Abstract. We present a calculation of the grand canonical partition function of a serial metallic island system by the imaginary-time path integral formalism. To this purpose, all electronic excitations in the lead and island electrodes are described using Grassmann numbers. The Coulomb charging energy of the system is represented in terms of phase fields conjugate to the island charges. By the large channel approximation, the tunneling action phase dependence can also be determined explicitly. Therefore, we represent the partition function as a path integral over phase fields with a path probability given in an analytically known effective action functional. Using the result, we also propose a calculation of the average electron number of the serial island system in terms of the expectation value of winding numbers. Finally, as an example, we describe the Coulomb blockade effect in the two-island system by the average electron number and propose a method to construct the quantum stability diagram.

Keywords: mesoscopic systems, quantum dots, quantum Monte Carlo simulations
1. Introduction

Single-electron tunneling devices are standard tools in nano-science [1, 2]. They continue to attract attention because of their nanoscopic scale, low power dissipation, and new functionalities [3]. A single-electron tunneling device allows us to control the tunneling current at the single electron level. Electron transport is strongly affected by the charging effect at temperatures in the sub-Kelvin range [4, 5]. It is therefore crucial to include the charging energy into the tunneling processes in the single-electron tunneling devices [6]. The most widely studied device is the single-electron transistor (SET), consisting of a single island, two tunnel junctions, and a gate electrode controlling the electrostatic potential of the island. In theoretical studies, the imaginary-time path integral formalism is a powerful tool for describing the experimental data of the SETs with high accuracy [7–9]. The findings on the SETs indicate that a close match between the theoretical model and its experimental realization exists for the SET. In addition, one can apply the path integral Monte Carlo simulation [10–13] to study the systems as the SET without the restriction of coupling parameters and temperature as perturbation theory [14–16] and semiclassical approximation [8, 17], respectively. However, since the complexity of the single-electron tunneling devices depends on the number of the island, it is still
unclear whether the theoretical calculation would agree with more complex experiments than that of the SET, i.e. the systems consist of many islands [18–20].

Due to the quantum statistical properties that can be obtained from the system’s partition function, this paper aims to calculate the grand canonical partition function of a finite serial metallic island system by the imaginary-time path integral approach [14, 21, 22]. The paper is organized as follows: section 2 introduces the Hamiltonian of the serial metallic island system and some basic notations. This section deals with the path integral representation of the grand canonical partition function of the serial island system. To this purpose, we describe all electronic excitation in the lead and island electrodes employing Grassmann numbers and Coulomb charging of the island electrodes in terms of phase fields conjugate to the island charges. The general form of the path integrals over the phase and Grassmann fields is discussed. In section 3, for further application, we propose a suitable form of the average electron number of the island system for the quantum Monte Carlo simulation and apply it to describe the Coulomb blockade effect in the two-island system as an example. Finally, we conclude and discuss possible extensions in section 4.

2. Model and the imaginary-time path integral

In this section, the grand canonical partition function and the effective action of a finite serial metallic island are derived. In section 2.1, we first introduce the Hamiltonian model used to describe a serial metallic island system. Section 2.2 deals with the imaginary-time path integral to represent the partition function of the system. The Coulomb action is then evaluated in section 2.3. The path integral over Grassmann fields and the integration are discussed in sections 2.4 and 2.5, respectively. Finally, in section 2.6, the tunneling action is evaluated by the large channel approximation [14, 23].

2.1. Hamiltonian model

A circuit diagram of the finite serial island system is depicted in figure 1. Microscopically, this system can be theoretically modeled by the Hamiltonian [1]

\[ H = H_B + H_T + H_C, \]

where the term \( H_B \) describes the conduction electrons of the leads and the islands

\[ H_B = \sum_{J\kappa\sigma} \epsilon_{J\kappa\sigma} c_{J\kappa\sigma}^\dagger c_{J\kappa\sigma} + \sum_{I\kappa\sigma} \epsilon_{I\kappa\sigma} d_{I\kappa\sigma}^\dagger d_{I\kappa\sigma}, \]

respectively. Here, \( \epsilon_{J\kappa\sigma} \) is the energy of an electron with longitudinal wave vector \( k \) in channel \( \sigma \) of lead \( J \), where \( J \in \{ S, D \} \). The channel index \( \sigma \) includes the transversal and spin quantum numbers. \( c_{J\kappa\sigma} \) and \( c_{J\kappa\sigma}^\dagger \) are the corresponding electron annihilation and creation operators, respectively. Likewise, \( \epsilon_{I\kappa\sigma} \) denotes the energy of an electron with the longitudinal wave vector \( k \) in channel \( \sigma \) of island \( I \), where \( I \in \{ 1, 2, \ldots, N \} \), and \( d_{I\kappa\sigma} \) and \( d_{I\kappa\sigma}^\dagger \) are the associated electron annihilation and creation operators, respectively.
Grand canonical partition function of a serial metallic island system

Figure 1. This arrangement is biased by the voltage difference $V_S - V_D$, where $V_S$ and $V_D$ are the source and drain voltage, respectively. The external gate voltage $V_{gl}$, which couples directly to the island by the capacitance $C_{gI}$. The average excess electron number on the island $I$ is denoted by $\langle n_I \rangle$. All tunneling junctions are represented by a conductor connected in parallel with a capacitor.

The second term in equation (1) describes the tunneling of electrons across the finite tunneling junctions of the circuit as shown in figure 1,

$$H_T = \sum_{kq\sigma} d_{1kq\sigma}^\dagger t_{1Skq\sigma} e^{-i\varphi_1} c^\dagger_{S\sigma} + \sum_{l=2}^{N} d_{1kq\sigma}^\dagger t_{II-1kq\sigma} e^{-i(\varphi_I - \varphi_{l-1})} c_{I-1kq\sigma}$$

$$+ c^\dagger_{Dkq\sigma} t_{DNkq\sigma} e^{i\varphi_N} d_{Nq\sigma} + h.c.$$,  (3)

where $t_{1Skq\sigma}$, $t_{II-1kq\sigma}$, and $t_{DNkq\sigma}$ denote the electron tunneling amplitude of the tunneling junctions labeled by 1S, II - 1, and DN, respectively. For example, $t_{1Skq\sigma}$ is the amplitude for an electron in state $|q\sigma\rangle$ on lead S to tunnel onto island 1 with final state $|k\sigma\rangle$. In addition, we have introduced the phase operators $\varphi_I$ conjugate to the number operators $n_I$ of excess charges on the islands I, i.e. $[n_I, \varphi_I] = i$. Accordingly, the charge shift operator $e^{-i\varphi_I}$ add one charge to the island $I$. Here and in the following, we have defined $\varphi_S = \varphi_D = 0$ since $V_S = V_D = 0$.

