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Coulomb blockade in a non-thermalized quantum dot

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We investigate non-equilibrium transport properties of a quantum dot in the Coulomb blockade regime under the condition of negligible inelastic scattering during the dwelling time of the electrons in the dot. Using the quantum kinetic equation we show that the absence of thermalization leads to a double-step in the distribution function of electrons on the dot, provided that it is symmetrically coupled to the leads. This drastically changes nonlinear transport through the dot resulting in an additional (compared to the thermalized case) jump in the conductance at voltages close to the charging energy, which could serve as an experimental manifestation of the absence of thermalization.

Many-body localization (MBL), predicted for disordered many-electron systems which are not thermalized with the environment [1, 2], has attracted a lot of theoretical and experimental attention (for a review see [3]) and has been observed in systems of ultracold atoms [4]. One of the defining properties of MBL is the absence of thermalization [5, 6].

Prior to the MBL papers [1, 2], a similar regime of localization in Fock space was predicted for quantum dots [7] where electrons fail to mutually equilibrate as their dwelling time on the dot, τ_{dw} , is much shorter than the equilibration time τ_{eq} . Alternatively, this condition can be formulated as

$$\gamma \ll \Gamma, \quad (1)$$

where $\gamma \sim 1/\tau_{\text{eq}}$ is the equilibration rate and $\Gamma \sim 1/\tau_{\text{dw}}$ is the tunneling rate. For a zero-dimensional diffusive dot, the electron-electron equilibration rate [7–9],

$$\gamma \approx \Delta \left(\frac{\varepsilon}{g\Delta} \right)^2, \quad (2)$$

can be sufficiently small provided that $\sqrt{g}\Delta < \varepsilon < g\Delta$, where Δ is the mean level spacing on the dot, and $g\Delta$ is the Thouless energy of the dot with dimensionless conductance $g \gg 1$.

In this Letter, we show that such an absence of thermalization leads to striking changes in nonlinear transport in the Coulomb blockade regime, where electrons are loaded one-by-one into a quantum dot due to the charging energy, $E_c = e^2/C$, of a dot of capacitance C , preventing a continuous flow. We assume the separation of scales typical for the classical Coulomb blockade at a temperature T (see [10–12] for reviews):

$$\Gamma \ll \Delta \ll T \ll E_c. \quad (3)$$

Typically, the study of quantum dots in the Coulomb blockade regime has been focused on the regime where complete thermalization is assumed. This regime is characterized by peaks in the conductance as a function of gate voltage [13, 14] that can be attributed to interesting features in the tunneling density of states [15], and –

in case of strong asymmetry in the coupling to the leads – by a staircase in the current as a function of the bias voltage V [16–19]. When the coupling is approximately symmetric, $\Gamma_L \sim \Gamma_R$, the Coulomb staircase practically vanishes in the thermalized case. But it is precisely in this case when the absence of thermalization reveals itself by an additional jump in the nonlinear differential conductance, as we show in this Letter by solving the quantum kinetic equation. The absence of thermalization on a dot, therefore, can be detected by this jump which occurs within the first step of the Coulomb staircase.

The jump arises due to the change in the distribution function of the dot; going from a Fermi function in the fully thermalized case to a double-step form. Such a structure has previously been observed in one-dimensional wires where the distribution function was a linear combination of the two Fermi functions of the leads due to insufficient time for equilibration [20].

