Ultrasmall double junction in terms of orthogonal polynomials

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The “orthodox theory” of a single electron double junction is dealt with. It is shown that
the stationary solution of the underlying master equation allows the construction of any time–
dependent solution in terms of orthogonal polynomials. The approach pays off if the stationary
solution becomes simple. Two special cases are considered. We use the time–dependent solution to
calculate the current noise in these cases.

73.40Gk, 73.40Rw

I. INTRODUCTION

Due to its simplicity the normal metal single electron
double junction (1E2J, shown schematically in Fig. 1) is
one of the best–studied systems of single electronics, both experimentally and theoretically. The common theoretical
approach uses “orthodox theory” to find a master equation for the charge probability of the island between
the two junctions. The stationary solution of this master equation is known analytically. Since the derivation of
the equation itself restricts its solution to slow processes on the time scale of $R_S C_S = (R_1 + R_2)(C_1 + C_2)$ the system appears more or less transparent within “orthodox theory.”

However, if one applies “orthodox theory” to the 1E2J
one realizes that the structure of the stationary solution restricts its practical use to both low voltages and
temperatures where the energy scale is the Coulomb energy $E_C = e^2/(2C_S)$. Therefore the investigation of n–
level systems, taking into account the most important charge states only, was introduced. Using this method, main features of single electron tunneling (SET), such as Coulomb blockade or the Coulomb staircase, can be understood theoretically.

Here we present an alternative method of solving the master equation that is mainly applicable at either high
voltage and negligible temperature or high temperature and small voltage. In these cases the stationary solution
of the master equation simplifies and provides access of the full time–dependent solution. In this regard the pre-
tened approach is complementary to that of a n–level system. We use this solution for the calculation of the current and the current noise in a 1E2J for frequencies $f \ll (R_S C_S)^{-1}$.

The physical relevance of our results lies in clarifying the asymptotic behavior of the 1E2J rather than in un-
veiling new SET effects. In fact, the latter can not be
expected in the considered domain. Furthermore, the treatment may be used as an easy–to–handle approxi-
mation in specific cases.

In Sec. I we present the general approach. In Secs. II and III this general approach is applied to the case of a high voltage at low temperature (ohmic limit) and low voltage but high temperature (thermal limit), respectively. Both stationary mean current through a 1E2J and current noise power spectrum are calculated. The results are discussed and limiting cases are compared with known results.

II. METHOD

Let $r_{\mu}(x)$ and $l_{\mu}(x)$ denote the tunneling rates in right
and left direction (see Fig. 1) across the $\mu$–th junction if $x$
excess charges reside on the island between the junctions.

Then the matrix

$\mathbf{W}(y, x) = (-1)^{1+x+y} \left\{ \begin{array}{c} [r_1(x) + l_2(x)] [\delta_{y+1} + \delta_{y}] \\ [r_2(x) + l_1(x)] [\delta_{y} + \delta_{y+1}] \end{array} \right\}$

enables to write the “orthodox” master equation

$|\dot{\sigma} \rangle = \mathbf{W}|\sigma \rangle,$

with the probability $\sigma(x)$ of $x$ excess charges on the island as the $x$–th component of the vector $|\sigma \rangle$. Due to the underlying tunneling of charges $x$ is integer. The left and right eigenfunctions are given by

$\mathbf{W}|\phi_n \rangle = -\lambda_n |\phi_n \rangle,$

$\langle \psi_n | \mathbf{W} = -\lambda_n \langle \psi_n |$

with the eigenvalues $\lambda_n \geq 0$. It can be shown that one of the eigenvalues equals zero (let it be $\lambda_0$). The corre-
sponding eigenfunction $|\phi_0 \rangle$ describes the stationary solution of the master equation (1). It obeys the detailed balance condition
\[ W(x, x + 1) \phi_0(x + 1) = W(x + 1, x) \phi_0(x) \]  

Left and right eigenfunctions are related through:

\[ \phi_n(x) = \psi_n(x) \phi_0(x). \]  

From Eq. (3) we see that \( \psi_0(x) = 1 \). The orthogonality relation of the left eigenfunctions reads

\[ \sum_x \psi_m(x) \psi_n(x) \phi_0(x) = \delta_{mn}. \]  

Thus, the eigenfunctions \( \psi_n(x) \) form a set of orthogonal polynomials with the weight function \( \phi_0(x) \) (“SET polynomials”). As an example, these polynomials are shown in Table I for a special case. In general, \( \psi_n(x) \) is a polynomial of order \( n \) in \( x \).