The last term in equation (1) is the Coulomb charging energy expressed as [1, 24]

$$H_C = \sum_{I=1}^{N} E_{II}(n_I - n_{0I})^2 + 2 \sum_{I < I'}^{N} E_{II'}(n_I - n_{0I})(n_{I'} - n_{0I'}),$$  (4)

where $n_I$ is the (excess) electron number in the island $I$. For the island $I$ the continuous charge induced by the gate voltage $I$ is denoted by $n_{0I}$ expressed by $n_{0I} = C_{gI} V_{gl}/e$. The variable $n_{0I}$ is non-integer and just a parameter of the external voltage. The coefficients $E_{II}$ and $E_{II'}$ are the matrix elements of the matrix $E_{CN}$ defined by

$$E_{CN} = \frac{e^2}{2} C_{N}^{-1},$$  (5)

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where $C^{-1}_N$ is the inverse matrix of $C_N$

$$C_N = \begin{pmatrix} C_{11} & C_{12} & \ldots & C_{1N} \\ C_{21} & C_{22} & \ldots & C_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ C_{N1} & \ldots & \ldots & C_{NN} \end{pmatrix},$$  

and the matrix elements of $C_{II'}$ are defined by the conditions:

$$C_{II'} = \begin{cases} 0, & \text{if } |I - I'| > 1 \\ C_{\Sigma I}, & \text{if } I = I' \\ -C_{I'}, & \text{if } |I - I'| = 1, \end{cases}$$

where $C_{\Sigma I}$ is the sum of all capacitors connected with the island $I$, i.e. $C_{\Sigma I} = C_I + C_{I-1} + C_{gI}$. According to the conditions in equation (7), one obtains $C_{II'} = C_{I'I}$.  

### 2.2. Path integral representation of the partition function

The goal of this section is a path integral representation of the grand partition function

$$Z = \text{tr} \{ e^{-\beta (\hat{H} - \mu \hat{N})} \}$$

of the island system suitable for the evaluation, where $\mu$ denotes the chemical potential of the system and $\hat{N}$ is the particle number operator. The Hilbert space of the Hamiltonian in equations (1)–(4) is the product of the space spanned by the state $|n\rangle$, or equivalently the phase state $|\varphi\rangle$, and the Fock space of the quasi-particles. In order to trace over the quasi-particle excitation, we introduce Grassmann numbers $\zeta_{Jk}\sigma$ and $\theta_{Ik}\sigma$ corresponding to the electron annihilators $c_{Jk}\sigma$ and $d_{Ik}\sigma$, respectively. For notation convenience, the Grassmann numbers for electronic lead states are combined to a single vector $\vec{\zeta} = (\zeta_{Sk}\sigma, \zeta_{Dq}\sigma)^T$. Likewise, $\vec{\theta} = (\theta_{1q}\sigma, \theta_{2q}\sigma, \ldots, \theta_{Nq}\sigma)^T$ combines all Grassmann numbers for electronic island states. To trace over the island charges, we work in the phase representation and introduce the vector $\vec{\varphi} = (\varphi_1, \ldots, \varphi_N)^T$. The partition function in equation (8) may then be written as

$$Z = \int D\mu(\vec{\varphi}) D\mu(\vec{\zeta}) D\mu(\vec{\theta}) e^{-\vec{\zeta} \cdot \vec{\zeta} - \vec{\theta} \cdot \vec{\theta}} \langle \vec{\varphi}, -\vec{\zeta}, -\vec{\theta} | e^{-\beta H} | \vec{\varphi}, \vec{\zeta}, \vec{\theta} \rangle,$$  

where we have dropped the term $(\mu \hat{N})$ in the partition function. This term is further discussed in section 2.4. Here, $|\vec{\varphi}\rangle$ stands for the product of phase states $|\varphi_I\rangle$. The shorthand notations $|\vec{\zeta}\rangle$ and $|\vec{\theta}\rangle$ stand for the product of fermion coherent states $|\zeta_{Jk}\sigma\rangle$ and $|\theta_{Ik}\sigma\rangle$, respectively. The shorthand integration

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\[ \int D\mu(\vec{\zeta}) \equiv \int \prod_{Jk\sigma} d\zeta^*_J\zeta_J d\zeta_{Jk\sigma}, \] (10)

and

\[ \int D\mu(\vec{\theta}) \equiv \int \prod_{Iq\sigma} d\theta^*_I\theta_I d\theta_{Iq\sigma} \] (11)

are overall Grassmann numbers related with the lead and island states, respectively. The short-hand integration

\[ \int D\mu(\vec{\phi}) \equiv \left( \frac{1}{2\pi} \right)^2 \int \prod_I d\phi_I \] (12)

integrates over the phases \( \phi_I \) that are \( 2\pi \)-periodic. Further, we have introduced the notations

\[ \vec{\zeta}^* \cdot \vec{\zeta} = \sum_{Jk\sigma} \zeta^*_J\zeta_J, \] (13)

and

\[ \vec{\theta}^* \cdot \vec{\theta} = \sum_{Iq\sigma} \theta^*_I\theta_I. \] (14)

The derivation of the path integral expression can be done as usual by multiple insertions of the closure relation \([21]\)

\[ 1 = \int D\mu(\vec{\varphi}) \int D\mu(\vec{\zeta}) \int D\mu(\vec{\theta}) e^{-\vec{\zeta}^* \cdot \vec{\zeta} - \vec{\theta}^* \cdot \vec{\theta}} |\vec{\varphi}, \vec{\zeta}, \vec{\theta}| \langle \vec{\varphi}, \vec{\zeta}, \vec{\theta} |, \] (15)

in the product space. The imaginary-time step is introduced as \( \Delta = \beta/P \), where we have used \( \hbar = 1 \) through this paper, and \( P \) denotes the Trotter number. For each imaginary time segment \( \Delta_j = \tau_j - \tau_{j-1} \), one can calculate the short-time propagator

