Phase property of the transmission through a quantum dot

2001 J. Phys.: Condens. Matter 13 3599

(http://iopscience.iop.org/0953-8984/13/15/304)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **13** (2001) 3599–3606 www.iop.org/Journals/cm PII: S0953-8984(01)21224-7

Phase property of the transmission through a quantum dot

H Q Xu[1,3] and Ben-Yuan Gu[2]

[1] Solid State Physics, Lund University, Box 118, S-221 00 Lund, Sweden
and Physics Department, Dalian University of Technology, Dalian 116023, China
[2] Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China

E-mail: Hongqi.Xu@ftf.lth.se

Received 22 January 2001

Abstract
We present a theoretical study of the phase property of the transmission coefficient of a quantum dot. We model the quantum dot by a cross-bar structure and take account of electron–electron interactions in the dot in a self-consistent mean-field approximation. We find that the phase acquired by electrons traversing the dot increases smoothly by π along a resonance peak and drops abruptly by π in the tail of the resonant peak, where the probability of the transmission vanishes. We also show that this sharp phase change cannot be seen in a model that assumes a single-particle, double-barrier structure only for the quantum dot.

Recently, a research group at the Weizmann Institute of Science [1, 2] reported two measurements of the phase of the transmitted electron wave through a quantum dot (QD). A knowledge of this phase, in addition to the transmission amplitude which can be found from the conductance [3], is required in order to characterize fully the nature of the electron transport in such a small quantum system. The first measurement [1] was made using an Aharonov–Bohm (AB) ring with the QD embedded in one of its arms. Two interesting features were observed in this measurement: first, the phase of the AB oscillations is discontinuous, i.e. it changes sharply by π, at every resonance; second, the AB oscillations at various resonances are in phase. In the beginning, the feature of the phase discontinuity was thought to be striking, since it cannot be explained by applying the standard Breit–Wigner formula [4] of the transmission to the QD. However, theoretical investigations [5, 6] motivated by this observation showed that the phase discontinuity is not an intrinsic property of the QD: it results from the fact that the measurement was set up with a two-terminal configuration in which the phase of the AB oscillations is restricted to be either 0 or π by current conservation and time reversal symmetry and, therefore, an observation of the continuous phase evolution of the transmission of the QD is not possible. To avoid this phase rigidity, Schuster *et al* [2] made the second phase measurement via a four-terminal, double-slit-like interference experiment. This improved measurement led to the following important observations: (i) The phase acquired by electrons

[3] Corresponding author.

traversing the QD increases smoothly by π along a resonance peak, in agreement with the prediction for the QD using the Breit–Wigner formula. (ii) The phase drops sharply by π in the tail of the resonant peak, where the probability of the transmission through the QD vanishes. This abrupt phase drop is now indeed striking and cannot be explained by a theory that predicts an abrupt change in the phase of the AB oscillations at a transmission peak, but not at a transmission zero.

Several theoretical models [7–13] have been proposed to explain the phase drops observed by Schuster *et al*. It was shown [7], based on an analytical and numerical calculation for QDs embedded in a narrow quantum wire, that the sharp phase drops occur exactly when the transmission amplitude vanishes. The result was attributed to the interference between two different transmission channels with one through a localized state in the dot and the other one through a continuous state of the quantum wire [7]. Later, it was shown that identical vanishing of the transmission amplitude occurs generically in quasi-1D systems if the time reversal is a good symmetry and that the Friedel sum rule is not strictly valid for quasi-1D systems due to the appearance of the transmission zeros [10, 11]. Very recently, models that take some special properties of the dot states in a semi chaotic situation were also proposed and a mechanism for the phase drops based on large differences in the coupling of the dot states to the continuous states of the leads was discussed [12, 13]. In spite of all these theoretical efforts, the question about a well-accepted, fundamental model for the phase property observed in the experiment by Schuster *et al* still remains.

In this paper, we study the phase property of the transmission through a quantum dot based on the real-space Hubbard Hamiltonian. To be relevant to the experiment by Schuster *et al*, it is clear that in the formulation we should avoid using a model that employs an AB ring with a two-terminal configuration. In principle, the problem can be formulated using a double-slit-like interference device with a four-terminal configuration. However, this is not necessary. The central physical issue to be addressed here is actually only the phase evolution of the transmission coefficient of the QD. Thus, the model we consider is a simple one that consists of two ideal, non-interacting leads coupled to an interacting QD. We will model the QD by a quantum cavity, instead of a double-barrier (DB) structure used in, e.g. [14]. As we will show, this is essential for understanding the phase properties measured by Schuster *et al*. The electron–electron interactions in the QD will be treated in a self-consistent mean-field approximation. This approximation simplifies the problem to the one that can be solved straightforwardly by using the Fisher–Lee relation [15].

