aim of this paper is to answer this question.

To this end, we employ the semiclassical theory. The advantage of the semiclassical theory is as follows. (a) We can understand the quantum phenomena in terms of the underlying classical dynamics. We fully use the classical-quantum correspondence in some sense. (b) Recent development of ''chaos theory'' in classical mechanics provides us with a large amount of useful information. (c) If the semiclassical theory is employed in an appropriate way, we obtain high accuracy compared with a quantum exact result.

Here we briefly comment on point (b). To calculate the transport coefficient from the microscopic levels is still the main subject of nonequilibrium statistical mechanics. The recent progress of ''chaos theory'' and the related numerical simulation of molecular dynamics show that for hard chaotic systems, the transport coefficient can be explicitly expressed in terms of the dynamical characteristic quantities such as Lyapunov exponents, escape rates, etc. There are three fundamental contributions. First is the escape rate formalism by Gaspard *et al.* [12,13]. Second is the cycle expansion by Cvitanović [14,15]. As is shown later, this formalism is particularly useful for our semiclassical analysis. Third is the mathematical rigorous proof by Chernov *et al.* [16]. From these contributions, we now know that ''chaos'' indeed plays an important role for the foundation of nonequilibrium statistical mechanics. At the same time, the validity of the classical Kubo formula was reconsidered from the aspect of chaos theoretically [16] and numerically since van Kampen's objection [17].

Turning our attention from a classical object to a quantum object in the context of transport phenomena, what changes? Recently the semiclassical Kubo formula was derived and applied to the magnetoconductivity and de Haas–van Alphen effect by several authors [18,19]. In their work, the Kubo formula is expressed in terms of the characteristics of the periodic orbits for quantized chaotic systems. As well as the Kubo formula, another formula for the transport coefficient as mentioned before can be semiclassically analyzed. The derived semiclassical expression directly enables us to eluci-

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date the process of the quantum interference in transport phenomena. In order to derive the semiclassical expression for the Thouless formula Eq. (1), we use a formal analogy of the zeta function formalism (i.e., cycle expansion). As we will show later in Sec. III, for quantized chaotic systems with the periodic boundary condition, it turns out that the semiclassical expression of level curvature (i.e., the inverse of effective mass) is a quantum analog of the classical diffusion coefficient derived in [14,15].

This paper is organized as follows. In Sec. II, we introduce the Thouless formula along the original Thouless argument. In Sec. III, we derive the semiclassical expression for the level curvature (i.e., the inverse of the effective mass) for both autonomous Hamiltonian systems and kicked Hamiltonian systems. In Sec. IV, we compare the Thouless formula with the Kubo formula in a semiclassical way. In Sec. V, the numerical calculation is reported. For the quantized kicked rotator, Akkermans's relation and the semiclassical level curvature derived here are tested. In Sec. VI, we summarize the results.

II. THOULESS FORMULA

In this section, we derive the Thouless formula along the original Thouless's argument and reexamine it under the consideration of the application to quantized chaotic systems. Consider the d-dimensional cubic fraction of a random alloy whose size is L. This fraction is described by the Schrödinger equation:

$$\hat{H}=\frac{\hat{\mathbf{p}}^2}{2m}+V(\hat{\mathbf{r}}), \tag{2}$$

$$\hat{H}\psi_\alpha(\mathbf{r})=E_\alpha\psi_\alpha(\mathbf{r}). \tag{3}$$

To measure the tendency of the localization for a given eigenstate, we introduce the change of the boundary condition:

$$\psi_\alpha(\mathbf{r}+L\mathbf{e}_x)=\exp(i\phi)\psi_\alpha(\mathbf{r}). \tag{4}$$

Here we only consider the x direction. The generalization to all directions is easy. This boundary condition is equivalent to solving the following Hamiltonian:

$$\begin{aligned}\hat{H}'&=\frac{1}{2m}\left(\hat{\mathbf{p}}+\frac{\hbar\phi}{L}\mathbf{e}_x\right)^2+V(\hat{\mathbf{r}})\\&=\hat{H}+\frac{\hbar\phi}{mL}\hat{\mathbf{p}}_x+\frac{\hbar^2\phi^2}{2mL^2}.\end{aligned} \tag{5}$$

For localized state, this change of the boundary condition does not affect the eigenwave function because the exponentially damped tail of it near the boundary of the alloy cannot transfer this perturbation to the other side. This would correspond to no conduction of electrons. However, for the extended eigenstate, this perturbation by the boundary condition does affect its wave function. The perturbation can be transformed to the other side without large loss. Thus, the extended state contributes to the conduction of electrons. This effect would appear in the change of the corresponding eigenenergy. Let us introduce the following quantity:

$$\Delta E_\alpha\equiv\frac{1}{2}\left|\left[\frac{\partial^2E_\alpha(\phi)}{\partial\phi^2}\right]_{\phi=0}\right|=\frac{\hbar^2}{L^2}\left[\frac{1}{2m}+\frac{1}{m^2}\sum_{\beta\neq\alpha}\frac{|\langle\alpha|\hat{p}_x|\beta\rangle|^2}{E_\alpha-E_\beta}\right]. \tag{6}$$

Now we assumed that there is no degeneracy. This is consistent with the later analysis for quantized chaotic systems.

For the localized state, it can be shown that $\Delta E_\alpha=0$ as $L\to\infty$ by using $i\hbar(d\hat{x}/dt)=[\hat{x},\hat{H}]$. However, for the extended state, since the eigenwave function is extended in the whole range, the evaluation for the localized state cannot work as $L\to+\infty$, namely, we cannot use the Heisenberg equation of motion above. So we choose another route to evaluate ΔE_α. The order of the energy difference is given as

$$E_\alpha-E_\beta\sim\mathcal{O}\left(\frac{1}{\left|\frac{dN}{dE}\right|}\right). \tag{7}$$

This replacement implies that the energy levels are uncorrelated. ΔE_α can be approximated by

$$\Delta E_\alpha\sim\frac{\hbar^2}{L^2}\frac{1}{m^2}\overline{p^2}\frac{dN}{dE}, \tag{8}$$

where $\overline{p}$ is the average of $\langle\alpha|\hat{\mathbf{p}}|\beta\rangle$. Here we assume that the $\overline{p^2}$ in Eq. (8) is same as that which appears in the Kubo formula. This implies that the value of the matrix elements is well-approximated by a single average value. In other words, the matrix element is statistically well-distributed. From the Kubo conductivity and the above formula, we obtain

$$\begin{aligned}\sigma&=\frac{\pi e^2\hbar}{L^d}\left\langle\sum_{\alpha,\beta}|\langle\alpha|\hat{p}_x|\beta\rangle|^2\delta(E-E_\alpha)\delta(E-E_\beta)\right\rangle\\&\sim\frac{e^2h}{2m^2L^d}\overline{p^2}\left(\frac{dN}{dE}\right)^2\\&=\frac{e^2h}{2L^{d-2}}\left(\frac{dN}{dE}\right)\langle\Delta E_\alpha\rangle\end{aligned} \tag{9}$$

(here the bracket in the first line is an appropriate average over energy levels). Since the conductivity G_d for a d-dimensional system may obey the scaling law, $G_d=\sigma L^{d-2}$, then

$$g_d=\frac{G_d}{(e^2/h)}\sim\frac{1}{\Delta}\langle\Delta E_\alpha\rangle=\frac{1}{\Delta}\left\langle\left|\frac{\partial^2E_\alpha}{\partial\phi^2}\right|_{\phi=0}\right\rangle, \tag{10}$$

where $\Delta\equiv1/(dN/dE)$ is the mean level spacing. Note that to let "$\sim$" become "$=$," we have to know the prefactor on the right-hand side (rhs) of Eq. (10).

We would like to make three points. (i) The derivation of the Thouless formula is based on the time-independent Schrödinger equation. On the other hand, for the Kubo formula, it is based on the time-dependent Schrödinger equation and the adiabatic process is assumed [20,1,2]. (ii) The Thouless conductance is the average conductance. Then, the Thouless conductance may be proportional to the usual Kubo conductivity, only if all assumptions above, which assure the averaging, are satisfied. (iii) For classically chaotic systems,

TABLE I. The situation for the derivation of the Thouless formula and the Kubo formula.

Thouless formula	↔	Time-independent Hamiltonian Equilibrium property
Kubo formula	↔	Time-dependent Hamiltonian (adiabatic process) Nonequilibrium property

the average over energy levels should be $\langle|\cdots|\rangle$ in the metallic regime rather than $\langle|\cdots|^2\rangle^{1/2}$ in the other definition [21]. (See Table I.) It is shown, by random matrix theory, that the tail of the curvature distribution obeys the power law [22]:

$$P(\kappa)\sim|\kappa|^{-(\beta+2)}\begin{cases}\beta=1, & \text{GOE (COE)}\\ \beta=2, & \text{GUE (CUE)}\\ \beta=4, & \text{GSE (CSE)},\end{cases} \tag{11}$$

where $\kappa\equiv\partial^2E(\lambda)/\partial\lambda^2$ $[\kappa\equiv\partial^2\omega(\lambda)/\partial\lambda^2]$ is the level curvature, and λ is the system parameter. These expressions are for the type of Hamiltonian $\hat{H}=\hat{H}_0+\lambda\hat{V}$, $\hat{H}\psi_n=E_n(\lambda)\psi_n$ $[\hat{H}=\hat{H}_0+\lambda\hat{V}\Sigma_{j=-\infty}^{\infty}\delta(t-j)$, $\hat{U}=e^{-(i/\hbar)\hat{H}_0}e^{-(i/\hbar)\lambda\hat{V}}$, $\hat{U}\psi_n=e^{i\omega_n(\lambda)}\psi_n]$. If we take $\langle|\cdots|^2\rangle^{1/2}$, the mean value of it will become divergent. Therefore, we should take the absolute value of the curvature in the bracket.

III. SEMICLASSICAL LEVEL CURVATURES

In the preceding section, we have introduced the Thouless formula in connection with the parameter dependence of energy levels to the Bloch parameter. In this section, using the semiclassical theory, we show that the level curvature is a quantum analog of classical diffusion coefficient. Then, it turns that the Thouless formula uses this analogy for measuring the transport property. To show this analogy, first we shall look at the result for the classical diffusion coefficient in hard chaotic systems with periodic lattice symmetry. Next, we start the derivation of the semiclassical expression for the Thouless formula for both the autonomous Hamiltonian system and the kicked Hamiltonian system.

