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Periodic conductance resonance in a constricted channel

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Abstract. The measurement of conductance through a narrow channel interrupted by two controlled potential barriers has been reported recently. Reproducible periodic osicllations of the conductance as a function of the gate voltage were observed. By including the change in resonant levels with chemical potential, we have used a tunnelling mechanism through localized changing levels in a modified Coulomb blockade model to explain this effect. In order to get rid of any unknown model parameters so as to justify our modified Coulomb blockade model, instead of the direct comparison of the period of conductance oscillations, we directly compare the box capacitances both from our calculation and from the value derived from the experiment.

1. Introduction

In a recent paper, Meirav *et al* [1] have announced their experimental discovery of the controlled conductance oscillations, which are periodic in the electron density of a narrow channel interupted by two intentional barriers on a GaAs–$Al_xGa_{1-x}As$ heterostructure. This experiment, in which the locations of two barriers are known exactly, has established the relation between the period of the oscillations and the length of an isolated segment between the barriers. They have partially confirmed a previous conjecture [2] of the electron-density-related conductance oscillations in one-dimensional quantum wires, based upon the assumption of the existence of two dominant charged impurities along hte narrow channel. However, the precise nature of these resonances has not been clear. By including the change in resonant levels with chemical potential in a modified Coulomb blockade model (MCB), we use a tunnelling mechanism through localized charging levels to explain this remarkable effect.

The related conductance oscillation phenomenon was first discovered by Scott-Thomas *et al* [3] who attributed it to the formation of a charge-density wave. Later, it was pointed out by Van Houten and Beenakker [4] in a comment that this effect could be accounted for by the Coulomb blockade (CB) of electron tunnelling. Unfortunately, as was argued in the replay from Kastner *et al* [5], the calculated energy scale was 16 times larger than that measured in the experiment. This looks like casting doubt on the explanation using the CB model. Glazman and Shekhter [6] presented a more detailed

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theoretical study on a similar situation. However, as will be shown below, their theory also suffers from an energy scale three times larger than that measured in the experiment [1]. Does this mean that the conclusive experimental evidence completely rules out the possibility of the CB model as an explanation for this phenomenon? Furthermore, where does this large discrepancy come from? In this letter, we argue that, if we properly include the change in resonant levels with the chemical potential in a MCB model, our prediction can quantitatively agree with the experimental observation [1].

In section 2, the theoretical model is presented and, in section 3, the numerical estimations and the comparison with the experimental results are carried out. The last section is devoted to the related discussions.

2. Modified Coulomb blockade model

Let us first assume U_n to be the total energy of the ground state with n electrons in an isolated box between two barriers. Within the framework of density functional theory [7], the topmost electron state (associated with the energy cost of the last electron added to the box) is assigned an energy

$$E_n = U_n - U_{n-1}. \tag{1}$$

Then we obtain a set of so-called resonant levels $\{E_n\}$ ($n = 1, 2, 3, \ldots$). Also, when $L_0 \geqslant 500$ nm and $W_0 \geqslant 200$ nm, the kinetic energies of the electrons in a box can be ignored compared with their interaction energies. As far as the interaction energies of the electrons are considered, U_n can be expanded as [7]

$$U_n = (\alpha n^2/2 + \beta n + \eta) + \lambda \rho_L n \tag{2}$$

where α, β, η and λ are constants, in which α is related to the capacitance of the box and is quite independent of the detailed structure of the electronic states in the box, and λ is the coupling constant between the box and the one-dimensional system outside the box. n is the number of electrons within the box, and ρ_L is the average linear electron density outside the box. From equations (1) and (2) we have

$$E_n = (\alpha n - \alpha/2 + \beta) + \lambda \rho_L. \tag{3}$$

These resonant levels $\{E_n\}$ will depend on the chemical potential μ only through the linear electron density ρ_L. Therefore, we get

$$\partial E_n(\mu)/\partial \mu = \lambda \, \partial \rho_L/\partial \mu = \lambda g_{1D}(\mu). \tag{4}$$

It is customary to choose the bottom of the electronic energy dispersion as the energy reference point in an *ab-initio* calculation. Then eV_g can be regarded as the difference between the chemical potential μ_m of the conductive substrate, which is fixed, and the electron chemical potential μ of the interface between the top layer of GaAs and the $Al_xGa_{1-x}As$ layer. We can set, therefore, $\delta\mu = \gamma e \, \delta V_g$, where $\gamma < 1$ is a ratio parameter determined by the self-consistent calculation.

