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Trace formula of quantum Liouville operator

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The spectral property of quantum Liouville operators ($\hat{\hat{L}}$) is investigated by introducing its trace formula. It is shown that this trace formula coincides with the two-point level correlator $R_2(-is)$ except some coefficients for quantized maps on a torus. Using semiclassical theory, for quantized chaotic systems, this enables us to write the trace formula (i.e., the spectrum of $\hat{\hat{L}}$) in terms of Pollicott-Ruelle resonances. Consequently, it is shown that the decay rates of density matrix is just semiclassically determined by the Pollicott-Ruelle resonances for the classical counterpart. [S1063-651X(99)50304-8]

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Recently, the spectral statistics for a system whose classical counterpart exhibits chaos has attracted the attention of physicists. The research area of this subject is now widely spread, i.e., mesoscopic, nuclear, and atom-molecular systems. As a first approximation, the behavior of such systems agrees well with the prediction of random matrix theory (RMT) [1]. It basically neglects details of a given system, for instance, many degrees of freedom with unknown interaction between particles. Thus one assumes randomness in the RMT, i.e., ensemble of Hamiltonian matrices.

However, a quantized chaotic system is deterministic. It is natural to question the compatibility of the behavior of such a system with the prediction of the RMT. To answer this, one of the important quantities usually investigated is the two-point level correlator $R_2(s)$, which characterizes spectral correlation of a given system. For semiclassical analysis of such systems, periodic orbits of the classical counterpart play an essential role [2]. Periodic orbits determine the semiclassical behavior of $R_2(s)$. This approach is powerful for short time behavior, however, not for long time behavior (i.e., the severe convergence problem). In fact, applicability of semiclassical theory will be limited up to a characteristic time scale, i.e., the Heisenberg time $\tau_H=2\pi\hbar\bar{d}$, which is the time scale in which the system starts to feel the discreteness of the spectrum. Here $\bar{d}$ is the mean density of states. Despite this difficulty, in [3–5] it has been shown that $R_2(s)$ is semiclassically written in terms of Pollicott-Ruelle resonances $\{\gamma_n\}_{n=0}^{\infty}$ which are the eigenvalues e^{γ_n} of $\mathcal{L}$,

$$(\mathcal{L}^t\rho)(\mathbf{x})=\int d\mathbf{y}\,\delta(\mathbf{x}-\phi^t(\mathbf{y}))\rho(\mathbf{y}), \tag{1}$$

where $\mathbf{x}=(\mathbf{q},\mathbf{p})$ is a pair of position and momentum coordinates, $\rho(\mathbf{x})$ is the phase space density, and ϕ is the classical flow. Note that the contribution from the leading resonance γ_0 to $R_2(s)$ coincides with the RMT universality and the nonuniversal character is encoded in higher resonances γ_n $(n\neq 0)$.

The achievement of [3–5] encourages us to extend their result to the spectrum of the quantum Liouville operator $\hat{\hat{L}}$ for von Neumann-Liouville equation

$$\frac{\partial\hat{\rho}}{\partial t}=\frac{1}{i\hbar}[\hat{H},\hat{\rho}]=\hat{\hat{L}}\hat{\rho}. \tag{2}$$

The real part of eigenvalues ($\{\Gamma_n\}_{n=0}^{\infty}$) of $\hat{\hat{L}}$ governs the decay rate of the density matrix. The determination of the spectrum of $\hat{\hat{L}}$ is a rather old problem [6–8]. One can expect that the spectral property of $\hat{\hat{L}}$ is also strongly influenced by the nature of underlying classical dynamics, i.e., regular or chaotic. For a system whose density matrix is decaying to the equilibrium state, chaotic nature of the underlying classical dynamics is essential there. In this Rapid Communication, we address a question about the relation between the eigenvalues of $\mathcal{L}$ and $\hat{\hat{L}}$ for a chaotic case. We will show indeed that Γ_n coincides with γ_n in the leading order of $\hbar$ for the chaotic case. Hence in some sense, we will show the classical-quantum correspondence between classical Liouville equation and quantum Liouville equation. This is done by introducing the trace formula for $\hat{\hat{L}}$ and relating this formula to $R_2(s)$ with the help of the results in [3–5]. The detailed calculation is in preparation [9].

