Non-linear Coulomb blockade microscopy of a correlated one-dimensional quantum dot

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Abstract

We evaluate the chemical potential of a one-dimensional quantum dot coupled to an atomic force microscope tip. The dot is described within the Luttinger liquid framework, and the conductance peak positions as a function of the tip location are calculated in the linear and non-linear transport regimes for an arbitrary number of particles. The differences between the chemical potential oscillations induced by the Friedel and Wigner terms are carefully analysed in the whole range of interaction strengths. It is shown that Friedel oscillations, unlike the Wigner ones, are sensitive probes for detecting excited spin states and collective spin density waves involved in the transport.

(Some figures may appear in colour only in the online journal)
especially in the charge sector. Therefore, we treat the total number of charges and spin. The repulsive electron density modulations which can also be detected in the quantum dot. In the non-linear case, where higher excited spins are involved, Friedel oscillations increase their number, reaching that of the Wigner case for a fully polarized dot. Collective spin density excitations also induce additional density modulations which can also be detected in the chemical potential traces.

We consider an interacting 1D quantum dot, treated as a Lifshitz liquid with open boundaries. The reference state is set with an even electron number $N^0$ and Fermi momentum $k_F = N^0/2L$ (L. dot length). The low-energy Hamiltonian takes the form [18] $(h) = E_{\nu} = \frac{\nu}{2} \Delta F_{\nu}^2 + \frac{\nu}{2} \Delta N_{\nu}$, \hspace{1cm} (1)

Here $E_{\nu}, q$ are the boson operators of the collective charge $(\nu = \rho)$ and spin $(\nu = \sigma)$ density waves, with quantized wavenumber $q = \pi n_\nu/L, n_\nu \in \mathbb{N}$ and energy $E_{\nu} = \pi n_\nu/L$, where $n_\nu = \pi v_c/L$. They propagate at a renormalized velocity $v_c = v_{\rho}/g_\rho$ (where $v_{\rho}$ being the Fermi velocity) without change in the total number of charges and spin. The repulsive electron interaction strength is represented by $g_\rho = g < 1$, while $g_\sigma = 1$ for an SU(2) invariant theory [16]. The second part of the Hamiltonian represents the zero-mode contributions with $\Delta N_{\rho,\sigma} = \Delta N_{\rho} \pm \Delta N_{\sigma}$, where $\Delta N_{\rho} = N_{\rho} - N^0$ are the extra electron per spin direction ($s = \pm$) with respect to the reference $N^0$ state. The total charge and spin are $N_{\rho} = \Delta N_{\rho} + N^0$ and $N_{\sigma} = \Delta N_{\sigma}$, with energies $E_{\rho}$ and $E_{\sigma}$. Despite the microscopic model providing their quantitative estimates ($E_{\nu} = \pi v_c/Lg_\nu$), several effects, e.g. coupling with the external gates or long range interactions, cause deviations, especially in the charge sector. Therefore, we treat $E_{\rho}$ as a free parameter, with $E_{\rho} \gg E_{\sigma}$, while keeping $E_{\sigma} = \pi v_c/2L = \pi/2$. Let us denote the eigenstates of the above Hamiltonian as $|S\rangle = |N_\rho, N_\sigma, \{n_\rho\}, \{n_\sigma\}\rangle$ with energies

$E(S) = \sum_{\rho,\sigma} \sum_{q \geq 0} \left[ E_{\rho} \Delta F_{\rho}^2 + \frac{\nu}{2} \Delta N_{\rho} \right]$, \hspace{1cm} (2)

where $\{n_\rho\}$ are the occupation numbers for the collective mode $v$ at momentum $q$. The electron operator $\Psi_{s}(x)$, with boundary conditions $\Psi_{s}(0) = \Psi_{s}(L) = 0$, is represented in terms of right-moving electrons as $\Psi_{s}(x) = e^{i k_F x} \psi_{s,R}(x) - e^{-i k_F x} \psi_{s,L}(x)$ [18]. In bosonized form

$\psi_{s,R}(x) = \frac{\eta_\rho}{\sqrt{2\pi} \alpha} e^{-i \theta_0} e^{i \Delta F_{\rho} x} e^{\frac{\nu}{2} \frac{\pi}{\lambda} x} e^{-i k_F x \psi_{s,R}(x) - e^{-i k_F x} \psi_{s,L}(x)}$. \hspace{1cm} (3)