If the stationary solution of the master equation (11) is known, an arbitrary time dependent one follows readily from Eqs. (3) and (4):

\[ |\sigma(t)\rangle = \sum_n b_n e^{-\lambda_n(t-t_0)} |\phi_n\rangle, \]

where the \( b_n \) are adjusted to meet the initial probability distribution \( |\sigma(t_0)\rangle \), \( b_n = \langle \psi_n | \sigma(t_0) \rangle \). The eigenvalues \( \lambda_n \), which determine the time–dependence, result from Eq. (11):

\[ \lambda_n = \beta(x-1,x) \left[ 1 - \frac{\psi_n(x-1)}{\psi_n(x)} \right] + \beta(x+1,x) \left[ 1 - \frac{\psi_n(x+1)}{\psi_n(x)} \right], \forall x. \]  

In summary, the stationary solution of the master equation complemented with an initial condition determines the full time–dependent solution.

III. OHMIC LIMIT

Now we turn to the case of zero temperature. Then the detailed balance property (12) causes the ratio \( \phi_0(x+1)/\phi_0(x) \) to be a rational function of the bias voltage \( v = V C_1/e \), and of the dimensionless charges \( q = Q/e \) and \( x \). Whereas \( x \) describes the integer part of the charge, which is altered during tunneling processes, the parameter \( q \) expresses the influence of background charges and/or an applied gate voltage. In the following we will make use of the additional dimensionless parameters \( \kappa_m = C_3 - \mu / C_1 \) and \( \vartheta_m = R_m / R_{\Sigma} \), \( \mu = 1, 2 \). If \( v \) is integer and obeys

\[ \kappa_2 v + q - 1/2 = m - 0^+ \]  

for an arbitrary other integer \( m \), the ratio \( \phi_0(x+1)/\phi_0(x) \) can be written as

\[ \frac{\phi_0(x+1)}{\phi_0(x)} = \frac{\vartheta_2}{\vartheta_1} \frac{N - k}{k + 1}. \]

with \( N = v - 1 \) and \( k = x - x_{\text{min}} = x + m - 1 \). \( x_{\text{min}} \) denotes the lowest of all accessible charge states, \( x_{\text{min}} = -[\kappa_2 v + q + 1/2] \), and \([\ldots]\) the integer part of . . . . Therefore \( \phi_0(x) \) is a binomial distribution in these cases:

\[ \phi_0(x) = \binom{N}{k} \vartheta_2^k \vartheta_1^{N-k}. \]

The given condition (12) defines a number of points in the \( V-Q \) plane, as shown in Fig. 3 (“binomial points”). However, if \( 1 \leq k \leq N \), the condition (12) is fulfilled for all \( v \) and \( q \). This is the case for high bias voltage \( V \).

For the binomial distribution the polynomials \( \psi_n(x) \) are known. They can be expressed in terms of Krawtchouk polynomials as follows:

\[ \psi_n(x) = K_n(x-x_{\text{min}}; \vartheta_2, N) \left( \frac{\vartheta_2}{\vartheta_1} \right)^n. \]

The eigenvalues are determined from Eq. (11), which is the difference equation (1.10.4) of Ref. [1], yielding

\[ \lambda_n = \frac{n}{R_{\Sigma} C_1} \frac{1}{\vartheta_1 \vartheta_2} = \frac{n}{R_{\parallel} C_{\Sigma}} \]

with \( R_{\parallel} = R_1 R_2 / R_{\Sigma} \).

The calculation of the stationary current follows the standard procedure and yields

\[ \langle I \rangle = \frac{e(v - 1)}{R_{\Sigma} C_1}. \]

One verifies that this formula describes the asymptotic behavior for large bias correctly. For lower bias the “binomial points” of Fig. 3 correspond to voltages where the \( \langle I \rangle-V \) characteristic of the 1E2J touches the asymptotic line. For the symmetric 1E2J with \( q = 0 \) this happens for \( v = 2m + 1 \) with integer \( m \).

Next we present our result of the current noise of a 1E2J. The method of calculation has been described in Refs. [1] and [11]. It takes advantage of the representation of the conditional probability \( p(m; t; m', t') \) and the matrix elements of \( W \) in terms of the eigenfunctions \( \psi_n(m) \).