The standard Hamiltonian of a Coulomb-blockaded quantum dot coupled to two leads is $H = H_{\text{dot}} + H_1 + H_{\text{tun}}$, where

$$H_{\text{dot}} = \sum_n \varepsilon_n d_n^\dagger d_n + \frac{1}{2} E_c (\hat{N} - N_g)^2, \quad (4a)$$

$$H_1 = \sum_{k,\alpha} (\varepsilon_k - \mu_\alpha) c_{k,\alpha}^\dagger c_{k,\alpha}, \quad (4b)$$

$$H_{\text{tun}} = \sum_{k,n,\alpha} (t_\alpha c_{k,\alpha}^\dagger d_n + \text{h.c.}). \quad (4c)$$

Here $\alpha=L, R$ labels the leads, $d_n^\dagger(d_n)$, $c_{k,\alpha}^\dagger(c_{k,\alpha})$ are the creation (annihilation) operators for electrons with energies ε_n and ε_k in the dot and leads respectively, $\hat{N} = \sum_n d_n^\dagger d_n$ is the number operator for the dot, and N_g is the preferred number of electrons on the dot set by the gate voltage. The leads have chemical potentials $\mu_L = \mu + eV$ and $\mu_R = \mu$. The k - and n -independent tunneling amplitudes between the dot and leads, t_α , define, along with the density of states of the leads ν_α (taken to be constant), the tunneling rates $\Gamma_\alpha = 2\pi\nu_\alpha |t_\alpha|^2$ with the total $\Gamma = \Gamma_L + \Gamma_R$.

In addition to inequalities (3), we assume that the Fermi energy of the dot is much larger than the charging energy, $\varepsilon_F \gg E_c$, to ensure that only electrons in a relatively narrow energy strip around ε_F contribute the transport properties of the system. This assumption is

$$I = e \frac{\Gamma_L \Gamma_R}{\Gamma} \sum_{N,n} p_N \left(F_N(\varepsilon_n) [f_L(\varepsilon_n + \Omega_{N-1}) - f_R(\varepsilon_n + \Omega_{N-1})] + (1 - F_N(\varepsilon_n)) [f_L(\varepsilon_n + \Omega_N) - f_R(\varepsilon_n + \Omega_N)] \right). \quad (5)$$

Here p_N is the probability of N electrons being on the dot, $F_N(\varepsilon_n)$ is their distribution function, and $f_{L,R}(\varepsilon_n)$ are Fermi functions in the leads with chemical potentials $\mu_L = \mu + eV$ and $\mu_R = \mu$ respectively. The presence of the charging energy is encapsulated by

$$\Omega_N = E_{N+1} - E_N = E_c \left(N + \frac{1}{2} - N_g \right), \quad (6)$$

where $E_N = \frac{1}{2} E_c (N - N_g)^2$.

The current through a thermalized quantum dot is usually considered with the help of a master equation [13, 14, 16–19] involving electrons of all energies. In the non-thermalized regime (1), the electrons with different energies are not mixed. Hence, the probabilities and distribution functions can be found from the energy-conserving quantum kinetic equation (QKE), which is formulated using the Keldysh formalism (see, e.g., [22–24]) in terms of the “greater”, $g^>(t)$, and “lesser”, $g^<(t)$, Green’s function of the dot. In the regime (3), where the mean level spacing is much larger than the level broadening due to tunneling, they are split into a sum over the energy levels, with Green’s function for the n^{th} level given by $g_n^>(t) = -i \langle d_n(t) d_n^\dagger(0) \rangle$ and $g_n^<(t) = i \langle d_n^\dagger(0) d_n(t) \rangle$, where $d_n(t) = e^{iHt} d_n e^{-iHt}$. Then, to linear order in tunneling, the QKE is reduced to [22–24],

$$g_n^>(\varepsilon) \Sigma^<(\varepsilon) = g_n^<(\varepsilon) \Sigma^>(\varepsilon). \quad (7)$$

