A new type of quantum size effect (QSE) oscillations is predicted for films with a relatively large correlation radius of surface inhomogeneities. The effect replaces usual QSE for random inhomogeneities with Gaussian and exponential power spectra. The well-pronounced oscillations of conductivity $\sigma$ as a function of channel width $L$ separate two distinct regions with different indices in the power-law dependence $\sigma(L)$. The oscillations are explained and their positions identified. The effect is reminiscent of magnetic breakthrough and can simplify observation of QSE in metals.

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Progress in nanofabrication reignited studies of ultrathin films with quantum size effect (QSE). QSE describes quantization of motion of particle across the film, $p_x \rightarrow \pi j/L$ (below $\hbar = 1$), and leads to a split of the 3D energy spectrum $\epsilon(p)$ into a set of minibands $\epsilon_j(q)$ ($q$ is the $2D$ momentum along the film). QSE is routinely observed by various spectroscopic and STM methods (see, e.g., [1] and references therein). QSE also leads to a pronounced saw-like dependence of conductivity $\sigma$ on, for example, film thickness $L$. Though only few transport measurements exhibit QSE directly [2], it has been known for a long time that the saw-like curves $\sigma(L)$ should exist for both bulk [3] and surface [4] scattering.

"Usual" QSE singularities in $\sigma(L)$ correspond to abrupt changes in the number $S = \text{Int}(L/\lambda_F \pi)$ of the occupied minibands $\epsilon_j$ in the points when the film thickness $L$ becomes equal to $L = k\pi \lambda_F$ with integer $k$ (the Fermi wavelength $\lambda_F = 1/p_F$). The drops in $\sigma(L)$ in these points are explained by an opening of $\kappa$ new scattering channels associated with the scattering-driven transitions to and from the newly accessible highest miniband $\epsilon_\kappa$. The amplitude of these drops ("saw teeth") is determined by comparison of the interband transition probabilities $W_{j\neq j'}(q-q')$ with the intraband scattering $W_{jj'}(q-q')$. When the off-diagonal $W_{j\neq j'}$ become small, the amplitude of QSE jumps decreases reducing, eventually, the saw teeth to barely visible kinks on $\sigma(L)$.

If elastic wall scattering is the main scattering mechanism, the usual QSE oscillations can always be observed for random surface inhomogeneities with small correlation radius ("size") $R$, $R < L$. For larger $R$ the interband transitions are often suppressed making $\sigma(L)$ smooth, almost power-law curve. Below we demonstrate that there exists a new type of QSE oscillations at $R > L$ between two distinct monotonic parts of $\sigma(L)$. These new oscillations can be observed only if the Fourier image $\zeta(q)$ of the correlation function of random surface inhomogeneities $\zeta(s)$ (the so-called power spectrum) is rapidly going to zero at large $q$. This finding is illustrated in Figure 1. Curves 1 and 2, which show $\sigma(L)$ for correlators with exponential power spectra, consist of two smooth parts separated by an oscillation region. Curves 3 and 4 for the power-law spectral functions exhibit usual saw-like QSE. The explanations for the new QSE and the disappearance of the usual saw-like QSE are interrelated.

The results are based on the formalism [5] that unites earlier approaches [5] to transport in systems with random rough walls with or without bulk scattering. Elastic wall scattering leads to transitions between the states $\epsilon_j(q) \leftrightarrow \epsilon_{j'}(q')$ with the probability $W_{j\neq j'}(q,q')$ which is proportional to the power spectrum of surface inhomogeneities $\zeta(q_j - q_{j'})$ ($q_j$ is the Fermi momentum for the miniband $\epsilon_j, \epsilon_j(q_j) = \epsilon_F$). The rate of decrease of $\zeta(q_j - q_{j'})$ at large $q$ depends on the correlation length $R$ via parameters $\nu_{j\neq j'} = R|q_j - q_{j'}|$.
\[ \nu_{jj'} = \sqrt{z^2 - \pi^2 j^2} - \sqrt{z^2 - \pi^2 j'^2} \frac{R}{L} \]  

(1)

where \( z = L/\lambda_F \). The diagonal \( \nu_{jj} = 0 \). The faster \( W_{j\neq j'} \) go to zero with increasing \( \nu_{j\neq j'} \), the earlier the transport signs of the usual QSE disappear.

