Universal phase lapses in a noninteracting model

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Abstract. We calculate the transmission probability and phase through a quantum dot using a noninteracting toy model consisting of a ladder of narrow levels and a wide level. We find that the interference of the electron waves transmitted through such a dot induce universal phase lapses between consecutive peaks. The reason for this universality can be related to a Fano-type interference pattern and is explained in a simple analytic analysis of the model. Temperature effects and possible relevance of the model to interacting systems are discussed towards the end of the paper.

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1. Introduction

Phase measurements on relatively large quantum dots show that the phase evolution of electrons traversing the dots exhibit a universal behaviour, independent of dot size, and electron occupancy. Specifically, for quantum dots in the Coulomb blockade regime, the transmission phase of electrons increases monotonically by $\pi$ throughout each conductance peak; in the conductance valleys, the phase returns sharply to its starting value.

The theoretically expected mesoscopic features in the phase evolution related to the dots’ shape and spin degeneracy were observed recently in small dots containing less than ten electrons. However, after a transition region, for dots with more than 14 electrons a universal behaviour was observed [1].

In this paper, we study a toy model\(^1\) of noninteracting spinless electrons. Our analysis shows that when the model has a set of narrow resonant levels and a single nonresonant wide level a phase lapse occurs between successive peaks. The universal occurrence of a phase lapse between consecutive peaks does not depend on the sign or the size of the coupling matrix elements of each narrow level to the left and right leads (except for nongeneric situations of high symmetry).

The nonresonant wide state may arise due to a direct semiclassical trajectory between the two point contacts that define the dot [3, 4]. Alternatively, it may arise due to the formation of a super-radiance state. This state is formed when a linear combination of a few nearly degenerate levels is coupled well to the lead while the other orthogonal linear combinations form very narrow levels [5, 6]. Recent works [5, 7] showed that interactions in the dot do not significantly modify this behaviour. In this paper we will assume that such a wide nonresonant level exists and show that the interference between the nonresonant level and a ladder of resonant levels leads to universal phase lapses. Only a small fraction of the density of an electron that occupied the wide level is concentrated in the dot. Hence, we expect it to be less sensitive to an external gate potential and to interact weakly with electrons that occupied the narrow levels. We will therefore assume that the position of the level does not change with the gate potential.

Although we cannot show it rigourously, it is not inconceivable that when plunger gates attract more electrons to the dot a wide nonresonant level appears and causes the occurrence of the universal lapses after an initial mesoscopic region. The effect of interactions between the electrons, the inclusion of spin effects and the exact origin of a nonresonant level require a more elaborate study which is postponed for future research.

The ideas that levels with different widths [8] are responsible for the phase lapses was considered in several publications. The reader can consult the Hackenbroich review from 2001 [9] and references therein. For later versions that concentrate on interaction effects see [10]–[12]. Our focus in this paper is on the interference pattern of one wide level and a ladder of narrower levels in a noninteracting model.

2. Modelling the dot–leads system

We use a tight binding model to describe a system that consists of two leads and a dot. A schematic view of the model is depicted in figure 1. Formally, the Hamiltonian of the system is written as:

$$
\mathcal{H} = V\sum_{i=-1}^{\infty} L_{i-1}^\dagger L_i + V\sum_{i=1}^{\infty} R_i^\dagger R_{i+1} + \sum_n \epsilon_n d_n^\dagger d_n + V_{L_n} d_n^\dagger L_n + V_{R_n} d_n^\dagger R_n + \text{h.c.,}
$$

(1)

\(^1\) A similar model was considered in [2].
with $L_i$, $R_i$, the creation and annihilation operators on the left and right leads whose band width is $2V$; and $d_n^\dagger$, $d_n$ the creation and annihilation operators of the $n$th level of the dot, with energy $\epsilon_n$. In the absence of magnetic field we can choose the coupling constants $V_{Ln}$, $V_{Rn}$ to be real.

