Deterministic Weak Localization in Periodic Structures

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The weak localization is found for perfect periodic structures exhibiting deterministic classical diffusion. In particular, the velocity autocorrelation function develops a universal quantum power law decay at 4 times Ehrenfest time, following the classical stretched-exponential type decay. Such deterministic weak localization is robust against weak enough randomness (e.g., quantum impurities). In the 1D and 2D cases, we argue that at the quantum limit states localized in the Bravis cell are turned into Bloch states by quantum tunnelling.

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The remarkable phenomenon of strong localization (SL)\textsuperscript{1} nowadays has been fully appreciated in aperiodic\textsuperscript{1} and periodic\textsuperscript{2} disordered electronic systems and disordered dielectric materials\textsuperscript{2}. The weak localization (WL), as the precursor of SL\textsuperscript{1} has been confirmed by tremendous experiments in the last two decades, e.g., the negative magnetoresistance\textsuperscript{1}, the coherent backscattering of light\textsuperscript{2}, etc. All these systems are strongly scattered, i.e., $\lambda \gtrsim a$, where $\lambda$ is the wavelength involved and $a$ is the typical scale over which the potential varies substantially. Yet, in nineties unprecedented degree of control reached in experiments with mesoscopic quantum dots\textsuperscript{3} allows to investigate the semiclassical region: $\lambda \ll a$, where quantum interference is suppressed, and classical chaotic motion prevails. Among central issues is the classical-to-quantum crossover. A long time ago\textsuperscript{4} it was established that appears the so-called Ehrenfest time marking the proliferation of quantum interference. However, the quantitative crossover had not been found until recently\textsuperscript{5}, in the context of quantum corrections to the Drude conductivity of disordered ballistic systems.

It is well known\textsuperscript{1,6} that in disordered time-reversal symmetric systems, WL originates from the quantum interference between two counter-propagating trajectories, and the diffusive nature of trajectories arises from the randomness, regardless of classical or quantum potentials. In contrast, the deterministic diffusive motion may take place on a classical periodic potential, where the extended Bloch state develops at the quantum limit. Transport properties in such system remains unexplored. On the other hand, the so-called periodic Lorentz gas, as a prototype has been well understood mathematically\textsuperscript{10,11,12}, where the interaction with the potential is simplified as “mirror reflection”. Essential properties are encapsulated in a series of theorems\textsuperscript{11,11,12}. To summarize, (i) the flow is $K$ mixing\textsuperscript{11}; (ii) for piecewise Hölder continuous (PHC) functions the correlation decay [e.g., the velocity autocorrelation function (VCF)] is fast of stretched exponential type, i.e., $\sim \exp(-t^\gamma)$, $0 < \gamma < 1$\textsuperscript{11}; and (iii) the diffusive dispersion relation is identified as a Pollicott-Ruelle resonance with an exact Green-Kubo relation for the diffusion constant established\textsuperscript{12}. A finite diffusion constant is ensured by a priori, so-called finite horizon condition\textsuperscript{10}. To explore quantum manifestations of these features naturally becomes a fundamental problem.

The main finding of the present work is to show that such deterministic classical diffusion leads to WL (to distinguish from the usual WL in disordered systems, here we may term it deterministic WL). In particular, at the one-loop level, we find the frequency-dependent quantum correction to the diffusion constant to be

$$\delta D(\omega) = -\frac{D_{cl}}{\pi \hbar \nu} \Gamma(\omega) \int \frac{dk}{(2\pi)^2} \frac{1}{-i\omega + D_{cl} k^2},$$ \hspace{1cm} (1)$$

where $\nu$ is the density of states, and the renormalization factor

$$\Gamma(\omega) = \exp\left(4i\omega t_E - \frac{4\omega^2 \lambda_2^2 E}{\lambda^2}\right).$$ \hspace{1cm} (2)$$

The Ehrenfest time, say $t_E$ is

$$t_E = \lambda^{-1} \ln \sqrt{\frac{a}{\chi_f}}.$$ \hspace{1cm} (3)$$

Here $\lambda$ is the Lyapunov exponent and can be expressed in the form of Abramov formula\textsuperscript{12}. Depending on initial conditions, $t_E$ may fluctuate, characterized by $\lambda_2$ with the characteristic scale $\delta t_E = \lambda_2 t_E / \lambda^2$. Results similar to Eqs.\textsuperscript{11,11,12} were found for disordered ballistic systems earlier\textsuperscript{6}. However, we emphasize that throughout the derivation below no quantum impurities will be introduced. Therefore, the main problem surrounding the result of Ref.\textsuperscript{6}, namely the possibility of removing auxiliary quantum impurities is solved. On the other hand, for the first time we see that at the quantum limit WL leads to extended states rather than SL.