First we introduce the definition of the trace of usual operator (indicated by a single hat) and superoperator (indicated by double hats) $\mathrm{tr}(\hat{A})=\Sigma_\alpha\langle E_\alpha|\hat{A}|E_\alpha\rangle$ and $\mathrm{Tr}(\hat{\hat{A}})=\Sigma_{\alpha,\beta}\langle E_\alpha|\{\hat{\hat{A}}|E_\alpha\rangle\langle E_\beta|\}|E_\beta\rangle$, where $|E_\alpha\rangle$ is the eigenket for $\hat{H}$. The notations ''Tr'' and ''tr'' are for superoperator and usual operator, respectively.

Let us separately consider two cases, namely, quantum maps on torus and autonomous systems.

Quantum maps on torus. In this case, the time evolution of the wave function is governed by successive multiplications of the Floquet operator $\hat{U}$ with the finite dimension N, where $N=\mathcal{A}/2\pi\hbar$ ($\mathcal{A}$: the area of torus). The eigenvalue problem is now $\hat{U}\psi_n=e^{i\omega_n}\psi_n$. The two-point level correlator $R_2(s)$ that characterizes the statistical property of spectrum is defined as

$$R_2(s)=\frac{1}{2\pi}\int_0^{2\pi}d\omega\left[d\left(\omega+\frac{s}{2}\right)-\bar{d}\right]\left[d\left(\omega-\frac{s}{2}\right)-\bar{d}\right]$$
$$=\frac{1}{2\pi^2}\mathrm{Re}\sum_{n=1}^{\infty}|\mathrm{tr}(\hat{U}^n)|^2e^{isn}, \tag{3}$$

where $d(\omega)=\Sigma_{n=1}^{N}\Sigma_{l=-\infty}^{\infty}\delta(\omega-\omega_n-2\pi l)$ is the density of states, $\overline{d}=N/2\pi$ is the mean density of states, and in the second line the Poisson sum formula was used. On the other hand, the resolvent of the quantum Liouville operator for quantized map systems is given as

$$\mathrm{Tr}\left(\frac{1}{1-e^{s-\hat{\hat{L}}}}\right)=\sum_{\alpha,\beta}\frac{1}{1-e^{s-i(\omega_\alpha-\omega_\beta)}}. \tag{4}$$

If $\mathrm{Re}(s)<0$, we can use the geometrical series. Then we obtain

$$\mathrm{Re}\,\mathrm{Tr}\left(\frac{1}{1-e^{s-\hat{\hat{L}}}}\right)=\mathrm{Re}\sum_{n=0}^{\infty}|\mathrm{tr}(\hat{U}^n)|^2e^{sn}=2\pi^2R_2(-is)+N^2. \tag{5}$$

This is the first main result of this paper. Note that Eq. (5) is quantum mechanically exact. The trace of $\hat{\hat{L}}$ for quantized maps on a torus coincides with $R_2(-is)$ except for the proportionality constant and the additional factor N^2. The sum in $R_2(s)$ starts from $n=1$, while that for the trace starts from $n=0$. Note that as $N\to\infty$, $\mathrm{Tr}(\cdots)$ diverges due to the part of the mean density of states. In order to obtain approximate pole structure of Eq. (5), we need the semiclassical analysis below.

Now we employ the semiclassical analysis for $R_2(s)$ and write its semiclassical expression as $R_2^{(sc)}(s)$. Here we assume that the corresponding classical dynamics is chaotic and the actions of periodic orbits do not systematically degenerate. If this assumption is violated, the system might have systematic degeneracy of eigenenergies and does not decay in time. Carrying out the same type of analysis in [3–5] to $R_2(s)$ of non-time-reversal systems for quantized maps on torus which have chaotic classical counterpart [10], we have

$$R_2^{(sc)}(s)=-\frac{1}{4\pi^2}\frac{\partial^2}{\partial s^2}\ln\mathcal{D}(s)+\frac{\cos(2\pi\overline{d}s)}{2\pi^2\overline{d}}\mathcal{D}(s), \tag{6}$$

where

$$\mathcal{D}(s)=\exp\left[2\sum_p\sum_{n=1}^{\infty}\frac{1}{n^2}\frac{1}{|\det(M_p^n-I)|}e^{inT_ps}\right]. \tag{7}$$