A. Classical transport phenomena

Recently, in the framework of classical mechanics, the connection between transport coefficient and dynamical chaos was discovered in the escape rate formalism [12,13], the cycle expansion [14,15], and the Gaussian thermostat model [16]. In particular, the cycle expansion will be used for the semiclassical evaluation of level curvature in the next subsection. It is based on the information of periodic orbits of the system with discrete geometrical symmetry (periodic lattice symmetry). Here we briefly show the derivation for later use. Readers should to consult Refs. [14,15].

To evaluate the diffusion coefficient, here we define the generating function $Q(\boldsymbol{\beta})$ formally:

$$Q(\boldsymbol{\beta})\equiv\lim_{t\to\infty}\frac{1}{t}\ln\langle e^{\boldsymbol{\beta}\cdot(\hat{\mathbf{x}}_t-\mathbf{x})}\rangle, \tag{12}$$

where $\langle\;\rangle$ denotes the ensemble average with respect to the initial points $\mathbf{x}$ in certain initial cell, $\hat{\mathbf{x}}_t\equiv\phi_t(\mathbf{x})$, and ϕ_t is the time-evolution operator. Here the caret represents the position in the whole space. We denote the positions in the initial cell by $\mathbf{x},\mathbf{y},\ldots$ without the caret. The diffusion coefficient D is written as

$$D=\frac{1}{2d}\sum_{j=1}^{d}\frac{\partial^2}{\partial\beta_j^2}Q(\boldsymbol{\beta})\bigg|_{\boldsymbol{\beta}=0}=\lim_{t\to\infty}\frac{1}{2dt}\langle(\hat{\mathbf{x}}_t-\mathbf{x})^2\rangle. \tag{13}$$

To express the diffusion coefficient in terms of the dynamical characteristic quantities, here we define the weighted Perron-Frobenius operator:

$$\mathcal{L}^t(\hat{\mathbf{y}},\mathbf{x})=e^{\boldsymbol{\beta}\cdot(\hat{\mathbf{y}}-\mathbf{x})}\delta[\hat{\mathbf{y}}-\phi_t(\mathbf{x})]. \tag{14}$$

The associated Fredholm determinant for this operator is

$$Z(\boldsymbol{\beta},s)\equiv\det(\mathbf{1}-z\mathcal{L}), \tag{15}$$

where $z=e^s$. By using the usual technique (see [23]) and reducing the symmetry, we rewrite $Z(\boldsymbol{\beta},s)$ in terms of the information of periodic orbits. Now the periodic orbits are described in the fundamental cell with the winding numbers which determine how many cells they pass through. The resulting expression is

$$Z(\boldsymbol{\beta},s)=\prod_p\exp\left[-\sum_{r=1}^{\infty}\frac{1}{r}\frac{e^{(\boldsymbol{\beta}\cdot\mathbf{w}_p-s\tau_p)r}}{|\det(\mathbf{M}_p^r-\mathbf{1})|}\right], \tag{16}$$

where p represents the prime periodic orbits, $\mathbf{w}_p$ is the winding vector of p (see Fig. 1), τ_p is the period of p, r is the repetition of p, and $\mathbf{M}_p$ is the monodromy matrix for p.

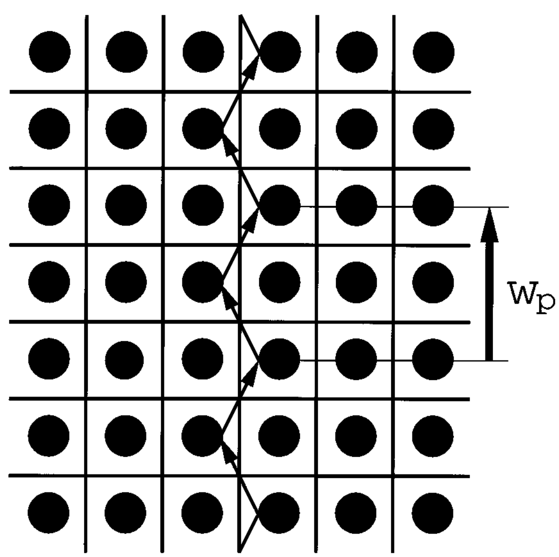

FIG. 1. The lattice symmetry and the winding vector for a ballistic periodic orbit (two-dimensional Sinai billiard).

$Z(\boldsymbol{\beta},s)$ can be further reduced to the infinite product of the associated Ruelle zeta functions. To see the leading zero of $Z(\boldsymbol{\beta},s)$ which corresponds to the equilibrium state, we only need the corresponding Ruelle zeta function among them:

$$\frac{1}{\zeta(\boldsymbol{\beta},s)}=\prod_p\left(1-\frac{e^{\boldsymbol{\beta}\cdot\mathbf{w}_p-s\tau_p}}{|\Lambda_p|}\right), \tag{17}$$

where $\Lambda_p=\Pi_e\lambda_{p,e}$, the product of the expanding eigenvalues. Here we must note that the generating function $Q(\boldsymbol{\beta})$ is a solution of $Z(\boldsymbol{\beta};Q(\boldsymbol{\beta}))=0$ [or $1/\zeta(\boldsymbol{\beta},Q(\boldsymbol{\beta}))=0$]. This is easily confirmed by the large deviation property [15,24,25]. Finally we expand the Euler product and differentiate it with respect to β_i two times. Then we get

$$\frac{\partial^2}{\partial\beta_i^2}Q(\boldsymbol{\beta})=\frac{\sum_k\left(\mathbf{w}_{p_1+p_2+\cdots+p_k,i}-\frac{\partial Q}{\partial\beta_i}\tau_{p_1+p_2+\cdots+p_k}\right)^2 t_{p_1+p_2+\cdots+p_k}}{\sum_k\tau_{p_1+p_2+\cdots+p_k}t_{p_1+p_2+\cdots+p_k}}. \tag{18}$$

Here the sum over k is taken over all combinations of the prime periodic orbits. If the system possesses the symmetry so that

$$\frac{\partial}{\partial\beta_i}Q(\boldsymbol{\beta})\bigg|_{\boldsymbol{\beta}=\mathbf{0}}=0, \tag{19}$$

then the diffusion coefficient is given as

$$D=\frac{1}{2d}\times\frac{\sum_k(-1)^k(\mathbf{w}_{p_1}+\mathbf{w}_{p_2}+\cdots+\mathbf{w}_{p_k})^2/|\Lambda_{p_1}\Lambda_{p_2}\cdots\Lambda_{p_k}|}{\sum_k(-1)^k(\tau_{p_1}+\tau_{p_2}+\cdots+\tau_{p_k})/|\Lambda_{p_1}\Lambda_{p_2}\cdots\Lambda_{p_k}|}. \tag{20}$$

B. Level curvature in terms of periodic orbits: Autonomous Hamiltonian systems

Let us start the derivation of the semiclassical expression for the Thouless formula. First, we have to rewrite the usual Gutzwiller trace formula into that for the periodic lattice system with the Bloch parameter. Next, we shall use the associated Gutzwiller-Voros zeta function (the associated Selberg-type zeta function). In that time, the formalism for the classical diffusion coefficient in the preceding subsection will be helpful for us.

1. Gutzwiller trace formula for the system with the periodic boundary condition (autonomous system)

Let us consider the d-dimensional systems with the periodic potential: $V(\mathbf{q}+n_i\mathbf{a}_i)=V(\mathbf{q})$, where $\mathbf{a}_i$ $(i=1,2,\ldots,d)$ is the primitive lattice vector along the ith direction and $n_i\in\mathbf{Z}$. In general, the associated quantum system has the Bloch parameter $\boldsymbol{\phi}\equiv(\phi_1,\phi_2,\ldots,\phi_d)$, namely, $\psi(\mathbf{q}+\mathbf{a}_i)=e^{i\phi_i}\psi(\mathbf{q})$. The eigenenergies for the system depend on the Bloch parameter $\boldsymbol{\phi}$. If the fundamental cell is the d-dimensional hypercubic, the corresponding Hamiltonian is given as

$$\hat{H}(\hat{\mathbf{p}},\hat{\mathbf{q}})=\frac{\left(\hat{\mathbf{p}}+\frac{\hbar\boldsymbol{\phi}}{L}\right)^2}{2m}+V(\hat{\mathbf{q}}), \tag{21}$$

where L is the size of the fundamental cell. This periodic condition for the potential is interpreted in the condition for the wave function: $\psi(\mathbf{q}+N\mathbf{a}_i)=\psi(\mathbf{q})$. For simplicity, we consider the simplest case, i.e., periodic cubic lattices in three-dimensional space. With this condition for the three-dimensional case, the system has the symmetry group $C_N\otimes C_N\otimes C_N$. N^3 irreducible representations of this symmetry are labeled by the reciprocal lattice vectors $\mathbf{k}$ in the first Brillouin zone. Each character is given as $\chi_{\mathbf{k}}(\mathbf{w})=e^{i\mathbf{k}\cdot\mathbf{w}}$. The Gutzwiller trace formula for the system with discrete symmetry was investigated in [26,27] and [28] for the zeta function form. The symmetry projected Gutzwiller trace formula is given as

$$g(E)=\sum_{m\in g}g_m(E), \tag{22}$$

$$g_m^{sc}(E)=\frac{d_m}{i\hbar}\sum_p\frac{T_p}{|K_p|}\sum_{r=1}^{\infty}\chi_m(g_p^r)\frac{\exp\left[ir\left(\frac{S_p}{\hbar}-\frac{\mu_p\pi}{2}\right)\right]}{|\det(\mathbf{M}_p^r-\mathbf{I})|^{1/2}}, \tag{23}$$

where m is the index for the irreducible representation, d_m is the dimension of the mth irreducible representation, $|K_p|$ is the order of the subgroup K_p of the group G, and $\chi_m(g_p)$ is the character of the symmetry operation g_p for the mth representation. For the system considered here, the irreducible representations are labeled by the vector $\mathbf{k}$ and the symmetry operation is represented by the vector $\mathbf{w}_p$ for the primitive periodic orbit p. Thus, the character $\chi_m(g_p)$ becomes $\chi_{\mathbf{k}}(\mathbf{w}_p)$. Equations (22) and (23) are rewritten as

$$g(E)=\sum_{\mathbf{k}\in g} g_{\mathbf{k}}(E), \tag{24}$$

$$g_{\mathbf{k}}^{sc}(E)=\frac{d_{\mathbf{k}}}{i\hbar}\sum_{p}\frac{T_p}{|K_p|}\sum_{r=1}^{\infty}\frac{\exp\left[ir\left(\frac{S_p}{\hbar}-\frac{\mu_p\pi}{2}+\mathbf{k}\cdot\mathbf{w}_p\right)\right]}{|\det(\mathbf{M}_p^r-\mathbf{I})|^{1/2}}. \tag{25}$$

