Scar State on Time-evolving Wavepacket

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Abstract. The scar-like enhancement is found in the accumulation of the time-evolving wavepacket in stadium billiard. It appears close to unstable periodic orbits, when the wavepackets are launched along the orbits. The enhancement is essentially due to the same mechanism of the well-known scar states in stationary eigenstates. The weighted spectral function reveals that the enhancement is the pileup of contributions from scar states on the same periodic orbit. The availability of the weighted spectrum to the semiclassical approximation is also discussed.

1. Introduction
The time-average of absolute squares of a time-evolving wavefunction in the stadium billiard is investigated, launching a Gaussian wavepacket as the initial state. It’s been an unique tool to detect dynamical properties of quantum systems. Nowadays nano-electronic devices, e.g. single electron transisters, quantum ratchets etc., are getting more and more realistic. Then dynamical behavior of an electron inside the (sub)nano-structure has been actively studied to clarify the physical properties of the structure[1, 2].

The novel feature of the nodal pattern of the stationary eigenstates in closed quantum systems was found about three decades ago[3]. It is drastically different in chaotic and integrable systems. In particular, the eigenstates of the chaotic systems often have the scars, which are the enhancement of quantum wavefunctions along classical unstable isolated periodic orbits.

Soon after the discovery, the semiclassical approximation has paved the way to understand the scars. Theories in phase space [4, 5] and in coordinate space[6] elucidated the contribution of the unstable periodic orbits in the scar states. Furthermore, in the theory of Heller[4], the propagation of a wavepacket near the unstable periodic orbit also uncovers the nature of the scar.

2. Gaussian Wavepacket
To investigate the properties of the time-evolution, the Gaussian wavepacket has been often used[7, 8, 9, 10]. Its initial form in 2D region is

$$\Psi_0(r) = \frac{1}{\sigma_0 \sqrt{\pi}} exp \left[ \frac{i}{\hbar} p_0(r-r_0) - \frac{(r-r_0)^2}{2\sigma_0^2} \right], \quad (1)$$
Figure 1. An example of the time-evolution of the Gaussian wavepacket is presented. The initial Gaussian wavepacket (Eq.1) is located at the center of the stadium. The launching angle is $30^\circ$. The angle is measured in the counterclockwise direction from the long axis of the stadium. After about 50000 steps the wavefunction almost diffuses all over the stadium.

Figure 2. The accumulation $A(r)$ of the time-evolving wavepacket in stadium billiard under the condition $|p_0|=50$, $\sigma_0=0.1$. It is launched from $(1, 0.5)$ and the launching angle $\theta$ is set by $\tan\theta = -1/2$, which is defined in the counterclockwise direction from the long axis of the stadium. The broken lines represents the corresponding unstable periodic orbit. It shows a rhombus shape.

where $r = (x, y)$ is a point inside the nano-structure and $r_0 = (x_0, y_0)$ is the initial location of the center of the wavepacket, and $p_0 = (p_{0x}, p_{0y})$ is the initial momentum of the center. The standard deviation of the Gaussian: $\sigma_0$ determines the size of the wavepacket. The time-average of the absolute square of the evolving wavepacket serves its coordinate-dependence. Therefore the scar-like phenomena, i.e. the weak localizations, are much easier to be detected.

The wavepacket has to follow the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V\right)\Psi = H\Psi. \quad (2)$$

Adopting the $2 \times 4$ stadium billiard [11] as the 2D structure, the potential is set $V = 0$ inside the billiard and $V = \infty$ outside. The length of its long horizontal axis is 4 and the diameters of the circular parts are 2. For numerical calculation, the Schrödinger equation has to be discretized in both space and time, then the Hamiltonian $H$ is realized by a large sized and yet very sparse matrix. We prepare the rectangle that circumscribes the stadium and install a lattice in it. The numbers of lattice points in the horizontal direction and the longitudinal direction are $N_x = 400$ and $N_y = 200$. Thus the lattice constant is $d = 0.01$. The time step is set $\Delta t = 10^{-4}$. Then the very short time-evolution can be well approximated as

$$\Psi(r, t + \Delta t) = \exp(-i \frac{\hbar}{\hbar} H \Delta t)\Psi(r, t) \approx \{1 - i \frac{\hbar}{\hbar} H \Delta t\}\Psi(r, t). \quad (3)$$

We also checked that absence of the higher order does not affect the result of this work. The potential in the rectangle and outside the stadium billiard is set $V = 10^{300}$, instead of infinity.
which is unrealizable in numerical computation. This is almost the largest number for a double-precision floating-point number.