M_p is the monodromy matrix of a periodic orbit labeled by p and T_p is the period of p. If the system is very unstable, we can approximate $\mathcal{D}(s)\approx|Z_{cl}(is)|^{-2}$ by neglecting the repetition of periodic orbits [3–5]. $Z_{cl}(s)$ is the Fredholm determinant for the associated Perron-Frobenius operator $\mathcal{L}$. (For its derivation and applications, see [11,12].)

$$\begin{aligned}Z_{cl}(s)&=\det(1-e^{-s}\mathcal{L})=\prod_n(s-\gamma_n),\\&=\prod_p\prod_{l=0}^{\infty}\left(1-\frac{e^{-sT_p}}{|\Lambda_p|\Lambda_p^l}\right)^{l+1},\end{aligned} \tag{8}$$

where the expression of $Z_{cl}(s)$ in the second line was derived by the periodic orbit expansion for the two-dimensional case and Λ_p is the largest eigenvalue of monodromy matrix for the primitive periodic orbit p, respectively. Note that the leading resonance is $\gamma_0=0$ corresponding to the equilibrium state and $\mathrm{Re}(\gamma_n)<0$ for $n\neq0$. In the second line, since for the quantized map system on a torus the dimension of the Hilbert space is finite, the product over periodic orbits should be truncated up to the Heisenberg time $T_p<\tau_H=N$ by the bootstrap effect. By Eq. (6), the spectrum of $\hat{\hat{L}}$ is expressed in terms of the Pollicott-Ruelle resonances,

$$\mathrm{Re}\,\mathrm{Tr}\left(\frac{1}{1-e^{s-\hat{\hat{L}}}}\right)-N^2=\sum_n\frac{1}{|s-\gamma_n|^2}+\frac{\cosh(2\pi\overline{d}s)}{\overline{d}}\prod_n\frac{A_n^2}{|s-\gamma_n|^2}, \tag{9}$$

where $A_n=1$ $(n=0)$ or γ_n $(n\neq0)$. This is the second result. The poles on the left-hand side are determined by the Pollicott-Ruelle resonances (i.e., the eigenvalues of $\mathcal{L}$). Therefore, it can be regarded as an approximate spectral decomposition by semiclassical theory. Formally, the eigenvalues Γ_n of $\hat{\hat{L}}$ can be expanded in terms of $\hbar$ and the repetition of periodic orbits,

$$\Gamma_n=\sum_{k=0}^{\infty}\sum_{r=0}^{\infty}\hbar^k\Gamma_n^{(r,k)}. \tag{10}$$

Therefore, the result implies $\Gamma_n\approx\Gamma_n^{(0,0)}=\gamma_n$. Originally, the Bohr frequency $i(\omega_i-\omega_j)$ is purely imaginary. Readers might see a contradiction, since the result obtained (i.e., Pollicott-Ruelle resonances) involves the real part. However, the obtained result only expresses diffusive behavior up to the Heisenberg time τ_H. Thus, we emphasize here that the validity of this result is limited in the range $0<t<\tau_H$. Beyond τ_H, the off-diagonal part might become significant. Its role is, however, still unexplored.

Autonomous systems. Compared with the case of a quantized map system on a torus, two difficulties arise. One is a problem due to the dimension of the associated Hilbert space. The other is nonlinearity of the action with respect to energy. We will see these problems below. For discrete spectra, the density of states is given as

$$d(E)=\sum_n\delta(E-E_n)=-\frac{1}{\pi}\mathrm{Im}\,\mathrm{tr}\frac{1}{E-\hat{H}}. \tag{11}$$