Next we consider how the Bloch parameter modifies the above-trace formula. If we define the translation operator $U(\boldsymbol{\phi})$ as $U(\boldsymbol{\phi})\equiv e^{i\boldsymbol{\phi}\cdot\mathbf{q}/L}$, then we get $U^{\dagger}(\boldsymbol{\phi})H(\mathbf{p},\mathbf{q})U(\boldsymbol{\phi})=H(\mathbf{p}+\hbar\boldsymbol{\phi}/L,\mathbf{q})$. The propagator

$$K(\mathbf{x},\mathbf{y};t)\equiv\langle\mathbf{x}|e^{-iHt/\hbar}|\mathbf{y}\rangle \tag{26}$$

is modified as

$$K(\mathbf{x},\mathbf{y};t;\boldsymbol{\phi})=e^{-i\boldsymbol{\phi}\cdot(\mathbf{x}-\mathbf{y})/L}K(\mathbf{x},\mathbf{y};t). \tag{27}$$

Then concerning the Guztwiller trace formula, the contribution of each periodic orbit to the density of states is weighted by the factor $\exp(-i\boldsymbol{\phi}\cdot\mathbf{w}_p)$, where $\mathbf{w}_p$ is the winding vector. Therefore, the Gutzwiller trace formula for the system with the Bloch boundary condition is given as

$$g_{\mathbf{k}}^{sc}(E;\boldsymbol{\phi})=\frac{d_{\mathbf{k}}}{i\hbar}\sum_{p}\frac{T_p}{|K_p|}\times\sum_{r=1}^{\infty}\frac{\exp\left\{ir\left[\frac{S_p}{\hbar}-\frac{\mu_p\pi}{2}+(\mathbf{k}-\boldsymbol{\phi})\cdot\mathbf{w}_p\right]\right\}}{|\det(\mathbf{M}_p^r-\mathbf{I})|^{1/2}}. \tag{28}$$

2. Semiclassical evaluation of level curvature

Rewriting the Gutzwiller trace formula into the zeta function form [29,30], the corresponding Selberg-type zeta function for the irreducible representation $\mathbf{k}$ is given as

$$Z_{\mathbf{k}}(E;\phi)=C\exp[-i\pi N_0(E)]\prod_{j_1,\ldots,j_{f-1}=0}^{\infty}\prod_{p}\left(1-\frac{\exp\left\{i\left[\frac{S_p}{\hbar}-\frac{\mu_p\pi}{2}+(\mathbf{k}-\boldsymbol{\phi})\cdot\mathbf{w}_p\right]\right\}}{\prod_{k-1}^{f-1}|\lambda_p^{(k)}|^{1/2}\lambda_p^{(k)j_k}}\right)^{m_p}, \tag{29}$$

where $m_p=d_{\mathbf{k}}/|K_p|$ is the multiplicity of the prime periodic orbits, C is an appropriate constant, and $\lambda_p^{(k)}$ $(k=1,\ldots,f-1)$ is the expanding eigenvalue of the monodromy matrix. The relation to the density of states is achieved by

$$d_{\mathbf{k}}(E;\boldsymbol{\phi})=-\frac{1}{\pi}\Im\sum_{n}\frac{1}{E-E_n(\boldsymbol{\phi})}=-\frac{1}{\pi}\Im\frac{Z_{\mathbf{k}}'(E;\boldsymbol{\phi})}{Z_{\mathbf{k}}(E;\boldsymbol{\phi})}. \tag{30}$$

From here on, by using this zeta function, we obtain the Thouless formula in terms of periodic orbits. The argument developed here is completely parallel to the classical case [14,15] in the preceding section.

First we assume that the zeta function is expanded near the eigenvalue $E_n(\boldsymbol{\phi})$, namely there is no degeneracy (this condition is relevant to classically chaotic quantum system), as [31]

$$Z_{\mathbf{k}}(E;\boldsymbol{\phi})=[E-E_n(\boldsymbol{\phi})]\{c_0(\boldsymbol{\phi})+c_1(\boldsymbol{\phi})[E-E_n(\boldsymbol{\phi})]+\cdots\}, \tag{31}$$

where

$$c_0(\boldsymbol{\phi})=\left.\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial E}\right|_{E=E_n(\boldsymbol{\phi})}, \tag{32}$$

$$c_1(\boldsymbol{\phi})=\frac{1}{2!}\left.\frac{\partial^2 Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial E^2}\right|_{E=E_n(\boldsymbol{\phi})}. \tag{33}$$

Differentiating the zeta function with respect to ϕ_i and setting $E=E_n(\boldsymbol{\phi})$, we obtain

$$\frac{\partial E_n(\boldsymbol{\phi})}{\partial\phi_i}=-\frac{1}{c_0(\boldsymbol{\phi})}\left.\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i}\right|_{E=E_n(\boldsymbol{\phi})}. \tag{34}$$

In a similar way, once more differentiating the zeta function and using Eq. (34),

$$\frac{\partial^2 E_n(\boldsymbol{\phi})}{\partial\phi_i^2}=-\frac{1}{c_0(\boldsymbol{\phi})}\left[\left.\frac{\partial^2 Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i^2}\right|_{E=E_n(\boldsymbol{\phi})}-\frac{2}{c_0(\boldsymbol{\phi})}\frac{\partial c_0(\boldsymbol{\phi})}{\partial\phi_i}\left.\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i}\right|_{E=E_n(\boldsymbol{\phi})}+\frac{2c_1(\boldsymbol{\phi})}{c_0(\boldsymbol{\phi})^2}\left(\left.\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i}\right|_{E=E_n(\boldsymbol{\phi})}\right)^2\right]. \tag{35}$$

To evaluate the individual terms on the rhs of Eq. (35), we use the cycle expansion technique. In order to avoid the complicated formula which comes from $\lambda_p^{(k)}$, we consider a two-dimensional system. As in [23], we rewrite the zeta function in the Euler product as follows:

$$Z_{\mathbf{k}}(E;\boldsymbol{\phi})=C\exp[-i\pi N_0(E)]\prod_{l=0}^{\infty}\prod_p (1-t_{p,l})^{m_p}$$
$$=C\exp[-i\pi N_0(E)]\left(1-\sum_k \tilde{t}_{p_1'+p_2'+\cdots+p_k'}\right), \tag{36}$$

where

$$\tilde{t}_{p'}\equiv t_{p,l}=\frac{\exp\left\{i\left[\frac{S_p}{\hbar}-\frac{\mu_p\pi}{2}+(\mathbf{k}-\boldsymbol{\phi})\cdot\mathbf{w}_p\right]\right\}}{|\Lambda_p|^{1/2}\Lambda_p^l} \tag{37}$$

and

$$\tilde{t}_{p_1'+p_2'+\cdots+p_k'}=(-1)^{k+1}\tilde{t}_{p_1'}\tilde{t}_{p_2'}\cdots\tilde{t}_{p_k'}. \tag{38}$$

Here p' is the pair of (p,l). The system considered here is bounded by symmetry. Then the repetition of prime periodic orbits will be needed for the semiclassical calculation of eigenvalues, differing from the classical case. The derivative of the zeta function with respect to ϕ_i is given as

$$\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i}=C\exp[-i\pi N_0(E)]\frac{\partial}{\partial\phi_i}\left(1-\sum_k \tilde{t}_{p_1'+p_2'+\cdots+p_k'}\right)$$
$$=iC\exp[-i\pi N_0(E)]\sum_k$$
$$\times(w_{p_1}^i+w_{p_2}^i+\cdots+w_{p_k}^i)\tilde{t}_{p_1'+p_2'+\cdots+p_k'}, \tag{39}$$

and

$$\frac{\partial^2 Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i^2}=\frac{\partial^2}{\partial\phi_i^2}\left(1-\sum_k \tilde{t}_{p_1'+p_2'+\cdots+p_k'}\right)$$
$$=\sum_k (w_{p_1}^i+w_{p_2}^i+\cdots+w_{p_k}^i)^2\tilde{t}_{p_1'+p_2'+\cdots+p_k'}. \tag{40}$$

Here we assume that $N_0(E)$ is independent of ϕ_i. This holds for the leading order approximation in $\hbar$. $c_0(\boldsymbol{\phi})$ and $c_1(\boldsymbol{\phi})$ are evaluated as follows. The derivative of t_{p_i} with respect to E now becomes

$$\frac{\partial}{\partial E}\tilde{t}_{p_i'}=\tilde{t}_{p_i'}\left\{\frac{i}{\hbar}\frac{\partial S_{p_i}}{\partial E}-\frac{\partial}{\partial E}(|\Lambda_{p_i}|^{-(1/2)}\Lambda_{p_i}^{-l_i})\right\}. \tag{41}$$