As for calculation, the QD cavity is modelled by a finite piece of interacting (vertically placed) quantum wire and two ideal wires are placed horizontally on the left- and right-hand sides of the QD in a cross-bar configuration, We will assign index (0,0) to the cross site. The QD spans lattice sites $(0, -M_1), \ldots, (0, M_2)$, while the two ideal leads span sites $(-\infty, 0), \ldots, (-2, 0), (-1, 0)$ and sites $(1, 0), (2, 0), \ldots, (\infty, 0)$, respectively. The Hamiltonian of the system can be written as

$$\begin{aligned} H = & \sum_{n(\neq 0),\sigma} \varepsilon_{n,0} a^{\dagger}_{n,0;\sigma} a_{n,0;\sigma} - \sum_{n,\sigma} t \left(a^{\dagger}_{n+1,0;\sigma} a_{n,0;\sigma} + H.c. \right) \\ & + \sum_{m,\sigma} \varepsilon_{0,m} a^{\dagger}_{0,m;\sigma} a_{0,m;\sigma} - \sum_{m,\sigma} t \left(a^{\dagger}_{0,m+1;\sigma} a_{0,m;\sigma} + H.c. \right) \\ & + \sum_{m} U a^{\dagger}_{0,m;\uparrow} a_{0,m;\uparrow} a^{\dagger}_{0,m;\downarrow} a_{0,m;\downarrow} \,. \end{aligned} \tag{1}$$

In the above equation, σ is the spin index, $\varepsilon_{n,0}$ and $\varepsilon_{0,m}$ are the on-site energies, and t is the hopping integral which can be related to the lattice constant a and the electron effective mass m^* via $t = \hbar^2/2m^*a^2$. The last term, which contains the Hubbard U, describes the electron–

electron interactions in the QD. One can then write $\varepsilon_{n,0} = U_0 + 2t$ and $\varepsilon_{0,m} = U_0 + U_D + 2t$, where U_0 is the local potential and U_D is the shift of the potential in the QD due to the gate voltage applied. In the present model, the energy dispersion relation in the ideal leads reads $E(k) = U_0 + 2t[1 - \cos(ka)]$, while the electron velocity v in the leads can be found from $\hbar v = \partial E/\partial k = 2at\sin(ka)$. In this work, we shall take a as the unit of length and t as the unit of energy.

To link to the experiment, the transmission coefficient s_σ for electrons with spin σ needs to be calculated for the interacting system. In a self-consistent mean-field approximation (in which the system is described by an effective, single-particle Hamiltonian), the transmission coefficient s_σ can be evaluated using the Fisher–Lee relation [15]. In the present model, the relation reads

$$s_\sigma = i\hbar v[G(E)]_{-1\sigma,1\sigma} \tag{2}$$

where $G(E) = (E - H + i\eta)^{-1}$ is the effective, single-particle Green function of the interacting system in the mean-field approximation with its matrix element defined by $[G(E)]_{\ell'\sigma,\ell\sigma} \equiv <\ell', 0; \sigma|G(E)|\ell, 0; \sigma>$. In equation (2), we choose to evaluate the Green function $G(E)$ between the lattice site $(-1, 0)$ and the lattice site $(1, 0)$. It should be noted, however, that $G(E)$ can be evaluated between any pair of lattice sites chosen from the two leads. For the system with a cross-bar QD, we find that the Green function appearing in equation (2) can be written as

$$[G(E)]_{-1\sigma,1\sigma} = \frac{\Sigma(E)}{\Sigma^*(E)}[G(E)]_{0\sigma,0\sigma} \tag{3}$$

with

$$[G(E)]_{0\sigma,0\sigma} = \frac{[G^D(E)]_{0\sigma,0\sigma}}{1 - [G^D(E)]_{0\sigma,0\sigma}\,\Sigma(E)} \tag{4}$$