The scattering matrix through a similar mesoscopic system with many leads modelled by a tight binding model was derived in [13]. For the special case of two leads, it was used in a series of papers (see [14]–[16]). The transmission amplitude for electrons at the Fermi level, assumed to be at the middle of the bands of the leads, is given by:

$$ t \equiv t(0) = \frac{2iG_{LR}}{(G_{LL} - i)(G_{RR} - i) - |G_{LR}|^2}, \tag{2} $$

with

$$ G_{LL}(\epsilon) = \sum_n \frac{V_{nL}V_{nL}^*}{V(\epsilon - \epsilon_n)}, $$

$$ G_{RR}(\epsilon) = \sum_n \frac{V_{nR}V_{nR}^*}{V(\epsilon - \epsilon_n)}, $$

$$ G_{RL}(\epsilon) = \sum_n \frac{V_{nL}V_{nR}}{V(\epsilon - \epsilon_n)}, \tag{3} $$

and $G_{LL} \equiv G_{LL}(0)$, $G_{RR} \equiv G_{RR}(0)$ and $G_{LR} \equiv G_{LR}(0)$. In the proceeding sections, we will analyse the transmission $t$ for various physical situations.

### 3. The mesoscopic regime: a ladder of narrow levels with random parity

Throughout this paper, we will concentrate on a ladder with equidistant levels

$$ \epsilon_n = n\delta - V_g, \tag{4} $$

where $\delta$ is the level spacing and $V_g$ the plunger gate potential that, by assumption, rigidly shifts the levels.

In all cases we will assume that the sign of the matrix elements (i.e., of the coupling constants $V_{Ln}$, $V_{Rn}$) is random. In a one-dimensional dot we expect (due to the parity class of the eigenfunctions) the following sequence of signs of the coupling constants. The first eigenstate does not have any nodes, the second state—one node, the third state two and so on, so that the
relative signs of the left and right coupling constants alternate. However, as the dots in [1] (as well as dots in other measurements [17]) are not one-dimensional, we choose coupling constants with random sign.

We assume that when there are only few electrons in the dot, the negative potential on the plunger gate that repels electrons from the dot, also makes the barrier between the leads to the dot higher. Hence, the coupling constants are rather small (compared to the level spacing) and the dot levels are narrow. To simulate this situation we choose $|V_{L_n}| = |V_{R_n}| = |V|/40$, $\delta = V/100$. Since $V$ is inversely proportional to the density of states in the lead we find the levels width $\Gamma = 2 (|V_{L_n}|^2 + |V_{R_n}|^2) / V = \delta/4$. (This definition of the level width is a bit arbitrary. It is chosen so that for a single level we obtain the Bright–Wigner formula for a resonance (see the expression for $t_r(\epsilon)$ before equation (12)).)

In figure 2(a) we show the transmission probability $|t|^2$ (which according to the Landauer formula is proportional to the conductance through the dot) and the phase $\arg(t)$ for the case
$|V_{L_n}| = |V_{R_n}| = |V|/40, \ \delta = V/100$; the coupling constants have random sign. While few phase lapses occur they do not exhibit any universal or ordered features. In figure 2(b) we plot the same curve in a parametric presentation of the complex transmission amplitude $t$. The curve covers all four quarters of the complex plain, indicating the fact that the phase of $t$ evolves by more than $2\pi$.

4. The transition regime: a ladder of wider levels with random parity

In this section we assume that when the negative potential on the plunger gate is reduced, both the size and the coupling to the dot increase. As a result the ratio between the width of the levels and the level spacing becomes larger. To model this situation we assume that the level spacing does not change but the states are wider $|V_{L_n}| = |V_{R_n}| = V/10$, i.e., $\Gamma = 4\delta$. The sign of the matrix elements is kept random as before (with an identical sequence of random signs).

Figures 3(a) and (b) depict $|t|^2$, the phase arg$(t)$ and a parametric plot of $\text{Im}(t)$ versus $\text{Re}(t)$. The curves exhibit a completely irregular behaviour, which mimic the ‘transition region’ in [1].