\[ \langle \vec{\varphi}_j, \vec{\zeta}_j, \vec{\theta}_j | e^{-\Delta_j H} | \vec{\varphi}_{j-1}, \vec{\zeta}_{j-1}, \vec{\theta}_{j-1} \rangle = \langle \vec{\zeta}_j, \vec{\theta}_j | e^{-\Delta_j (H_B + H_T(\vec{\varphi}_{j-1}))} | \vec{\zeta}_{j-1}, \vec{\theta}_{j-1} \rangle \]
\[ \times \langle \vec{\varphi}_j | e^{-\Delta_j H_C} | \vec{\varphi}_{j-1} \rangle, \] (16)

where \( \vec{\varphi}_j = (\varphi_1(\tau_j), \varphi_2(\tau_j), \ldots, \varphi_N(\tau_j))^T \) and \( \vec{\varphi}_{j-1} = (\varphi_1(\tau_{j-1}), \varphi_2(\tau_{j-1}), \ldots, \varphi_N(\tau_{j-1}))^T \) and \( \vec{\zeta}_j \) and \( \vec{\theta}_j \) are the Grassmann variables at time \( \tau_j \). Further, \( H_T(\vec{\varphi}_j) \) refers to the Hamiltonian in equation (3) with the phase operators \( \varphi_I \) replaced by \( \varphi_I(\tau_j) \). Making use of the form in equation (16) of the short time propagator in the Trotter break-up for the partition function, we obtain

\[ Z = \int_0^{2\pi} \prod_{I=1}^N [d\varphi_{I,P} \ldots d\varphi_{I,0} \delta(\varphi_{I,P} - \varphi_{I,0})] \]
\[ \times \langle \vec{\varphi}_P | e^{-\Delta_P H_C} | \vec{\varphi}_{P-1} \rangle \ldots \langle \vec{\varphi}_1 | e^{-\Delta_1 H_C} | \vec{\varphi}_0 \rangle Z_{BT}[\vec{\varphi}], \] (17)

where \( Z_{BT}[\vec{\varphi}] \) is the trace over the Grassmann fields discussed in more detail in section 2.4.
2.3. Path integral over phase fields and Coulomb action

The representation of the partition function in equation (17) can be evaluated by inserting the closure relation

\[
1 = \int_0^{2\pi} d\varphi \langle \varphi | \varphi \rangle = \sum_{n=-\infty}^{\infty} |n\rangle \langle n|,
\]

where \( n \) is an integer number into the short time propagator in the last term in equation (16). We have

\[
\langle \vec{\varphi}_j | e^{-\Delta_j H_C} | \vec{\varphi}_{j-1} \rangle = \sum_{\vec{n}} \langle \varphi_{1,j} | n_1 \rangle \ldots \langle \varphi_{N,j} | n_N \rangle \\
\times e^{-\Delta_j H_{C}(n_1,\ldots,n_N)} \langle n_1 | \varphi_{1,j-1} \rangle \ldots \langle n_N | \varphi_{N,j-1} \rangle \\
= \frac{1}{(2\pi)^N} \sum_{\vec{n}} e^{-\Delta_j H_{C}(n_1,\ldots,n_N)} e^{-i \sum_{I=1}^{N} n_I (\varphi_{I,j} - \varphi_{I,j-1})},
\]

where we have defined

\[
\sum_{\vec{n}} \equiv \sum_{n_1=-\infty}^{\infty} \ldots \sum_{n_N=-\infty}^{\infty}.
\]

\( H_{C}(n_1,\ldots,n_N) \) is the Coulomb Hamiltonian in equation (4) for given eigenvalues of the electron number operators \( n_I \) and \( \langle n_I | a_j \rangle = (2\pi)^{-1/2} \exp(i n_I a_j) \). By means of the Poisson re-summation formula [21],

\[
\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} dn e^{-2\pi ikn} f(n),
\]

and the matrix in equation (5) corresponding with \( H_C \), the short time propagator can be transformed to read

\[
\langle \vec{\varphi}_j | e^{-\Delta_j H_C} | \vec{\varphi}_{j-1} \rangle = \frac{1}{(2\pi)^N} \sum_{\vec{k}_j} \int_{-\infty}^{\infty} d\tilde{n}_1 \ldots \int_{-\infty}^{\infty} d\tilde{n}_N \\
\times \exp \left[ -i \Delta_j \sum_{I=1}^{N} \tilde{n}_I \Delta \varphi_I - \Delta_j \tilde{n}_I^T E_{CN} \tilde{n}_I \right],
\]

where we have defined

\[
\sum_{\vec{k}_j} \equiv \sum_{k_1,j=-\infty}^{\infty} \ldots \sum_{k_N,j=-\infty}^{\infty},
\]

\( \tilde{n}_I = (\tilde{n}_1,\ldots,\tilde{n}_N)^T \) with \( \tilde{n}_I \equiv (n_I - n_{I0}) \), and \( \Delta \varphi_I = (\varphi_{I,j} - \varphi_{I,j-1} + 2\pi k_{I,j}) / \Delta_j \). Evaluating the Gaussian integrals for matrix form [21]
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\[
\int_{-\infty}^{\infty} dn_1 \ldots dn_N \exp[-\lambda (\vec{n}^T E_{CN} \vec{n} + \vec{n}^T \vec{J})] = \left( \frac{\pi}{\lambda} \right)^{N/2} \left[ \det E_{CN} \right]^{-\frac{1}{2}} \times \exp \left[ \left( \frac{\lambda}{4} \right) \vec{J}^T E_{CN}^{-1} \vec{J} \right],
\]

(24)

where \( \vec{n} = (\tilde{n}_1, \ldots, \tilde{n}_N)^T \), \( \vec{J} = (\Delta \varphi_1, \ldots, \Delta \varphi_N)^T \), and \( \lambda \) is a constant, one obtains

\[
\langle \varphi_j | e^{-\Delta_j H_c} | \varphi_{j-1} \rangle = \mathcal{N}_j \sum_{k_j} \exp \left[ -\frac{\Delta_j}{4} \Delta \varphi_j^T E_{CN} \Delta \varphi_j - i \Delta_j \vec{n}_g^T \Delta \varphi_j \right]
\]

(25)

where \( \mathcal{N}_j \) is the normalization constant for the time segment \( j \);

\[
\mathcal{N}_j = \frac{1}{(2\pi)^N} \left( \frac{\pi}{\Delta_j} \right)^{N/2} \left[ \det E_{CN} \right]^{-\frac{1}{2}},
\]

(26)

which can be incorporated into the path integral measure. We now use the freedom to relabel the summations over the winding numbers \( k_I \) and to transform the integrals over \( \varphi_I \). Instead of summations over \( k_{I,j}, \ldots, k_{I,P} \), we sum over

\[
k'_{I,n} = \sum_{j=1}^{n} k_{I,j} \quad \text{for} \quad n = 1, \ldots, P,
\]