where $G^D(E)$ denotes the effective, single-particle Green function of the interacting QD when there is no coupling to the leads, and $\Sigma(E) = (E - U_0 - 2t) - i[4t^2 - (E - U_0 - 2t)^2]^{1/2}$ represents the self-energy due to the coupling to the leads. Because of the finite imaginary term in the self-energy, we do not need to add an infinitesimal imaginary term $(i\eta)$ to $G^D(E)$ when evaluating equation (4). The Green function $G^D(E)$, in general, depends on the occupation of the dot and thus the Fermi energy of the system. The prefactor appearing in equation (3) can be written as $\Sigma/\Sigma^* = \exp(i2ka)$. Thus, it contributes to s_σ only a phase factor corresponding to that acquired by an electron traversing from site $(-1, 0)$ to site $(1, 0)$ in the system without the dot.

In the non-interacting case ($U = 0$), the Green function $G^D(E)$ does not depend on the electron occupation in the dot. It can simply be written as $G^D(E) = \sum_n |n><n|/(E - \lambda_n)$, where λ_n and $|n>$ are the energy eigenvalues and eigenstates of the non-interacting dot. Thus, $[G^D(E)]_{0\sigma,0\sigma}$ has poles at λ_n unless the projection $<0, 0; \sigma|n>= 0$. When the energy E sweeps over these poles, $[G^D(E)]_{0\sigma,0\sigma}$ changes its sign. This implies that $[G^D(E)]_{0\sigma,0\sigma}$ has zeros between its poles and, thus, the transmission through the QD exhibits zeros between resonances.

In the interacting case ($U \neq 0$), although equations (3) and (4) remain unchanged under a self-consistent mean-field approximation, the local Green function $[G^D(E)]_{0\sigma,0\sigma}$ now includes terms derived from the interactions. In this paper, we shall treat the interactions using the Hartree–Fock (HF) approximation. In this approximation, the on-site energies in the lattice sites of the QD in the effective, single-particle Hamiltonian H^{HF} are spin dependent, $E^{HF}_{0,m;\uparrow} = \varepsilon_{0,m} + U <n_{m\downarrow}>$ and $E^{HF}_{0,m;\downarrow} = \varepsilon_{0,m} + U <n_{m\uparrow}>$, where $<n_{m\sigma}>$ is the averaged occupation number at site $(0, m)$ with spin σ. It follows that the single-particle states are diagonal in spin space. However, $< n_{m\sigma} >$ must now be determined self-consistently from $< n_{m\sigma} >= \int_{-\infty}^{E_F} \rho_{m\sigma}(E) dE$ where, in terms of the Green function $G(E) = [E - H^{HF} + i\eta]^{-1}$, the local density of states is given by

$$\rho_{m\sigma}(E) = -\frac{1}{\pi}\mathrm{Im} < 0, m; \sigma|G(E)|0, m; \sigma > . \tag{5}$$

In searching for the self-consistent solutions, we have employed the recursion method. For the details of the procedure implemented in this work, we refer to [16].

The self-consistent HF solutions can be spin-polarized. However, as far as the phase measurement [2] is concerned, in which no effect of the spin polarization on the phase property was observed, it is reasonable to neglect the spin polarization. Thus, we shall, in the following, confine our discussion only to the spin-unpolarized solutions for which the self-consistent, single-particle states are spin degenerate and we shall drop the spin variable from now on.

Once the self-consistent solutions are obtained, the local Green function of the decoupled, interacting dot is calculated from

$$[G^D(E)]_{0,0} = \frac{1}{E - E_{0,0}^{HF} - \Sigma_{0,0}^{(-)} - \Sigma_{0,0}^{(+)}} \tag{6}$$

where $\Sigma_{0,0}^{(-)}$ and $\Sigma_{0,0}^{(+)}$ represent the contributions from the lower and upper arms of the QD, respectively. Using equations (2), (3) and (4), we find that the transmission probability is given by

$$T = |s|^2 = \frac{(E - U_0)\,[4t - (E - U_0)]\,[G^D(E)]_{0,0}^2}{\left\{1 - [G^D(E)]_{0,0}(E - U_0 - 2t)\right\}^2 + [G^D(E)]_{0,0}^2[4t^2 - (E - U_0 - 2t)^2]} \tag{7}$$

and the phase shift of the transmission coefficient due to the presence of the QD by

$$\theta = \tan^{-1}\frac{1 - [G^D(E)]_{0,0}(E - U_0 - 2t)}{[G^D(E)]_{0,0}\left[4t^2 - (E - U_0 - 2t)^2\right]^{1/2}}. \tag{8}$$