We assume that the second term is negligible. This holds for the case in which the corresponding periodic orbit is away from the bifuncation points. Thus,

$$c_0(E;\boldsymbol{\phi})=\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial E}$$
$$=\exp[-i\pi N_0(E)]\left\{-i\pi d_0(E)\right.$$
$$\times\left(1-\sum_k \tilde{t}_{p_1'+p_2'+\cdots+p_k'}\right)$$
$$\left.+\frac{1}{i\hbar}\sum_k (T_{p_1}+T_{p_2}+\cdots+T_{p_k})\tilde{t}_{p_1'+p_2'+\cdots+p_k'}\right\}, \tag{42}$$

where we used the relation

$$\frac{\partial S_p}{\partial E}=T_p. \tag{43}$$

Now we can interpret the individual terms on the rhs of Eq. (35). First,

$$\frac{\partial E_n(\boldsymbol{\phi})}{\partial\phi_i}=-\frac{1}{c_0(\boldsymbol{\phi})}\left.\frac{\partial Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i}\right|_{E=E_n(\boldsymbol{\phi})}=\hbar\left.\frac{\sum_k (w_{p_1}^i+w_{p_2}^i+\cdots+w_{p_k}^i)\tilde{t}_{p_1'+p_2'+\cdots+p_k'}}{\sum_k (T_{p_1}+T_{p_2}+\cdots+T_{p_k})\tilde{t}_{p_1'+p_2'+\cdots+p_k'}}\right|_{E=E_n(\boldsymbol{\phi})} \tag{44}$$

can be interpreted as the *drift term*, which is the group velocity. If the system possesses some symmetry, this term may vanish. We assume that the system has such symmetry. Now if $\partial E_n/\partial\phi=0$ (this holds for $\phi=0$ usually), Eq. (35) becomes

$$\frac{\partial^2 E_n(\boldsymbol{\phi})}{\partial\phi_i^2}=-\frac{1}{c_0(\boldsymbol{\phi})}\left.\frac{\partial^2 Z_{\mathbf{k}}(E;\boldsymbol{\phi})}{\partial\phi_i^2}\right|_{E=E_n(\boldsymbol{\phi})}=-i\hbar\left.\frac{\sum_k (w_{p_1}^i+w_{p_2}^i+\cdots+w_{p_k}^i)^2\tilde{t}_{p_1'+p_2'+\cdots+p_k'}}{\sum_k (T_{p_1}+T_{p_2}+\cdots+T_{p_k})\tilde{t}_{p_1'+p_2'+\cdots+p_k'}}\right|_{E=E_n(\boldsymbol{\phi})}, \tag{45}$$

TABLE II. Comparison between the classical and semiclassical results for the autonomous Hamiltonian systems: The Gutzwiller-Voros zeta function is for two-dimensional systems.

Classical result	Semiclassical result
Weighted Frobenius-Perron kernel	Feynman kernel for the system
$\mathcal{L}^t(\hat{\mathbf{y}},\mathbf{x})=e^{\boldsymbol{\beta}\cdot(\hat{\mathbf{y}}-\mathbf{x})}\delta(\hat{\mathbf{y}}-\phi_t(\mathbf{x}))$	$K(\mathbf{x},\mathbf{y};t)=e^{-i\boldsymbol{\phi}\cdot(\mathbf{x}-\mathbf{y})/L}\langle\mathbf{x}\|e^{-i\hat{H}t/\hbar}\|\mathbf{y}\rangle$ $\simeq e^{-i\boldsymbol{\phi}\cdot(\mathbf{x}-\mathbf{y})/L}\sum_b A_b e^{iS_b/\hbar-i\pi\mu/4}$
Fredholm determinant	Spectral determinant
$\det(\mathbf{1}-z\mathcal{L})=0$	$\det(E-\hat{H})=0$
Associated Ruelle zeta function	Gutzwiller-Voros zeta function
$\frac{1}{\zeta(\beta;s)}=\prod_p(1-t_p)$	$\frac{1}{\zeta_{\mathbf{k}}(E;\phi)}=\exp(-\pi N_0(E))\Pi_l\Pi_p(1-t_{p,l})$
$t_p=\frac{e^{\boldsymbol{\beta}\cdot\mathbf{w}_p-s\tau_p}}{\|\Lambda_p\|}$	$t_{p,l}=\exp\left[i\left(\frac{S_p}{\hbar}-\frac{\mu_p\pi}{2}+(\mathbf{k}-\boldsymbol{\phi})\cdot\mathbf{w}_p\right)\right]\times\|\Lambda_p\|^{-1/2}\Lambda_p^{-l}$
Generating function	Eigenenergy
$Q(\boldsymbol{\beta})=\lim_{t\to\infty}\frac{1}{t}\ln\langle e^{\boldsymbol{\beta}\cdot(\hat{\mathbf{x}}_t-\mathbf{x})}\rangle$	$E_n^{\mathbf{k}}(\phi)$
Condition: $1/\zeta(\boldsymbol{\beta},Q(\boldsymbol{\beta}))=0$	Condition: $1/\zeta_{\mathbf{k}}(E_n^{\mathbf{k}},\phi)=0$
Diffusion coefficient	Level curvature (inverse of effective mass)
$D=\frac{1}{2d}\sum_{j=1}^{d}\frac{\partial^2}{\partial\beta_j^2}Q(\boldsymbol{\beta})\Big\|_{\boldsymbol{\beta}=\mathbf{0}}$	$\frac{\partial^2E_n^{\mathbf{k}}}{\partial\phi^2}\left(=\frac{1}{m_*}\right)$

where we used in Eq. (42)

$$1-\sum_k \tilde{t}_{p_1'+p_2'+\cdots+p_k'}=0, \tag{46}$$

that is, the condition that $E_n(\boldsymbol{\phi})$ is a zero of the zeta function. Here it turns out that Eq. (45) is the semiclassical analog of the classical diffusion coefficient.

In order to compare it with the exact quantum result, we can use the result of level dynamics for the autonomous Hamiltonian system [32,33,22,34]. The Hamiltonian is now

$$\hat{H}(\boldsymbol{\phi})=\hat{H}_0+\frac{\hbar\boldsymbol{\phi}\cdot\hat{\mathbf{p}}}{mL}+\frac{\hbar^2\boldsymbol{\phi}^2}{2mL^2}. \tag{47}$$

Here we put

$$\hat{\mathbf{V}}=\frac{\hbar\hat{\mathbf{p}}}{mL}. \tag{48}$$

Then after some calculation, we obtain the following set of equations [32,33,22,34]:

$$\partial_{\phi_i}E_n(\boldsymbol{\phi})=V_{i,nn}=\langle n|\hat{V}_i|n\rangle, \tag{49}$$

$$\partial^2_{\phi_i}E_n(\boldsymbol{\phi})=2\sum_{m\neq n}\frac{|V_{i,nm}|^2}{E_n-E_m}, \tag{50}$$

$$\partial_{\phi_i}\partial_{\phi_j}E_n=2\sum_{m\neq n}\Re\frac{V_{i,nm}V_{j,mn}}{E_n-E_m}, \tag{51}$$

$$\partial_{\phi_i}|n\rangle=\sum_{m\neq n}|m\rangle\frac{V_{i,mn}}{E_n-E_m}, \tag{52}$$

$$\partial_{\phi_i}\langle n|=\sum_{m\neq n}\langle m|\frac{V_{i,nm}}{E_n-E_m}, \tag{53}$$

where $V_{i,nm}\equiv\langle n|V_i|m\rangle$. Equations (50) and (51) give the exact level curvatures. Here we subtract the term $\hbar^2\phi^2/2mL^2$ from the original eigenvalue:

$$E_n=E_n|_{org}-\frac{\hbar^2|\boldsymbol{\phi}|^2}{2mL^2}. \tag{54}$$

Finally, we summarize the relation between the classical case in Sec. III A and the semiclassical case in this section in Table II.

C. Semiclassical level curvature for kicked systems

In this section, we derive the semiclassical level curvature in terms of periodic orbits for the kicked systems.

1. The exact quantum result: Level dynamics

The one-dimensional kicked system has the following Hamiltonian:

$$\hat{H}=f(\hat{p})+g(\hat{q})\sum_{n=-\infty}^{+\infty}\delta(t-n). \tag{55}$$

The periodic boundary condition can be applied to both the p axis and q axis. If it is applied to both axes, setting period 1, then, due to the compactness of the phase space, the uncertainty principle is given by

$$\frac{1}{2\pi\hbar}=N, \tag{56}$$

where N is the number of lattice points. Throughout the present paper, we consider the case that the phase space is torus. The time evolution operator $\hat{U}$ is given as

$$\hat{U}=\exp\left(-\frac{i}{\hbar}f(\hat{p})\right)\exp\left(-\frac{i}{\hbar}g(\hat{q})\right). \tag{57}$$

Here according to the periodic boundary conditions, $f(\hat{p})$ and $g(\hat{q})$ should be

$$f(\hat{p}+1)=f(\hat{p}),$$

$$g(\hat{q}+1)=g(\hat{q}).$$

In a similar way to the Bloch boundary condition in solid states physics, we can introduce the following transformation:

$$\hat{q}\to\hat{q}+\hbar\beta, \tag{58}$$

$$\hat{p}\to\hat{p}+\hbar\alpha. \tag{59}$$

This transformation corresponds to the boundary condition for the wave functions,

$$\psi(q+1)=\exp(i\alpha)\psi(q), \tag{60}$$

$$\overline{\psi}(p-1)=\exp(i\beta)\overline{\psi(p)}. \tag{61}$$

For simplicity, we introduce the set $\boldsymbol{\theta}\equiv(\alpha,\beta)$ of the variables α and β. Then the time evolution operator $\hat{U}(\boldsymbol{\theta})$ becomes

$$\hat{U}(\boldsymbol{\theta})=\exp\left(-\frac{i}{\hbar}f(\hat{p}+\hbar\alpha)\right)\exp\left(-\frac{i}{\hbar}g(\hat{q}+\hbar\beta)\right). \tag{62}$$

It is related to $\hat{U}$ by the operator $\hat{R}=\exp[-i\beta\hat{p}]\exp[i\alpha\hat{q}]$ as

$$\hat{U}(\boldsymbol{\theta})=\hat{R}^{\dagger}\hat{U}\hat{R}. \tag{63}$$

The eigenvalue problem for our case is

$$\hat{U}(\boldsymbol{\theta})|n\rangle=e^{i\omega_n(\boldsymbol{\theta})}|n\rangle. \tag{64}$$