(27)

with the consequence that

\[
\Delta \varphi_{I,j} = \frac{\varphi_{I,j} + 2\pi k'_{I,j} - \varphi_{I,j-1} - 2\pi k'_{I,j-1}}{\Delta_j}
\]

(28)

Using \( \varphi'_{I,j} = \varphi_{I,j} + 2\pi k'_{I,j} \) and dropping the primes as a convenient integration variable, we can rewrite the partition function in equation (17) as

\[
\begin{align*}
Z &= \mathcal{N} \prod_{I=1}^{N} \left[ \sum_{k_{I,j}=-\infty}^{\infty} \int_{2\pi k_{I,j}}^{2\pi (k_{I,j}+1)} d\varphi_{I,j} \ldots \int_{2\pi k_{I,1}}^{2\pi (k_{I,1}+1)} d\varphi_{I,1} \int_{0}^{2\pi} d\varphi_{I,0} \right] \\
&\quad \times \delta(\varphi_{I,P} - \varphi_{I,0} - 2\pi k_{I,P}) \\
&\quad \times \exp \left[ \sum_{j=1}^{P} \Delta_j \left( \frac{1}{4} \Delta \varphi_j^T E_{CN}^{-1} \Delta \varphi_j + i \vec{n}_g^T \Delta \varphi_j \right) \right] \mathcal{Z}_{BT}[\vec{\varphi}],
\end{align*}
\]

(29)

where we have introduced the vectors

\[
\Delta \vec{\varphi}_j = \left( \frac{\varphi_{1,j} - \varphi_{1,j-1}}{\Delta_j}, \frac{\varphi_{2,j} - \varphi_{2,j-1}}{\Delta_j}, \ldots, \frac{\varphi_{N,j} - \varphi_{N,j-1}}{\Delta_j} \right)^T,
\]

(30)

and \( \vec{n}_g = (n_{01}, n_{02}, \ldots, n_{0N})^T \). The normalization factor \( \mathcal{N} \equiv \prod_{j=1}^{P-1} \mathcal{N}_j \).

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With the exception of \( k_p \), the sums over \( k_j \) can be incorporated in the integrals over \( \varphi_{I,j} \). This simplifies the expression in equation (29) further, and we get in the continuum limit, i.e. \( (P \to \infty, \Delta_j \to 0) \), which is a path integral over all imaginary-time paths \( \vec{\varphi}(\tau) = (\varphi_1(\tau), \varphi_2(\tau), \ldots, \varphi_N(\tau))^T \) in the time interval \((0, \beta)\) with arbitrary winding numbers

\[
Z = N^N \prod_{I=1}^{N} \left[ \sum_{k_I=-\infty}^{\infty} \int_{\varphi_I(0)}^{\varphi_I(\beta)} D[\varphi_I(\tau)] \right] e^{-S_C[\vec{\varphi}(\tau)]} Z_{BT}[\vec{\varphi}],
\]

and the Coulomb action of the serial island system is expressed by

\[
S_C[\vec{\varphi}(\tau)] = \int_0^\beta d\tau \left[ \frac{1}{4} \vec{\varphi}^T E_{CN}^{-1} \vec{\varphi} + i(\vec{n}^T \cdot \vec{\varphi}) \right],
\]

where \( \vec{\varphi}(\tau_j) = (\dot{\varphi}_1(\tau_j), \dot{\varphi}_2(\tau_j), \ldots, \dot{\varphi}_N(\tau_j))^T \) is the continuum limit of \( \Delta \vec{\varphi}_j \) for \( \Delta_j \to 0 \) and \( E_{CN}^{-1} \) is the inverse matrix of the matrix \( E_{CN} \) in equation (5).

### 2.4. Path integral over Grassmann fields

In this section, we have to evaluate the partition function in equation (31), wherein \( Z_{BT} \) involves the integration over the Grassmann numbers. In the Trotter break-up discussed in the previous section, the imaginary-time segment \( \Delta_j \) gives rise to the short time propagator in equation (16) with the fermions short time propagator

\[
\langle \vec{\zeta}_j, \vec{\theta}_j | e^{-\Delta_j [H_B + H_T(\vec{\varphi}_{j-1})]} | \vec{\zeta}_{j-1}, \vec{\theta}_{j-1} \rangle.
\]

Within this short time propagator, the electron annihilation (creation) operators in the Hamiltonians \( H_B \) in equation (2) and \( H_T \) in equation (3) can be replaced for small \( \Delta_j \) by the corresponding (conjugate) Grassmann numbers. Accordingly, one finds

\[
\langle \vec{\zeta}_j, \vec{\theta}_j | e^{-\Delta_j [H_B + H_T(\vec{\varphi}_{j-1})]} | \vec{\zeta}_{j-1}, \vec{\theta}_{j-1} \rangle = \langle \vec{\zeta}_j, \vec{\theta}_j | \vec{\zeta}_{j-1}, \vec{\theta}_{j-1} \rangle \exp \{ -\Delta_j [H_{B,j,j-1} + H_{T,j,j-1}(\vec{\varphi}_{j-1})] \},
\]

where

\[
H_{B,j,j-1} = \sum_{Jk,\sigma} \epsilon_{Jk,\sigma} \hat{\zeta}_{Jk,\sigma,j}^* \hat{\zeta}_{Jk,\sigma,j-1} + \sum_{I\kappa,\sigma} \epsilon_{I\kappa,\sigma} \hat{\theta}_{I\kappa,\sigma,j}^* \hat{\theta}_{I\kappa,\sigma,j-1},
\]

and

\[
H_{T,j,j-1}(\vec{\varphi}_{j-1}) = \sum_{kq,\sigma} [\theta_{1k,\sigma,j}^* t_{1skq,\sigma} e^{-i\varphi_{1k,\sigma,j} - \varphi_{s,\sigma,j-1}} \zeta_{Sqr,\sigma,j-1}^* + \sum_{l=2}^{N} \theta_{1k,\sigma,j}^* t_{I-1kq,\sigma} e^{-i(\varphi_{I-1k,\sigma,j-1} - \varphi_{I-1k,\sigma,j-1})} \theta_{I-1kq,\sigma,j-1} + \sum_{Dk,\sigma,j} \theta_{Dkq,\sigma} e^{i\varphi_{Dkq,\sigma,j-1}} \zeta_{Nqr,\sigma,j-1} + \text{h.c.}].
\]

