Numerical study of localization in antidot lattices

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Localization effects in antidot lattices in weak magnetic fields are numerically studied with the use of a Thouless-number method. In hexagonal antidot lattices, both conductance and inverse localization length oscillate as a function of a magnetic flux with the same period as an Al’A’shuler-Aronov-Spivak oscillation, in qualitative agreement with recent experiments. [S0163-1829(98)01440-4]

I. INTRODUCTION

An antidot lattice is a two-dimensional electron system modulated by a strong repulsive periodic potential. Recently, a metal-insulator transition was observed in hexagonal antidot lattices in magnetic fields.1 The temperature dependence of the resistivity exhibits Mott’s variable-range hopping and its analysis gave an interesting conclusion that the localization length itself oscillates with the period \( \Phi_0/2 \), a half of the flux quantum \( \Phi_0 = e\hbar/4 \), as a function of the total magnetic flux \( \Phi \) passing through a unit cell. The purpose of this paper is to study the Anderson localization in antidot lattices in a weak magnetic field.

Studies of localization effects in antidot lattices began with observation of Al’tshuler-Aronov-Spivak (AAS) oscillation2 with the period \( \Phi_0/2 \) as a function of \( \Phi \) in a weak localization regime.3–5 Numerical calculations revealed that fluctuations in the antidot potential play an essential role in suppressing irregular Aharonov-Bohm oscillations and giving a regular AAS oscillation in realistic antidot lattices where the mean-free path is much larger than a lattice constant.6,7

In this paper, we shall numerically study the localization effect in antidot lattices based on a Thouless-number method. Difficulties in theoretical treatment of antidot lattices with a large size and realistic potential can be overcome by a scattering (S) matrix method proposed previously.8 In Sec. II, the models and the method of numerical calculations are described. Results of explicit calculations are presented in Sec. III and discussed in Sec. IV. A summary is given in Sec. V.

II. MODEL AND METHOD

In this paper, we shall use a conventional Thouless-number method in order to study localization effects.9,10 This method is useful also in magnetic fields.11 According to a scaling argument,12 the Thouless number \( g(L) \) is a dimensionless conductance defined by the ratio of the strength of effective coupling \( V(L) \) and energy difference \( W(L) \) of two systems with size \( L \) when the systems are combined, i.e.,

\[
g(L) = \frac{V(L)}{W(L)},
\]

There can be various ways to estimate the effective coupling strength \( V(L) \) and the average energy difference \( W(L) \). In the present work, the effective coupling strength is estimated from a geometric average of the curvature of energy bands \( \frac{\partial^2 E}{\partial k^2} \) for periodic systems having a unit cell with size \( L \) and the energy difference is determined from the average energy spacing given by \( D(E)^{-1} \), where \( D(E) \) is the density of states at energy \( E \). We then have

\[
g(L) = \frac{\partial^2 E}{\partial k^2} D(E). \tag{2.2}
\]

The energy bands are calculated in an S-matrix method,8 in which an antidot lattice is replaced by an array of two-dimensional quantum-wire junctions characterized by S matrices. It was demonstrated previously8 that the inclusion of all traveling modes and only a few evanescent modes in the wire region between nearest-neighbor antidots gives accurate energy bands. This reduces the effective matrix size required in the calculation of energy levels considerably and makes calculations in a lattice having a very large unit cell possible. We shall choose quantum-wire junctions illustrated in Fig. 1(a) for a square lattice and Fig. 1(b) for a hexagonal lattice. The area of a junction for a hexagonal lattice is twice as large as a unit cell. The S matrix for a junction is calculated in a nearest-neighbor tight-binding model based on a recursive Green’s-function technique.13

In the S-matrix method, at a given energy, several \( k_x \) values are obtained for each \( k_y \) or several \( k_y \) values for each \( k_x \) on an equi-energy line in the \( k \) space. The second derivative of the energy bands is calculated numerically by varying the energy slightly. The curvature of the bands at each energy for a sample system can be estimated from an average over several such points in the \( k \) space.