5. The universal regime: the effect of a nonresonant level

In this section we consider what happens when we add a nonresonant level to the ladder of resonant levels with coupling constants of random sign. We expect such a level to appear when the potential is sufficiently positive, i.e., when the dot contains many electrons and the coupling constants are large. In addition, since an electron transported through the nonresonant level spends a short time at the dot area, it is expected to be less sensitive to the external gate potential. Possible origins for the nonresonant state were discussed extensively in [3]–[5], [18], we will model this level by a constant $\gamma$ added to the ladder of resonant levels, which gives:

$$
G_{LL}(0) = \gamma - \sum_n V_{nL}V_{nL}^* V_{e_n}/V_{e_n}, \quad G_{RR}(0) = \gamma - \sum_n V_{nR}V_{nR}^* V_{e_n}/V_{e_n},
$$

$$
G_{RL}(0) = \gamma - \sum_n V_{nL}V_{nR} V_{e_n}/V_{e_n}.
$$

(5)

In figure 4 we plot the transmission, $|t|^2$, and arg$(t)$ for a ladder of resonant levels with an addition of one nonresonant level with an effective width $\gamma = 5$. We find that the effect of the nonresonant level is striking. While few of the peaks disappear the phase does not exceed $\pi$ except at some isolated points where sharp features are observed.

5.1. Left–Right asymmetry

When the left and right barriers are asymmetric [14, 19], the transmission curves are even more regular. In figure 5 we plot the transmission properties using the same parameters as in figure 4 but now we assume $|V_{L_n}| = 4|V_{R_n}| = V/10$.

In the case of a single resonance level with left–right asymmetry the maximal transmission probability is smaller than one. In contrast, for the current case at certain gate potentials, despite the left–right asymmetry in the coupling constants, the transmission probability reaches

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Figure 3. The transition regime: a ladder of wider levels with coupling constants of random sign. (a) $|t|^2$ and arg$(t)$ as a function of the plunger gate potential $V_g$ (measured in units of the level spacing $\delta$). (b) Parametric plot of the complex variable $t$, notice that it still covers all four quarters of the complex plane. Therefore the phase of $t$ changes by more than $2\pi$.

6. Interpretation: analytic analysis

6.1. Comparison to a dot where all the levels have identical parities

It is not very difficult to understand analytically why the nonresonant level is so effective in producing universally ordered phase lapses. To understand how it happens let us first consider the case where all the levels have the same parity (and also equal values of the coupling constants).

a maximal value close to one. In addition, the shape of the peaks is not purely Lorentzian and has some skewing feature due to the Fano like interference effects.
Figure 4. Universal (symmetric) regime: a wide nonresonant level with $\gamma = 5$ is added in parallel to the ladder of levels. (a) $|t|^2$ and arg($t$): some of the original peaks disappear but there are clear phase lapses and very few sharp features. (b) Parametric plot of the complex variable $t$ (we note that for clarity the phase was shifted by $+\pi/2$). Now there are only a few isolated points with positive real parts, they correspond to the sharp features in the first panel. The proximity of the curve to the origin causes sharp phase lapses.

Then we have:

$$G_{LR} = G_{LL} = G_{RR} \equiv S$$

and we may assume that $S$ is real. The expression for the transmission amplitude becomes:

$$t_{\text{even}}(S) = \frac{2iS}{(S - i)^2 - S^2} = -\frac{(2S)^2}{1 + (2S)^2} - i\frac{2S}{1 + (2S)^2}. \quad (7)$$

An inspection of equation (7) reveals that Re($t_{\text{even}}$) < 0 always. We therefore conclude that when all the levels have the same parity the phase cannot evolve by more than $\pi$. Hence, phase lapses must occur.
Let us now examine what happens when we have matrix elements with random sign and a nonresonant level of width $\gamma$. The amplitude $t$ may be written in the form:

$$t_\gamma = \frac{2i(\gamma + G_{LR})}{-2i\gamma - 1 + \gamma(G_{LL} + G_{RR} - 2G_{LR}) - 1(G_{LL} + G_{RR}) + G_{LL}G_{RR} - |G_{LR}|^2}.$$  \hfill (8)

For

$$\gamma \gg G_{LL}G_{RR}, |G_{LR}|^2, G_{LR}, G_{LL}, G_{RR}, 1$$ \hfill (9)

we can neglect $G_{LR}$ in the numerator and the term $-1 + i(G_{LR} + G_{RR}) + G_{LL}G_{RR} - |G_{LR}|^2$ in the denominator to obtain:

$$-t_\gamma = \frac{i}{i - 2\tilde{S}} = 1 - \frac{(2\tilde{S})^2}{1 + (2\tilde{S})^2} - i\frac{2\tilde{S}}{1 + (2\tilde{S})^2}, \quad \tilde{S} = \frac{1}{4} \sum \frac{(V_{Ln} - V_{Rn})^2}{\epsilon_n}. \hfill (10)$$