If the Gaussian wavepacket(1) is launched in 2D infinite flat space, at first it travels as a bunch with the initial velocity of the center of the wavepacket \( \mathbf{v}_0 = (p/m) \). Then, observing the absolute value of the wavepacket, its shape is always the Gaussian, however, its size is getting broader as \( |\sigma(t)| = \sigma_0 \sqrt{1 + \left(\frac{\hbar}{m\sigma_0^2}\right)^2} \). If time is large enough, \( \sigma(t) \approx \frac{\hbar}{m\sigma_0} t \). In this work the wavepacket travels in the finite region, and repeated reflections on the boundary make the wavepacket eventually diffuse all around the billiard(Fig.1)(see also [12, 13]).

3. Dynamical Scar

Consequently, the time-evolving wavepacket seems to show no particular signature after diffusing all around the billiard(e.g., a snapshot of 5000th step in Fig.1). The wavefunction just billows all over and shows irregular and granular nodal patterns. On the contrary, the auto-correlation function already has revealed the long time recurrence[8]. Then we should turn to the accumulation, or the time-average of absolute square of the wavefunction:

\[
A(\mathbf{r}) = \lim_{T \to \infty} \frac{1}{T} \int_0^T |\Psi(\mathbf{r}, t)|^2 dt.
\]

Numerically it is discretized as

\[
A(\mathbf{r}_i) = \frac{1}{N_t} \sum_{j=1}^{N_t} |\Psi(\mathbf{r}_i, t_j)|^2,
\]

at each mesh point \( \mathbf{r}_i = (x_i, y_i) \), where the discretized time \( t_j = j\Delta t \) and \( \Delta t \) is a time step. The integer \( N_t \) represents the number of the time steps. For our simulations, the natural system of units \( \hbar = m = 1 \) are adopted. Fig.2 shows the numerical results of the accumulation during \( N_t = 10^6 \) steps.

In spite of no significant characteristics in the snapshots of the evolving wavepacket, the accumulation (4) shows clear enhancement along an unstable periodic orbit. It is apparently similar to the scars of stationary wavefunction[3]. In various cases with different launching conditions the same phenomena are also found(Fig.3). The enhancement appears around the periodic orbit, if the initial location of the center of the wavepacket and its velocity are on and along the orbit. We shall call them the "dynamical scars" to distinguish from the scar states in stationary eigenstates. It is the enhancement in the accumulation of time-dependent wavefunction.

4. Weighted Spectral Function

Any state in quantum systems can be expanded by its eigenfunctions as

\[
\Psi(\mathbf{r}, t) = \sum_n c_n \psi_n(\mathbf{r}, t) = \sum_n c_n \phi_n(\mathbf{r}) \exp(-i\frac{\hbar}{\tau}E_n t),
\]

where \( \psi_n(\mathbf{r}, t) = \phi_n(\mathbf{r}) \exp(-i\frac{\hbar}{\tau}E_n t) \) is the \( n \)-th eigenstate of the system with the energy \( E_n \). Then the time-average of \( |\Psi(\mathbf{r}, t)|^2 \) becomes

\[
A(\mathbf{r}) = \lim_{T \to \infty} \frac{1}{T} \int_0^T |\Psi(\mathbf{r}, t)|^2 dt
\]