In actual numerical calculations, \( g(L) \) is calculated for \( n \times n \) systems with \( n=4, 8, 12, \) and 16 for a square lattice and for \( 2n \times n \) systems with \( n=2, 4, 6, \) and 8 for a hexagonal lattice. The inverse localization length \( g(L) \) is determined by fitting the results to

\[
g(L) = g(0) \exp(-aL), \tag{2.3}
\]

with \( L=na \) and \( 2na \) for the square and hexagonal lattice, respectively, where \( a \) is a lattice constant.

We use the following model potential \( V(\mathbf{r}) \) of an antidot with its center at the origin:
ers and their strength is characterized by the mean free path corresponding to usual experiments.

The dot diameter and a lattice constant in the case of the Fermi energy is of the same order as the Fermi wavelength. This corresponds to the electron concentration $n_d$ being effective included by the dot-size fluctuations.

We consider antidots with several different diameters $d_i (i = 1, \ldots, n_d)$, whose distribution is characterized by average $\langle d \rangle$ and fluctuation $d_f$, given by

$$\langle d \rangle = \frac{1}{n_d} \sum_{i} d_i, \quad d_f^2 = \frac{1}{n_d} \sum_{i} (d_i - \langle d \rangle)^2. \quad (2.7)$$

We denote the average diameter of an antidot $\langle d \rangle$ as $d$ for simplicity. In the case of the square antidot lattice, we have to prepare $n^2_d$ junctions because each junction contains four antidots. In the hexagonal case, the number of different kinds of junctions is $n_d^2$ because of the presence of the central antidot. In order to construct a system with size $n \times n$, we should combine $n^2$ junctions in such a way that the antidots of adjacent junctions have the same sizes and the potential is continuous across all boundaries of junctions. Further, we have to prepare several samples with different short-range disorders for each junction in order to include the effects of impurity scattering.

For simplicity, we shall use $\beta = 1$ independent of the antidot diameter. This is likely to give channels between neighboring antidots wider than those in actual systems when the aspect ratio is larger, i.e., $d_f/a > 0.5$. In actual antidot lattices, the potential in the channel region is likely to be raised higher because of the overlapping of the potential of neighboring antidots with the increase of $d_f/a$. It is not easy to include effects of such potential overlapping in the hexagonal lattice in particular, because of the necessity to increase the number of different junctions considerably (the sample number becomes $n^4_d$ instead of $n^3_d$).

We consider the case $a/\lambda_F = 3.77$, where $\lambda_F$ is the Fermi wavelength. This corresponds to the electron concentration $n_i = 2.2 \times 10^{11}$ cm$^{-2}$ for $a = 2000$ Å, which is comparable to $n_i = 1.8 \times 10^{11}$ cm$^{-2}$ in the experiments.\textsuperscript{1} We shall consider two cases $d_f/a = 0.035$ and 0.07. This amount of fluctuation is necessary for the explanation\textsuperscript{6,7} of the AAS oscillation observed experimentally\textsuperscript{1,4,5} and is likely to be present in actual systems in which the experiments were carried out.\textsuperscript{1} We use $l_e/a = 4$, which is consistent with a real system with high mobility where the mean free path is much larger than the lattice constant. Further, we have $n_d = 5$ for the square lattice and $n_d = 3$ for the hexagonal lattice. The number of energy levels used for the determination of the Thouless number is 2000–3000 typically.

### III. Numerical Results

#### A. Hexagonal Antidot Lattices

The diagram shows some examples of the calculated Thouless number $g$ as a function of a magnetic field in hexagonal antidot lattices with size $4x2$ ($L = 4a$). They show an AAS oscillation with the period $\Phi_d/2$ as a function of the total magnetic flux passing through a unit cell given by $\Phi = \sqrt{3}B a^2/2$, where $B$ is the strength of the magnetic field. The amplitude of the oscillation $\Delta g$ normalized by the Thouless number at zero magnetic field $g_0$ is about $\Delta g/g_0 \sim 0.19$ almost independent of $d_f$. This is consistent with the results $\Delta g/g_0 \sim 0.15$ calculated for similar systems in a dif-

![FIG. 1. Schematic illustration of quantum-wire junctions for (a) a square antidot lattice and (b) a hexagonal antidot lattice. Dashed lines indicated boundaries of Wigner-Seitz cells.](image)
different method, i.e., through a direct calculation of the conductance from the transmission probability.\textsuperscript{6,7} Figure 3 shows calculated results of (a) the Thouless number and (b) the inverse localization length in antidot lattices with \(d/f/a=0.035\) in the absence of a magnetic field. It contains the energy of one-dimensional subbands in the quantum-wire region between nearest-neighbor antidots in the absence of the disorder. The figure shows that the localization is quite sensitive to the aspect ratio \(d/a\). In fact, the localization length is reduced from \(\alpha^{-1}\sim 50a\) for \(d/a=0.6\) to \(\alpha^{-1}\sim 8a\) for \(d/a=0.8\).