Let μ_n be the value of the chemical potential outside the box which is in resonance with the level E_n in the box. Then we have

$$\mu_n = E_n(\mu_n) \tag{5}$$

and the period of V_g (or μ) in the conductance oscillations will be given by

$$\delta\mu = \mu_{n+1} - \mu_n = \alpha + \lambda[\rho(\mu_{n+1}) - \rho(\mu_n)] = \alpha + \lambda g_{1D}(\mu)\,\delta\mu \tag{6}$$

or equivalently by

$$\delta\mu = \alpha/[1 - \lambda g_{1D}(\mu)] = \alpha/K \tag{7}$$

with $K = 1 - \lambda g_{1D}(\mu)$.

Assuming that the observed peaks in the conductance are due to the many-body resonant tunnelling mechanism through the resonant levels $\{E_n\}$, we can write down the conductance, at finite temperature, using the Landauer [8] formula

$$G(\mu, T_e) = \frac{e^2}{h}\sum_n A_n(\mu, T_e)\cosh^{-2}\left(\frac{E_n - \mu}{2k_B T_e}\right) \tag{8}$$

where we have assumed a Fermi–Dirac distribution for the electrons outside the box, the assumption also used for fitting in [1]. Furthermore, near a resonant peak position V_r, we can expand the argument of the cosh term in equation (8) as

$$[E_n(V_g) - \mu(V_g)]/2k_B T_e = [\partial E_n(V_g)/\partial V_g - \partial\mu(V_g)/\partial V_g][(V_g - V_r)/2k_B T_e]. \tag{9}$$

According to the experiment in [1], we can define the thermal peak width by

$$\delta V = k_B T_e/[\partial\mu(V_g)/\partial V_g - \partial E_n(V_g)/\partial V_g] \tag{10}$$

where T_e is the electron temperature. In [1], Meirav *et al*, by treating $\{E_n\}$ as a set of single-particle resonant energy levels, have implicitly set $\partial E_n/\partial V_g = 0$. We point out that the resonant levels $\{E_n\}$ in equation (3) results from the Coulomb interaction between the electrons within a box. The screening of Coulomb interaction changes with the number of electrons in the box, or equivalently the chemical potential in the leads. The change in screening will shift these resonant levels. The inclusion of this shfit is crucial for the MCB model. It leads to renormalization of the energy scale to reach quantitative agreement with the experiment [1, 9]. At high temperatures ($T_e \geqslant 500$ mK), the electron temperature approaches the measured temperature T.

The box-capacitance-related constant α can be easily estimated as

$$\alpha \sim [e^2/4\pi\varepsilon_0\varepsilon_{eff}L_0][\tfrac{3}{2} + \ln(L_0/W_0)] = e^2/C_{box} \tag{11}$$

where L_0 and W_0 are the length and width of the box, ε_{eff} is the effective dielectric constant of the box which is determined by the geometry-related screening of the ISIS structure (solving the Poisson equation) and the screening from the electrons within the box (using the Hartree–Fock approach). C_{box} is the bare box capacitance which is proportional to L_0 and weakly depends on the electric width of the channel as is expected [9].

For a non-interacting 1D electron gas, the density of states per unit length can be calculated from

$$g_{1D}(\mu) = \frac{\sqrt{2m^*}}{\pi\hbar}\sum_j^{\text{occupied}}\frac{1}{\sqrt{\mu - \varepsilon_j}} \tag{12}$$

where m^* is the effective mass of the electrons, and ε_j is the bottom of the jth subband.

Since $\delta g_{1D}(\mu)/g_{1D}(\mu) = \delta V_g/2(V_g - V_{th})$, we may regard $g_{1D}(\mu)$ as a constant in a range much smaller than $V_g - V_{th}$, where V_{th} is the threshold gate voltage, related to the bottom of the lowest subband energy dispersion.