\[
= \lim_{T \to \infty} \frac{1}{T} \int_0^T \left[ \sum_n |c_n|^2 |\phi_n(\mathbf{r})|^2 + \sum_{n \neq m} c_m^* c_n \phi_m^* \phi_n \exp\left\{i\frac{\hbar}{\tau}(E_m - E_n) t\right\} \right] dt
\]

\[
= \sum_n |c_n|^2 |\phi_n(\mathbf{r})|^2,
\]
The accumulations $A(r)$ of time-evolving wavepacket in stadium billiard with different launching angles are presented. In all cases the initial Gaussian wavepackets are located at the center of the stadium, with $|p_0| = 50$ and $\sigma_0 = 0.1$. The launching angles are (a) $30^\circ$ (the same as Fig.2), (b) $45^\circ$, and (c) $0^\circ$. The angles are measured in the counterclockwise direction from the long axis of the stadium. The broken lines represent the corresponding unstable periodic orbits.

Assuming $E_n \neq E_m$, if $n \neq m$. In other words, by eq.(6), if the coefficients $c_n$ have larger values for the scar eigenstates on the same periodic orbit, the "dynamical scars" of the periodic orbit in the accumulation $A(r)$ should be observed\cite{12, 13}. Obviously, also following eq.(6), it is expected to be persistent in longer time accumulation.

The accumulation has close relation to the weighted spectral function $C(E)$. The typical form of the function in chaotic systems has already been studied cautiously \cite{7, 8, 9, 10}. It may be expected as

$$C(E) \approx \sqrt{2\pi} \frac{\sigma_0}{v} \exp \left\{ -\frac{\sigma_0^2}{2v^2\hbar^2} (E - E_0)^2 \right\} \times \frac{\hbar}{\pi} \sum_{n=-\infty}^{+\infty} \frac{\lambda/2}{(E - E_n)^2 + (\lambda/2)^2}. \quad (7)$$

The Gaussian part forms the envelop function, whose shape is determined by the parameters of the initial wavepacket (1): $\sigma_0$, $v$ and $E_0 = \frac{p_0^2}{2m}$. The summation of Lorentzians corresponds to the weighted spectral function.
shaper peaks of dominant eigenstates. The energy peaks have almost the same energy spacings and \( E_n = E_p + n\Delta \) would represent the energies at the peaks. Here \( E_p \) is the highest maximum of the serial local peaks with width \( \lambda \), and \( \Delta \) is the energy spacing between local peaks. The Bohr-Sommerfeld quantization condition for the semiclassical action explains the nearly equal energy spacings [14]. The width parameter \( \lambda \) is just the Lyapnov exponent of the periodic orbit that we concern. This curve \( C(E) \) (7) is imposed on the histogram of \( |c_n|^2 \)'s in Fig.4. The setting is the same as Fig.2, in which the rombus shape of the "dynamical scar" appears clearly, and also the rombus-shaped scars can be observed in most of corresponding eigenstates at the local peaks of \( C(E) \).

The existence of the scar states in chaotic billiard systems makes relatively smaller mount of eigenstates, which represent scars along the corresponding periodic orbit, have dominant coefficients (Fig.4). Thus it turns out to be a "totalitarian" case of [9]. And simultaneously it also lets the "dynamical scars" emerge. Then the histogram must be spiky, though, it still has a clear remnant of the typical structure of \( C(E) \) (see Fig.4). Furthermore, by averaging over the energy range which is sufficiently larger than the energy spacing of levels and still much smaller than the energy that we concern, the smoothed shape of the histogram of \( |c_n|^2 \) becomes strikingly close to the weighted spectrum \( C(E) \) (Fig.5).

In Fig.4 (and also in Fig.5), the local peaks of the histogram are found to be located at almost equal energy intervals \( \Delta = 0.0337 \). It agrees well with the semiclassical estimation \( \Delta_{th} = \frac{\hbar^2}{m(2L^2)}|p_0| = 0.0351 \) for the rombus shaped periodic orbit, where \( L = 4.472 \) is its length.