The standard semiclassical theory [2] gives us the expression of $d(E)$ for f-dimensional systems whose classical dynamics exhibits chaos,

$$d(E)=\overline{d}(E)+d_{osc}(E), \tag{12}$$

where

$$\overline{d}(E)=\frac{1}{(2\pi\hbar)^f}\int\int d\mathbf{q}d\mathbf{p}\,\delta[E-H(\mathbf{q},\mathbf{p})]+\mathcal{O}(\hbar^{-(f-1)}),$$

$$d_{osc}(E)=\frac{1}{\pi\hbar}\sum_{p}\sum_{r=1}^{\infty}\frac{T_p}{|\det(\mathbf{M}_p^r-\mathbf{I})|^{1/2}}\times\cos\left[r\left(\frac{S_p(E)}{\hbar}-\frac{\pi\nu_p}{2}\right)\right]+\mathcal{O}(\hbar^0), \qquad (13)$$

where $\mathbf{M}_p$, S_p, and ν_p are the monodromy matrix, the action, and the Maslov index for the primitive periodic orbit p. The eigenvalues of $\hat{H}$ are also specified as zeros of the spectral determinant $D(E)=\det(E-\hat{H})$.

$$D(E)=C(E)\prod_n F_n(E)(E-E_n)=e^{-i\pi\bar{N}(E)}Z(E), \quad (14)$$

where in the first line functions $C(E)$ and $F_n(E)$ are introduced for the regularization, $Z(E)$ is defined in the above way, and $\bar{N}(E)$ is the mean staircase. Note that if E is real, $D(E)$ takes real value. The trace of the resolvent for $\hat{H}$ is related to the spectral determinant by

$$\mathrm{tr}\frac{1}{E-\hat{H}}=\frac{\partial}{\partial E}\ln D(E)=-i\pi\bar{d}(E)+\frac{\partial}{\partial E}\ln Z(E). \quad (15)$$

$Z(E)$ is semiclassically approximated by the Gutzwiller-Voros(GV-) zeta function $Z_{\mathrm{GV}}(E)$

$$Z(E)\simeq Z_{\mathrm{GV}}(E)=\prod_p\prod_{k=0}^{\infty}\left(1-\frac{e^{(i/\hbar)S_p(E)-(i\pi\nu_p/2)}}{|\Lambda_p|^{1/2}\Lambda_p^k}\right), \quad (16)$$

for the two-dimensional case.

The following relation for the resolvent of $\hat{\hat{L}}$ is the starting point of our analysis for autonomous systems [7,8]:

$$\frac{1}{s-\hat{\hat{L}}}=\frac{\hbar}{2\pi}\int_{\mathcal{C}}dz\frac{1}{z-\hat{H}}\frac{1}{z-i\hbar s-\hat{H}}. \quad (17)$$

The contour $\mathcal{C}$ is the semicircle contour with infinite radius in the upper half plane plus the line integral from $-\infty\pm i\epsilon$ to $+\infty\pm i\epsilon$ which is shifted in an appropriate way according to the value of s. The contribution from the semicircle contour vanishes.

Taking the trace of Eq. (17), the resolvent of $\hat{\hat{L}}$ is expressed as the integral of the product of two resolvents of $\hat{H}$,

$$\mathrm{Tr}\left(\frac{1}{s-\hat{\hat{L}}}\right)=\frac{\hbar}{2\pi}\int_{\mathcal{C}}dz\,\mathrm{tr}\left(\frac{1}{z-\hat{H}}\right)\mathrm{tr}\left(\frac{1}{z-i\hbar s-\hat{H}}\right)=\sum_{n,m=0}^{\infty}\frac{1}{s-\frac{1}{i\hbar}(E_n-E_m)}. \quad (18)$$

It is clear that in the second line the diagonal sum diverges, thus it does not belong to the trace class. This divergence corresponds to the fact that the contribution from the mean density of states has a problem of the divergence of the integral, since $N(E)\to+\infty$ as $E\to+\infty$. However, here we continue to employ formal manipulation. Substituting Eq. (15) into Eq. (18), we have

$$\mathrm{Tr}\left(\frac{1}{s-\hat{\hat{L}}}\right)=\frac{\hbar}{2\pi}\int_{\mathcal{C}}dE\frac{\partial}{\partial E}\ln D^*(E)\frac{\partial}{\partial E}\ln D(E-i\hbar s). \quad (19)$$