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Combining the exponential factor in equation (34) with the factor \(\exp \left( -\vec{\zeta}_j \cdot \vec{\zeta}_j - \vec{\theta}_j \cdot \vec{\theta}_j \right)\) stemming from the closure relation in equation (15), and the scalar product 
\[ \langle \vec{\zeta}_j, \vec{\theta}_j | \vec{\zeta}_{j-1}, \vec{\theta}_{j-1} \rangle = \exp \left( \vec{\zeta}_j \cdot \vec{\zeta}_{j-1} + \vec{\theta}_j \cdot \vec{\theta}_{j-1} \right), \]
we obtain for each time segment \(\Delta_j\) a factor
\[
\exp \left\{ -\Delta_j \left[ \vec{\zeta}_j \cdot \vec{\zeta}_j - \vec{\theta}_j \cdot \vec{\theta}_j \right] \right\}. \tag{37}
\]

In the continuum limit, these factors and the integration over the Grassmann numbers \(\vec{\zeta}_j\) and \(\vec{\theta}_j\) are combined to the path integral
\[
Z_{BT}[\vec{\varphi}] = \int D\mu(\vec{\zeta}) \int D\mu(\vec{\theta}) \exp \left[ -S_{BT}[\vec{\zeta}, \vec{\theta}, \vec{\varphi}] \right], \tag{38}
\]
where
\[
S_{BT}[\vec{\zeta}, \vec{\theta}, \vec{\varphi}] = S_{\text{lead}}[\vec{\zeta}] + S_{\text{isl}}[\vec{\theta}] + S_T[\vec{\zeta}, \vec{\theta}, \vec{\varphi}], \tag{39}
\]
with the lead action
\[
S_{\text{lead}}[\vec{\zeta}(\tau)] = \int_0^\beta d\tau \sum_{jk\sigma} \left[ \zeta_{jK\sigma}(\tau)(\partial_\tau - \mu + \epsilon_{jK\sigma})\zeta_{jK\sigma}(\tau) \right] \equiv \zeta^* g^{-1}_j \zeta, \tag{40}
\]
and the island action
\[
S_{\text{isl}}[\vec{\theta}(\tau)] = \int_0^\beta d\tau \sum_{lq\sigma} \left[ \theta^*_{lq\sigma}(\tau)(\partial_\tau - \mu + \epsilon_{lq\sigma})\theta_{lq\sigma}(\tau) \right] \equiv \theta^* G^{-1}_I \theta, \tag{41}
\]
where \(\partial_\tau \equiv (\vec{x}_j - \vec{x}_{j-1})/\Delta_j\) for any variable. We have defined the shorthand notations including the integration over imaginary-time in the vector multiplication. The inverse of the Green’s functions of electrons in the lead (\(J\)) and the island (\(I\)) are denoted by \(g^{-1}_j\) and \(G^{-1}_I\), respectively. We will discuss the Green’s functions in more detail in section 2.5. The tunneling term reads
\[
S_T[\vec{\zeta}, \vec{\theta}, \vec{\varphi}] = \int_0^\beta d\tau \left[ \sum_{kq\sigma} \theta^*_{1k\sigma} t_{1Skq\sigma} e^{-i\varphi_{1k\sigma}} \zeta_{Skq\sigma} \sum_{l=2}^N \sum_{kq\sigma} \theta^*_{lk\sigma} t_{II-1kq\sigma} e^{-i(\varphi_{lI} - \varphi_{lI-1})} \theta_{I-1q\sigma} \right.
\]
\[
+ \sum_{kq\sigma} \zeta^*_{DK\sigma} t_{DNkq\sigma} e^{i\varphi_N} \theta_{Nq\sigma} + \text{h.c.} \right]. \tag{42}
\]

Inserting the result in equation (38) into the representation of the partition function in equation (31), we obtain a path integral representation of the partition function that will be the basis for the analysis in the following section. We close this section with a

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summary of the path integral formulation for the partition function

\[
Z[\vec{\zeta}, \vec{\theta}, \vec{\varphi}] = \mathcal{N} \prod_{I=1}^{N} \left[ \sum_{k_I = -\infty}^{\infty} \int_{\varphi_I(0)}^{\varphi_I(\beta)} D[\varphi_I(\tau)] \right] \int D\mu(\vec{\zeta}) \int D\mu(\vec{\theta}) e^{-S[\vec{\zeta}, \vec{\theta}, \vec{\varphi}]},
\]

(43)

where

\[
S[\vec{\zeta}, \vec{\theta}, \vec{\varphi}] = S_C[\varphi] + S_{BT}[\vec{\zeta}, \vec{\theta}, \vec{\varphi}].
\]

(44)

Introducing vectors \( \vec{\zeta}_J = (\ldots, \zeta_{JK}\sigma, \ldots)^T \), \( \vec{\theta}_I = (\ldots, \theta_{IK}\sigma, \ldots)^T \) and combining equations (39)–(42), we found that

\[
S_{BT}[\vec{\zeta}, \vec{\theta}, \vec{\varphi}] = S_{\text{lead}}[\vec{\zeta}] + S_{\text{isl}}[\vec{\theta}] + \int_{0}^{\beta} d\tau \left[ \theta_1^* \Lambda_{1S} \zeta_S + \sum_{I=2}^{N} \left( \theta_I^* \Lambda_{II-1} \theta_{I-1} + \zeta_D^* \Lambda_{DN} \theta_N + \text{h.c.} \right) \right],
\]

(45)

where we have introduced the tunneling matrices

\[
\Lambda_{1S} = t_{1Sk}\sigma e^{-i\varphi_1},
\]

\[
\Lambda_{II-1} = t_{II-1k}\sigma e^{-i(\varphi_I - \varphi_{I-1})},
\]

(46)

\[
\Lambda_{DN} = t_{DNk}\sigma e^{i\varphi_N},
\]

and used \( \varphi_S = \varphi_D = 0 \).