After the some calculation, the derivatives of $\omega_n(\boldsymbol{\theta})$ are given as

$$\frac{\partial\omega_n}{\partial\alpha}=-\frac{1}{\hbar}\left\langle n\left|\frac{\partial}{\partial\alpha}[f(\hat{p}+\hbar\alpha)]\right|n\right\rangle, \tag{65}$$

$$\frac{\partial\omega_n}{\partial\beta}=-\frac{1}{\hbar}\left\langle n\left|\frac{\partial}{\partial\beta}[g(\hat{q}+\hbar\beta)]\right|n\right\rangle, \tag{66}$$

$$\frac{\partial^2\omega_n}{\partial\alpha^2}=\frac{1}{\hbar^2}\sum_{m\neq n}\left|\left\langle n\left|\frac{\partial}{\partial\alpha}[f(\hat{q}+\hbar\alpha)]\right|m\right\rangle\right|^2\cot[(\omega_n-\omega_m)/2] -\frac{1}{\hbar}\left\langle n\left|\frac{\partial^2}{\partial\alpha^2}[f(\hat{q}+\hbar\alpha)]\right|n\right\rangle, \tag{67}$$

$$\frac{\partial^2\omega_n}{\partial\beta^2}=\frac{1}{\hbar^2}\sum_{m\neq n}\left|\left\langle n\left|\frac{\partial}{\partial\beta}[g(\hat{q}+\hbar\beta)]\right|m\right\rangle\right|^2\cot[(\omega_n-\omega_m)/2] -\frac{1}{\hbar}\left\langle n\left|\frac{\partial^2}{\partial\beta^2}[g(\hat{q}+\hbar\beta)]\right|n\right\rangle, \tag{68}$$

$$\frac{\partial^2\omega_n}{\partial\alpha\partial\beta}=\frac{2}{\hbar^2}\Re\sum_{m\neq n}\left\langle n\left|\frac{\partial}{\partial\alpha}[f(\hat{p}+\hbar\alpha)]\right|m\right\rangle \times\left\langle m\left|\frac{\partial}{\partial\beta}[g(\hat{q}+\hbar\beta)]\right|n\right\rangle\frac{1}{1-\exp(i(\omega_n-\omega_m))}. \tag{69}$$

2. Semiclassical evaluation of level curvatures for kicked systems

To evaluate the curvature of the eigenangle semiclassically, we use the zeta function formalism again. As mentioned before, we consider the torus case. For this case, the formalism is greatly simplified. First, we must derive the Selberg-type zeta function for the quantum kicked system [35]. Since eigenangles are periodic with period 2π, then the density of states for eigenangles is given as

$$d(\omega;\boldsymbol{\theta})=\sum_{n=1}^{N}\sum_{l=-\infty}^{+\infty}\delta[\omega-\omega_n(\boldsymbol{\theta})-2\pi l]. \tag{70}$$

This density of states should be connected with the following spectral determinant:

$$P(z;\boldsymbol{\theta})=\det(z-\hat{U}(\boldsymbol{\theta}))=0, \tag{71}$$

where $z=e^{i\omega}$. The relation is achieved by

$$d(\omega;\boldsymbol{\theta})=-\frac{1}{\pi}\Im\frac{d}{d\omega}\ln P(e^{i(\omega+i\epsilon)}), \tag{72}$$

where $\epsilon>0$. Because of the finiteness of the time-evolution operator $\hat{U}(\boldsymbol{\theta})$, Eq. (71) is expressed in the finite series:

$$P(z;\boldsymbol{\theta})=\sum_{n=0}^{N}a_n z^n, \tag{73}$$

where the coefficients a_k for $k=1,\ldots,N$ satisfy the Newton relation [35],

$$a_{N-k}=-\frac{1}{k}\sum_{n=1}^{k}a_{N-k+n}\,\mathrm{Tr}(\hat{U}^n(\boldsymbol{\theta})). \tag{74}$$

To investigate the spectral property, it is convenient to consider the following zeta function:

$$Z(\omega;\boldsymbol{\theta})=e^{-i(\Theta+N\omega)/2}P(e^{i\omega}), \tag{75}$$

where

$$e^{i\Theta}=\exp i\left[\left(\sum_{j=1}^{N}\omega_j\right)-N\pi\right]=\det(-\hat{U}(\boldsymbol{\theta})), \tag{76}$$

and ω_j are the eigenangles. We can obtain this formula along the analog of the derivation of the Riemann-Siegel look-alike formula [30]. We note here that for real ω, this zeta function $Z(\omega)$ crosses on the real axis and a_k is related to a_{N-k} (self-inversive property):

$$a_k = a_{N-k}^* e^{i\Theta}. \tag{77}$$

The semiclassical analysis enables us to show that the trace of integer power of $\hat{U}$ is given as [36]

$$\mathrm{Tr}^{sc}(\hat{U}^n(\boldsymbol{\theta})) = i^n \sum_{p,n=n_p r} \frac{n_p}{\sqrt{|\det(M_p^r - I)|}} \exp\left[\frac{i}{\hbar} S_p + i w_{p,p}\beta - i w_{p,q}\alpha - \frac{i\pi\nu_p}{2}\right], \tag{78}$$

where the action S_p is

$$S_p = \sum_{i=0}^{n-1} \{-[f(p_i) + g(q_i)] + p_{i+1}(q_{i+1} - q_i) - w_p^{(i)} q_i + w_q^{(i-1)} p_i\} \tag{79}$$

and the total winding numbers w_q and w_p for the q and p coordinates are given as

$$w_p = \sum_{i=0}^{n-1} w_p^{(i)},$$
$$w_q = \sum_{i=0}^{n-1} w_q^{(i)}, \tag{80}$$

respectively. Since $\Theta \to 0$ as $\hbar \to 0$, then the semiclassical zeta function is given as follows [35]:

$$Z_{sc}(\omega;\boldsymbol{\theta}) = \sum_{l=0}^{[N/2]-\varepsilon_N} [A_{N-l}^* e^{i(l-N/2)\omega} + A_{N-l} e^{-i(l-N/2)\omega}] + \frac{1}{2}\varepsilon_N (A_{N/2} + A_{N/2}^*), \tag{81}$$

where $\varepsilon_N = 1$ for even N, 0 for odd N, and

$$A_k = -\frac{1}{k} \sum_{n=1}^{k} A_{N-k+n}\, \mathrm{Tr}^{sc}(\hat{U}^n(\boldsymbol{\theta})). \tag{82}$$

In a similar way as in Sec. III B 2, we obtain the semiclassical expression for the curvature of the eigenangle given as

$$\frac{\partial^2 \omega_n}{\partial \alpha^2} = -\frac{\partial^2 Z_{sc}(\omega;\boldsymbol{\theta})}{\partial \alpha^2}\bigg|_{\omega=\omega_n(\alpha)} \left(\frac{\partial Z_{sc}(\omega;\boldsymbol{\theta})}{\partial \omega}\bigg|_{\omega=\omega_n(\alpha)}\right)^{-1}. \tag{83}$$

Here we note that both denominator and divisor of Eq. (83) include the analytical bootstrap effect, although we do not write them explicitly.

IV. COMPARISON WITH KUBO FORMULA

In order to unify the theoretical understanding of the quantum transport process, the Thouless formula should be compared with the other formula on the conductivity, especially the Kubo formula:

$$\sigma_{\mu\nu} = \frac{n_e g_s}{\Omega} \int dE \left(-\frac{df}{dE}\right) \sigma_{\mu\nu}(E), \tag{84}$$

where

$$\sigma_{\mu\nu}(E) = \pi e^2 \hbar\, \mathrm{Tr}[\hat{v}_\mu \delta(E - \hat{H}) \hat{v}_\nu \delta(E - \hat{H})], \tag{85}$$

and $f(E)$ is an appropriate averaging function such as the Fermi-Dirac or Bose-Einstein distribution and Ω is the volume of the system. The Thouless formula represents the average conductance. Then, we need the averaging process for the Kubo formula. Using the appropriate averaging, Akkermans [37] found the relation between the Kubo conductivity and Thouless conductance within the framework of the random matrix theory. First remember the process of the derivation of both formulas. We know that if we start from the time-independent Hamiltonian (see the Appendix), the conductivity σ is proportional to the level curvature (i.e., equilibrium property). On the other hand, starting from the time-dependent approach (the adiabatic switching of the perturbation), the Kubo formula is obtained from the use of the von Neumann–Liouville equation (i.e., nonequilibrium property). The situation for the derivation of both formulas is summarized in Table I. The question here is as follows: Is the Thouless formula the same as the Kubo formula, or what is the common part in both formulas? Furthermore, we also question whether the underlying classical chaos positively plays an essential role for the relation between both Kubo and Thouless formulas or not. To answer these questions, the relation derived by Akkermans [37] is interesting, and is given as

$$\overline{\left\langle \left(\frac{\partial E}{\partial \phi}\right)^2 \right\rangle} = \pi^2 a \Delta \left\langle \frac{\partial^2 E}{\partial \phi^2}\bigg|_{\phi=0}^2 \right\rangle^{1/2}, \tag{86}$$

where the overbar represents the average over ϕ, Δ is the mean level spacing, the brackets represent the energy level average, and $a = 1/(\pi\sqrt{6})$. The lhs and rhs represent the Kubo formula (the current-current autocorrelation function) and the Thouless formula, respectively. However, the Kubo formula on the lhs is different from the usual Kubo formula. Here the current-current correlation function is time-averaged over the linearly time-dependent flux ϕ. On the other hand, the Kubo formula is evaluated at the $\phi = 0$ (see the derivation of the Kubo formula [20,38]). The assumption used here is essentially that the Hamiltonian belongs to GOE for $\phi = 0$ and GUE for $\phi \neq 0$.