**Figure 5.** Universal regime: in addition to the nonresonant level we add a left–right asymmetry in the coupling constants ($|V_{Ln}| = 4|V_{Rn}|$). (a) $|t|^2$ and arg($t$): the number of peaks is similar to the number of peaks in the absence of the nonresonant level, and between every consecutive peak we have a sharp phase lapse. (b) Parametric plot of $t$, notice that now all points are in the left part of the plane, this means that the phase never exceeds $\pi$ and phase lapses must occur.
Notice that the structure of $\tilde{S}$ does not depend on the sign of the matrix elements. Hence, for large $\gamma$, $t_{\gamma}$ has a structure very similar to the case when all the levels have identical parity, cf. equation (7). In addition, equations (10) show that in the symmetric case levels with even parity disappear (since the residue of $\epsilon_n$ for these levels is zero) but reappear in the asymmetric case. This explains the absence of a few of the peaks in figure 4, and their reappearance in a more regular fashion in figure 5.

6.1.1. How large should $\gamma$ be? To obtain equation (10) we have assumed that $\gamma \gg |G_{LL}|^2, |G_{LR}|^2, G_{LL}, G_{RR}, G_{LR}$. However, this condition is not fulfilled for any value of $\epsilon_n$. For $\epsilon_n$ near zero we can approximate the sums by a single term, for example $G_{RR}G_{LL} \approx V_{RR}V_{LL}/(V^2 \epsilon^2_n)$. In this case equation (9) is not satisfied when $|\epsilon_n| < V_{RR}V_{LL}/\sqrt{\gamma}$.

For large $\gamma$ these regions are very narrow and should show up as a sharp feature when the gate potential is swept. We expect that the observation of these regions would require a very fine tuning of the gate potential. In addition, as we will see in the proceeding section, temperature effects tend to smear sharp features.

6.2. Interpretation in terms of Fano-type resonances

We can obtain the conclusions of the previous section by considering a Fano-type interference pattern.

The classic Fano line shape [4]

$$|t_{\text{Fano}}(\epsilon)|^2 = G_d |2\epsilon + q \Gamma_F|^2,$$

arises from the interference of a nonresonant path, with transmission amplitude $t_d = e^{i\beta_d \sqrt{G_d}}$, and a resonance path, with transmission amplitude $t_r(\epsilon) = \frac{z_r \Gamma_F}{2\epsilon + i\Gamma_F}$, where

$$t_{\text{Fano}}(\epsilon) = t_d + t_r(\epsilon)$$

and $q = i + z_r e^{-i\beta_d} / \sqrt{G_d}$.

Let us now consider transmission through a dot with a wide (nonresonant) level and a single resonance level. The simple relation (12) does not trivially hold, as multiple scattering between the levels is possible. Despite this fact, we will see below that the transmission amplitude has the shape of a Fano line.

In this case the $G$’s take the form:

$$G_{LL}(0) = \gamma - \frac{V_L V_L^*}{\epsilon_f}, \quad G_{RR}(0) = \gamma - \frac{V_R V_R^*}{\epsilon_f}, \quad G_{RL}(0) = \gamma - \frac{V_L V_R}{\epsilon_f},$$

where $\epsilon_f$ is the position of the resonance and $V_L, V_R$ are the coupling constants of the resonance to the leads. Defining $s = \text{sign}(V_L V_R)$ the transmission amplitude is readily found to be:

$$t_{\text{Fano-type}}(\epsilon_f) = \frac{2i (\gamma V_{\epsilon_f} + s V_L V_R)}{i (2\gamma \epsilon_f V + V^2_L + V^2_R) + \epsilon_f V + (V^2_L + V^2_R - 2s V_L V_R) \gamma}.$$
The function $t_{\text{Fano-type}}(\epsilon_r)$ is a complex function of $\epsilon_r$ with a single pole. Therefore using the partial fraction expansion of complex functions we can write it as