2.5. Integration over Grassmann fields

The Green’s functions of the lead electrons are defined by

\[
(\partial_\tau - \mu + \epsilon_{JK}\sigma) g_{JK}\sigma(\tau, \tau') = \delta(\tau - \tau'),
\]

(47)

and

\[
g_{JK}\sigma(0, \tau') = -g_{JK}\sigma(\beta, \tau'),
\]

(48)

where \( \mu \) denotes the chemical potential of the lead \( J \). Correspondingly, for the island electrons we have

\[
(\partial_\tau - \mu + \epsilon_{1q}\sigma) G_{1q}\sigma(\tau, \tau') = \delta(\tau - \tau')
\]

(49)

and

\[
G_{1q}\sigma(0, \tau') = -G_{1q}\sigma(\beta, \tau'),
\]

(50)
where $\mu$ also denotes the chemical potential of the island $I$. The solution of the inhomogeneous differential equation in equation (49) with the boundary condition in equation (50) reads [21]

$$G_{Iq\sigma}(\tau, \tau') = \begin{cases} 
\frac{\exp[-\epsilon_{Iq\sigma}(\tau - \tau')]}{1 + \exp(-\beta \epsilon_{Iq\sigma})} & \text{for } \tau > \tau', \\
-\frac{\exp[-\epsilon_{Iq\sigma}(\tau - \tau')]}{1 + \exp(\beta \epsilon_{Iq\sigma})} & \text{for } \tau < \tau', 
\end{cases}$$ (51) with the analogous expression for $g_{Jk\sigma}(\tau, \tau')$. For convenience, hereafter, we have measured all energies from the chemical potential of the leads and islands.

The action in equation (43) is quadratic in the Grassmann fields $\bar{\zeta}$ and $\bar{\theta}$ as can be seen explicitly from equation (45). Hence, the corresponding path integral is Gaussian and can be performed analytically. Thus, we can integrate over the quasi-particle reservoirs in three steps as in the following. For the first step, using the general Gaussian’s integral formula as [21]

$$\int \prod_{i=1}^{N} \frac{dx_i^* \, dx_i}{2\pi i} e^{-\frac{1}{2} x_i^* \, \mathcal{H} \, x_i + \theta_i^* \Lambda_i^* \theta_i + \bar{\zeta}_i^* \Lambda_i \bar{\zeta}_i} = (\det (\mathcal{H}))^{-1} e^{\theta_i^* \Lambda_i^* \Lambda_i \theta_i},$$

(52) we can integrate over the fermion in the source electrode in equation (43) as

$$\int D\mu(\zeta_S) e^{-S[\bar{\zeta}, \bar{\theta}, \bar{\varphi}]} = \int D\mu(\zeta_S) e^{-\left(\bar{\zeta}_S^* \Lambda_1^* \Lambda_S \zeta_S + \theta_1^* \Lambda_1^* \Lambda_S \theta_1 + \bar{\zeta}_S^* \Lambda_S \Lambda_1 \bar{\zeta}_S + \zeta_1^* \Lambda_1 \zeta_1 + \bar{\theta}_1^* \Lambda_S \bar{\theta}_1 + \bar{\varphi}_1^* \Lambda_S \bar{\varphi}_1\right)} = Z_S e^{\theta_1^* \Lambda_1^* \Lambda_S \Lambda_1 \theta_1},$$

(53) where $Z_S = \det (g_S^{-1})$. In the second step, we integrate over $\theta_1$ as

$$\int D\mu(\theta_1) e^{-S[\bar{\zeta}, \bar{\theta}, \bar{\varphi}]} = \int D\mu(\theta_1) e^{-\left(\theta_1^* \Lambda_1^* \Lambda_1 \theta_1 + \theta_1^* \Lambda_S \theta_1 + \theta_1^* \Lambda_1 \Lambda_1 \theta_1 + \theta_1^* \Lambda_S \Lambda_1 \theta_1 + \bar{\theta}_1^* \Lambda_1 \Lambda_S \bar{\theta}_1 + \bar{\theta}_1^* \Lambda_S \Lambda_S \bar{\theta}_1\right)}$$

$$= \det (G_1^{-1} - \Lambda_S^* \Lambda_S) e^{\theta_1^* \Lambda_1^* \Lambda_S \Lambda_1 \theta_1}$$

$$= Z_I \det (1 - G_I \Lambda_1^* \Lambda_1 \Lambda_S) e^{\theta_1^* \Lambda_1^* \Lambda_S \Lambda_1 \theta_1},$$

(54) where $Z_I = \det (G_I^{-1})$ and $\tilde{G}_I^{-1} = G_I^{-1} - \Lambda_1^* \Lambda_1$. We have used the identity matrix properties $G_1^{-1} G_1 = I$, and the determinant matrix property, respectively. In the same way, one integrates over $\theta_I$ variable and then obtains

$$\int D\mu(\theta_I)e^{-S[\bar{\varphi}, \Lambda]} = Z_I \det(1 - G_I \Lambda_1^* \Lambda_S \Lambda_1) e^{\theta_I^* \Lambda_1^* \Lambda_S \Lambda_S \Lambda_1 \theta_I},$$

(55) where $Z_I = \det (G_I^{-1})$, and

$$\tilde{G}_I^{-1} = G_I^{-1} - \Lambda_1^* \Lambda_S \Lambda_1.$$

(56)
For the third step, the fermion in drain $\zeta_D$ can be integrated as
\[
\int D\mu(\zeta_D) e^{-S[\varphi,\Lambda]} = Z_D \det (1 - g_D\Lambda_D^\dagger \tilde{G}_N\Lambda_D),
\]
where $Z_D = \det (g_D^{-1})$ and $\tilde{G}_N^{-1} = G_N^{-1} - \Lambda_{NN}^* \tilde{G}_{N-1} \Lambda_{N-1}$. We may rewrite the partition function in equation (38) as
\[
Z_{BT}[\vec{\varphi}] = N_{BT} \det (1 - G_1\Lambda_{IS}^* g_S\Lambda_{IS}) \prod_{I=2}^N \det \left(1 - G_I\Lambda_{II-1}^* \tilde{G}_{I-1}\Lambda_{II-1}\right)
\times \det \left(1 - g_D\Lambda_D^* \tilde{G}_N\Lambda_D\right),
\]
where $N_{BT} = Z_S Z_D Z_1 Z_2 \ldots Z_N$. To simplify for future reference, we rewrite the partition function in equation (58) in terms of the trace of matrix as
\[
Z_{BT}[\vec{\varphi}] = N_{BT} e^{\text{tr}\left\{\ln(1 - G_1\Lambda_{IS}^* g_S\Lambda_{IS})\right\}}
\times e^{\text{tr}\left\{\ln(1 - G_I\Lambda_{II-1}^* \tilde{G}_{I-1}\Lambda_{II-1})\right\}}
\times e^{\sum_{I=2}^N \text{tr}\left\{\ln(1 - GI\Lambda_{II}^* \tilde{GI}_{II-1}\Lambda_{II-1})\right\}},
\]
where we have used the matrix property as
\[
\det A = e^{\text{tr}\ln A}.
\]
We can therefore rewrite the partition function of the system in terms of the effective action as
\[
Z[\vec{\varphi}] = N_{\text{sys}} \prod_{I=1}^N \left[\sum_{k_I = -\infty}^{\infty} \int \varphi_I(\tau) D[\varphi_I(\tau)] e^{-S_{\text{eff}}[\vec{\varphi},\Lambda]}\right],
\]
where $N_{\text{sys}} = N_{BT}$ and $S_{\text{eff}}[\vec{\varphi},\Lambda]$ is the effective action of the island system
\[
S_{\text{eff}}[\vec{\varphi},\Lambda] = S_C[\vec{\varphi}] + S_T[\vec{\varphi},\Lambda],
\]
with the Coulomb action $S_C[\vec{\varphi}]$ obtained in equation (32) and the tunneling action is expressed as
\[
S_T[\vec{\varphi},\Lambda] = -\text{tr}\left\{\ln(1 - G_1\Lambda_{IS}^* g_S\Lambda_{IS})\right\} - \sum_{I=2}^N \text{tr}\left\{\ln \left(1 - G_I\Lambda_{II-1}^* \tilde{G}_{I-1}\Lambda_{II-1}\right)\right\}
\times -\text{tr}\left\{\ln \left(1 - g_D\Lambda_{DN}^* \tilde{G}_N\Lambda_{DN}\right)\right\}.
\]