Here $\{\eta_\rho, \eta_\sigma\} = \delta_{s,s'}$, $\alpha = k_F^{-1}$ is the cutoff length, $[\theta_0, \Delta F_{\rho}] = i \delta_{s,s'}$ and

$\Phi_{s}(x) = \sum_{q \geq 0} \frac{e^{-\nu q/2}}{\sqrt{\nu q^2}} (\cos(qx) - i \eta_\rho \sin(qx)) d_{s,q}^\dagger + h.c.$, \hspace{1cm} (4)

The total electron density $\rho(x) = \sum_{\rho} \rho_{\rho}(x)$ with $\rho_{\rho}(x) = \Psi_{\rho}^\dagger(x) \Psi_{\rho}(x)$ consists of several contributions [25, 28]. Here we take into account the most relevant adopting a number-conserving formalism [29] for open boundaries. The smooth long-wave term $\rho_{LW}(x) = \sum_{\rho} \rho_{LW}(x)$ is given by

$\rho_{LW}(x) = \frac{k_F}{\pi} \Delta N_{\rho} \frac{2}{\pi} \delta_{s,s'} h(x)$, \hspace{1cm} (5)

with $\psi_{s}(x) = [\psi_{s}(x) + s \psi_{s}(x)]/\sqrt{2}$ where

$\psi_{s}(x) = \frac{1}{2} \phi_{s}(x) - \Phi_{s}(x)$, \hspace{1cm} (6)

and $h(x) = \frac{1}{2} \tan^{-1} \left[ \frac{\sin(\pi x/L)}{\cos(\pi x/L)} \right]$. The oscillating Friedel contribution is $\rho_{F}(x) \propto \sum_{\rho} \rho_{F}^\dagger(x)$ with $\rho_{F}^\dagger(x) = e^{-2i k_F x} \psi_{s,R}(x) \psi_{s,R}(-x) + h.c.$ in bosonic representation one has

$\rho_{F}(x) = -\frac{1}{2\pi} \frac{\partial x}{\partial h_{x}} \left[ L(\Delta N_{\rho}, x, g), 2 \psi_{s}(x) \right]$, \hspace{1cm} (7)

where

$L(n, x, g) = 2k_F x + \frac{2\pi n x}{L} - 2g^2 h(x)$. \hspace{1cm} (8)

In addition to these 'standard' terms we include the so-called Wigner contribution $\rho_{W}(x) \propto e^{-4i k_F x} \psi_{s,L}^\dagger(x) \psi_{s,L}(-x) \psi_{s,R}^\dagger(x) \psi_{s,R}(-x) + h.c.$ which may arise due to interaction effects, band curvature or other external perturbations [26, 28, 27]. In the bosonization language [25] one has

$\rho_{W}(x) = -\frac{1}{2\pi} \frac{\partial x}{\partial h_{x}} \left[ 2L \left( \Delta N_{\rho}^2, x, g \right) + 2\sqrt{2} \psi_{s}(x) \right]$. \hspace{1cm} (9)

Note that these terms constitute the most relevant contributions to the electron density, whose amplitudes are to be interpreted as model parameters [25, 28]. The total density, satisfying boundary conditions $\rho(0) = \rho(L) = 0$, can then be expressed as

$\rho(x) = \rho_{LW}(x) + (1 - \lambda) \rho_{F}(x) + \lambda \rho_{W}(x)$, \hspace{1cm} (10)

with $\lambda \in [0, 1]$ a free parameter.

We now analyse the expectation values $\rho_{GS}^\xi = \langle S | \rho_{\xi}(x) | S \rangle_{GS}$ on the ground state $|S \rangle_{GS} = |N_{\rho}^0, N_{\sigma}^0, \{n_\rho^0\}, \{n_\sigma^0\}\rangle$ for the different contributions $\xi = LW, F, W$. Note that, due to $N^0$ being even, one has $N_{\rho}^0 = N^0$ and $N_{\sigma}^0 = 0$ with $\Delta N_{\rho}^0 = 0$ for an even number of electrons, while $N_{\rho}^0 = N^0 + 1$ and $N_{\sigma}^0 = \pm 1$ with $\Delta N_{\rho}^0 = 1$ for the nearest larger odd electron number. Using the bosonization technique one obtains

$\rho_{LW}(x) = \frac{2k_F}{\pi} \left( \frac{\pi}{\lambda} \Delta N_{\rho}^0 \right) - 2g^2 \frac{\partial x}{\partial h_{x}}$. \hspace{1cm} (11)
contributions. Figure 2 shows of particles increases.