Here we used the fact that $D(E)$ is real for real E. To remove the contribution of the mean part, we replace $D(E)$ by $Z(E)$ and insert $Z_{GV}(E)$ into $Z(E)$ (semiclassical approximation),

$$\overline{\mathrm{Tr}}\left(\frac{1}{s-\hat{\hat{L}}}\right)=\frac{\hbar}{2\pi}\sum_{p,q}\sum_{r,k=0}\int_{\mathcal{C}}dz\frac{\partial_z t_{p,r}(z)}{1-t_{p,r}(z)}\frac{\partial_z t_{q,k}(z-i\hbar s)}{1-t_{p,k}(z-i\hbar s)}, \quad (20)$$

where $t_{p,k}(z)=e^{iS_p(z)/\hbar-i\pi\nu_p/2}/|\Lambda_p|^{1/2}\Lambda_p^k$ and we use the notation "$\overline{\mathrm{Tr}}$" after removing the mean part. We can approximate the latter action $S_p(z-i\hbar s)\simeq S_p(z)-i\hbar sT_p(z)$. The poles are determined by $1-t_{p,k}(z^*)=0$ and $1-t_{p,k}(z^*-i\hbar s)=0$ for all p. Therefore, the location of poles depends on the functional form of the action $S_p(z)$. We have to analytically continue the energy z into the complex domain and specify the location of poles by the above conditions. Among an infinite number of poles z^*, the poles in the upper half plane contribute to the integral. The determination of the analytical structure of the integrand is, in general, difficult.

However, the diagonal approximation by the same procedure of [3–5] can give us an approximate expression for the regularized trace. The result is

$$\overline{\mathrm{Tr}}^{(diag)}\left(\frac{1}{s-\hat{\hat{L}}}\right)=(+\infty)\frac{1}{2\pi\hbar}\frac{\partial^2}{\partial s^2}\ln\mathcal{D}(s). \quad (21)$$

The factor of infinity comes from the integration with respect to z. This means that the regularization is still needed besides removing the mean part of the density of states. Because of the nonlinearity in actions, the off-diagonal part cannot be expressed in a compact form. The result implies that the poles of the regularized trace are the Pollicott-Ruelle resonances in the same way for the case of quantized maps on a torus.

Here, in order to avoid the problem of the nonlinearity in actions, we consider the simplest case where the action is linear with respect to energy. One such case is the Riemann zeta function, which is a mathematical test field of quantized chaotic systems. The action is given as $S_p(E)=E\ln p$, where p is prime number. The Riemann zeta function is defined as $\zeta(z)=\Pi_p(1-1/p^z)^{-1}$, for Re(z)>1. We shall regard the nontrivial zeros $\frac{1}{2}+iz_n$ as eigenvalues of a hypothetical Hermitian operator, which is now actively investigated [13,14]. Here we formally consider the associated quantum Liouville operator $\hat{\hat{L}}_R$. For the Riemann zeta function, setting $Z(z)=\zeta(\frac{1}{2}+iz)$, Eq. (20) can be rewritten as (in this case, $\hbar=1$)

$$\overline{\mathrm{Tr}}\left(\frac{1}{s-\hat{\hat{L}}_R}\right)=\frac{1}{2\pi}\sum_{p,q}\int_{\mathcal{C}}dz\,\frac{\partial_z t_p(z)}{1-t_p(z)}\,\frac{\partial_z t_q(z-is)}{1-t_q(z-is)},\tag{22}$$

where $t_p(z)=e^{-iz\ln p}/p^{1/2}$. Notice that the analytical structure of $\zeta(x)$ is symmetric with respect to $\mathrm{Re}(x)=0$. Using the geometrical series and carrying out the integration, we get

$$\overline{\mathrm{Tr}}\left(\frac{1}{s-\hat{\hat{L}}_R}\right)=\sum_{p,q}\sum_{l,k=1}^{\infty}\frac{\ln p\ln q}{p^{l/2}q^{k/2}}e^{-sk\ln q}\delta(\ln p^l-\ln q^k).\tag{23}$$