Alternatively, according to the Green-Kubo formula one may view the result above from VCF $\langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$ [with the average over the primitive cell of the phase
space energy shell (for shorthand we will call primitive cell below)]. In the semiclassical limit, \( t_E \) satisfies \( \tau_{fi} \ll t_E \ll t_L \), where the localization time scale \( t_L \sim m d \sqrt{D_3 \hbar} \) and \( \tau_{fi} \) is the classical mean free time. Ignoring \( \hbar t_E \), we find that the VCF develops a power law decay at \( t \gtrsim 4t_E \) beyond the classical stretched-exponential type decay. Particularly, in the 2D case, the power law takes the form as \(- (4\pi^2\hbar \nu)^{-1} (t - 4t_E)^{-1}\) (see Fig. 1).

![FIG. 1: The velocity autocorrelation function of the motion in a 2D periodic Lorentz gas (with finite horizon) develops a power law decay at \( t \gtrsim 4t_E \).](image)

Remarkably, the standard WL correction acquires a dispersion \( \Gamma(\omega) \), prevaling at \( \omega \sim t_E^{-1} \). In fact, similar renormalization factors exist at all the higher order loop corrections. Such phenomenon originates from the interference nature of the localization. Indeed, two classical trajectories pass through (almost) the same position at (almost) the same momentum. Subsequently they diverge and eventually take counter-propagating routes. If these positions and momenta were strictly identical, the probability would be zero. The quantum uncertainty makes it possible. It takes, however, a long time \( \sim t_E \).

Having outline the qualitative picture, we turn to details of the proof. To be specific, let us focus on the 2D case. The model consists of an electron of mass \( m \) with the energy \( E \) (namely the Fermi wavelength \( \lambda_F = \hbar / \sqrt{2mE} \)) moving in a periodic Lorentz gas. The lattice constant is \( d \), while \( a \) is referred to the disk radius. Technically, to avoid the singularity of the hard core potential, the billiard is softened to be the potential \( V(r) \) around the boundary with the typical width \( b \ll W := d - 2a \). The Hamiltonian thereby is replaced by \( \mathcal{H} := \hat{p}^2 / 2m + V(r) \).

The basic tool that we will employ is the generalization of the diagrammatical technique developed in essentially different context—the kicked rotor [13]. We will skip parallel intermediate steps, with emphasis on the main difference. Let us start from the quantum four-point “density-density” correlator, defined as:

\[
\mathcal{D}(r_+, r_-, r_+', r_-'; t, t') := \langle r_+| \exp[i\hat{H}t / \hbar]|r_+\rangle \langle r_-| \exp[i\hat{H}t' / \hbar]|r_-\rangle^*,
\]

where \( r_\pm, r'_\pm \). A crucial step is to introduce an artificial “one-step” evolution operator \( \hat{U} := \exp[i\hat{H}t / \hbar] \), and consider the density-density correlator at times of multiple \( t_* \), i.e., \( t = nt_*, t' = nt_* \). Here \( t_* \) is a time scale such that \( t_* \ll \tau_{fi} \). Passing to the frequency representation \( \langle \omega, E \rangle \), the density-density correlator is

\[
\mathcal{D}(r_+, r_-; r'_+, r'_-; \omega) = \sum_{n, n'} \langle r_+| \hat{U}_n^* | r'_+\rangle \langle r_-| \hat{U}_{n'} | r'_-\rangle^* \times e^{i\omega t\frac{(n-n')}{2}} e^{i\frac{E t^2}{2m}}.
\]

Now we consider the classical limit of the exact quantum density-density correlator. First let us sum over all the diagrams such that \( |r_+ - r_-|, |r'_+ - r'_-|, |r_{k+} - r_{k-}| \sim \lambda_F \ll W \), \( k = 1, 2, \cdots \) [see Fig. 2 (a)] and denote it as \( \mathcal{D}_0 \). To proceed further, we perform Wigner transform the quantum density-density correlator with respect to \( r_+ - r_- \), \( r'_+ - r'_- \) and pass to the \( (p, p') \) representation. As a result, we find that \( \mathcal{D}_0 \) evolves following the classical Perron-Frobenius equation according to \( \omega \) will be ignored to shorten notations.