reversed. This fact is particularly evident when the number for strong interactions (panels (b) and (d)), the situation is Wigner ones for weak interactions (panels (a) and (c)), while easily see that Friedel oscillations are dominant over the number of observed peaks. Concerning amplitudes one can equation (13)) and depends on \( N \) (\( \lambda \)).

\[
\rho_{GS}^F(x) = -\frac{1}{2\pi} \partial_x \left\{ K^F \sum_{s=\pm} \sin[L(\Delta N_{GS}^F, x, g)] \right\},
\]

\[
\rho_{GS}^W(x) = -\frac{1}{2\pi} \partial_x \left\{ K^W \sin \left[ 2L\left( \frac{\Delta N_{GS}^W}{2}, x, g \right) \right] \right\}
\]

with the enveloping functions (\( \eta_F = \frac{1+g}{2}; \eta_W = 2g \)).

\[
K^F(x) = \left[ \frac{\sinh \left( \frac{\pi x}{2\pi} \right)}{\sqrt{\sin^2 \left( \frac{\pi x}{2\pi} \right) + \sin^2 \left( \frac{\pi x}{2\pi} \right)}} \right]^N_{\lambda}. \tag{14}
\]

Let us now study the Friedel and Wigner contributions separately. Figure 1 shows the electron density (see equation (10)) in the ground state with the long-wave part and the Friedel (\( \lambda = 0 \)) or the Wigner (\( \lambda = 1 \)) terms. In both cases it exhibits an oscillatory behaviour but with different patterns and amplitudes. The Friedel contribution shows oscillations related to the two different electron spin populations. In particular, for even electrons one has \( N_{GS}^F = \frac{N_{GS}^F}{2} \) and thus the superposition results in \( N_{GS}^F/2 \) peaks. For odd numbers, one of the two sub-populations has \( (N_{GS}^F + 1)/2 \) electrons, while the other has \( (N_{GS}^F - 1)/2 \). The superposition for both spin directions then has \( (N_{GS}^F + 1)/2 \) peaks. The Wigner correction, on the other hand, is insensitive to spin (see equation (13)) and depends on \( N_{GS}^W \) only, which is also the number of observed peaks. Concerning amplitudes one can easily see that Friedel oscillations are dominant over the Wigner ones for weak interactions (panels (a) and (c)), while for strong interactions (panels (b) and (d)), the situation is reversed. This fact is particularly evident when the number of particles increases.

Let us now consider the combined effects of both contributions. Figure 2 shows \( \rho_{GS}(x) \) as a function of \( x \) and \( g \) for \( \lambda = 0.5 \) (see equation (10)). For weak interactions (\( g \approx 1 \)) one can distinguish \( (N_{GS}^F + 1)/2 \) peaks (in both panels \( N_{GS}^F \) is odd). At strong interactions (\( g \to 0 \)), Wigner correlations grow and eventually the density exhibits sharp oscillations with \( N_{GS}^F \) peaks. Thus, even when Wigner correlations are mixed along with Friedel ones, the presence of strong interactions makes the Wigner channel the relevant one. The above behaviour can be attributed to the enveloping functions \( K^F(x) \) and \( K^W(x) \) in equation (14). For \( g \to 1 \), the weaker power law in \( K^F(x) \) (namely, \( x^{-1(1+g)/2} \)) in comparison to that of \( K^W(x) \) (namely, \( x^{-2g} \)) leads to a suppression of the Wigner channel. On the other hand, when \( g \to 0 \) one has \( K^W(x) \to 1 \) and \( K^F(x) \ll 1 \) away from the borders. Thus, for strong interactions Friedel oscillations are damped, while the Wigner ones are still fully developed.

We would now like to show how to probe electron density correlations in the presence of a movable AFM tip. This has already been considered as a powerful tool for investigating the electronic correlated state for linear transport in dots with few electrons [13]. Here we will consider the more general non-linear regime, without any constraint on the number of electrons.

The charged AFM tip is capacitively coupled to the dot at position \( x \), with coupling \( H_{tip} = V_0 \rho(x) \), assuming a tip narrower than the average wavelength of the density oscillations. In the sequential regime, for a given transition \( |S \rangle \to |S' \rangle \), electrons tunnel between the dot and the leads and the number of dot charges oscillates between \( N_{\rho} \) and \( N_{\rho} + 1 \), with the spin constraint \( |N_{\rho} - N_{\rho}| = 1 \). The onset of a transition is signalled by peaks in the differential conductance.