Equations (7) and (8) establish a relationship between the transmission probability and the phase shift of the transmitted wave via the local Green function $[G^D(E)]_{0,0}$ of the decoupled dot. It can be shown, in general, that at the poles of $[G^D(E)]_{0,0}$, both the transmission (T) and the phase shift (θ) are finite and continuous. It can also be shown that when $[G^D(E)]_{0,0} = 0$, $T = 0$ but $|\theta| = \pi/2$ (with $\theta = -\pi/2$ when $[G^D(E)]_{0,0} = 0^-$ and $\theta = \pi/2$ when $[G^D(E)]_{0,0} = 0^+$). As a result, the phase shift θ is discontinuous (i.e. it changes abruptly by π) at the transmission $T = 0$ and changes smoothly by π in its passage through a whole resonant region between two transmission zeros. This property of the phase shift is the same as measured by Schuster *et al*.

We first illustrate in figure 1 these fundamental features by the calculations for the system with a non-interacting QD modelled by a vertical wire of 13 lattice sites. It is seen in the top panel of figure 1 that the local Green function $[G^D(E)]_{0,0}$ has poles of type $(E - \lambda_n)^{-1}$ at the energy eigenvalues λ_n of the decoupled, non-interacting dot and changes its sign when passing through a zero. It is seen in the middle and bottom panel that the transmission zeros and the phase drops of π co-occur precisely at the zeros of $[G^D(E)]_{0,0}$. At this point, we note that the formulation presented in this work can easily be generalized to the case where a DB structure is included in the system. However, the feature of the abrupt phase drops of π cannot be obtained in a calculation that assumes a DB structure only for the QD. This is demonstrated in figure 2, where the calculations for a non-interacting QD, defined only by a DB structure (i.e. a wire of 13 sites placed horizontally, as opposed to the structure in figure 1, between two single-site barriers), are plotted. Here, a series of transmission resonances with

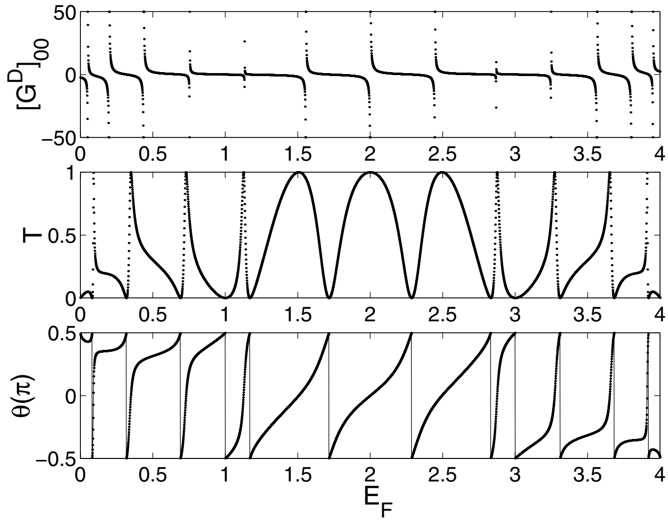

Figure 1. Real part of the local Green function of the decoupled dot (top panel), the transmission probability (middle panel), and the phase acquired by electrons traversing the dot (bottom panel), all as a function of the Fermi energy E_F in the non-interacting case. The dot modelled by a quantum wire of 13 lattice sites ($M_1 = 2$ and $M_2 = 10$) is attached to the leads in a cross-bar configuration. The calculations are done for $U_0 = 0$ and $U_D = 0$. The thin line in the bottom panel is only a guide for the eyes.

the peak value of one are clearly seen, and when the transmission passes a whole resonant region the phase changes continuously by π. This property of the phase is well described by the Breit–Wigner formula. However, no physically meaningful drops in the phase of the transmission coefficient exist. (The phase drops of 2π seen in the figure are simply due to the fact that we have folded the calculated phase to the region between 0 and 2π.) This leads us to conclude that a calculation based on a pure DB model for the QD cannot be used to explain the phase measurement by Schuster *et al.* In contrast, we show in figure 3 that the measured phase property can be obtained when a finite vertical wire is included inside the DB. Here we see that the shape of the phase evolution is remarkably similar to that measured by Schuster *et al.* In fact, the DB structure has a very singular geometry of very little physical relevance to the measurement. Any slight widening of the region between the barriers leads to a cross-bar-like geometry. The calculation presented in this paper shows that the electron wave transmitted through it can exhibit a π-discontinuity in its phase shift, as long as the region is wide enough so that the local Green function at a site of the QD has two or more poles and zeros between the poles.