Figure 4 shows the magnetic-field dependence of the Thouless number and the inverse localization length for \(d/a=0.7\) and \(d/f/a=0.035\). The Thouless number for each system size oscillates with the period of about \(\Phi_0/2\) like an AAS oscillation. The localization length also exhibits a clear oscillation with the same period in good qualitative agreement with the experiments.\textsuperscript{1} The localization length oscillates in the range between \(\sim 20a\) to \(\sim 70a\).

Figure 5 shows calculated results for \(d/a=0.7\) and \(d/f/a=0.07\). The Thouless number for each system size oscillates with the period of about \(\Phi_0/2\) and at the same time the localization length oscillates with the same period. Due to the presence of larger fluctuations, the localization has become strong in comparison with the results shown in Fig. 4. The amount of the oscillation of the localization length is slightly smaller, i.e., \(\alpha^{-1}\) lies in the range between \(\sim 20a\) to \(\sim 50a\).

Figure 6 shows the calculated results for \(d/a=0.8\) and \(d/f/a=0.035\). In this case, the channel width between neighboring antidots is small and only a single traveling channel is present [see Fig. 3(b)]. The localization effect is enhanced considerably and the AAS oscillation of the localization length is reduced significantly. In fact, the localization length varies only in the range \(\sim 8a\) to \(\sim 10a\) and the tendency corresponding to a negative magnetoresistance that the localization effect becomes weaker with the increase of the magnetic field can be more clearly identified.
B. Square antidot lattices

Figure 7 shows some examples of the results for a square lattice. The parameters are \( d/a = 0.8 \) and \( d_f/a = 0.035 \), which are the same as those of Fig. 6. In the square lattice the Thouless number is much larger and the inverse localization length is significantly smaller than those of the hexagonal lattice shown in Fig. 6. The Thouless number for each system size oscillates very weakly with the period of about \( \Phi_0/2 \) as a function of \( \Phi = B \alpha^2 \) like an AAS oscillation in agreement with a previous numerical simulation and with the experiments. An AAS oscillation cannot clearly be identified in the inverse localization length, while a monotonic decrease of the localization effect with the increase of the magnetic field is much more apparent.

IV. DISCUSSIONS

The origin of the AAS oscillation is known to be quantum interferences of a path encircling an antidot with its time-reversal path in the weak localization regime. In fact, the quantum correction of the conductivity obtained perturbationally from so-called maximally crossed diagrams takes a maximum when the flux \( \Phi \) passing through the area is surrounded by the path is an integer multiple of a half of the flux quantum. The AAS oscillation of the conductance does not necessarily mean the presence of the oscillation of the localization length itself, however.

The localization depends strongly on the symmetry of the system. In usual systems in the absence of a magnetic field, the Hamiltonian is chosen as a real symmetric matrix and the corresponding wave function is real except for an unimportant phase factor. In this orthogonal case the effective coupling \( V(L) \) is given by a real number and an effective dimension of \( V(L) \) is given by \( \eta = 1 \). In the presence of a magnetic field, the Hamiltonian is given by a complex unitary matrix and the corresponding wave function becomes complex. In this unitary case, \( V(L) \) is given by a complex number and consequently \( \eta = 2 \). In the presence of a strong
spin-orbit interaction in the absence of a magnetic field, states are always doubly degenerate (Kramers degeneracy) and $V(L)$ is given by a quaternion number. In this symplectic case we have $\eta = 4$. This $\eta$ is the exponent characterizing level repulsion effects in the random-matrix theory.\textsuperscript{16}

It is clear that the localization effect becomes weaker with the increase of $\eta$. In fact, the localization length in quasi one-dimensional systems is known to be approximately given by $N_c \eta l_e$,\textsuperscript{17\textendash}20 where $N_c$ is the number of channels and $l_e$ is the mean free path. The AAS oscillation of the conductivity is closely related to the fact that the system belongs to an orthogonal ensemble for $\Phi = n \Phi_0 / 2$ with an integer $n$ and to a unitary ensemble in other cases.

