Electron Scattering Through a Quantum Dot: A Phase Lapse Mechanism

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Abstract

The scattering phase shift of an electron transferred through a quantum dot is studied within a model Hamiltonian, accounting for both the electron–electron interaction in the dot and a finite temperature. It is shown that, unlike in an independent electron picture, this phase may exhibit a phase lapse of $\pi$ between consecutive resonances under generic circumstances.
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In a recent elegant experiment Yacoby et al. [1] investigated phase coherence in the Coulomb blockade regime. They have introduced a new ingredient concerning the physics of a quantum dot, namely, the scattering phase shift of an electron transmitted through a dot. Information about this phase could be obtained by incorporating the dot in a two probe Aharonov–Bohm interferometer. The experiment resulted in a remarkable observation: as the gate voltage on the dot is varied (keeping the Fermi energy of the leads attached to the dot unchanged), it is possible to scan the phase of the transmission amplitude over consecutive resonances (in energy). Changing the location of the Fermi energy from below resonance 1 (denote this situation by $1^-$) to above resonance 1 ($1^+$), the phase shift, $\theta$, is expected to increase by $\pi$, i.e., $\theta(1^+) - \theta(1^-) = \pi$. Similarly $\theta(2^+) - \theta(2^-) = \pi$ etc. The results of the experiment, consistent with these expectations, are clearly born out by the zero temperature Friedel sum rule [2,3]. The unexpected part of the observation was the indication that $\theta(2^-) - \theta(1^+) = \pm \pi$. In other words, the experiment suggests that there is a phase lapse of $\pi$ between two consecutive resonances. This phase lapse has been observed directly in a recent four probe measurement [4], and has been discussed in a few theoretical works [5–7].

In the present work we propose a mechanism that produces such an inter–resonance phase lapse. To what extent this is relevant to the the Coulomb blockade interference experiments [1,4,8] is left for future discussion. We stress, though, that the phase lapse discussed here, being an inherently finite temperature many body effect, has no analogue in an independent electron system, and is not born out by the Friedel sum rule. The phase lapse mechanism discussed here can be tested in experiments which include tunneling through a two or a few level system, e.g. a quantum spin.

The first step in our analysis is to construct a simple model for the dot and the leads attached to it, underlining the essentials required to observe the phase lapse alluded to above. Consider the following Hamiltonian (our Hamiltonian is a special case of the one employed in Ref. [3])
\[ H = H_L + H_{DL} + H_D + H_{DR} + H_R. \]  

(1)

Here \( H_L (H_R) \) describes the leads on the left (right), with the corresponding Fermi operator \( \hat{L} (\hat{R}) \):

\[
H_L = \sum_k \varepsilon_L(k) \hat{L}^\dagger(k) \hat{L}(k) \quad \text{(2)}
\]

\[
H_R = \sum_k \varepsilon_R(k) \hat{R}^\dagger(k) \hat{R}(k)
\]

where \( k \) runs over the single electron momentum states of the leads. The dot is modeled as a two–level system

\[
H_D = \varepsilon_a a^\dagger a + \varepsilon_b b^\dagger b + U a^\dagger ab^\dagger b,
\]

(3)

where \( U \) is an interaction term [9]. Coupling to the leads is described by

\[
H_{DL} = V_{aL} a^\dagger L(x_1) + V_{bL} b^\dagger L(x_1) + h.c.,
\]

(4)

\[
H_{DR} = V_{aR} a^\dagger R(x_2) + V_{bR} b^\dagger R(x_2) + h.c.,
\]

where \( x_1, x_2 \) are two coordinates on the left and on the right leads respectively, near the contacts to the dots. Here \( a^\dagger, b^\dagger \) are the creation operators of the two single electrons states on the dot. We assume that the coupling to the leads (through tunneling), given by the quantum hopping terms, is weak. Transfer of an electron through the dot may be classified into several, qualitatively different, processes [10,11]. These include sequential tunneling and inelastic cotunnelling, which do not play a role in an interference experiment since a transfer of an electron through the dot is accompanied by a change in its quantum state. Here we shall focus on coherent processes, so called elastic cotunneling.