\[
\left\{ 1 - \exp \left[ t_* \left( i\omega - \hat{L} \right) \right] \right\} \mathcal{D}_{E0}(r, p; r', p')
\]

\[
= (2\pi\hbar)^2 \delta (r - r') \delta (p - p') \delta \left( E - \frac{p^2}{2m} \right),
\]

where \( \hat{L} = \nabla_r \nabla_r V(r) \cdot \nabla_p \) is the Liouvillian. Note that in most region of the phase space the Liouvillian is free except near the boundary of the billiard, where the potential is involved. According to Eq. 5, the modified Hamiltonian induces a flow restricted on the energy shell: \( E = p^2 / 2m \). We assume that for this flow, the essential properties (i), (ii) and (iii) for the periodic Lorentz gas hold. To be specific, in the PHC functional space, the Fourier transform of the operator \( \{ 1 - \exp[t_* (i\omega - \hat{L})] \}^{-1} \) admits the diffusive poles: \( \omega = -iD_3 k^2 \) (\( k \) the wave number taken from the first Brillouin zone of the reciprocal lattice). Moreover, the classical diffusion constant, \( D_{cl} \) is given by the Green-Kubo formula, i.e.,

\[
D_{cl} = \frac{1}{4} \frac{t_*}{m^2} \sum_{j=-\infty}^{\infty} \langle p(j) \cdot p(0) \rangle
\]

with the average over the primitive cell. We point out that \( D_{cl} \) is finite due to the nature of the finite horizon, although we leave the problem of calculating Eq. 6 open. Based on this conjecture, despite of the deterministic nature of Eq. 5, one may work on distributions with the smoothness admitted by the PHC condition. Define \( \mathcal{D}_{E0}(r, p; r', p') := D_0(r, n; r', n') \delta(E - p^2 / (2m)) \delta(E -
\[ D_\nu(k; \omega) = \frac{2\pi}{\nu} \frac{1}{-it_\omega + t_\nu D_{\text{cl}}k^2} \]  

(a)

(b)

(c) \[ \hat{D}_0 \quad \hat{C} + \hat{C}_* \quad \hat{D}_0 \]

\[ = \exp[ it \omega ] \hat{U} \hat{U}^* - 1 \]

\[ : \text{retarded propagator} \]

\[ : \text{advanced propagator} \]

FIG. 2: Typical diagrams lead to the Diffuson (a) and the Cooperon (b). The difference of two coordinates connected by the dot-dashed line denotes is order of \( \lambda_F \ll W \). The one loop correction is given by (c). The retarded (advanced) propagation line is \( \exp[it_\omega] \hat{U} \) (\( \exp[-it_\omega] \hat{U}^\dagger \)). See Eq. (14) for the definition of \( \hat{C} \) and \( \hat{C}_* \).

We note that in fact, to sum over all the diagrams such that \( |\mathbf{r}_+ - \mathbf{r}_-|, |\mathbf{r}'_+ - \mathbf{r}'_-|, |\mathbf{r}_{k+} - \mathbf{r}_{(n+1-k)-}| \sim \lambda_F \ll W, k = 1, 2, \cdots, n \) [Fig. 2 (b)] yields another classical object, so-called Cooperon (denoted as \( \hat{C}_c \)). In fact, one may Wigner transform the quantum density-density correlator with respect to \( \mathbf{r}_+ - \mathbf{r}_-, \mathbf{r}'_+ - \mathbf{r}'_- \) and arrive at Eq. (15).