The coupling constant λ can be evaluated from

$$\lambda \sim [e^2/2\pi\varepsilon_0\varepsilon_{eff}]\{\tfrac{8}{2} + \tfrac{1}{6}[W_0/(L - L_0 - 2L_b)]^2 + \ln[(L - L_0 - 2L_b)/W_0]\} \tag{13}$$

where L is the length of the 1D channel. From the above discussions, we know that $g_{1D}(\mu)$ is a constant only in the asymptotic region $V_g \gg V_{th}$. When $V_g - V_{th}$ is small, $g_{1D}(\mu)$ usually increases with V_g. In this asymptotic region, we can define the so-called asymptotic gate capacitance $C_{asymptotic}$ by the maximum box-related capacitance C_{max} [9]:

$$\begin{aligned} e(L - L_0 - 2L_b)\rho_L &= C_{asymptotic}(V_g - V_{th}) \\ &= [(L - L_0 - 2L_b)/L_0]\{[\tfrac{8}{3} + \ln(L_0/W_0)]/\{\tfrac{8}{3} + \ln[(L - L_0 - 2L_b)/W_0]\}\} \\ &\times C_{max}(V_g - V_{th}) \end{aligned} \tag{14}$$

where $C_{max} \sim A\varepsilon_0\varepsilon_{eff}L_0W_0/d$ is mainly determined by the geometrical structure of the box, and L_b is the barrier width. Here, d is the thickness of the $Al_xGa_{1-x}As$ layer, and A is the local correction factor due to the existence of the top gate. The calculation of A is rather complicated. We shall adopt the numerical result in [9] to fix C_{max} directly. The estimations of equations (11) and (13) could be much more accurate if the condition $L \gg L_0 \gg W_0$ is well satisfied.

3. Numerical estimations

Using the experimental data given in [9], i.e. $L_0 = 700$ nm, $W_0 = 500$ nm for sample 2 and $L_0 = 600$ nm, $W_0 = 450$ nm, for sample 3, we estimate from equation (11) that the values of α for sample 2 and sample 3 are 0.301 meV and 0.343 meV, respectively (taking $\varepsilon_{eff} = 12.5$). The experimental measurement, i.e. $\alpha = K\,\delta\mu = e\gamma K\,\delta V_g$ with $e\,\delta V_g = 0.95$ meV, $1/\gamma K = 2.6$, for sample 2 and $e\,\delta V_g = 2.0$ meV, $1/\gamma K = 3.5$, for sample 3 [9], gives the values of α as 0.365 meV and 0.571 meV, respectively. By using the theory of Glazmann and Shekhter [6], it is easy to show that $\alpha = (1 - K)\,\delta\mu = e\gamma(1 - K)\,\delta V_g$. Because we know from the experiment [9] only the values of γK and $e\,\delta V_g$, we cannot quantitatively compare the prediction in [6] with experiment. Clearly, our present MCB model has successfully removed the large discrepancy between the theory and the experiment compared with the previous CB model [4]. The variation in V_g shifts the chemical potential and the resonant levels at the same time. The small value of K indicates that the change in the resonant levels with V_g is quite considerable. We must emphasize that we can directly compare only the bare box capacitance both from our calculation and from the value derived from the experiment to validate our MCB model because in our model we do not know the exact value of the parameter K. This approach is expected to be quite reliable since no adjustable parameters go into our calculation. We can see from this simple comparison that the agreement is reasonably good. We thus believe that the phenomenon observed in [1] can be explained by our present theory.

Furthermore, from equation (14) we can calculate the density of states per unit length:

$$\begin{aligned} g_{1D}(\mu) &= C_{asymptotic}/e^2(L - L_0 - 2L_b) = (1/e^2L_0) \\ &\times \{[\tfrac{8}{3} + \ln(L_0/W_0)]/\{\tfrac{8}{3} + \ln[(L - L_0 - 2L_b)/W_0]\}\}C_{max}/\gamma \end{aligned} \tag{15}$$

Table 1. Calculation results.