Here, the conservation of particle number for an isolated dot allows one to represent the single-level Green’s functions as

$$\begin{aligned} g_n^>(\varepsilon) &= -2\pi i \sum_N \delta(\varepsilon - \varepsilon_n - \Omega_N) p_N (1 - F_N(\varepsilon_n)), \\ g_n^<(\varepsilon) &= 2\pi i \sum_N \delta(\varepsilon - \varepsilon_n - \Omega_{N-1}) p_N F_N(\varepsilon_n), \end{aligned} \quad (8)$$

with the normalization $\sum_N p_N = 1$. The self-energy functions of the leads in Eq. (7) are assumed to be n -independent and are given by

$$\Sigma^>(\varepsilon) = i \sum_{\alpha=L,R} \Gamma_\alpha (f_\alpha(\varepsilon) - 1), \quad \Sigma^<(\varepsilon) = i \sum_{\alpha=L,R} \Gamma_\alpha f_\alpha(\varepsilon). \quad (9)$$

also utilized in the orthodox theory of the Coulomb blockade [14, 16–19] and is achievable in experiments [10, 21]. Assuming current conservation, the current across the quantum dot is given by [22]

Substituting Eqs. (8) and (9) into Eq. (7) leads to the QKE reflecting the detailed balance equations, coinciding with those derived in [14] for $\Delta \gg T$,

$$\begin{aligned} p_{N+1} F_{N+1}(\varepsilon_n) \left(1 - \tilde{f}(\varepsilon_n + \Omega_N) \right) \\ = p_N (1 - F_N(\varepsilon_n)) \tilde{f}(\varepsilon_n + \Omega_N), \quad (10) \\ \tilde{f}(\varepsilon) = (\Gamma_L/\Gamma) f_L(\varepsilon) + (\Gamma_R/\Gamma) f_R(\varepsilon). \end{aligned}$$

It is this equation along with the normalization conditions, $\sum_N p_N = 1$ and $\sum_n F_N(\varepsilon_n) = N$, that can be used to obtain the probabilities and distribution functions required in Eq. (5) to calculate the current. The results for full thermalization are recovered by summing Eq. (10) over n and making the replacement $F_N(\varepsilon_n) \rightarrow f(\varepsilon_n - \varepsilon_F)$.

As we show in *Supplemental Material*, this equation has an exact solution providing there are only two relevant states (N and $N + 1$) for a given voltage. In the case of approximately equal coupling, this condition can be satisfied only for a finite bias window, i.e. within the first step of the Coulomb staircase. For higher bias, there are more states with different numbers of particles that are not being exponentially suppressed (in contrast to the asymmetric case when $\Gamma_L/\Gamma_R \gg 1$ [25]).

Assuming that the chemical potential in the dot is of order of the unbiased chemical potential in the (right) lead, we show that the current and, hence, the differential conductance has an additional peak in the window $0 \leq eV \lesssim \Omega_{N+1}$ as compared to the thermalized case [16–19]. In this window, where only two levels are relevant, the kinetic equation (10) has the solution $F_N(\varepsilon_n) \approx F_{N+1}(\varepsilon_n) \approx F(\varepsilon_n)$ in the limit $N \gg 1$, leading to

$$F(\varepsilon_n) = \frac{\tilde{f}(\varepsilon_n + \Omega_N)}{[1 - \tilde{f}(\varepsilon_n + \Omega_N)] A_N + \tilde{f}(\varepsilon_n + \Omega_N)}, \quad (11)$$

where $A_N = p_{N+1}/p_N$. This ratio of probabilities is found from normalization, $N = \sum_n F(\varepsilon_n) = (1/\Delta) \int_0^\infty F(\varepsilon) d\varepsilon$, while $p_N + p_{N+1} = 1$ when only two states are relevant.