**2.6. The tunneling action**

In order to evaluate the tunneling action in equation (63) explicitly, we have followed the ideas of Ambegaokar et al [22] and Grabert [14]. We expand the first term in equation (63) as
- \text{tr} \left\{ \ln (1 - G_1 \Lambda_{1S}^* g_S \Lambda_{1S}) \right\} = \text{tr} \left\{ \ln (1 - G_1 \Lambda_{1S}^* g_S \Lambda_{1S})^{-1} \right\}
= \text{tr} \left\{ \sum_{n=1}^{\infty} \left( \frac{G_1 \Lambda_{1S}^* g_S \Lambda_{1S}}{n} \right)^n \right\}.
\quad (64)

For the metallic oxide-layer tunnel junctions, the tunneling conductance arises from a large number, i.e., \( M = \sum_{\sigma} 1 \) of available tunneling channels while the tunneling amplitude and, accordingly, the matrix element of the tunneling matrices (\( \Lambda \)) introduced in equation (46) are very small. It is sufficient that one may keep only the first term in the expansion in equation (64) as

\[- \text{tr} \left\{ \ln (1 - G_1 \Lambda_{1S}^* g_S \Lambda_{1S}) \right\} \approx \text{tr} \left\{ G_1 \Lambda_{1S}^* g_S \Lambda_{1S} \right\}.\quad (65)\]

This approximation is known as the large channel number approximation \([14]\), and will be discussed in more detail later. To evaluate the trace of the matrix in equation (65), we substitute \( \Lambda_{1S} \) and \( \Lambda_{1S}^* \) from (46) into (65) as

\[\text{tr} \left\{ G_1 \Lambda_{1S}^* g_S \Lambda_{1S} \right\} = \sum_{kq\sigma} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' |t_{1Skq\sigma}|^2 e^{i(\varphi_1(\tau) - \varphi_1(\tau'))} G_{1k\sigma}(\tau, \tau') g_{S\sigma}(\tau, \tau'),\quad (66)\]

where \( |t_{1Skq\sigma}|^2 = t_{1Skq\sigma}^* t_{1Skq\sigma} \). We introduce the electron–hole-pair propagator as

\[\Pi_{1S}(\tau, \tau') = \sum_{kq\sigma} |t_{1Skq\sigma}|^2 G_{1k\sigma}(\tau, \tau') g_{S\sigma}(\tau, \tau').\quad (67)\]

By inserting the Green’s function \( G_{1k\sigma}(\tau, \tau') \) in equation (51) and the analogous expression for \( g_{S\sigma}(\tau, \tau') \), the propagator \( \Pi_{1S} \) becomes

\[\Pi_{1S}(\tau, \tau') = -\sum_{kq\sigma} |t_{1Skq\sigma}|^2 \frac{\exp \left[ -\epsilon_{1k\sigma}(\tau - \tau') \right]}{1 + \exp \left( \mp \beta \epsilon_{1k\sigma} \right)} \frac{\exp \left[ -\epsilon_{S\sigma}(\tau' - \tau) \right]}{1 + \exp \left( \pm \beta \epsilon_{S\sigma} \right)},\quad (68)\]

where the upper and lower sign holds for \( \tau > \tau' \) and \( \tau < \tau' \), respectively. Here we have measured all energies from the chemical potential of the leads and islands. Clearly, \( \Pi_{1S}(\tau, \tau') = \Pi_{1S}(\tau - \tau') \) depends only on \( \tau - \tau' \).

The tunnel matrix elements may be approximated as a constant in the relevant energy range, closed to the Fermi energy at low temperature. Thus, the energy dependence of the tunneling amplitudes can be neglected for energies near the Fermi energy, which contribute to the energy integrals. The propagator \( \Pi_{1S} \) can be transformed to read

\[\Pi_{1S}(\tau - \tau') = -|t_{1S}|^2 \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon' \sum_{\sigma} \rho_\sigma \rho_\sigma' \frac{e^{-\epsilon(\tau - \tau')}}{1 + e^{\pm \beta \epsilon}} \frac{e^{\epsilon'(-\tau - \tau')}}{1 + e^{\pm \beta \epsilon'}},\quad (69)\]

where the summation over wave vectors were transformed as the integration over energies. We have used a constant density of state per channel, i.e., \( \rho_\sigma \equiv \rho_\sigma(0) \) and extended
the limit of the integration since the metallic bandwidth is much larger than the relevant energy scales, $E_C$ and $k_B T$ [14]. The integration over the energies can be performed [25] and by replacing $\rho_\sigma$ and $\rho'_\sigma$ with the average densities of state per channel $\rho$ and $\rho'$ of the island and the lead, one gets

$$\Pi_{IS}(\tau - \tau') = -g_{1S} \alpha(\tau - \tau'),$$

where we have introduced the tunneling kernel

$$\alpha(\tau - \tau') = \frac{1}{4\beta^2 \sin^2 \left( \frac{\pi}{\beta}(\tau - \tau') \right)},$$

and the dimensionless tunneling conductance

$$g_{1S} = 4\pi^2 |t_{1S}|^2 M \rho \rho'$$

of the tunnel junction between the source electrode and the first island. Accordingly, the tunneling conductance $g_{1S}$ can be treated as a constant and we insert (70) into equation (66) to yield

$$\text{tr}\{G_1 \Lambda_{IS}^* g_S \Lambda_{IS}\} = -g_{1S} \int_0^\beta d\tau \int_0^\beta d\tau' \alpha(\tau - \tau') \cos[\varphi_1(\tau) - \varphi_1(\tau')],$$

where the imaginary part vanishes because of $\alpha(\tau - \tau')$ being an even function.