We compared \( \sigma (L) \) for several realistic correlation functions \[ \xi \]: the Gaussian correlator,

\[ \zeta (s) = \ell^2 \exp \left( -s^2 / 2R^2 \right) , \]  

(2)

power-law correlators with various \( \mu \),

\[ \zeta (s) = 2\mu \ell^2 \left[ R^2 / (s^2 + R^2) \right]^{1+\mu} , \]  

(3)

including the Staras correlator \( \mu = 1 \), the Lorentzian

\[ \zeta (s) = 2\ell^2 R^2 / (s^2 + R^2) , \]  

(4)

and the correlators with a power-law Fourier image,

\[ \zeta (q) = 2\pi \ell^2 \left[ R^2 / (1 + q^2 R^2) \right]^{1+\lambda} . \]  

(5)

The last group includes the Lorentzian in momentum space \( \lambda = 0 \) (see experiment \[ \xi \]) and the exponential correlator \( \zeta (s) = \ell^2 \exp \left( -s/2R \right) \) at \( \lambda = 1/2 \). All the correlators describe the surface inhomogeneities of the same average amplitude \( \ell \) and, except for \[ \xi \], lead to the same conductivity \( \sigma \) in the long-wave limit \( R/\lambda_F \to 0 \) in which \( \sigma \) should not depend on details of the inhomogeneities. The Fourier image of the Lorentzian \[ \xi \] contains the function \( K_0 (qR) \) and diverges logarithmically at \( R/\lambda_F \to 0 \). We do not want to get into the discussion to what extent this correlator is "physical". The fact that this correlator is used in some calculations \[ \xi \] is sufficient enough to consider it. To deal with the divergence, one can truncate this correlator at large distances (commonly, at about 0.1 of the system length \[ \xi \]). The divergence, by itself, does not lead to any singularities in \( \sigma \). Sometimes, the divergence of the power spectrum \( \zeta (q) \) is associated with a fractal nature of the surface \[ \xi \]; to what extent our approach can be used for films with fractal surfaces is an open question.

In all four Figures below curve 1 corresponds to the Gaussian correlator \[ \xi \], curve 2 to Eq. \[ \xi \] with \( \mu = 1/2 \), and curves 3 and 4 to Eq. \[ \xi \] with \( \lambda = 1/2 \) and 0.

The power spectrum of the Gaussian \[ \xi \] decays at large \( qR \) as \( \exp \left( -q^2 R^2 / 2 \right) \) and the off-diagonal \( W_{jj'} \) go to zero faster than the diagonal ones by the factor \( \exp \left( -\nu_{jj}^2 / 2 \right) \). The power spectra of the correlators \[ \xi \] contain \( (qR)^\mu K_\mu (qR) \) and \( W_{jj'} \) go to zero as \( \nu_{jj'}^{\mu-1/2} \exp \left( -\nu_{jj'} \right) \). The slowest, power-law decay of the power spectrum corresponds to inhomogeneities \[ \xi \].

The amplitudes of the QSE drops of \( \sigma (L) \) in the points \( z = L/\lambda_F = k\pi \) decrease with increasing \( \nu_{jj} \) with the rate that reflects the dependence \( W_{kz} (\nu_{kz}) \). Accordingly, the QSE saw disappears, with increasing \( R \), first for the surfaces with Gaussian inhomogeneities, then for the correlators \[ \xi \], \[ \xi \], and almost never for \( \xi \). This different rate of suppression of QSE is illustrated in Figure 1 at \( x = R/\lambda_F = 200 \). The 2D conductivity \( \sigma (L) \) is parameterized as

\[ \sigma (L) = \frac{2e^2}{\hbar} \frac{R^2}{L} f_L (z, x) . \]  

(6)

Since \( f_L (z, x = 200) \) for correlators \[ \xi \] with the same values of \( \ell \) and \( R \) have different orders of magnitude, functions \( f_L \), for better comparison, are normalized by their values at \( z = 110 \), \( f_L (z) / f_L (110) \). At \( x = 200 \), \( \exp \left( -\nu_{jj'}^{2} / 2 \right) \) and \( \exp \left( -\nu_{jj'} \right) \) are small and QSE is suppressed for Gaussian \[ \xi \] and power-law \[ \xi \] (\( \mu = 0.5 \)) correlators (curves 1,2), but still persists for the slowly decaying power spectra \[ \xi \] with \( \lambda = 0.5 ; 0 \) (curves 3,4).

What is unexpected is the appearance of a new oscillation structure on curves 1,2 for \( x \) between 20 and 90 for the Gaussian and power-law correlators. It looks as if there are two distinct regimes with large oscillations in-between. These oscillations are not related to the usual QSE, i.e., to abrupt changes in the number of occupied minibands \( S (z) = \text{Int}(z/\pi) \): the oscillations are less sharp, have a larger period roughly proportional to \( z^2 \), and appear only at relatively large \( z \) and \( S \).