In the regime characterized by the inequalities (1) and (3), $\tilde{f}(\varepsilon_n + \Omega_N)$ can be split into three regions, (i) $\varepsilon_n <$

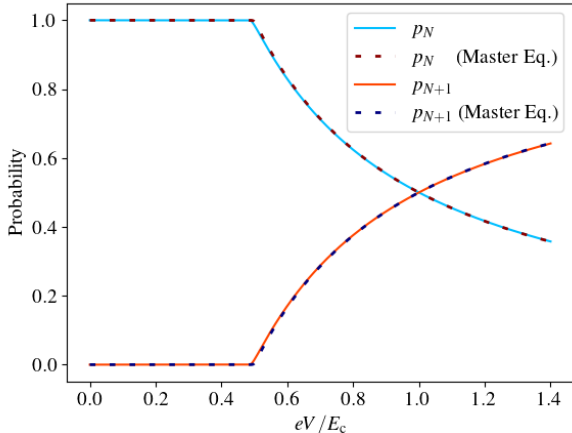


FIG. 1. The occupation probabilities of the two states of the dot as a function of bias voltage, V , for $\Gamma_L = \Gamma_R$ and $\Omega_N = E_c/2$. The solid lines are our results and the dashed lines are those obtained in the case of full thermalization using the master equation approach [16–19]. In the low-temperature limit shown, the results are practically indistinguishable.

$\mu - \Omega_N$, (ii) $\mu - \Omega_N < \varepsilon_n < \mu - \Omega_N + eV$, and (iii) $\varepsilon_n > \mu - \Omega_N + eV$, as follows

$$\tilde{f}(\varepsilon_n + \Omega_N) \approx \begin{cases} 1 - (\Gamma_R/\Gamma)e^{\beta(\varepsilon_n - (\mu - \Omega_N))}, & \text{(i)} \\ \Gamma_L/\Gamma, & \text{(ii)} \\ (\Gamma_L/\Gamma)e^{-\beta[\varepsilon_n - (\mu - \Omega_N + eV)]}. & \text{(iii)} \end{cases} \quad (12)$$

Using the normalization of $F(\varepsilon_n)$ with $\varepsilon_F = N\Delta$ and splitting up Eq. (11) into these three regions results in the following equation to determine A_N :

$$\beta\varepsilon_F = \frac{\beta eV}{A_N \frac{\Gamma_R}{\Gamma_L} + 1} + \ln \left(\frac{\Gamma}{\Gamma_R A_N} e^{\beta(\mu - \Omega_N)} + 1 \right) + \ln \left(\frac{\frac{\Gamma_L}{\Gamma} + A_N}{\frac{\Gamma}{\Gamma_R} + A_N} \right). \quad (13)$$

Solving this equation numerically across the entire voltage range, $0 \leq eV \lesssim \Omega_{N+1}$ gives the probabilities p_N and p_{N+1} as shown in Fig. 1. They are practically the same as in the standard theory of the Coulomb blockade of completely thermalized quantum dots [16–19].

The absence of thermalization, however, drastically changes the distribution function. By substituting the solution of Eq. (13) into Eq. (11), we obtain the double-step distribution function for $A_N \sim 1$ (i.e. $p_N \sim p_{N+1}$), in contrast to the Fermi function $f(\varepsilon - \varepsilon_F)$ in the case of full thermalization. The steps in $F(\varepsilon_n)$ occur in the same three regions as in Eq. (12),

$$F(\varepsilon_n) \approx \begin{cases} 1, & \text{(i)} \\ \left(1 + \frac{\Gamma_R}{\Gamma_L} A_N\right)^{-1}, & \text{(ii)} \\ 0. & \text{(iii)} \end{cases} \quad (14)$$

which is depicted in Fig. 2. It is possible to write this as a linear combination of two Fermi functions, directly reflecting the lack of thermalization between electrons coming from the left and right leads. In a steady state, electrons from both leads enter the dot at two different chemical potentials and thermalize with the opposite lead only after exiting the dot. The ratio of the two contributions is determined by the relative tunneling probabilities so that the double-step is washed out only in the case of extreme anisotropy, e.g. $\Gamma_R/\Gamma_L \ll 1$.