Equation (86) suggests that there is some relation between the classical results. First, from another route (see [11]), using the diagonal approximation and assuming the Gaussian distribution of winding numbers, the rhs of Eq. (86) can be shown to be

$$\overline{\left\langle \left(\frac{\partial E}{\partial \phi}\right)^2 \right\rangle} = \left(\frac{w^*}{\hbar T^*}\right)^2, \tag{87}$$

where $w^* = \sqrt{2\pi\hbar d_0 \xi / T_0}$, T_0 is the shortest period of periodic orbits, and $\xi T/T_0$ is the variance of the winding number for the periodic orbits around period T. If we put $T^* = 2\pi\hbar d_0$, the rhs of Eq. (87) is the variance of the winding number with period T^*. On the other hand, from the expression of the level curvature Eq. (45), the rhs of Eq. (86) can be considered as the fourth cumulant of winding numbers. Therefore, Eq. (86) implies that the flatness factor of the winding numbers is constant. This may be related to the distribution of the winding numbers (e.g., Gaussian distribution), although we do not show this explicitly within our theory because of the complicated formula for the level velocity and curvature. However, it is clear that the validity of Akkermans's relation depends on the validity of the diagonal approximation [11] for the energy average in both sides of Eq. (86), that is, how the decoherence in the off-diagonal terms is realized. The decoherence is assured for the quantized chaotic systems, since the actions of the periodic orbits around a certain value of action are distributed randomly (for instance [39], for a dispersing billiard system). Note that Akkermans's relation is also valid for diffusive mesoscopic systems [37]. In short, it seems that the Gaussian distribution of the winding number and the decoherence is responsible for the validity of Akkermans's relation. Conversely, in general cases, the underlying classical dynamics affects the validity of Eq. (86). This will be shown in the next section.

V. NUMERICAL TEST

In Sec. III, we have derived the semiclassical expression for the level curvature formally. Naturally, the following questions arise: (i) How can the expression obtained here work? Do we need the higher order corrections? (ii) Where do we find the localization property? In order to answer these questions, we have to test the expression obtained on an appropriate model. We choose the quantized kicked rotator system as a model system. The next aim of this section is to check Akkermans's relation.

A. The test of semiclassical curvature

We use the kicked rotator system for the test of semiclassical curvature. The kicked rotator system is a well known and well investigated model [40–42]. The classical dynamics is defined as a simple two-dimensional map:

$$q_{n+1}=q_n+p_{n+1}, \quad \mathrm{mod}\ 2\pi,$$

$$p_{n+1}=p_n+K\sin(q_n). \tag{88}$$

Here the phase space is a cylinder. However, we can also impose the periodic boundary condition to the momentum axis. For this case, the phase space is T^2. It is known by the numerical experiment and the rough estimation [43] that the diffusion coefficient in the momentum space behaves like

$$D\sim\frac{K^2}{4} \quad \text{for large } K. \tag{89}$$

The corresponding quantum system is defined by the following Hamiltonian:

$$\hat{H}=\frac{\hat{p}^2}{2}+K\cos(\hat{q}+\hbar\alpha)\sum_{n=-\infty}^{\infty}\delta(t-n), \tag{90}$$

where α is the Bloch parameter $(-\pi\leqslant\alpha<\pi)$. The time evolution operator is defined as

$$\hat{U}=e^{-(i/\hbar)(\hat{p}^2/2)}e^{-(i/\hbar)K\cos(\hat{q}+\hbar\alpha)}. \tag{91}$$

For simplicity, we choose $\hbar$ as $\hbar=2\pi/N$, where N is a positive integer. Using the Fourier bases, the matrix elements of the time evolution operator Eq. (91) are given as

$$U_{nm}=\frac{1}{N}e^{-i\hbar(m^2/2)}\sum_{j=1}^{N}e^{i(m-n)\theta_j}e^{-iy\cos(\theta_j)}, \tag{92}$$

where

$$\hbar=\frac{2\pi}{N}, \quad y=\frac{KN}{2\pi}, \quad \theta_j=\frac{2\pi j+\alpha}{N}. \tag{93}$$

Now we evaluate the level curvature for the quantized kicked rotator system. However, the kicked rotator system is a nonhyperbolic system. The enumeration of the periodic orbit including the complex one is very hard. Then, as the first step, we consider the case $N=2$, namely an extremely deep quantum regime. The secular determinant for this case is given as

$$\begin{aligned}P(\omega;\alpha)&=\det(z-\hat{U}(\alpha))\\&=e^{2i\omega}-\mathrm{Tr}(\hat{U}(\alpha))e^{i\omega}+\det(\hat{U}(\alpha))\\&=(e^{i\omega}-e^{i\omega_+(\alpha)})(e^{i\omega}-e^{i\omega_-(\alpha)}),\end{aligned} \tag{94}$$

where $z=e^{i\omega}$. We know that the determinant $\det(\hat{U}(\alpha))$ is given as

$$\det(\hat{U}(\alpha))=-i \tag{95}$$

and the eigenangles are explicitly given as

$$\omega_\pm=\log\left(\frac{1}{2}\{(1-\eta i)\pm\sqrt{2i\eta^2+4i\gamma^2}\}\right), \tag{96}$$

where

$$\eta=\sin\left[\frac{K}{\pi}\cos\left(\frac{\alpha}{2}\right)\right], \quad \gamma=\cos\left[\frac{K}{\pi}\cos\left(\frac{\alpha}{2}\right)\right]. \tag{97}$$

The trace of $\hat{U}(\alpha)$ can be expressed as

$$\begin{aligned}\mathrm{Tr}(\hat{U}(\alpha))&=\sqrt{\frac{1}{2i}}\sum_{j=1}^{2}e^{-iz\cos(\theta_j)}\\&=\sqrt{\frac{2}{i}}\left(J_0(z)+2\sum_{m=1}^{\infty}J_{2m}(z)e^{-im\pi}\cos(m\alpha)\right).\end{aligned} \tag{98}$$

The semiclassical evaluation of the trace $\mathrm{Tr}(\hat{U})$ can be found in [44]. We omit the details here. However, we only note that each Bessel function corresponds to a contribution of one (real or complex) periodic orbit. Then, the number of all periodic orbits is infinite. Furthermore, since each contribution from a real periodic orbit is the oscillating one with respect to α, the number of real periodic orbits controls the nodal pattern of the parametric motion of eigenangles. In other words, the topological richness of the underlying classical dynamics determines the complexity of the band structure. (See Fig. 2 for $K=1,15,25$.) The exact and semiclassical band structure for $K=10.0$ are depicted in Fig. 3. In this

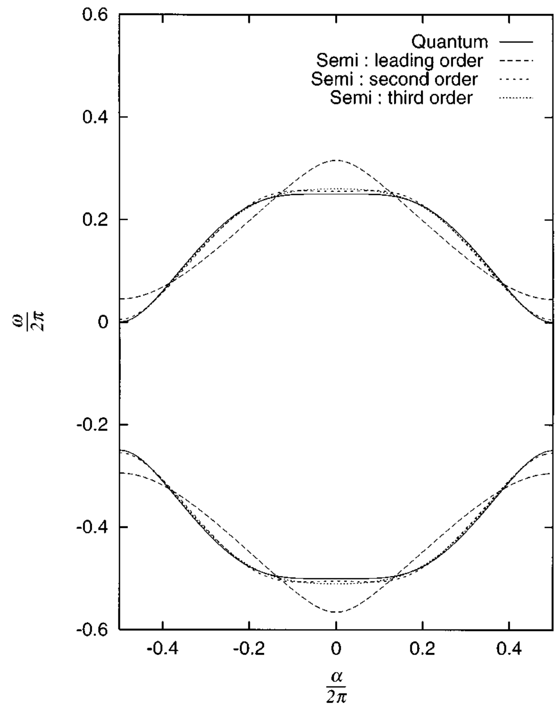

FIG. 2. Band structure for $K=1,15,25$.

calculation, we did not need a uniform approximation for real periodic orbits but we did need one for some complex periodic orbits and used the result of the asymptotic approximation of the Bessel function [45,46]. The agreement is excellent for the case of including the complex orbits. In Table III, the value of the level curvature for each order of approximationis listed. It was shown that the complex orbits play an important role for the semiclassical evaluation of the level curvature.

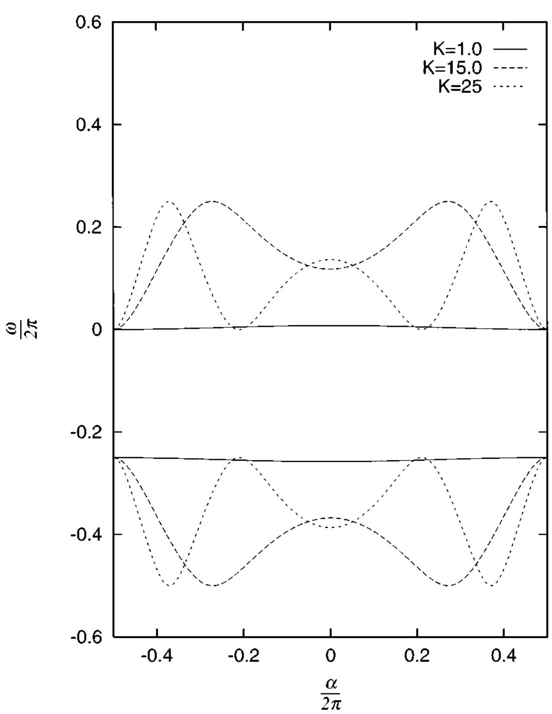

FIG. 3. Band structure: exact and semiclassical (from the leading to third orders) $K=10.0$.

TABLE III. Level curvature for $N=2$: exact and semiclassical results (from the leading to fifth orders) for $K=10.0$: Two eigenangles are symmetric to each other. Then we list one value only.