We now focus on the effect of the electron–electron interactions on the phase property of the transmission. Figure 4 shows a calculation based on the self-consistent formulation described in this work. Here, we present the calculation only for the structure in figure 1 without a DB. The calculation shows that transmission peaks, when compared with their corresponding peaks in the non-interacting case (not shown in this paper), are broadened by the interactions, as we expected. However, the characteristic phase property of the transmitted wave remains unchanged: the phase changes continuously by π when the transmission passes a whole peak region and drops sharply by π when it passes a zero. This is in good agreement with the measurement by Schuster *et al* and we expect that the inclusion of a DB in the calculation will only further improve the agreement (cf figure 3).

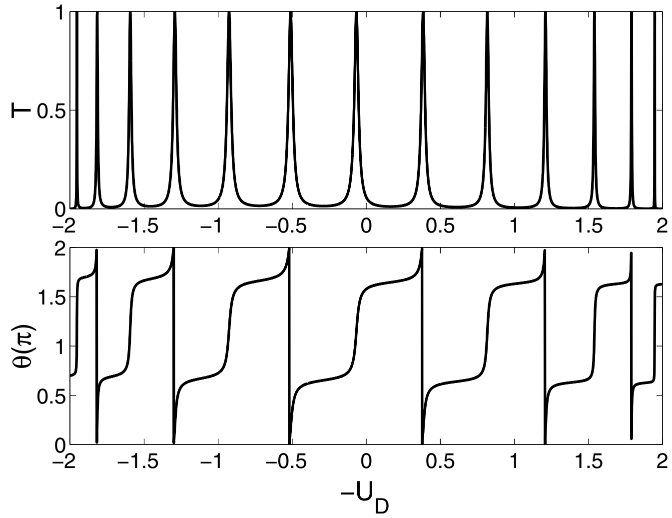

Figure 2. Transmission probability and phase acquired by electrons traversing a non-interacting dot modelled by a conventional, double-barrier structure as a function of the dot potential ($-U_D$) at the Fermi energy $E_F = 2$. Each barrier is modelled by a single site with a local barrier potential $U_B = 4$. The wire placed between the barriers in an in-line configuration has 13 lattice sites with the local potential $U_0 = 0$.

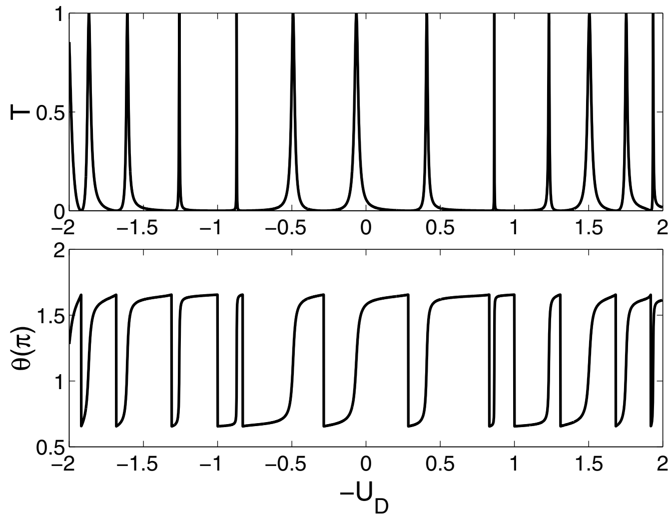

Figure 3. Transmission probability and phase acquired by electrons traversing a non-interacting dot modelled by a cross bar plus a double barrier as a function of the dot potential ($-U_D$) at the Fermi energy $E_F = 2$. The cross-bar structure is the same as in figure 1, while the two single-site barriers with a local barrier potential $U_B = 4$ are located at lattice sites immediately to the left and right of the cross bar.