The explanation involves the interchange transitions. It seems that at large \( x \) the off-diagonal \( \nu_{jj'} \) are large and the interchange transitions are suppressed. However, for large \( z \) few of the elements \( \nu_{jj'} \) with small \( j \), which are close to the main diagonal, could become relatively small even for large \( x \), \( \nu_{jj+1} (j \ll z/\pi) \pi^2 x (2j+1)/2 z^2 \). Then the transitions \( j \leftrightarrow j + 1 \) become noticeable,

\[ W_{jj+1} (x, z) \sim W_{jj} (0, z) - W_{jj} (1, z) , \]  

(7)

\( (W_{jj}) \) are the angular harmonics of \( W (q_j - q_{j''}) \) over the angle \( q_j q_{j''} \). The opening of such transition channels is accompanied by drops in conductivity. Eqs. \[ \xi \] define the positions \( z_j (x) \) of such drops in \( \sigma (L) \). At \( z = z_1 (x) \), \( W_{12} \) is the first of transition probabilities to acquire the "normal" order of magnitude. At \( z = z_2 (x) \), \( W_{23} \) becomes noticeable, then \( W_{34} \). The amplitudes of the drops rapidly decrease with increasing \( j \). In the end, when all interband channels with \( j \ll z/\pi \) are open, \( \sigma (L) \) becomes smooth, but with a much lower slope than in its initial part. The transitions \( j \leftrightarrow j + 1 \) with high \( j \) always remain suppressed at large \( x \) and the usual saw-like QSE does not reappear. The growth of transition probabilities for transitions \( j \leftrightarrow j + 2 \) does not result in new oscillations in \( \sigma (L) \). In the points \( z \) \( x \) where \( W_{jj+2} \) becomes large, \( W_{jj+2} \sim W_{jj} - W_{jj+2} \), the states \( j \) and \( j + 2 \) are already strongly coupled via \( W_{jj+1} \) and \( W_{jj+1} \).

According to \[ \xi \], for Gaussian inhomogeneities

\[ W_{jj'}^{(0,1)} = \frac{4\pi^5 \ell^2 R^2}{m^2 L^6} \left[ e^{-QQ'} I_{0,1} (QQ') \right] e^{-(Q-Q')^2 / 2} , \]  

(8)

\( Q = q_j R, Q' = q_{j'} R \). The asymptotic solution of \[ \xi \] is
The values \( z_j(x = 200) = 24.3; 31.7; 37.7; \ldots \) agree well with the positions of the drops on curve 1 of Fig.1. For the surface with the power-law correlations of inhomogeneities (1) with \( \mu \lesssim 1 \), the solution of Eq. (7) is not sensitive to \( \mu \). With logarithmic accuracy

\[
z_j(x) = \frac{\pi}{2} \sqrt{(2j+1)x} \left[ \ln \left(x\sqrt{2}\left(1+1/j\right)\right) \right]^{-1/4}.
\]

(9)

The saw-like drops in conductivity for usual QSE correspond to opening of transitions to and from the newly accessible, highest miniband while all other interband transitions are also allowed. The drops are equidistant with the period \( \pi \) along the \( z \) axis. The new QSE oscillations in Fig. 1 correspond to the opening of transitions between the lowest minibands while the transitions in and out of higher minibands are suppressed. The peaks are almost equidistant if plotted against \( z^2 \).

The initial part of the curves 1,2 for \( \sigma(L) \) is described analytically by equations of Ref. [5] and is close to the power law \( \sigma \propto L^{5+\alpha} \) (small \( \alpha \) depends on \( x \)) and to experimental data of the first Ref. [2]. After the region of new QSE oscillations, the curves are again smooth, but with a much smaller tangent. We do not have an analytical description for this regime. The numerical analysis yields either \( \sigma = A + B \cdot L^{1+\beta} \) with small \( \beta \) or \( a + b \cdot L + c \cdot L^2 \). This is close to experimental data [4] and is different from the known behavior of \( \sigma(L) \) at \( x = p_F R \ll 1 \) (see second references in [2,4]).

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The dependence of the conductivity on the correlation radius of surface inhomogeneities, \( \sigma(R) \), is best illustrated by the function \( f_R(y, z = \text{const}) \),

\[
\sigma(R) = \frac{2e^2 L^2}{\hbar^2} f_R(y, z = \text{const}),
\]

(11)

with \( y = R/L \). The number of the occupied minibands \( S \) does not depend on the correlation radius of inhomogeneities, and \( f_R(y, z = \text{const}) \) does not exhibit any saw-like QSE. However, these curves exhibit the step-like structure that corresponds to the new QSE oscillations of Fig. 1.