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In the following we will determine their positions as a function of the tip. The key quantity to evaluate is the generalized chemical potential

$$\mu_{S \rightarrow S'}(x) = E_{\text{tot}}(S', x) - E_{\text{tot}}(S, x),$$

(15)
defined in terms of the total energy $E_{\text{tot}}(S, x)$ in the presence of the tip. Indeed, whenever $\mu_{S \rightarrow S'}(x) \approx \mu_\chi$, where $\mu_\chi$ is the electrochemical potential of the lead $\chi$, the given transition becomes allowed. We will evaluate equation (15) in the weak tip-coupling regime, namely $E_{\text{tot}}(S, x) = E(S) + \delta E(S, x)$ with $\delta E(S, x)$ the lowest order correction.

We will consider only non-degenerate energy levels, whose corrections to the energy $E(S)$ in equation (2) are given by $\delta E(S, x) = V_0|\delta\mu(x)|(|S|)$. This is a relevant case since it applies to zero-mode spin excited states (the degeneracy on $\pm |N_\sigma|$ is explicitly diagonal and does not cause problems) and to the lowest lying spin density waves with a singly occupied bosonic state. The latter is indeed non-degenerate in the presence of interactions since $\varepsilon_\sigma < \varepsilon_{\bar{\sigma}}$. Generalizing the results obtained for the ground state one has

$$\delta E_{\text{FW}}(S, x) = \delta E_{\text{FW}}^L(S, x) + (1 - \lambda)\delta E_{\text{FW}}^S(S, x) + \lambda \delta E_{\text{FW}}^W(S, x),$$

(16)

and $\delta E_{\text{W}}(S, x) = V_0 \left[ \frac{2\varepsilon_\sigma}{\pi} \right]$, $\lambda = \frac{\sigma}{\sum_{\lambda} \lambda}$, $\sigma = \frac{\lambda|\delta\mu(x)|(|S|)}{\sum_{\lambda} \lambda}$. The corresponding chemical potential is then decomposed as $\mu_{S \rightarrow S'}(x) = G^F(x) + G^W(x)$. The linear regime corresponds to the bare one, $\mu_{S \rightarrow S'}(x) = E(S') - E(S)$ (see equation (2)), and the tip correction, $\delta \mu_{S \rightarrow S'}(x) = \delta E_{\text{FW}}^L(S, x) + \delta E_{\text{FW}}^W(S, x)$ (see equations (16)–(18)). In short notation, omitting the states, one has

$$\mu(x) = \mu_0 + \delta \mu(x)$$

(19)

and

$$\delta \mu(x) = \delta \mu_{\text{FW}}^L + (1 - \lambda)\delta \mu_{\text{FW}}^S + \lambda \delta \mu_{\text{FW}}^W.$$  

(20)

We are now in a position to investigate the chemical potential variation as a function of the tip position for a given transition. We start by considering the linear regime where only the ground states are involved: $|S⟩_{\text{GS}}$ with total number of particles $N_\rho$, and $|S'⟩_{\text{GS}}$ with total number $N_\rho'$. The Friedel term, shown in panel (a) for even $N_\rho' = 0$, displays 1 maxima and 2 minima. The number of these maxima is related to the spin population of the final state of the dot. Indeed, the initial spin populations are $N_\sigma = N_\rho/2$. When an extra electron, with spin up, enters into the dot, the state with $N_\rho = 1$ is reached with $N_\rho' = 1 + N_\rho/2$. These are indeed the values which correspond to the number of maxima and minima exhibited. A similar behaviour holds for an odd number $N_\rho$ (not shown) where one finds $(N_\rho + 1)/2$ maxima and $(N_\rho - 1)/2$ minima. Thus, in the Friedel case the oscillations of the chemical potential are a sensitive probe to detect the spin sub-populations of the electron involved in the linear transport process. The Wigner case, on the other hand, is not sensitive to the spin direction. As shown in panel (b), it always displays $N_\rho + 1$ maxima and $N_\rho$ minima, allowing us to count the total number of electrons only. Panels (c) and (d) show the combined effect of equally weighted Friedel and Wigner corrections. For strong interactions (panel (d)), Wigner corrections are clearly well pronounced, differently from the weak interactions case (panel (c)). These results are in agreement with those obtained for few particles with an exact diagonalization procedure [13].