Finally, we note that we have so far presented the analysis only for the situation in which only one propagating channel is open for conduction in the left- and right-hand leads. The analysis can be generalized to the situation of having multiple open channels in the leads

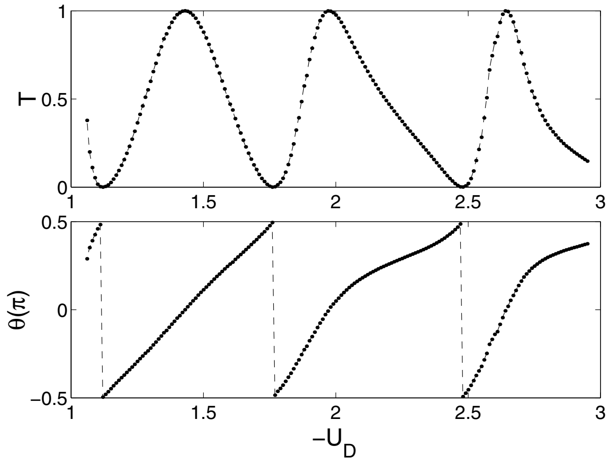

Figure 4. Transmission probability and phase acquired by electrons traversing an interacting quantum dot with the Hubbard $U = 1.5$ as a function of the dot potential $(-U_D)$ at the Fermi energy $E_F = 0.6$. The dot structure is exactly the same as in figure 1 and the electron–electron interaction in the dot is included in the Hartree–Fock approximation. The marks are calculations, while the dashed lines are only guides for the eyes.

by introducing, in equation (1), multiple-valued on-site energies, various additional hopping integrals between the leads and QD, as well as various additional interactions within the QD. We would also like to comment on the role of the spin correlation, which is not included in the present model. Very recently, the phase evolution of electrons as they traverse a Kondo-correlated system was measured [17]. It was found that the phase evolution shows a specific feature which is highly sensitive to the onset of Kondo correlation. Generalization of the present model towards an explanation of this very recent observation is in progress.

In summary, we have presented a theoretical study for the phase of the transmission coefficient of a QD embedded in a quantum channel. We have modelled the QD with a multiple energy-level system and have taken account of electron–electron interactions in the dot in a self-consistent mean-field approximation. Our study has shown that the phase acquired by electrons traversing the QD increases smoothly by π along a transmission resonance and has a discontinuity of π in the tail of the resonance where the transmission probability through the QD vanishes. We have also shown that the physical phase discontinuity does not appear in a calculation using a single-particle DB model for the QD.

Acknowledgments

One of us (H Q X) is grateful to Professor M Büttiker for helpful discussions. This work has been supported by the Swedish Foundation for Strategic Research (SSF) and the Swedish Research Council for Engineering Sciences (TFR). H Q X also gratefully acknowledges the support of the K C Wong Education Foundation, Hong Kong.

References

[1] Yacoby A, Heiblum M, Mahalu D, Umansky V and Shtrikman H 1995 *Phys. Rev. Lett.* **74** 4047
[2] Schuster R Buks E, Heiblum M, Mahalu D, Umansky V and Shtrikman H 1997 *Nature* **385** 417
[3] Landauer R 1957 *IBM J. Res. Dev.* **1** 223

[4] Breit G and Wigner E 1936 *Phys. Rev.* **49** 519
[5] Yeyati A L and Büttiker M 1995 *Phys. Rev.* B **52** R14 360
[6] Yacoby A, Schuster R and Heiblum M 1996 *Phys. Rev.* B **53** 9583
[7] Xu H Q and Sheng W D 1998 *Phys. Rev.* B **57** 11 903
[8] Ryu C M and Cho S Y 1998 *Phys. Rev.* B **58** 3572
[9] Xu H Q and Sheng W D 1999 *Superlatt. Microstruct.* **25** 79
[10] Lee H W 1999 *Phys. Rev. Lett.* **82** 2358
[11] Taniguchi T and Büttiker M 1999 *Phys. Rev.* B **60** 13 814
[12] Silverstrov P G and Imry Y 2000 *Phys. Rev. Lett.* **85** 2565
[13] Yeyati A L and Büttiker M 2000 *Phys. Rev.* B **62** 7307
[14] Wu J *et al* 1998 *Phys. Rev. Lett.* **80** 1952
[15] Fisher D S and Lee P A 1981 *Phys. Rev.* B **23** 6851
[16] Xu H Q and Lindefelt U 1990 *Phys. Rev.* B **41** 5979
[17] Ji Y, Heiblum M, Sprinzak D, Mahalu D and Shtrikman H 2000 *Science* **290** 779