The coherent transmission amplitude through the dot is given by a single electron retarded propagator from the l.h.s lead to the lead on the r.h.s., \( G_{RL} \). The corresponding imaginary time propagator is given by

\[
\mathcal{G}_{RL}(\epsilon_n) = -\int_0^\beta e^{i\epsilon_n \tau} \text{Tr} \left\{ \exp \left( \beta (\Omega - H) \right) \mathcal{T} \left( R(x_R, \tau) L^\dagger(x_L, 0) \right) \right\} d\tau
\]

\[
\equiv -\int_0^\beta e^{i\epsilon_n \tau} \left\langle \mathcal{T} \left( R(x_R, \tau) L^\dagger(x_L, 0) \right) \right\rangle d\tau.
\]

(5)
Here \( \Omega \) is the Gibbs potential, \( \tau = it \) is imaginary time, \( \beta \) is the inverse temperature, \( \{ \epsilon_n \} \) are fermionic Matsubara frequencies and \( \mathcal{T} \) is the imaginary time ordering operator. The operators \( R \) and \( L \) are taken at points \( x_R, x_L \) on the r.h.s and l.h.s leads respectively. The retarded propagator \( G_{RL} \) is obtained by performing the analytical continuation \( i\epsilon_n \to \varepsilon + i\gamma \)\(^+\) [12]. The propagator \( G_{RL} \), corresponding to the coherent transmission amplitude, is now calculated within a perturbation theory with respect to \( H_{DL} \) and \( H_{DR} \). To second order in the coupling it is given by [13]

\[
G_{RL}(\varepsilon_n) = G_R(\varepsilon_n;x_R,x_2) \left[ V_{aR}^* G_a(\varepsilon_n)V_{aL} + V_{bR}^* G_b(\varepsilon_n)V_{bL} \right] G_L(\varepsilon_n;x_1,x_L),
\]

(6)

Here \( G_L \) (\( G_R \)) is the propagator associated with the l.h.s. (r.h.s) lead when it is uncoupled from the dots; \( G_a \) is the propagator of an electron prepared at the state \( a \) in the uncoupled dot. One is allowed to consider low order in perturbation theory since the coupling is weak and we refer to energies \( \varepsilon \) far from the resonances [14]. The factors \( G_R, G_L \) in Eq. (6) are given by \(-i\pi\nu e^{-ik_F(x_R-x_2)}, -i\pi\nu e^{-ik_F(x_L-x_1)} \) where \( \nu \) is the density of states in the leads and \( k_F \) is the Fermi momentum. The phase factors \( e^{-ik_Fx_2} \) and \( e^{ik_Fx_1} \) cancel out similar phase factors in the coupling potential amplitudes.

This yields

\[
G_{RL}(\varepsilon_n) = -e^{i\theta_g} \pi^2 \nu^2 \left[ \tilde{V}_{aR}^* G_a(\varepsilon_n)\tilde{V}_{aL} + \tilde{V}_{bR}^* G_b(\varepsilon_n)\tilde{V}_{bL} \right],
\]

(7)

where \( \theta_g = k_F(x_R - x_L) \) is a geometrical phase. The coupling amplitudes \( \tilde{V} \) are equal to the coupling amplitudes \( V \) divided by the respective phase factors \( e^{-ik_Fx_2} \) and \( e^{ik_Fx_1} \).

In the absence of a magnetic field \( \tilde{V} \) can be chosen to be real. The Green functions associated with the dot are obtained from definitions similar to Eq. (3), summing over all relevant many body states in the dot. We adopt the notation \( |0\rangle \) (no electron in the dot),

\[
|a\rangle \equiv a\dagger |0\rangle, \quad |b\rangle \equiv b\dagger |0\rangle, \quad |ab\rangle \equiv a\dagger b\dagger |0\rangle
\]

for these states with the respective energies \( E_0 = 0, E_a = \epsilon_a - \mu, E_b = \epsilon_b - \mu, E_{ab} = \epsilon_a + \epsilon_b - 2\mu + U \). The factor \( \mu \) appears in the expression for the grand canonical energies since populating a state in the dot is associated with the removal of an electron from the leads whose electrochemical potential is \( \mu \). We now define the probabilities of the dot to be found (at equilibrium) in either of the states

\[
|i\rangle = |0\rangle, |a\rangle, |b\rangle, |ab\rangle,
\]

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\[ P_i = e^{-E_i/T} / \sum_i e^{-E_i/T}. \] (8)