The double-step distribution in the dot drastically changes the differential conductance, $G = dI/dV$, in comparison with the thermalized case [16–19]. Substituting p_N and $F(\varepsilon_n)$ into Eq. (5) with $F_N(\varepsilon_n) \approx F(\varepsilon_n)$, we find G as shown in Fig. 3. For small voltages, $eV \lesssim E_c$, the absence of thermalization has little impact in the low- T limit. However, at $eV \approx E_c$, there appears a secondary jump in the non-thermalized case. It is robust as long as the tunneling is symmetric, $\Gamma_L \approx \Gamma_R$, when there are three distinct regions for the distribution, Eq. (14). Rewriting the current in the low- T limit makes this clearer,

$$I = \frac{e}{\Delta} \frac{\Gamma_L \Gamma_R}{\Gamma} \left(p_N \int_{\mu - \Omega_{N-1}}^{\mu - \Omega_{N-1} + eV} F(\varepsilon) d\varepsilon + \int_{\mu - \Omega_N}^{\mu - \Omega_N + eV} [p_N(1 - F(\varepsilon)) + p_{N+1}F(\varepsilon)] d\varepsilon + p_{N+1} \int_{\mu - \Omega_{N+1}}^{\mu - \Omega_{N+1} + eV} (1 - F(\varepsilon)) d\varepsilon \right). \quad (15)$$

The second integration over the middle step always gives a non-zero contribution. For $eV < E_c$, the remaining in-

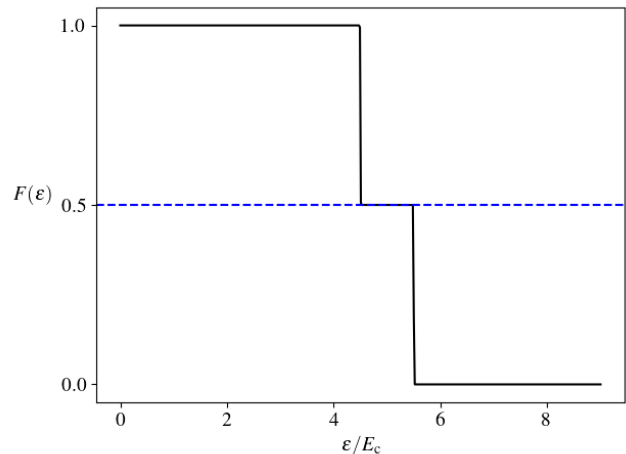


FIG. 2. The distribution function of the dot for $eV = E_c$, $\Gamma_L = \Gamma_R$ and $N = N_g$, where $A_N = 1$. The double-step structure is a direct consequence of the absence of equilibration of electrons coming from the left and right leads, and it remains qualitatively the same for other values of parameters, as long as $\Gamma_L \sim \Gamma_R$ and $eV \sim E_c$.

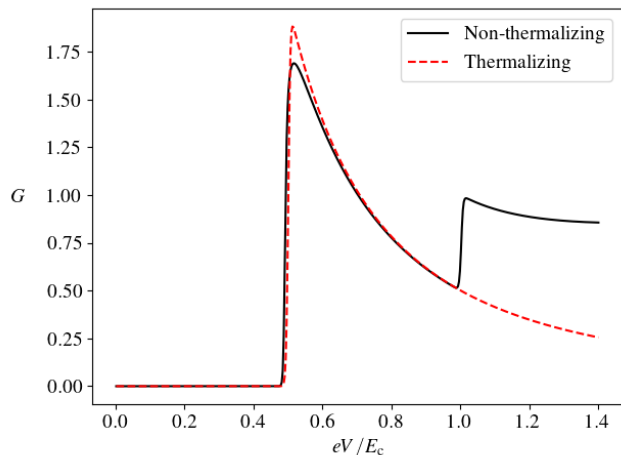


FIG. 3. The differential conductance, G , (in units of $\frac{e^2}{\Delta} \frac{\Gamma_L \Gamma_R}{\Gamma}$) as a function of V for $\Gamma_L = \Gamma_R$ and $\Omega_N = E_c/2$. Due to the distribution function of the dot having a double-step form, there is an extra jump in the conductance compared to the fully thermalized case (red dashed line) [16–19].