After several steps (see Appendix) we obtain

\[ S(0) = 2 e \langle I \rangle (1 - 2 \vartheta_1 \vartheta_2) \]

for zero frequency. Since a realistic estimation shows that \( (R_{\Sigma} C_1)^{-1} \geq 1 \text{GHz} \) typically, the result (13) is valid in a wide range of frequencies, down to the regime where \( 1/f \)-noise becomes predominant.

Eq. (13) yields the ordinary shot noise formula in the limit of an extremely asymmetric 1E2J (\( \vartheta_1 \rightarrow 1 \wedge \vartheta_2 \rightarrow 0 \) or vice versa), where the current across both junctions is uncorrelated. The shot noise is halved for a symmetric 1E2J in agreement with earlier results [9, 14].

Additional noise suppression in double junctions in dependence on the bias voltage was both theoretically predicted [11] and experimentally observed [12]. Our result
decreases very rapidly with increasing temperature we find its use is justified by the binomial points” are located at bias values where this suppression does not occur.

In Fig. 3 and Fig. 4 the results for symmetric and asymmetric 1E2J are shown. For the symmetric system the noise is suppressed. An additional suppression occurs between the “binomial points” in comparison to $2e/I$. For higher bias the use of Eq. (9) as approximation improves. This improvement is best for the symmetric 1E2J.

**IV. THERMAL LIMIT**

Let us now consider the case of dominating temperature $k_BT \equiv 1/\beta \geq E_C$. The equilibrium distribution is then a Gaussian with mean $(\kappa_1 - \varphi_1)v$ and width $(2\beta E_C)^{-1/2}$

$$\phi_0(x) = \sqrt{\frac{\beta E_C}{\pi}} \exp\left(-\frac{(x - (\kappa_1 - \varphi_1)v)^2}{2\beta E_C}\right), \quad (10)$$

which follows from detailed balance (4), or equivalently, from a thermodynamic consideration. In order to determine the eigenvalues, we consider Eq. (3) in the limit $x \rightarrow \pm \infty$, where it yields again the temperature independent values of Eq. (7). While our consideration has been exact within orthodox theory so far, the treatment requires several approximations from now on. Since many states are significantly occupied, the above charge state sums can be replaced by integrals $\sum_x \rightarrow \int dx$. Then, the SET polynomials are given in terms of Hermite polynomials

$$\psi_n(x) = \frac{H_n\left((x - (\kappa_1 - \varphi_1)v)\sqrt{2\beta E_C}\right)}{\sqrt{2^n n!}}. \quad (11)$$

For the calculation of the stationary current let us introduce a current vector $\langle \iota \rangle$ by

$$\langle I \rangle = \langle \iota | \sigma \rangle$$

$$\iota(x) = \sum_{\mu=1}^{2} \kappa_\mu \left[r_\mu(x) - I_\mu(x)\right]$$

$$\langle \iota \rangle = \sum_n a_n \langle \psi_n \rangle,$$

where a Taylor expansion in $(\beta E_C)$ is used to approximate the high temperature behavior of $\langle \iota \rangle$. Even if this expansion yields positive powers in $x$, which are integrated later on, its use is justified by $\phi_0(x)$ of Eq. (10), which decreases very rapidly with increasing $|x|$. For the stationary current we find

$$\langle I \rangle = \langle \iota | \phi_0 \rangle = a_0 \xrightarrow{\beta \rightarrow 0} \frac{V}{R_S} \left(1 - \frac{\beta E_C}{3}\right).$$

This high temperature result is independent of the double junction’s symmetry. It agrees with the known result from SET thermometry.

The calculation of the noise follows again Refs. [10][11]. In terms of Eq. (10) we use

$$\phi_0(x \pm 1) = \phi_0(x) e^{-\beta E_C \{1 \pm 2[x - (\kappa_1 - \varphi_1)v]\}}.$$

Furthermore, high temperature expansions are used again to simplify the calculation which is lengthy, but straightforward. Restricting to the leading term and its first order correction results in contributions from the eigenvalues $\lambda_{0,1}$ only. After carefully collecting all relevant contributions the zero frequency noise power

$$S(0) = \frac{4k_B T}{R_S} \left[1 - \frac{\beta E_C}{3} \left(2 - \frac{\kappa_1^2}{\varphi_1} - \frac{\kappa_2^2}{\varphi_2}\right)\right] \quad (12)$$

is found. This result coincides with the high temperature limit of Ref. [10], but gives a correction to the known expression as well. In case of symmetric 1E2J (or more generally: for $\kappa_1 = \varphi_1$) the term $(\ldots)$ in (12) simplifies to unity and it becomes clear that the Nyquist formula yields an upper bound of the noise of a 1E2J. This fact expresses the partial coherence between tunneling events on both junctions. At high temperature, however, this coherence get lost. This behavior does not correspond to the coth–formula [14].

$$S(0) = 2e/I \coth \left(\frac{eV}{2k_B T}\right),$$

using the current $I$ through the system and the bias voltage $V$, which predicts elevated noise above $4k_B T/R_S$. We want to point out that the coth–formula was derived for the single junction (1E1J) and does not allow for coherence effects of both junctions.