We thus find
\[ G_a(\epsilon_n) = (P_0 + P_a) \frac{1}{i\epsilon_n - (\epsilon_a - \mu)} + (P_b + P_{ab}) \frac{1}{i\epsilon_n - (\epsilon_a - \mu + U)} \] (9a)
\[ G_b(\epsilon_n) = (P_0 + P_b) \frac{1}{i\epsilon_n - (\epsilon_b - \mu)} + (P_a + P_{ab}) \frac{1}{i\epsilon_n - (\epsilon_b - \mu + U)} \] (9b)

To obtain the phase shift we need to measure the interference of the transmitted amplitude with a reference beam, \( t_{ref} \). The latter is assumed to be energy independent. The magnitude of this interference term is thus given by \( 2\Re\left(t_{ref}^* t_{RL}\right) \) where
\[ t_{RL} = -\frac{1}{\pi \nu} \int d\epsilon G_{RL}(\epsilon) \frac{\partial f(\epsilon)}{\partial \epsilon}, \] (10)
and \( f \) is the Fermi–Dirac distribution. The retarded propagator \( G_{RL} \) is obtained by evaluating the expression in Eq. (6) (assuming that the coupling parameters are practically constant over an energy scale of the order of the temperature). Analytically continuing to real energies and performing the energy integration in Eq. (10) we obtain
\[ t_{RL} = e^{i\theta_g \nu} \frac{1}{2 iT} \left\{ \tilde{V}_{aR}^* \tilde{V}_{aL}(P_0 + P_a)\psi'((-E_a + i\gamma)/(2\pi iT) + 1/2) \right. \] (11)
\[ \left. + \tilde{V}_{aR}^* \tilde{V}_{aL}(P_a + P_{ab})\psi'((-E_a + U + i\gamma)/(2\pi iT) + 1/2) \right. \]
\[ + \tilde{V}_{bR}^* \tilde{V}_{bL}(P_0 + P_b)\psi'((-E_b + i\gamma)/(2\pi iT) + 1/2) \]
\[ \left. + \tilde{V}_{bR}^* \tilde{V}_{bL}(P_b + P_{ab})\psi'((-E_b + U + i\gamma)/(2\pi iT) + 1/2) \right\} , \]
where \( \psi'(z) \) is the trigamma function.

Trying to mimic real systems, the states \( a \) and \( b \) may represent two consecutive single particle levels in the dot’s spectrum. Their energies may depend (linearly) on the gate voltage applied on the dot. Below we employ the parameterization
\[ E_a = V_g, \quad E_b = V_g + \Delta. \] (12)

Before we proceed with detailed results, we present a qualitative discussion pertaining to the essential physics which leads to the interresonance phase lapse. Fig. [1] presents the
various occupation probabilities as a function of the gate voltage $V_g$, for $\Delta < T \ll U$. The range of $V_g$ depicted in Fig. 1 corresponds to two resonances that occur near $V_g = 0$ and near $V_g = -U$, respectively. These resonances, in turn, correspond to a change in the state of the dot from 0–occupied to singly occupied, and from singly to doubly occupied, respectively.

FIG. 1. Equilibrium probabilities of the four many-body dot states as a function of $V_g$, $\Delta < T \ll U$ ($\Delta = 10 \mu eV$, $T = 20 \mu eV$ and $U = 500 \mu eV$.)

We note that there are four terms which correspond to four channels through which an electron transfer through the dot can take place. We refer to these terms as $A_1$, $A_2$ (these correspond to the two terms of $G_a$, Eq. (12)) and $B_1$, $B_2$. These four terms also correspond to the four terms of the transmission amplitude, Eq. (11). We further notice that the terms $A_1$, $B_1$ ($A_2$, $B_2$) appear in connection with resonance 1 (resonance 2). If $T \geq \Delta$ the thermal factors associated with $A_1$ and $B_1$ are of comparable magnitude for the whole range of $V_g$ (a similar statement holds for $A_2$, $B_2$). At the same time, if our model represents a dot with a random potential (or of a chaotic shape), the coupling parameters exhibit strong level–to–level fluctuations [6,15]. Let us assume, for example, that for a given sample $|V_{aR}^*V_{aL}|$...
is significantly larger than $|V_{bR}V_{bL}|$. The main contribution to the transmission is then due to $A_1$, $A_2$. The term $A_1$ (cf. first term in Eq. (9a), and in Eq. (11)), represents the sum of two different second order processes: (1) an electron from the left hops to level $a$ (which was vacant) and then hops to the right; (2) an electron from level $a$, (which originally was occupied while level $b$ was empty) hops to the right, and then an electron from the lead on the left hops to state $a$. (i.e., a transfer of a hole from right to left.) Schematically, these two processes are described by the two following time sequences of the dot: (1) $|0\rangle \rightarrow |a\rangle \rightarrow |0\rangle$, (2) $|a\rangle \rightarrow |0\rangle \rightarrow |a\rangle$. In either process the transfer of an electron through the dot involves the single electron level $a$. A similar analysis applies to the term $A_2$, with two time sequences (1) $|b\rangle \rightarrow |ab\rangle \rightarrow |b\rangle$, (2) $|ab\rangle \rightarrow |b\rangle \rightarrow |ab\rangle$. Again the electron transfer takes place through the very same single particle state $a$. This is unlike an independent electron picture, whereby two consecutive resonances are associated with two different single particle states \cite{16}.