tegrals are negligible as the integrations are over a region where the respective integrands are exponentially small at low temperatures. For $eV > E_c$ this is no longer true, and non-zero contributions results in a sudden change in the current revealed as a jump in the differential conductance at $eV = E_c$. In the region around the jump, the ratio of probabilities is found from Eq. (13) at sufficiently low temperatures as

$$A_N \equiv \frac{p_{N+1}}{p_N} \approx \frac{\Gamma_L}{\Gamma_R} \left(\frac{eV - \Omega_N}{\Omega_N} \right). \quad (16)$$

Then, calculating the current from Eq. (15) on both sides of the jump we find that the jump in the differential conductance has a magnitude:

$$\delta G = \frac{e^2}{2\Delta} \frac{\Gamma_L \Gamma_R}{\Gamma}, \quad (17)$$

As the temperature is increased, while still obeying inequalities (3), the jump is smeared across a wider range of voltages and has a smaller height. Nevertheless, this jump should be experimentally observable and give a clear indication of the absence of thermalization within a quantum dot.

In conclusion, we have shown that the absence of thermalization in quantum dots manifests itself as a jump in the differential conductance. This is a direct consequence of the lack of equilibration between electrons coming from the left and right leads so that the distribution function on the dot has a double-step form. We anticipate this jump to be experimentally accessible at voltages comparable to the charging energy and therefore could be used as a method of identifying the absence of thermalization in the dot.

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Supplemental material for Coulomb blockade in a non-thermalized quantum dot

FULL SOLUTION TO THE QUANTUM KINETIC EQUATION

In order to calculate the current through the quantum dot using Eq. (5) of the main text, it is necessary to find the probability that it has N electrons, p_N , and the distribution function given that it has N electrons, $F_N(\varepsilon)$. To do this, we make use of the quantum kinetic equation (QKE) which for a quantum dot in the Coulomb blockade regime coupled to two leads is given by Eq. (10) in the main text

$$p_N (1 - F_N(\varepsilon_n)) \tilde{f}(\varepsilon_n + \Omega_N) = p_{N+1} F_{N+1}(\varepsilon_n) \left(1 - \tilde{f}(\varepsilon_n + \Omega_N)\right). \quad (\text{S1})$$

In this equation, $\tilde{f}(\varepsilon) = \frac{\Gamma_L}{\Gamma} f_L(\varepsilon) + \frac{\Gamma_R}{\Gamma} f_R(\varepsilon)$ and the absence of thermalization on the dot has been assumed. Providing there are only two states whose probabilities aren't exponentially suppressed this has a solution in which $F_N(\varepsilon_n) \approx F_{N+1}(\varepsilon_n) \approx F(\varepsilon_n)$. The probabilities are then found from the normalization conditions,

$$\int_0^\infty F_N(\varepsilon) d\varepsilon = N\Delta \equiv \varepsilon_F, \quad \sum_N p_N = 1, \quad (\text{S2})$$

where the energies in the dot are counted from the bottom of the band and the normalization of the probabilities can be written as $p_N + p_{N+1} \approx 1$. This solution is valid in the limit $N \gg 1$ and here we demonstrate how this solution is obtained using the saddle point approximation as we achieved in [S1]. When there are only two relevant probabilities, Eq. (S1) has an exact solution

$$p_N = \frac{Z_N}{Z_N + Z_{N+1}}, \quad p_{N+1} = \frac{Z_{N+1}}{Z_N + Z_{N+1}}, \quad (\text{S3})$$

$$F_N(\varepsilon_n) = \frac{Z_N(\varepsilon_n)}{Z_N}, \quad F_{N+1}(\varepsilon_n) = \frac{Z_{N+1}(\varepsilon_n)}{Z_{N+1}}.$$