Order of Approximation	Curvature
Exact	$3.2991718206349899\times10^{-2}$
Leading	$1.6290961810539495\times10^{0}$
Second	$2.8162351851093587\times10^{-1}$
Third	$1.0965217236333496\times10^{-2}$
Fourth	$3.5433553408994005\times10^{-2}$
Fifth	$3.4298978252502783\times10^{-2}$

B. The test of Akkermans's relation

First we confirm the validity of the proportional relation between the Kubo and Thouless formula derived by Akkermans [37]. We choose the quantized kicked rotator system as a model system and consider the transport phenomena in the momentum space. In Fig. 4, the typical behavior of the level dynamics for the kicked rotator system with respect to the Bloch parameter is depicted. Comparing Fig. 4(a) with 4(b), the motion of the energies of 4(b) is much more complicated. This behavior may correspond to the topological richness (i.e., the topological entropy) of the classical dynamics. For $\mathrm{Tr}(\hat{U})$, this is easily confirmed as mentioned in Sec. III. In Fig. 5, we depict the N-dependence of the ratio A for several values of K, where

$$A=\frac{\overline{\left\langle\left(\frac{\partial\omega_n}{\partial\alpha}\right)^2\right\rangle}}{\Delta\left\langle\left|\frac{\partial^2\omega_n}{\partial\alpha^2}\right|^2_{\alpha=0}\right\rangle^{1/2}}, \tag{99}$$

and $\hbar=2\pi/N$. As we can see from Fig. 5, for large values of K in which the corresponding classical dynamics exhibits global chaos, Akkermans's relation is observed in the semiclassical regime (large $\hbar=2\pi/N$). On the other hand, for small values of K, Akkermans's relation breaks down. Its qualitative behavior can be summarized as

$$\text{(i) } A\sim \text{ constant} \quad \text{for large } K, N,$$

$$\text{(ii) } A\sim N^{-\gamma(K)} \quad \text{for small } K. \tag{100}$$

It seems that the transition of this behavior actually corresponds to the breakup of the last KAM tori. The breakup of the KAM torus occurs at $K\sim0.97$. Regime (i) can be regarded as the metallic regime. In this regime, the classical dynamics exhibits globally chaotic motion. On the other hand, regime (ii) corresponds to the localization regime. This regime is a classically integrable regime. The localization is due to the fact that the eigenwave function has the support of the tori in classical dynamics. The intermediate regime corresponds to the transition to the global diffusion. Akker-

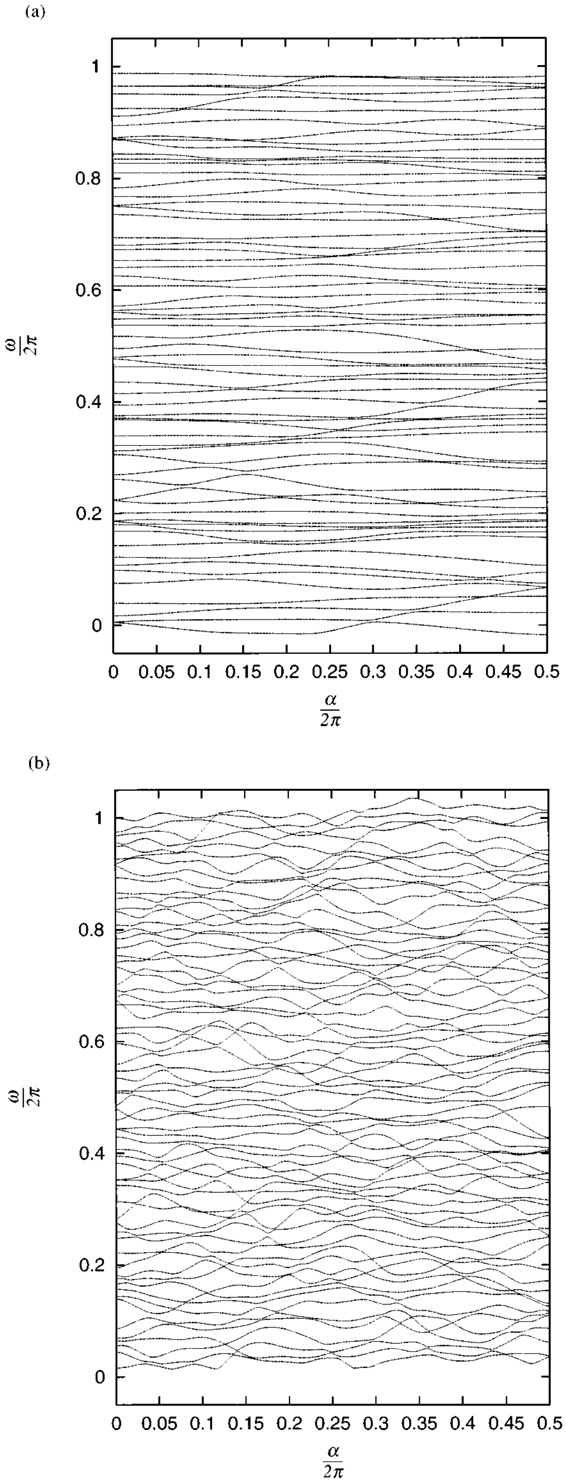

FIG. 4. Level dynamics for the kicked rotator system: The vertical and horizontal axes represent the eigenangle $\omega/2\pi$ and the Bloch parameter $\alpha/2\pi$. The parameters are chosen as (a) $K=5.0$, $N=2\pi/\hbar=64$; (b) $K=20.0$, $N=2\pi/\hbar=64$.

mans's relation Eq. (86) is valid for a globally chaotic (K large) and semiclassical ($\hbar$ small) regime. Akkermans used the Thouless conductance

$$g=\frac{1}{\Delta}\left\langle \left.\frac{\partial^2\omega_n}{\partial\alpha^2}\right|^2_{\alpha=0}\right\rangle^{1/2}. \tag{101}$$

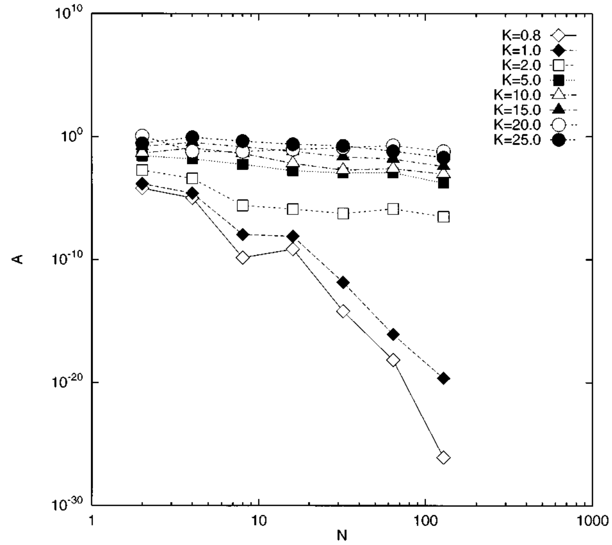

FIG. 5. Check of Akkermans's relation: The vertical axis represents the ratio A. The horizontal axis represents $N=2\pi/\hbar$ in the log scale. We plot the data for $K=0.8,1.0,2.0,5.0,10.0,15.0,20.0,25.0$.

Another definition of the Thouless conductance is

$$g'=\frac{1}{\Delta}\left\langle \left|\frac{\partial^2\omega_n}{\partial\alpha^2}\right|_{\alpha=0}\right\rangle. \tag{102}$$

We plot the following relation, which is similar to Akkermans's relation

$$A'=\frac{\overline{\left\langle\left(\frac{\partial\omega_n}{\partial\alpha}\right)^2\right\rangle}}{\Delta\left\langle\left|\frac{\partial^2\omega_n}{\partial\alpha^2}\right|_{\alpha=0}\right\rangle} \tag{103}$$

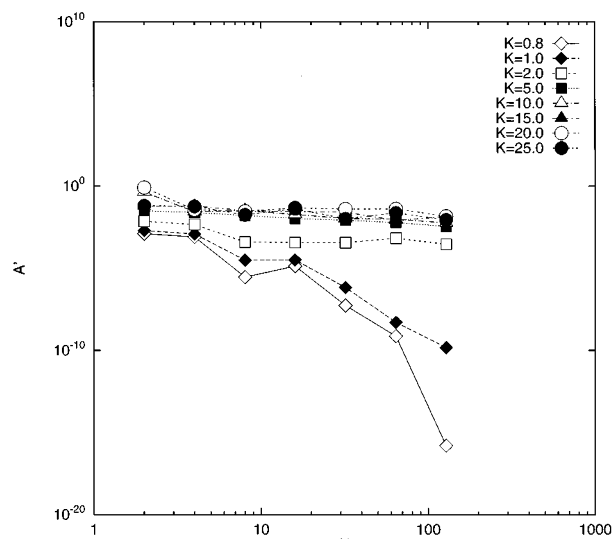

FIG. 6. Check of Akkermans's relation: The vertical axis represents the ratio A'. The horizontal axis represents $N=2\pi/\hbar$ in the log scale. We plot the data for $K=0.8,1.0,2.0,5.0,10.0,15.0,20.0,25.0$. The behavior is similar to Fig. 5.

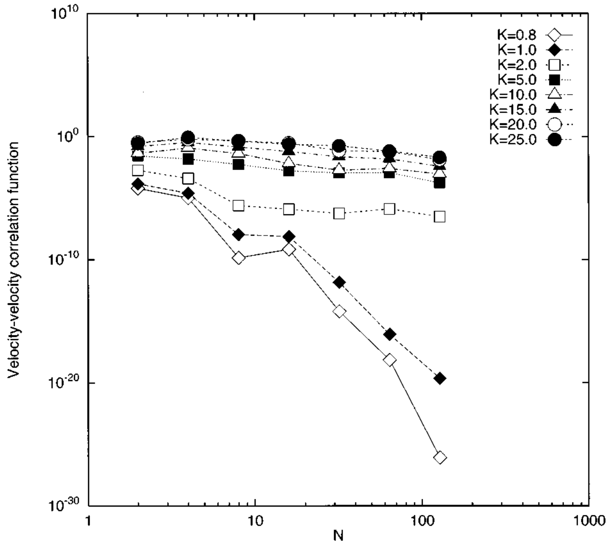

FIG. 7. Velocity-velocity correlation function vs N.

in Fig. 6. There is no drastic change compared with Fig. 5. A and A' tend to be constant. However, since the fluctuation is very large, we cannot determine the universal constant from the numerical data. Figure 7 shows the N dependence of the velocity-velocity correlation function. For large N, we see the tendency of the slow decay with respect to N. In Fig. 8, we depict the K dependence of the velocity-velocity correlation function. After the breakup of the classical tori, it behaves like

$$\overline{\left\langle \left(\frac{\partial \omega_n}{\partial \alpha} \right)^2 \right\rangle} \sim K^2. \tag{104}$$

In Fig. 9, the K dependence of the Thouless conductance g and g' are depicted, respectively. Their behavior is similar to the velocity-velocity correlation function, i.e.,

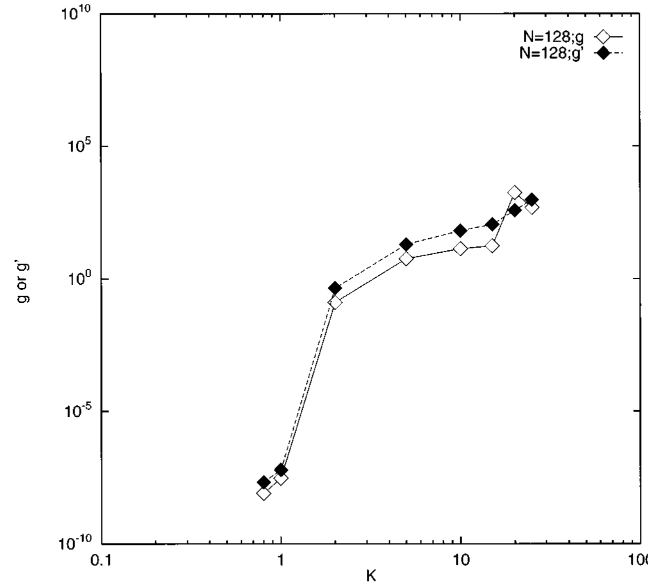

FIG. 9. g or g' vs K: the solid line (dashed line) is for g (g').

g (or g')$\sim K^2$. In Fig. 10 and Fig. 11, the N dependences of the Thouless conductance g and g' are depicted, respectively. This shows that g and $g' \sim \hbar^{-1}$. The numerical calculation here suggests that the Thouless formula essentially measures the classical diffusion coefficient.