The coupling factor, $V_{aR}^*V_{aL}$ in our example, is common to both $A_1$ and $A_2$. Between the resonances (and far from them) the thermal factors are practically constant, but the denominators involved in $A_1$ and $A_2$ (Eq. (9a)) do vary with $V_g$. The one in $A_1$ (practically real positive) decreases as $V_g$ becomes more negative, while the second denominator (practically real negative) increases in magnitude. At a certain point between the resonances $A_2$ takes over $A_1$, which introduces a phase lapse of $\pi$.

Fig. 2a depicts the phase and the magnitude of the transmission amplitude for the case $T > \Delta$, when the coupling to level $a$ is stronger than the coupling to level $b$. An opposite case, where the coupling to level $b$ is stronger, is presented in Fig. 2b. For $T > \Delta$ the phase lapse between the resonances is clearly seen and is robust to changes in the values of the parameters as long as

$$\Delta/U \ll 1 \quad \text{and} \quad \frac{(\tilde{V}_{aR}^*\tilde{V}_{aL} - \tilde{V}_{bR}^*\tilde{V}_{bL})}{(\tilde{V}_{aR}^*\tilde{V}_{aL} + \tilde{V}_{bR}^*\tilde{V}_{bL})} < \frac{2T}{\Delta}. \quad (13)$$
FIG. 2. The argument of $t_{RL}$ (Eq. (11)) (solid line) and its magnitude (dashed line) for $U = 500 \mu eV$, $T = 20 \mu eV$, $\Delta = 10 \mu eV$ and $\gamma = 5 \mu eV$ (a) $\tilde{V}_{bL} = - \tilde{V}_{bR} = 0.3 \tilde{V}_{aL} = 0.3 \tilde{V}_{aR}$ (b) $0.3 \tilde{V}_{bL} = -0.3 \tilde{V}_{bR} = \tilde{V}_{aL} = \tilde{V}_{aR}$. The perturbative result (second order the couplings) should not be trusted close to the resonances. The interresonance phase lapse is apparent.

Note that the width of the phase lapse is $\sim \gamma$ and is hardly affected by a finite temperature. The reason is that $G_{RL}(\epsilon)$ is a linear function of $\epsilon$ (in the vicinity of the phase lapse). Performing the energy integration in Eq. (10) results in a virtually temperature independent $t_{RL}$. 

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This phase lapse disappears in the non–generic case where the coupling to level $a$ and $b$ are exactly equal in magnitude $[17]$. This is depicted in Fig. 3 where no interresonance phase lapse is observed $[18]$.

\[ \tilde{V}_{bL} = -\tilde{V}_{bR} = \tilde{V}_{aL} = \tilde{V}_{aR}, \quad U = 500\mu eV, \quad T = 10\mu eV, \quad \Delta = 10\mu eV \quad \text{and} \quad \gamma = 5\mu eV \quad \text{no phase lapse is observed.} \]

FIG. 3. The argument of $t_{RL}$ (solid line) and its magnitude (dashed line) for the non generic case $\tilde{V}_{bL} = -\tilde{V}_{bR} = \tilde{V}_{aL} = \tilde{V}_{aR}$, $U = 500\mu eV$, $T = 10\mu eV$, $\Delta = 10\mu eV$ and $\gamma = 5\mu eV$ no phase lapse is observed.