**Figure 5.** The weighted spectrum of the Gaussian wavepacket \( \tilde{w}(E) \) (a red curve) and the averaged behavior of the expansion coefficients \( |c_n|^2 \) (a blue curve) are presented. Here the averaging is performed in the energy range of 20\( \epsilon \). These lines matches considerably well.

5. Discussion
The Green’s function provides the expression for the accumulation

\[
A(r) = \int \sum_n |c_n|^2 |\phi_n(r)|^2 \delta(E - E_n) dE \approx \int w(E) \sum_n |\phi_n(r)|^2 \delta(E - E_n) dE
\]

\[
= -\frac{1}{\pi} \int_{-\infty}^{\infty} w(E) \text{Im}G(r, r; E) dE,
\]

where the window function \( w(E) \) is introduced [15]. Mathematically, if the condition \( w(E) = |c_n|^2 \) at \( ^*E = E_n \) is exactly satisfied, the approximation (8) becomes an exact equation. Practically it is concluded that the window function can be approximated by the weighted spectrum: \( w(E) \approx C(E) \), assuming that \( A(r) \) is estimated in wide energy range which covers at least several serial scar states.

If we choose the window size small enough to suppose that the only one eigenstate would be in the window simultaneously. It is essentially the result of ref. [6] for the scar states. In this work the window size is much larger, because the initial wavepacket has to take the contribution of eigenstates in broader energy range. Thus we may not see the scar in the snapshot of time-dependent wavefunctions. The "dynamical scar" is the superposition of many states in the window.
Then the semiclassical expansion [6] is still available as

$$A(r) = \langle \rho_0(r, E) \rangle + \text{Im}(G_{osc}(r, r; E)),$$  \hspace{1cm} (9)

where

$$\langle G_{osc}(r, r; E) \rangle = \frac{1}{i(2\pi)^{1/2}h^{3/2}} \sum_n \int C(E) \frac{D_n(\xi)^{1/2}}{\int} \left\{ \exp \left[ \frac{i}{h}(S_n(\xi; E) + W_n(\xi) - \frac{\pi}{2} \mu_n) \right] - i\frac{\pi}{2} \right\} dE,$$  \hspace{1cm} (10)

and the notation $\langle \cdots \rangle$ stands for the average over the energy range that the window function covers, $\rho_0(r, E)$ is just the averaged density of states derived by the Thomas-Fermi approximation. The $\xi$ axis is set along the orbit, and the $\eta$ axis perpendicular to it at the point $\xi$. The classical action $S(\xi; E) = \frac{1}{2} \int_{p} p dr$ of the $n$-fold repeated orbit can be derived $S_n = nS$ from the action $S(\xi; E)$ of the primitive orbit $C$. Then its period is $T_n(r, E) = nT(r, E)$, and $T$ is the period of the primitive orbit. Its maximal number of conjugate points $\mu_n = n\mu$ on the orbit can be derived from the primitive one $\mu$. And also $D = -\left(\frac{\partial^2 S_n}{\partial \eta_n \partial \eta''_n}\right)_{\eta''=0}$ and $W(\xi) = \left(\frac{\partial^2 S}{\partial \eta \partial \eta''} + \frac{\partial^2 S}{\partial \eta' \partial \eta''} + \frac{\partial^2 S}{\partial \eta'' \partial \eta'''}\right)_{\eta''=0}$ of the $n$-fold periodic orbit $W_n(\xi)$. $D_n(\xi)$ can be derived from $D$ of the primitive $D_n(\xi) = D_{n} \lambda_1^2$; $W_n = D_n(\lambda_1^2 + \lambda_2^2 - 2)$. Note that $\lambda_1$, $\lambda_2$ are the eigenvalues of the monodromy matrix of the orbit.

Therefore, following the semi-classical approximation[6, 15], it can be expected that the enhancement that is similar to the scar also in the accumulation $A(r)$. Its argument is also close to the discussion for the scar states. The time average emphasizes the periodic orbit contribution and washes away just oscillatory part of the wavefunctions. The “dynamical scars” emerge from just the billowing texture.

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