VI. CONCLUSION

In this paper, we have derived the semiclassical expression of the level velocity (the group velocity or crystal velocity) and level curvature (the effective mass for $\phi = 0$) for systems with the periodic lattice symmetry. Using the semiclassical expression, the theoretical foundation of the Thouless conductance was reconsidered. It turned out that the Thouless conductance essentially measures the classical dif-

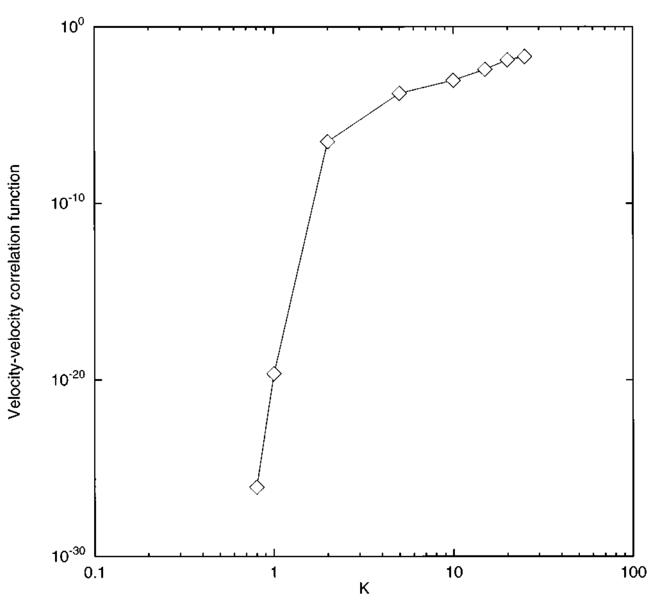

FIG. 8. Velocity-velocity correlation function vs K.

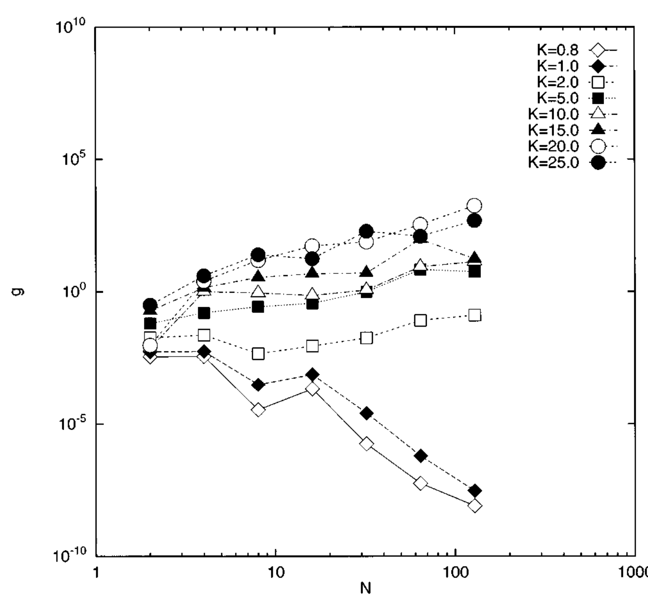

FIG. 10. g vs N.

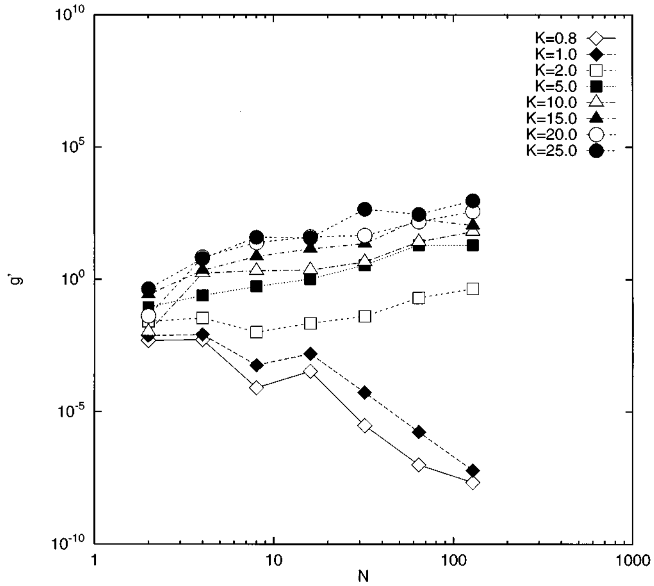

FIG. 11. g' vs N.

fusion coefficient and the underlying chaos plays a very important role as a decoherent effect. The decoherence originated in the classical counterpart allows us to wash out the quantum fluctuation by the energy averaging. The numerical calculation supports this. By this work, the intuitive approximation in solid state physics, such as the replacement of the Thouless conductance by the diffusion coefficient, is surely justified. Conversely, the author hopes that this work stimulates the study of the localization problem, which was the original motivation of Thouless. In addition, the Thouless formula can be regarded as a variant of the semiclassical sum rule [47,31]. In Sec. IV, it was roughly speculated that this may be related to the distribution of the winding numbers of periodic orbits, perhaps the Gaussian distribution [48,49]. The author hopes there will be a numerical check of this by a simple system and much more rigorous derivation of it from the Gutzwiller-Voros zeta function or Ruelle's dynamical zeta function. Beside the mean behavior of the conductance, the fluctuation of the conductance is also accessible from the method here. It may provide us with the previous result found in [50].

From the numerical test and the theoretical aspect, we found several interesting points. (i) In the numerical test of the semiclassical level curvature, we found that the inclusion of complex trajectories makes a drastic change. Furthermore, our test was limited to the contribution of fixed points. The interference of periodic orbits was not investigated here. Recently the contribution of complex trajectories to wave packet dynamics was investigated and the fine structure of the quantum interference was elucidated [51]. Concerning the transport property, the investigation for the interference of periodic orbits will be needed. More generally, the investigation of higher-order $\hbar$-correction is required not only for the oscillation part but also for the mean part in the density of states. The $\hbar$-correction sometimes becomes important. For instance, the next leading order term in the Weyl term affects the magnetization of two-dimensional noninteracting electron gas [52]. The effect of higher $\hbar$-correction (to both the mean and oscillation parts) for level curvatures is now in preparation [53]. (ii) The topological richness of the underlying classical dynamics complicates the band structure, that is, the oscillation of the parametric motion of the given ith energy is determined by the number of the periodic orbits. If the one-body description of the system is supported and spin-orbit interaction is negligible, this suggests the possibility of finding the signature of the underlying classical dynamics from the experimental data. (iii) Using Akkerman's relation, we conjecture the sum rule on the winding number of periodic orbits. From this observation, it is suggested that the universal constant in the random matrix theory might be related to the universal relation in the underlying classical chaotic dynamics. It is worth investigating the other universal constant of the random matrix theory.

Finally, before closing this paper, I must mention an excellent review on the subject of this paper from the random matrix theory [54]. I strongly recommend that readers consult this review.

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APPENDIX

Consider the following Hamiltonian describing the system in the static electric field:

$$\hat{H}=\hat{H}_0+\hat{\mathbf{J}}\cdot\mathcal{E}. \tag{A1}$$

By using the usual perturbation theory, we can show that the current operator $\hat{\mathbf{J}}(t)\equiv e\Sigma\hat{\mathbf{v}}\approx\hat{\mathbf{J}}_0+\delta\hat{\mathbf{J}}$ from the electron occupying the nth eigenenergy (Fermi energy) in the linear order of the electric field $\mathcal{E}$ is expressed as

$$\langle\hat{\mathbf{J}}\rangle=-2\mathcal{E}\sum_{m\neq n}\frac{|\langle n|\hat{\mathbf{J}}|m\rangle|^2}{E_n-E_m}\left\{1-\cos\left(\frac{(E_n-E_m)t}{\hbar}\right)\right\}, \tag{A2}$$

where we assumed that $\hat{\mathbf{J}}_0=\mathbf{0}$ and there is no degeneracy which corresponds to our case. If the level degeneracy exists, the perturbation theory should be modified. This implies that the theory is modified by whether the underlying classical mechanics is chaotic or not. The bras and kets are the eigenstates for the Hamiltonian H_0. The second term will vanish in the time average. Thus the current $\langle \hat{\mathbf{J}} \rangle$ becomes

$$\langle \hat{\mathbf{J}} \rangle = -\mathcal{E} \frac{\partial^2 E_n}{\partial \mathcal{E}^2} \bigg|_{\mathcal{E}=0}. \tag{A3}$$

Then the conductivity σ is

$$\sigma = -d(E_n) \frac{\partial^2 E_n}{\partial \mathcal{E}^2} \bigg|_{\mathcal{E}=0}, \tag{A4}$$

where we multiply the density of states at the nth eigenenergy E_n. From this, we see that the Thouless formula represents the equilibrium property of the system [55–57].

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