Having identified the classical normal diffusive modes, we come to analyze WL. For this purpose, the essential step is to show that in the semiclassics, the one-loop quantum correction is given by the diagram shown in Fig. 2 (c). In the exact quantum operator representation, it may be expressed as

\[ \delta \hat{D} = \hat{D}_{E0} (\hat{P} - 1) \left( \hat{C} + \hat{C}_* \right) (\hat{P} - 1) \hat{D}_{E0} \]  

with

\[ \hat{C} := \sum_{n=1}^{\infty} \hat{P}^{n+1} \hat{C}_{E0} \hat{P}^n, \quad \hat{C}_* := \sum_{n=1}^{\infty} \hat{P}^n \hat{C}_{E0} \hat{P}^{n-1} \]  

Here \( \hat{P} = e^{it_\omega \mathbf{U}} \mathbf{U}^\dagger \). Notice that in Eq. (15) the operator \( \hat{P} \) in \( (\hat{P} - 1) \) is chosen in the way such that it describes the free motion. As usual, we then perform the Wigner transform for \( \hat{D}_{E0}, \hat{C}, \hat{C}_* \) and \( \hat{P} \), respectively. Now we assume that the initial distribution is PHC. Furthermore, the appearance of diffusive poles allows us to make the so-called hydrodynamic expansion, \( \omega t_\nu \ll 1 \) and \( \exp[t_\nu (i\omega - \hat{C})] - 1 \approx -t_\nu \mathbf{v} \cdot \nabla \). Eventually in the PHC functional space, the one-loop quantum correction to the Diffuson is reduced into

\[ \delta \hat{D}(\mathbf{r}, \mathbf{n}; \mathbf{r}', \mathbf{n}') = \frac{t_\nu^2 E}{m} \mathbf{V} \left[ \sum_{j=-\infty}^{\infty} \mathbf{n}''(j) \mathbf{n}''(0) \right] : \nabla_{\mathbf{r}} \nabla_{\mathbf{r}_2} \hat{D}_0 \left( \mathbf{r}, \mathbf{n}; \mathbf{r}_1 + r_2, \mathbf{n}'' + \frac{\mathbf{n}_1}{2}, \mathbf{r}', \mathbf{n}' \right) \right|_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}''} \]  

where \( \mathbf{n}(0) := \mathbf{n}'' \). The vertex operator \( \mathbf{V} \) is an integral operator defined as

\[ (\mathbf{V} f)(\cdot) := \int \frac{d\mathbf{r}'' d\mathbf{n}''}{2\pi \hbar} \int \frac{d\mathbf{r}_1 d\mathbf{n}_1}{2\pi \hbar} \int \frac{d\mathbf{r}_2 d\mathbf{n}_2}{2\pi \hbar} \]  

\[ \times \mathcal{C}_0 \left( \mathbf{r}'' + \frac{\mathbf{r}_1}{2}, \mathbf{n}'' - \frac{\mathbf{n}_2}{2}, \mathbf{r}' - \frac{\mathbf{r}_1}{2}, -\mathbf{n}'' - \frac{\mathbf{n}_2}{2} \right) \mathcal{X} \]  

\[ \times f(\cdot; \mathbf{r}'', \mathbf{n}'', \mathbf{r}_2, \mathbf{n}_1) \]  

where

\[ \mathcal{X} = \exp \left[ \frac{i}{F} \left( \mathbf{r}_1 \cdot \mathbf{n}_1 + \mathbf{r}_2 \cdot \mathbf{n}_2 \right) \right] \]  

Above the dot is the shorthand of \( (\mathbf{r}, \mathbf{n}; \mathbf{r}', \mathbf{n}') \). The interference factor \( \mathcal{X} \) originates from the phase difference of two paths underlying the Cooperon, and technically results from the difference of performing Wigner transform for the Diffuson and the Cooperon. \( \mathcal{X} \) can be also obtained in the Moyal formalism [14]. In the diffusive limit, Eq. (16) leads to the standard WL in disordered systems. For ballistic systems like periodic Lorentz gases, the two legs of the Cooperon must propagate together for \( 2t_\nu \) in the Lyapunov region in order to develop the universal quantum limit of Cooperon develops, which stands for the probability of returning to the origin via the random walk. Such a crossover picture, encapsulated in the renormalization factor \( F(\omega) \) was proposed earlier [3]. Here the essential difference is that, due to the absence of quantum impurities the motion equation of Cooperon does not involve any regularizers. Consequently the Ehrenfest time is fully determined by the size of the minimal quantum wave packet, as read out from \( \mathcal{X} \), i.e., \( \delta \mathbf{r}_{1,\text{min}} \sim \lambda_F \).
and $\delta n_{\min} \sim \lambda_F/W$. Then following the procedure of Ref. [13] one ends up with Eqs. (2) and (3).