**V. CONCLUSIONS**

We have presented a method allowing access to the time–dependent solution of the master equation that is used in the semiclassical “orthodox theory” to describe the behavior of an ultrasmall single electron double junction. This method is based on general properties of master equations. We can show that the stationary solution of the master equation is sufficient to determine any time–dependent solution by quadratures on the range of allowed charge states. For special cases of the stationary solution this procedure simplifies to an approximatively analytically solvable problem. Two of these cases are presented in this paper in detail. After calculating the respective mean currents the time–dependent solution is used to find expressions for the current noise power spectra. The obtained results are discussed. It turns out that the presented method together with the usual $n$–level approach enable access to time–dependent solution in a wide parameter range of the bias voltage $V$ and the temperature $T$. 

3
The term corresponding to 

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\[ \text{tions of their arguments. Hence, they can be expanded} \]

\[ \text{property (2). With the rates} \]

\[ \text{diagonal terms of} \]

\[ \text{is calculated. Due to the vanishing temperature} \]

\[ \text{is obeyed at} \]

\[ \text{we see that the correct initial condition of} \]

\[ \text{is finally the noise power spectrum of the current that is} \]

\[ \text{considered in the zero frequency limit} \]

\[ \text{The conditional probability} \]

\[ \text{can be expressed in terms of the eigenfunctions of} \]

\[ \text{is transformed into} \]

\[ \text{is obtained at} \]

\[ \text{Now the different noise contributions are calculated. Due to the vanishing temperature one finds} \]

\[ \text{independent of the junction number} \]

\[ \text{The non-diagonal terms of} \]

\[ \text{simplify using the detailed balance property} \]

\[ \text{With the rates} \]

\[ \text{the current direction has to be considered only) } \]

\[ \text{is transformed into} \]

\[ \text{The term corresponding to} \]

\[ \text{results in} \]

\[ \text{which cancels against the same term in the noise expression (A3). The rates} \]

\[ \text{are linear functions of their arguments. Hence, they can be expanded} \]

\[ \text{into the left eigenfunctions} \]

\[ \text{with contributions of} \]

\[ \text{exp}\]

\[ \text{using the self–duality property of the Krawtchouk polynomials. Finally, assemblage of the noise follows the line of} \]

\[ \text{straightforwardly. For zero frequency we obtain} \]

\[ \text{where the stationary current is expressed via} \]

\[ \text{are found for} \]

\[ \text{yielding the same result.} \]

\[ \text{The calculation of the mean current starts from the} \]

\[ \text{of the stationary solution} \]

\[ \text{of Ref.} \]

\[ \text{In detail, we find} \]

\[ \text{using the self–duality property of the Krawtchouk polynomials. Finally, assemblage of the noise follows the line of} \]

\[ \text{straightforwardly. For zero frequency we obtain} \]

\[ \text{where the stationary current is expressed via} \]
The relevant expansion of the current operator \( \ell(x, v) \) is simplified by the use of the shifted charge \( y = [x - (\kappa_1 - \varrho_1)]v \): 
\[
\ell(x, v) \xrightarrow{\beta \rightarrow 0} \left( \frac{V}{R_S} - \frac{e(\kappa_1 - \varrho_1)}{R_{\parallel}C_S} \right) \left( 1 - \frac{\beta E_C}{3} \right).
\]

The determination of \( a_i \) results in contributions to \( a_{0,1} \), in detail 
\[
a_0 = \frac{V}{R_S} \left( 1 - \frac{\beta E_C}{3} \right)
\]
\[
a_1 = \frac{e(\kappa_1 - \varrho_1)}{R_{\parallel}C_S\sqrt{2\beta E_C}} \left( 1 - \frac{\beta E_C}{3} \right).
\]

The calculation of the stationary current makes use of \( a_0 \) only.