$$t_{\text{Fano-type}}(\epsilon_r) = \frac{r_F}{\epsilon_r - z_F} + c_F.$$ 

Here $z_F$ is the pole, $r_F$ the residue of the pole and $c_F = 2i\gamma/(1 - 2i\gamma)$ a constant. Comparing to the Fano shape (12) and using the relations $\epsilon = \epsilon_r - \text{Re}z_F$, $\Gamma_F = 2 \text{Im}z_F$, $z_r = r_F \text{Im}z_F$, $\beta_d = \text{arg}c_F$ and $G_d = |c_F|^2$, we find that the shapes are identical. Since $t_{\text{Fano-type}}(\epsilon_r)$ has a zero (at $\epsilon_r = -sV/LV_R/(V\gamma)$) the parameter $q$ of $t_{\text{Fano}}$ is real.

As was explained earlier in this paper a zero in the transmission amplitude leads to a phase lapse. Hence for large $\gamma$ we have a zero near the position of the original resonance. The zero exists both for positive and negative $s$. Away from the zero $t_{\text{Fano}}$ is close to $c_F$ which for large $\gamma$ is close to 1. This result does not depend on the left–right asymmetry of the coupling constants to the lead. Notice, however that for the symmetric case and $s = 1$ the last term in the denominator vanishes. This makes the line shape of the $s = 1$ case very different from the $s = -1$ case. An asymmetry between left and right coupling will lead to more similar resonances.

To have isolated resonances that interfere one by one with the wide nonresonant level the distance between the zero and the original position of the resonance has to be much smaller than the average level spacing $\delta$. In other words to obtain the universal behaviour the condition:

$$V_LV_R/(V\gamma) < \delta$$

has to be fulfilled.

This condition clarifies why it is sufficient to take only relatively small $\gamma$ (of the order of 5) to see the universal behaviour.

7. Finite temperature effects

To find the temperature effects on the linear conductance $G = \frac{e^2}{\pi\hbar} |t|^2$ and phase $\text{arg}(t)$ we have to convolute the transmission probability and the transmission amplitude with the derivative of the Fermi function $f(\epsilon)$ [10]:

$$\text{arg}(t(T)) = \text{arg} \left( -\int_{-\infty}^{\infty} f'(\epsilon)t(\epsilon)d\epsilon \right),$$

(15)

$$|t|^2(T) = -\int_{-\infty}^{\infty} f'(\epsilon)|t(\epsilon)|^2d\epsilon.$$ 

(16)

At low temperature the energies $\epsilon$ are close to the Fermi level. Therefore, we can neglect the changes in the density of states and substitute $G_{LR}(0)$, $G_{RR}(0)$ and $G_{LL}(0)$ by $G_{LR}(\epsilon)$, $G_{RR}(\epsilon)$ and $G_{LL}(\epsilon)$ in the expression for the transmission in equation (2). The integrals can be performed analytically with the help of partial fraction expansion, presentation of the Fermi–Dirac function in terms of the digamma function and a contour integration, see appendix A and B.

For illustration we plot in figure 6 the result with the same parameters as before but now with $T$ equal to one twentieth of the level spacing. We see that the phase lapses are smeared. The analysis of the width of the phase lapse should be very similar to that in [10].

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Figure 6. Effect of finite temperature $T = \delta/20$ (a) $|t|^2$ and $\arg(t)$ for matrix elements with random sign and a parallel wide nonresonant level with $\gamma = 5$ and an asymmetry between the left and right coupling constants. The number of peaks is similar to the number of peaks in the absence of the nonresonant level, and between consecutive peaks we have sharp phase lapses. The temperature leads to a smearing of the phase lapses. (b) Parametric plot of $t$. Notice that the temperature average shifts the curve away from the origin and causes the phase lapse to smear. As all points are in the left part of the complex plane, the phase never exceeds $\pi$ and phase lapses must occur.

8. Conclusions

To summarize we have analysed a toy model consisting of a ladder of resonant levels with matrix elements of random sign. We showed that the addition of a parallel nonresonant level and left–right asymmetry in the coupling to the leads, causes universal phase lapses between consecutive peaks. Smearing due to finite temperature tends to average out sharp features and makes the phase lapses appear even more similar.