Introducing

$$\varphi(\varepsilon) = \frac{\tilde{f}(\varepsilon)}{1 - \tilde{f}(\varepsilon)}, \quad (\text{S4})$$

Z_N and Z_{N+1} are defined as

$$Z_N = \sum_{\{n_j=0,1\}} \prod_{j=1}^{\infty} [\varphi(\varepsilon_j + \Omega_N)]^{n_j} \delta_{(\sum_j n_j), N}, \quad (\text{S5})$$

$$Z_{N+1} = \sum_{\{n_j=0,1\}} \prod_{j=1}^{\infty} [\varphi(\varepsilon_j + \Omega_N)]^{n_j} \delta_{(\sum_j n_j), N+1}.$$

Then $Z_N(\varepsilon_n)$ and $Z_{N+1}(\varepsilon_n)$, required for calculating the distribution functions in Eq. (S3), are found by restricting the sums in Eq. (S5) to terms where the level ε_n is occupied. We stress that in these definitions the relevant N dependence enters only via the Krönecker delta's as both Z_N and Z_{N+1} contain $\varphi(\varepsilon_j + \Omega_N)$, reflecting the fact that the two states are coupled via the QKE, Eq. (S1), which contains $\tilde{f}(\varepsilon_n + \Omega_N)$. In the large N limit ($N \gg 1$), the Krönecker delta can be written as an integral due to its equivalence to a delta function,

$$\delta_{(\sum_j n_j), N} = \int \frac{d\theta}{2\pi} e^{i\theta(\sum_j n_j - N)}, \quad (\text{S6})$$

meaning that Z_N can be written in a form which we evaluate using the saddle-point approximation.

$$Z_N = \int \frac{d\theta}{2\pi} e^{Nf(\theta)}, \quad f(\theta) = \frac{1}{N} \sum_j \ln(1 + \varphi(\varepsilon_j + \Omega_N) e^{i\theta}) - i\theta. \quad (\text{S7})$$

Recalling that the density of states in the dot is approximately the inverse of the mean level spacing, Δ^{-1} , we write the sum in the definition of $f(\theta)$ as an integral, so that the saddle point, θ_0 , is determined by the equation

$$\varepsilon_F = \int_0^\infty d\varepsilon \frac{\varphi(\varepsilon + \Omega_N)}{\varphi(\varepsilon + \Omega_N) + e^{-i\theta_0}}. \quad (\text{S8})$$

Despite the presence of Ω_N , the relevant N dependence of θ_0 enters only via $\varepsilon_F \equiv N\Delta$, as there is no change in Ω_N going from Z_N to Z_{N+1} . Therefore we write $Z_N = g(\theta_0)e^{-iN\theta_0}$, where $g(\theta_0)$ is a function depending on N only through ε_F . In the limit $N \gg 1$, $N\Delta \approx (N+1)\Delta$, so that ε_F is approximately a constant and consequently $g(\theta_0)$ is approximately the same for Z_N and Z_{N+1} . Therefore we find, after using Eq. (S3), that

$$\frac{p_{N+1}}{p_N} = e^{-i\theta_0}, \quad F_N(\varepsilon_n) \approx F_{N+1}(\varepsilon_n) \approx \left(\frac{e^{-i\theta_0}}{\varphi(\varepsilon + \Omega_N)} + 1 \right)^{-1}. \quad (\text{S9})$$

This solution is equivalent to assuming $F_N(\varepsilon_n) \approx F_{N+1}(\varepsilon_n)$ in the QKE, Eq. (S1), with the ratio of probabilities then being given by the normalization of $F_N(\varepsilon_n)$, Eq. (S2) (or equivalently Eq. (S8)). This is the solution presented in the main text.

[S1] G. McArdle, R. Davies, I. V. Lerner, and I. V. Yurkevich, Coulomb staircase in an asymmetrically coupled quantum dot (2023), arXiv:2304.09665 [cond-mat.mes-hall].