The calculation of the noise follows a similar, though more complicated, line of the current calculation above in the evaluation of the expression (A3)–(A5). By use of (10) we find
\[
r_{1,2}(x \pm 1)\phi_0(x \pm 1) = l_{1,2}(x)\phi_0(x) \exp(2\beta E_Cg_{1,2}v)
\]
\[
l_{1,2}(x \pm 1)\phi_0(x \pm 1) = r_{1,2}(x)\phi_0(x) \exp(-2\beta E_Cg_{1,2}v).
\]

Furthermore, the abbreviations
\[
\ell_\mu(x) = e[r_\mu(x) - l_\mu(x)]
\]
\[
\sigma_\mu(x) = e[l_\mu(x) \exp(2\beta E_Cg_\mu v) - r_\mu(x) \exp(-2\beta E_Cg_\mu v)]
\]
\[
k_\mu(x) = e[r_\mu(x) + l_\mu(x)],
\]

allow the transformation of the correlation function into 
\[
S^e_{\mu\nu}(t - t') = \sum_n \exp[-\lambda_n(t - t')] \langle \ell_\mu|\phi_n \rangle \langle j_\nu|\phi_n \rangle \quad (B2)
\]

and the Shottky value is expressed as \( S^S_{\mu} = e(k_\mu|\phi_0) \).

The representation of the relevant high temperature expansion of \( \ell_\mu, j_\mu, \) and \( k_\mu \) in terms of the left eigenfunctions \( \psi_n \) reads
\[
\langle \ell_\mu | \approx \frac{2E_C}{eR_S} \langle \psi_0 | + \frac{2E_C}{eR_S} \frac{1}{\varrho_\mu \sqrt{2\beta E_C}} \left( 1 - \frac{\beta E_C}{3} \right) \langle \psi_1 |.
\]
\[
\langle j_\mu | \approx \frac{2E_C}{eR_S} \langle \psi_0 | + \frac{2E_C}{eR_S} \frac{1}{\varrho_\mu \sqrt{2\beta E_C}} \left( 1 - \frac{\beta E_C}{3} \right) \langle \psi_1 |.
\]
\[
\langle k_\mu | \approx \frac{2}{eR_\parallel \varrho_\mu} \left( 1 - \frac{E_C}{3\beta} \right) \langle \psi_0 | + \frac{E_C \sqrt{3}}{3eR_\parallel \varrho_\mu} \langle \psi_2 |.
\]

The calculation of the zero frequency noise power follows directly (A3)–(A5). Keeping the leading two orders in \( \beta E_C \) only results in the expression (12) given in the text.

\[\text{FIG. 1.} \quad \text{Circuit diagram of the ultrasmall double–tunnel junction, consisting of two tunnel junctions connected in series} \quad \text{(with resistances} R_{1,2} \text{and capacitances} C_{1,2} \text{, respectively)} \quad \text{and an excess charge} \ Q \text{on the island.}\]
FIG. 2. V–Q plane for $C_2/C_1 = 1.5$. The tiles correspond to regions of fixed $N$ and the black corners indicate the points where the stationary charge distribution is binomial.

FIG. 3. Noise in a symmetric 1E2J ($R_\Sigma = 200k\Omega$, $C_\Sigma = 0.2fF$). The full line represents Eq. (9) and the dashed line displays the $2e\langle I \rangle$. The arrows indicate the “binomial points” for this system.

FIG. 4. Noise in an asymmetric ($\kappa_1 = \varrho_1 = 0.9$) 1E2J ($R_\Sigma = 200k\Omega$, $C_\Sigma = 0.2fF$). The full line represents Eq. (9) and the dashed line displays the $2e\langle I \rangle$. The arrows indicate the “binomial points” for this system.

| $n$ | $c_{n0}$ | $c_{n1}$ | $c_{n2}$ |
|-----|---------|---------|---------|
| 0   | 1       |         |         |
| 1   | 0       | $-\sqrt{3v-1}$ |         |
| 2   | $-\sqrt{\frac{v-1}{v+1}}$ | 0       | $\sqrt{2v^2-2}$ |

TABLE I. Coefficients $c_{nm}$ of the SET polynomials for a symmetric 1E2J with $Q = T = 0$ at dimensionless voltages $v$ in units of $e/C_\Sigma$ so that $v \in (1; 3]$. The polynomials are built from these coefficients via $\psi_n(x) = \sum_m c_{nm}x^m$. 