Our toy model does not include spin and electron–electron interaction. It should therefore be considered with a grain of salt. A few remarks are nevertheless due. It is possible to treat as a first approximation an interaction term within a self-consistent Hartree scheme. This approximation
is justified for a degenerate point [12], when the proper symmetries are utilized. The validity of such an approximation in the presence of the wide nonresonant level is, however, unclear. For a level width smaller than the level spacing, the main effect of including the interactions is the replacement of the bare levels \( \epsilon_n \) by the self consistent Hartree levels. The level spacing is then roughly \( \delta + U \) with \( U \) being the Coulomb energy.

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**Appendix A. Pole integrals involving Fermi functions**

To perform the integral

\[
 g(T) = - \int_{-\infty}^{\infty} f'(\epsilon) g(\epsilon) d\epsilon,  \tag{A.1}
\]

we first use the partial fraction expansion of the function \( g \) in terms of its poles \( \{z_i\} \), residues \( \{r_i\} \) and a constant \( c \):

\[
 g(\epsilon) = \sum_i \frac{r_i}{\epsilon - z_i} + c.  \tag{A.2}
\]

To integrate

\[
 - \int_{-\infty}^{\infty} f'(\epsilon) \frac{1}{\epsilon - z_0} d\epsilon,
\]

we use the presentation [20] of the Fermi function in terms of the digamma function \( \psi(z) \)

\[
 f(z) = \frac{1}{2\pi i} \left[ \psi \left( \frac{1}{2} + \frac{z}{2\pi iT} \right) - \psi \left( \frac{1}{2} - \frac{z}{2\pi iT} \right) + \pi i \right],
\]

the fact that \( \psi(\frac{1}{2} + \frac{z}{2\pi iT}) \) (and its derivatives) is analytic in the upper half plane of the complex plane, and perform a contour integration. For example when \( \text{Im} \ z_0 > 0 \) the second term does not contribute since we may close the contour of integration in the lower half plane, and the first term is easily integrated by closing the contour of integration in the upper half plane encircling only the pole \( z_0 \). The final result is

\[
 g(T) = c - \sum_i \frac{r_is_i}{2\pi iT} \psi' \left( \frac{1}{2} + \frac{s_i z_i}{2\pi iT} \right)  \tag{A.3}
\]

with \( s_i = \text{sign} \ (\text{Im}(z_i)) \).
Appendix B. Partial fraction expansion of \( t \) and \( |t|^2 \)

Following appendix A we perform partial fraction expansion for \( t(\epsilon) \) in equation (2)

\[
t(\epsilon) = c + \sum_i \frac{r_i}{\epsilon - z_i}.
\]  

(B.1)

Noticing that \( \forall i \text{ Im} z_i < 0 \) we find:

\[
t(T) = c + \sum_i \frac{r_i}{2\pi i T} \psi' \left( \frac{1}{2} - \frac{z_i}{2\pi i T} \right)
\]  

(B.2)

with \( z_i, r_i \) the poles and the residues of the function \( t(\epsilon) \).

The partial fraction expansion of the transmission probability is:

\[
|t|^2(\epsilon) = |c|^2 + 2 \text{Re} \left[ \sum_i \frac{c^* r_i}{\epsilon - z_i} \right] + \sum_{ij} \frac{r_i^* r_j}{z_i - z_j} \left( \frac{1}{\epsilon - z_i} - \frac{1}{\epsilon - z_j^*} \right).
\]  

(B.3)

The use of equation (A.3) yields:

\[
|t|^2(T) = |c|^2 + 2 \text{Re} \left[ \sum_i \frac{c^* r_i}{2\pi i T} \psi' \left( \frac{1}{2} - \frac{z_i}{2\pi i T} \right) \right]
\]

\[+ \sum_{ij} \frac{1}{2\pi i T} \frac{r_i^* r_j}{z_i - z_j^*} \left[ \psi' \left( \frac{1}{2} - \frac{z_i}{2\pi i T} \right) + \psi' \left( \frac{1}{2} + \frac{z_j^*}{2\pi i T} \right) \right].
\]  

(B.4)

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