The positions of singularities \( y_j(z) \) on \( f_R(y, z = \text{const}) \) are identified by Eqs. (9) with \( x = y z \). The functions \( f_R(y, z = 64.4) \) are plotted in Figure 2 for several correlators. The steps on curve 1 in the points \( y = 25; 14; 8; \ldots \) agree well with the solution \( y(z) \) of Eq. (10). The same feature, though barely discernible, is also observed for the power-law correlators. [Minima in all curves near the vertical axis describe the region of the most effective surface scattering at \( p_F R \sim 1 \)].

The dependence of the conductivity \( \sigma \) on the density of fermions \( N \) or their Fermi momentum \( p_F \) is best displayed by the function \( f_N(z) \),

\[
\sigma(p_F) = \frac{2e^2 L^2}{\hbar^2} f_N(z, y = \text{const}).
\]

(12)

Function \( \sigma(p_F) \) exhibits usual saw-like QSE at not very high \( y \) for all types of correlators. With increasing \( y \), the saw teeth disappear, first for the Gaussian and later for the power-law correlators, and persist for the power-law correlators in the momentum space.

![Figure 2](image-url)

**FIG. 2.** Functions \( f_R(y) \) for \( \sigma(R) \), Eq. (11), at \( z = 64.4 \). Curves 1 and 2 (correlators (2) and (3) with \( \mu = 0.5 \)) exhibit new QSE (steps). Curves 3,4 (correlators (3), (4), \( \lambda = 0.5; 0 \)) are smooth in accordance with usual QSE.

![Figure 3](image-url)

**FIG. 3.** Normalized functions \( f_N(z) \) for \( \sigma(p_F) \), Eq. (12), \( f_N(z) \) for \( z = 44 \), at \( y = R/L = 1 \). Curves 1 and 2 (correlators (2), (3) with \( \mu = 0.5 \); \( f_N(44) = 5 \cdot 10^{-3}; 2.5 \cdot 10^{-2} \)) exhibit suppressed usual QSE peaks at small \( z \) that gradually transform at higher \( z \) into the new QSE oscillations with larger period. Curve 4 for surfaces with power spectrum (4) \( (\lambda = 0; f_N(44) = 20.2) \) exhibits usual QSE.

Curves \( f_N(z) \) exhibit the effect related to the new QSE oscillations of Figure 1 for \( \sigma(L) \) and to the steps in Figure 2 for \( \sigma(R) \). Figure 3 shows normalized (by the highest value) functions \( f_N(z) \) for the correlators (3) (curve 1),
\[ \mu = 1/2, \text{ curve } 2, \] and \[ \lambda = 0.5, \text{ curve } 4. \] The correlation radius \( R \) is small, \( y = 1 \), and the figure illustrates the transition from usual to new QSE. The correlators \[ \text{ have a slowly decaying power spectrum and the functions } \] \( f_N(z) \) reveal usual saw-like QSE. Curve 2 starts as a usual QSE curve, but, with increasing \( z \), the oscillations lose the saw-like shape and increase the period. Curve 1 for the Gaussian correlator with a much faster decaying power spectrum does not exhibit, even for the smallest \( z \), neither the shape nor the periodicity of usual QSE.

Curves \( f_N(z) \) for the same correlators, but at \( y = 20 \), are shown in Figure 4. Curves 3,4 still exhibit usual QSE, while curves 1,2 show the well-developed oscillations of the new type. The peaks on curve 1 at \( z_j(y = 20) = 19.8; 50.3; 83.6; \ldots \) are in good agreement with Eq. (1) with \( x = yz \).

FIG. 4. \( f_N(z) / f_N(z = 126) \) for \( y = R/L = 20. \) Curves 1,2 (correlators \( \text{ and } \lambda = 0.5; f_N(126) = 1.1 \times 10^9; 4.5 \times 10^7 \) ) exhibit well-developed new QSE oscillations. Curves 3,4 for correlators \( \lambda = 0.5; 0 \) \( f_N(126) = 1.4 \times 10^9; 47 \) still exhibit usual saw-like QSE.

In summary, we predict new type of QSE in conductivity of films with random rough walls. The effect is reminiscent of magnetic breakthrough. The positions of the peaks \( \text{ are determined by the angular harmonics of the correlation function of surface inhomogeneities. These new QSE singularities replace usual QSE for surface inhomogeneities with large correlation radius and with rapidly (exponentially) decaying power spectra such as for Gaussian or power-law correlation functions. Surfaces with the power-law decay of the Fourier image of the correlation functions exhibit persistent standard QSE and do not exhibit new singularities. Dependences of the conductivity on the film thickness, correlation radius of inhomogeneities, and the particle density (Fermi momentum) display these new QSE anomalies in consistent, but somewhat different, ways. Analysis of transport along surfaces with large \( R \) by equations for usual QSE can result in misinterpretation of experimental data. Large period of new oscillations can make the observation of QSE in metal films easier (cf. the last of Refs. \( \text{[3]} \)).

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