Let us turn to the non-linear case, with excited zero-mode spin states and for the moment without collective modes. This has never been investigated in literature to our knowledge. The transitions are between states of the form $|S⟩ = |N_\rho, N_\sigma⟩$ and $|S'⟩ = |N_\rho', N_\sigma'⟩$, with $N_\rho, N_\rho'$ and no longer restricted to the ground state values. We select, in particular, $N_\rho' = N_\rho + 1$ and $N_\rho = 2k$ with $k \in \mathbb{N}$, focusing on the Friedel contribution only. The Wigner contribution is indeed insensitive to the total spin (see equation (18)) and will give, for each of the above transitions, a contribution equal to that of the linear case. The possible spin transitions are $|N_\rho, 0⟩ \rightarrow |N_\rho + 1, 1⟩; |N_\rho + 1, 1⟩ \rightarrow |N_\rho, 2⟩; \ldots; |N_\rho', N_\sigma'⟩ \rightarrow |N_\rho + 1, N_\rho' + 1⟩$. Namely, the dot starts in the ground state with $N_\rho = N_\rho'/2$, eventually becoming fully polarized. As a representative example we show in figure 4(a) the position dependence of the chemical potential in equation (19) with

![Figure 3](image_url)
of coupling with a moving AFM tip. As a general trend, traces of an interacting 1D quantum dot in the presence due to the different contribution of the function $G$. Figure 4.

Even. Figure 4(b) shows the corresponding chemical potential $\mu$ two transitions have the same bare chemical potential corresponding to the overall behaviour is similar to the green trace in figure 4(a). $|6, 0, |n^q = 0, |n^\rho = 0,\rangle \rightarrow |7, 1, |n^q = 0,\rangle \rightarrow |7, 1, |n^\rho = 0,\rangle$ involving a spin density wave (black) and $|6, 2 \rightarrow |7, 3$ involving zero-modes only (green). In both panels $g = 0.7, E_\rho = 10E_\sigma, V_0 = 0.08E_\sigma$ and $a^{-1} = 3\pi/L$.

the Friedel contribution for the tunnel-in transitions. Starting with $N_\rho/2 + 1$ maxima in the ground states (blue trace), an increasing number of oscillations appear as higher spin states get involved. Eventually, the transition involving fully polarized dot state is reached and the chemical potential shows with $N_\rho + 1$ maxima (red trace). Note that this is the same number of maxima that one would obtain from the Wigner corrections.

The sensitivity of the Friedel corrections to spin suggests the employment of non-linear transport experiments in the presence of an AFM tip to explore highly excited spin states of quantum dots. This seems particularly desirable for interactions that are not too strong, when the Wigner corrections do not dominate over the Friedel ones. It is also possible to conclude that the observation of $N_\rho + 1$ peaks in the chemical potential for an excited transition does not alone provide clear-cut evidence of the presence of Wigner correlations.

We close our discussion by briefly addressing how the above effect can be obtained also for transitions involving excited spin density waves, previously neglected. In general, and in contrast to zero-mode excitations, collective modes are assumed to relax to the ground state over a time shorter than the average tunnelling time of electrons due to several possible types of dissipative coupling. This implies excitations only in final states. To be more specific we consider a transition from the ground state to the lowest lying collective spin excitation with $q = \pi/L$. The two involved states are $|N_\rho, 0, |0_\sigma, |0_\rho\rangle \rightarrow |N_\rho + 1, 1, |0_\sigma, |n^q = \delta_{q, \pi/L}\rangle$ with $N_\rho$ even. Figure 4(b) shows the corresponding chemical potential with Friedel corrections for $N_\rho = 6$. It exhibits five peaks and the overall behaviour is similar to the green trace in figure 4(a) corresponding to $|6, 2 \rightarrow |7, 3$. Indeed since $2E_\rho = E_\sigma$, the two transitions have the same bare chemical potential $\mu_0 = E_\rho(2N_\rho + 1)/2 + 5E_\sigma/2$ but different corrections $\delta \mu(x)$, also due to the different contribution of the function $G^2(x)$ in equation (17).

In conclusion, we have studied the chemical potential traces of an interacting 1D quantum dot in the presence of coupling with a moving AFM tip. As a general trend, we have found that Friedel modulations dominate for weak interactions and are sensitive to spin populations, while the Wigner oscillations become relevant at strong interactions and depend on the total charge sector only. We demonstrated that this results in markedly different behaviours. In the linear regime, Friedel correlations exhibit half the number of oscillations of the Wigner ones. On the other hand, in the non-linear case, when higher excited spin are involved, they increase the number of oscillations, reaching that of the Wigner case for a fully polarized dot. We expect that predicted oscillations of the chemical potential traces as a function of the AFM tip will be observed in transport experiments.

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