Our results may be generalized to an $n$–level dot. To observe an interresonance phase lapse between every two consecutive resonances, we require large enough statistical fluctuations of the couplings $\{V\}$ and a finite temperature, which satisfies a generalization of Eq. (13).

Finally, it is interesting to compare our findings with the Friedel sum rule $[2,3]$. The latter, addressing the scattering phase shift right at the Fermi energy (hence at zero temperature), predicts that as we sweep through $n$ resonances, the phase shift increases by $n\pi$. Our present analysis addresses a finite temperature scenario, and therefore is not in contradiction with the Friedel sum rule. (The interresonance phase lapse disappears at $T = 0$).
In summary, we have considered a few level model Hamiltonian describing a dot connected to leads, accounting for a finite temperature and an electron–electron interaction. The latter leads to a separation of consecutive resonances. The same single electron level may dominate the electron transfer in two resonances that are consecutive in energy. This leads to an interresonance phase lapse in the scattering phase shift, hence two consecutive resonances are in–phase vis–a–vis the scattering phase shift. We propose that this effect may be observed in a transmission experiment through a few level system (e.g. a quantum spin).

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REFERENCES

[1] A. Yacoby, M. Heiblum, D. Mahalu, and H. Shtrikman, Phys. Rev. Lett. 74, 4047 (1995), see also A. Yacoby, R. Schuster and M. Heiblum Phys. Rev. B 53, 9583 (1996).

[2] J. Friedel, Philos. Mag. 43, 153 (1952).

[3] J. S. Langer and V. Ambegaokar, Phys. Rev. 121, 1090 (1961).

[4] R. Schuster, E. Buks, M. Heiblum, D. Mahalu, V. Umansky and H. Shtrikman, (preprint).

[5] A. L. Yeyati and M. Büttiker, Phys. Rev. B 52, 14360 (1995).

[6] G. Hackenbroich and H. A. Weidenmüller, Phys. Rev. Lett. 76, 110 (1996).

[7] See also C. Bruder, R. Fazio and H. Schoeller, Phys. Rev. Lett. 76, 114 (1996).

[8] E. Buks, R. Schuster, M. Heiblum, D. Mahalu, V. Umansky and H. Shtrikman, (preprint).

[9] U can be thought of as a capacitance term, or, when a and b stand for spin states, as a Hubbard term.

[10] D. V. Averin and Y. Nazarov, Phys. Rev. Lett. 65, 2446 (1990).

[11] I. L. Aleiner and L. I. Glazman, cond–mat 05, 29 (1996).

[12] Physically the factor γ represents a finite width of a resonance.

[13] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, in Methods of Quantum Field Theory in Statistical Physics, edited by R. A. Silverman (Prentice-Hall, Inc. Englewood Cliffs, New-Jersey, 1963).

[14] Far on the scale \( V = \max \{ \nu|V_{aL}|^2, \nu|V_{bL}|^2, \nu|V_{aR}|^2, \nu|V_{bR}|^2, \gamma \} \). To be specific the small parameter of the expansion is \( V/\delta E \) where \( \delta E \) is the distance from the resonances. The parameters of the problem will not be renormalized due to multiple tunneling processes.
as long as $\frac{V}{\delta E} \log(D/V) \ll 1$, where $D$ is the band width \[13\]. We stress that the problem addressed here is that of the phase–slip between resonances, not the more trivial effect of a phase–shift by $\pi$ as one sweeps through a resonance.

[15] Y. Alhassid and C. H. Lewenkopf, Phys. Rev. Lett. 75, 3922 (1995).

[16] Note that a sequence such as $|a\rangle \rightarrow |0\rangle \rightarrow |b\rangle$ does not contribute to coherent transmission since it involves a change of the quantum state of the dot. Such inelastic cotunneling processes are not accounted for by the single particle Green’s function.

[17] We have chosen the relative sign of the parameters $V_{aR}^*V_{aL}$ with $V_{bR}^*V_{bL}$ to be opposite. As was noted in Refs. $[13,15]$ this may not always be the case, but it does not affect our generic results outlined here.

[18] Our picture is also modified in the low temperature, $T < \Delta$ limit, where the inter–resonance phase slip may interfere with the phase jump at the resonance. This more intricate picture goes beyond the second order analysis presented here.

[19] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).