This symmetry change can lead to an oscillation of the localization length with a period of $\Phi_0 / 2$ in a tight-binding lattice also. However, a numerical study showed a dominant $\Phi_0$ oscillation rather than $\Phi_0 / 2$ oscillation.\textsuperscript{19} Tight-binding lattices exhibit self-similar spectra called Hofstadter’s butterfly\textsuperscript{21} and the effective band width itself oscillates as a function of the magnetic flux with period $\Phi_0$. In antidot lattices, on the other hand, the oscillation in the total band-width as a function of the flux is not important because the butterfly spectrum is destroyed due to strong mixing among many different bands. This is presumably the reason that an AAS oscillation in the localization length is not appreciable in tight-binding lattices but is clearly observed in antidot lattices.

The present results show that the amplitude of localization-length oscillation for strong localization shown in Fig. 6 is much smaller than that for weaker localization shown in Fig. 4. This is consistent with the fact that the AAS oscillation requires interferences between the paths encircling an antidot in different directions. In fact, with the increase in the localization effect the probability amplitude for an electron to circle around an antidot is reduced. In the strong localization limit where the localization length is smaller than the antidot period, in particular, the oscillation amplitude should be reduced considerably because the interference between paths rounding an antidot is almost completely suppressed.

The large difference between the square and hexagonal lattices is considered to arise from the nature of the electron motion in these lattices. In fact, electrons are more frequently scattered by antidots and perform more complicated trajectories in hexagonal lattices than in square lattices. As a result, electrons circle around a dot more frequently in hexagonal lattices than in square lattices, leading to a possible reduction of the conductance.

According to our results on hexagonal antidot lattices with $d_o / 2 = 0.035$, the oscillation amplitude $\Delta \alpha$ of the inverse localization length normalized by that at zero magnetic field $\alpha_0$ is $\Delta \alpha / \alpha_0 \sim 0.37$ for $d_o / a = 0.7$. This is in reasonable agreement with experimental results $\Delta \alpha / \alpha_0 \sim 0.20$.\textsuperscript{1} However, the absolute magnitude of the localization length obtained in the present calculation is $\alpha_0^{-1} \sim 20a$, which is much larger than $\alpha_0^{-1} \sim a$ estimated experimentally. The localization length can be much smaller for larger aspect ratio, but the amplitude of the AAS oscillation of the localization length becomes smaller with the increase of the oscillation effect ($\Delta \alpha / \alpha_0 \sim 0.11$ for $d_o / a = 0.8$ for which $\alpha_0^{-1} \sim 8a$).

When the confinement is strong, the system is considered as a quantum-dot array rather than an antidot lattice. The hopping of electrons to neighboring dots can be considerably suppressed by a Coulomb blockade if effects of electron-electron interactions are considered. In a weak localization regime, effects of electron-electron interactions give another quantum correction to the conductivity.\textsuperscript{22} Further, when such a charging effect is important in a strong localization regime, the system exhibits a Coulomb gap.\textsuperscript{23} In the case, however, the temperature dependence of hopping resistivity $\rho$ obeys $\rho(T) = \rho_0 \exp[(T_o / T)^{1/2}]$ different from Mott’s variable-range hopping observed in the experiments.\textsuperscript{1}

V. SUMMARY

The Anderson localization in antidot lattices has been numerically studied with the use of a Thouless-number method. The localization is very sensitive to the aspect ratio between the antidot diameter and the lattice constant. In a hexagonal antidot lattice, the Thouless number oscillates with the period equal to that of the AAS oscillation and the localization length oscillates also with the same period. The AAS oscillation of the localization length has a large amplitude when the localization length is much larger than the lattice constants but becomes smaller in the stronger localization regime. In a square lattice, the AAS oscillation of the Thouless number itself is quite small and that of the localization length has not been identified clearly.

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