The diagonal approximation $(p=q,l=k)$ gives us the following formula:

$$\overline{\mathrm{Tr}}^{(diag)}\left(\frac{1}{s-\hat{\hat{L}}_R}\right)=\delta(0)\frac{1}{2}\frac{\partial^2}{\partial s^2}\ln\mathcal{F}(s),\tag{24}$$

where

$$\mathcal{F}(s)=\exp\left[2\sum_p\sum_{l=1}^{\infty}\frac{1}{l^2}\left(\frac{e^{-s\ln p}}{p}\right)^l\right].\tag{25}$$

If we use the approximation $\Sigma_{n=1}(1/n^2)x^n\approx x$ for $|x|<1$, we can replace $\mathcal{F}(s)$ as $\mathcal{F}(s)\approx|\zeta(1+s)|^2$. Next consider the off-diagonal part. Since the argument of the δ function does not become zero, therefore, the off-diagonal part of this case vanishes. Compared with the result in [4], for the Riemann zeta function, although another regularization for the factor of infinity is needed, the trace formula for $\hat{\hat{L}}_R$ surely coincides with the diagonal part of $R_2(-is)$. The difference is the absence of the off-diagonal part, which for $R_2(s)$ is related to Hardy-Littlewood conjecture on the two-point correlation of primes [15]. We hope that this also holds for general autonomous systems after unfolding of spectrum and appropriate regularization.

In summary, we have investigated the trace formula for $\hat{\hat{L}}$ by employing semiclassical theory. For a quantized map on a torus, the trace formula for $\hat{\hat{L}}$ is exactly related to $R_2(s)$. As a result, by semiclassical theory for systems which exhibit chaos in $\hbar\to0$, an approximate spectral decomposition was obtained. It has been shown that in the leading order, the decay rate Γ_n of $\hat{\hat{L}}$ coincides with γ_n of $\mathcal{L}$. For general autonomous systems, we encountered two difficulties, i.e., the contribution from mean density of states and the nonlinearity in actions. However, for the case of the Riemann ζ function, thanks to the linear energy dependence of actions we could evaluate the semiclassical expression for the trace of $\hat{\hat{L}}$ for this system, although the regularization is still needed besides the contribution from the mean part of the density of states. For general autonomous systems, it is unclear whether or not this approach gives the same result. Finally, although our approach is the semiclassical treatment, the relation between the result obtained here and the work by the Brussels school (for instance, see recent review [16]) would be interesting for future investigation.

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[1] M. L. Mehta, *Random Matrices* (Academic Press, San Diego, 1991).
[2] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, New York, 1990).
[3] O. Agam, B. Altshuler, and A. V. Andreev, Phys. Rev. Lett. **75**, 4389 (1995).
[4] E. Bogomolny and J. P. Keating, Phys. Rev. Lett. **77**, 1472 (1996).
[5] M. M. Sano, J. Phys. Soc. Jpn. **67**, 2678 (1998).
[6] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience Publishers, New York, 1962).
[7] B. C. Eu, J. Chem. Phys. **63**, 298 (1975), Eq. (41).
[8] C. George, F. Mayné, and I. Prigogine, Adv. Chem. Phys. **LXI**, 223 (1985), Appendix F, Eq. (5).
[9] M. M. Sano (unpublished).
[10] In [3,4], autonomous systems are treated. But an extension to quantized maps on a torus is easy.
[11] R. Artuso, E. Aurell, and P. Cvitanović, Nonlinearity **3**, 325 (1990); **3**, 361 (1990).
[12] P. Cvitanović and B. Eckhardt, J. Phys. A **24**, L237 (1991).
[13] A. Connes, C.R. Acad. Sci. **A323**, 1231 (1996).
[14] S. Okubo, J. Phys. A **31**, 1049 (1998).
[15] G. H. Hardy and J. E. Littlewood, Acta Math. **44**, 1 (1923).
[16] *Resonances, Instability, and Irreversibility*, edited by I. Prigogine and S. A. Rice, Advances in Chemical Physics Vol. XCIX (Wiley, New York, 1997).