At the time $\sim t_F$, if $\mathbf{V}$ is smeared out over the primitive cell surrounding the entries (if thereby obtained is denoted as $f$). Consequently it can be shown that the interaction vertex $\mathbf{V}$ can be simplified as (denoted as $\mathbf{V}_f$) $$(\mathbf{V}_f) \rightarrow \left(\mathbf{V}_f, f\right) := \mathbf{V} \int dr'' f(r, r'; r'') ,$$
$$V = \frac{\Gamma(\omega)}{n\hbar} \int \frac{dk}{(2\pi)^2} \frac{1}{-i\omega + D_0 k^2} . \quad (13)$$

Now let us identify the Diffusons in the right hand side of Eq. (10) as deterministic diffusive modes. Technically, we may average $(r, n)$ and $(r', n')$ over the primitive cell surrounding them. With the application of Eq. (13), we thereby obtain the one-loop quantum correction as

$$\delta D(r, r') = t_n D_{cl} \mathbf{V} \int dr'' \left(\nabla^2 r_1 + \nabla^2 r_2\right)$$
$$\left[D_{\nu}(r_1) D_{\nu}(r_2, r')\right]|_{r_1=r_2=r''} , \quad (14)$$

where we take into account the isotropy of the Bravis lattice. Then we perform the Fourier transform and substitute Eq. (7), as well as the renormalized interaction vertex $\mathbf{V}$ [see Eq. (13)] into it. As a result, we find that the diffusive modes are modified as $[-it_\omega + t_n(D_{cl} + \delta D(\omega))k^2]^{-1}$ with $\delta D(\omega)$ given by Eq. (11).

An important question is how WL develops into extended states in the quantum limit. For qualitative discussions, it may be instructive to discuss the quasi-1d case. For $\lambda_F \ll W < d$, each Bravis cell has a well defined mean level spacing, say $\Delta \sim \hbar^2/md^2$, with a tunnelling energy, say $t$ between them. Increasing the size of the cell $n$ times larger then we rescales the mean level spacing as $\Delta_n \sim \Delta/n$. For $t_n$, we note that the Thouless energy of the rescaled cell is of the order of the total tunnelling energy, namely $hD_{cl}/(nd)^2 \sim t_n/\Delta_n$, yielding $t_n \sim h(D_{cl}\Delta_n)^{1/2}/nd$. Localization states develop at $\Delta_n \gtrsim t_n$, namely $n \gtrsim n_c$ with $n_c \sim mD_{cl}/h \sim W/\lambda_F$ the localization length. In contrast to the usual disordered system, these localization states (with the same energy) are exactly identical because of the periodic feature, and thus, serves as Wannier function in the electronic band theory. The tunnelling between these states turns them into the extended state. In particular, at the quantum limit, $W \sim \lambda_F$, $n_c \sim 1$, the energy band takes the form of Bloch band, i.e., $\varepsilon + t_n \cos(\hbar k/2\pi)$.

In realistic environments randomness (e.g., quantum impurities) dooms to exist. Bloch states are unstable against randomness. Indeed, in the 1D and 2D cases arbitrarily weak randomness leads to SL at the long time (or large size) limit. In contrast, the deterministic WL is robust. In fact, any randomness results in a scattering rate $\tau_q^{-1}$. As far as it is weak enough, namely $\tau_q^{-1} \ll (h\nu)^{-1}$, the Ehrenfest time is dominated by the size of the initial quantum wavepacket due to the logarithmic accuracy. This conclusion, indeed is consistent with an important conjecture made in Ref. [6]. That is, although auxiliary quantum impurities may be introduced artificially, the strength of the scattering rate $\tau_q^{-1}$ must be adjusted to be $\sim (h\nu)^{-1}$ in order to mimic quantum diffractions. Thus, an estimation for the Ehrenfest time was established [4], which is the same as Eq. (8). In the present work, this essential conjecture is proved.

To conclude, we find WL for periodic Lorentz gases with finite horizon. The result is applicable for any systems exhibiting deterministic diffusive motion, regardless whether the underlying potential is ordered or disordered. Finally since WL is responsible for coherent backscattering [4], we expect that the result here may be confirmed by experiments on coherent backscattering of light in state-of-art periodic photonic materials, where the semiclassical condition: $\lambda \ll a$ may be met.

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