	Theory	Experiment
Bare box capacitance $C_{box} = (e^2/\alpha)$ (10^{-16} F)	5.316	
Scaled density of states $\gamma g_{1D}(\mu)$ (10^{22} μm^{-1} J^{-1})	0.558	
Coupling constant λ (10^{-22} μm J)	1.084	
Slope of thermal width $e\,\delta V/k_B T_e = 1/\gamma K$		2.6
Ratio parameter $\gamma = \gamma K + \gamma\lambda g_{1D}(\mu)$	0.99	
1D density of states $g_{1D}(\mu)$ (10^{22} μm^{-1} J^{-1})	0.564	
Effective capacitance $C_{eff} = \gamma K C_{box}$ (10^{-16} F)	2.101	
Period of oscillations $e\,\delta V_g = \delta\mu/\gamma = \alpha/\gamma K$ (meV)	0.78	0.95

which is in accordance with the experimental fact that the slope $d\rho_L/dV_g$ is a constant in this region. As discussed in [6], it is also the pre-condition for observing the periodic conductance oscillations in the experiment.

On the other hand, from equations (4) and (7) we can get

$$\partial E_n(V_g)/\partial\mu = 1 - K = \lambda g_{1D}(\mu). \tag{16}$$

Furthermore, from equation (10) we know that this constant $1/\gamma K$ is, in fact, the slope $e\,\delta V/k_B T_e$ given by experiment in [1, 9]. This confirms from the experiment the soundness of the approximation in equation (15). From equation (7) we thus conclude that the period of conductance oscillations is a constant which is in agreement with the experiment in [1, 9].

As a numerical example, we consider sample 2 in [9]. We take $m^* = 0.067m_e$, $C_{max}/e = 1.0\,mV^{-1}$, $\varepsilon_{eff} = 12.5$, $L = 3\,\mu m$, $L_0 = 700\,nm$, $L_b = 100\,nm$ and $W_0 = 500\,nm$. We list all the calculation results in table 1.

The theoretical prediction of $e\,\delta V_g$ is close to the experimentally measured value. Considering that equations (11) and (13) are not the exact estimations, we thus believe that our MCB model is at least qualitatively applicable. Unfortunately, the direct calculation of γ is rather complicated, which needs the self-consistent calculation of both Schrödinger's and Poisson's equations; we have used the experimental value of γK from the slope of thermal width and our theoretical value of $\gamma\lambda g_{1D}(\mu)$ to calculate γ above.

4. Discussion

Compared with the usual CB model [4] in which $e\,\delta V_g = e^2/\gamma C_{box}$, our theory predicts that the period of the observed conductance oscillations is determined by an effective box capacitance, defined by $C_{eff} = \gamma K C_{box}$, instead of the bare box capacitance C_{box}. C_{eff} is also the capacitance measured in the experiment [1, 9].

From the experiment [1, 9] we know that the variation in peak heights is unpredictable. This may be ascribed to the effect of impurity disorder since thermal cycling changes the height of conductance peaks but not the period of the conductance oscillations. We can infer from equation (8), therefore, that $A_n(\mu, T_e)$ ($n = 1, 2, 3, \ldots$) are affected by the impurity distribution. Because a magnetic field can change only the height of conductance peaks but not the peak width, and because α, or the Coulomb interaction between the electrons in the box, is insensitive to the magnetic field, we conclude from equation (7) that the period of conductance oscillations should not be

affected by a variation in the magnetic field. This has been proved in a recent experiment [10].

When the electron density is high, the kinetic energy term, which is ignored in equation (2), will become important compared with the interaction energy term. We expect that these overlapping broad oscillation peaks will be greatly weakened and even disappear at high electron density. When the electron temperature is low ($T_e \leq 500$ mK), the experimental observation of the saturation of the thermal peak width [9] may be attributed to the electron heating in the system. Considering that $\partial \rho_{2D}(V_g)/\partial V_g = em^*/\pi\hbar^2$ is a constant over a larger range of chemical potential μ or gate voltage V_g, we believe that the one-dimensionality (of the narrow wire) outside the box may not be essential in this experiment. If the gate voltage $V_g - V_{th}$ is very small, there will be several periods overlapping since the density of states generally cannot be a constant within this region. This has been confirmed by experiment [10]. Furthermore, from this theory, we see that the discretization of $\{E_n\}$ is essentially a classical electrostatic phenomenon. On the other hand, resonant tunnelling is a quantum phenomenon. It is remarkable that the experiment shows such a combination of these two. The calculation on the magnetic field and temperature dependences of the conductance peaks will be published elsewhere.

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