Analogous to the calculation of the first term above, one can evaluate the second and third terms in equation (63) with the approximation of $\tilde{G}_I$ as

$$\tilde{G}_I = (1 + G_I \Lambda_{I-1}^* G_{I-1} \Lambda_{I-1}) G_I,$$

where we have approximated $\tilde{G}_I^{-1}$ in equation (56) by the inverse matrix property and

$$\frac{1}{1 - x} = \sum_{n=0}^\infty x^n \approx (1 + x).$$

Using the definition of $\Lambda_{I-1}$ in equations (46) and (74), one can obtain the propagators

$$\Pi_{I-1}(\tau - \tau') = -g_{I-1} \alpha(\tau - \tau'),$$

and

$$\Pi_{DN}(\tau - \tau') = -g_{DN} \alpha(\tau - \tau'),$$

with

$$g_{I-1} = 4\pi^2 |t_{I-1}|^2 M \rho \rho',$$

and

$$g_{DN} = 4\pi^2 |t_{DN}|^2 M \rho \rho'.$$

At this point, we will explain the large channel number approximation in more detail, clarifying why the higher order terms in the expansion of the logarithm in equation (63)

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may be neglected in the limit of $M \gg 1$. The form the definitions in equations (70), (76), and (77) shows that by keeping only the first order of the expansion, the dimensionless conductance is proportional to $M|t_{II-1}|^2$. It is easy to see that for the higher order terms, the term $M|t_{II-1}|^n$ is proportional to $g_{II-1}^n M^{-n/2}$ for any even number $n \geq 2$, which is negligible for the large $M$ [23]. The dimensionless conductance can be related to the conductance of the tunnel junction between two conductors $I$ and $I-1$ as

$$g_{II-1} = \frac{2\pi}{e^2} G_{NN-1},$$

with $g_{IS}$ and $g_{DN}$ are related to $G_{IS}$ and $G_{DN}$, respectively.

By the large channel number approximation, the tunneling action in equation (63) can be rewritten as

$$S_T[\vec{\varphi}] = -\int_0^\beta d\tau \int_0^\beta d\tau' \alpha(\tau - \tau') \left\{ g_{IS} \cos[\varphi_1(\tau) - \varphi_1(\tau')] + \sum_{I=2}^N g_{II-1} \cos[(\varphi_{I-1}(\tau) - \varphi_{I-1}(\tau')) - (\varphi_I(\tau) - \varphi_I(\tau'))] + g_{DN} \cos[\varphi_N(\tau) - \varphi_N(\tau')] \right\},$$

where the imaginary parts were vanished due to the integrands being odd functions. We close this section with the expressed of the partition function as

$$Z[\vec{\varphi}] = N_{sys} \prod_{I=1}^N \left[ \sum_{k_I=-\infty}^{\infty} \int_{\varphi_I(0)}^{\varphi_I(\beta) + 2\pi k_I} D[\varphi_I(\tau)] \right] e^{-S_{\text{eff}}[\vec{\varphi}]},$$

where the effective action reads

$$S_{\text{eff}}[\vec{\varphi}] = \int_0^\beta d\tau \left\{ \frac{1}{4} \dot{\vec{\varphi}}^T E_{CN}^{-1} \dot{\vec{\varphi}} - i n_y^T \cdot \dot{\vec{\varphi}} \right\} - \int_0^\beta d\tau' \alpha(\tau - \tau') \left\{ g_{IS} \cos[\varphi_1(\tau) - \varphi_1(\tau')] + \sum_{I=2}^N g_{II-1} \cos[(\varphi_{I-1}(\tau) - \varphi_{I-1}(\tau')) - (\varphi_I(\tau) - \varphi_I(\tau'))] + g_{DN} \cos[\varphi_N(\tau) - \varphi_N(\tau')] \right\},$$

with $E_{CN}^{-1}$ is related to the matrix defined in equation (5).

3. Applications

The previous section found that the partition function corresponding to the path integral is a non-Gaussian integral and cannot be performed analytically. However, since all possible paths are expressed in imaginary time, the quantum mechanical propagator
turns into a quantum statistical density matrix to perform the quantum Monte Carlo method [13, 21, 26, 27]. Therefore, to show an application of the partition function in equation (82) with the effective action in equation (83), we will propose the calculation of average electron numbers of the serial island system and its application in the following.

3.1. Dimensionless energies

For more convenience in numerical calculations, such as the quantum Monte Carlo simulation of the SET [9], one may measure all energies in the relevant charging energy scale unit. Thus, in principle, one is free to choose the reference energy scale. However, this paper will use the charging energy that may be defined as

$$E_C = G^{cl} \sum_{I=1}^{N+1} \frac{E_{II-1}}{G_{II-1}},$$  \hspace{1cm} (84)

for the serial island system in figure 1. $G^{cl}$ denotes the total of high-temperature conductance of all tunneling junctions, i.e.

$$G^{cl} = \left( \sum_{I=1}^{N+1} \frac{1}{G_{II-1}} \right)^{-1},$$ \hspace{1cm} (85)

where $G_{II-1}$ stands for the high-temperature conductance between island $I$ and $(I-1)$ with $G_{10} = G_{1S}$ and $G_{N+1N} = G_{DN}$. The coefficient $E_{II}$ is the element of the matrix $E_N$ defined in equation (5). In the unit of the charging energy ($E_C$) given in equation (84), one can rewrite the Coulomb action in equation (32) as

$$S_C[\vec{\phi}(\tau)] = \int_0^{\beta E_C} d\tau \left\{ \frac{1}{4} \dot{\vec{\phi}}^T E_N \dot{\vec{\phi}} + i (\vec{\eta}^T \cdot \dot{\vec{\phi}}) \right\},$$ \hspace{1cm} (86)

where

$$E_N = 2E_C e^2 C_N \equiv \begin{pmatrix} E_{11} & E_{12} & \cdots & E_{1N} \\ E_{21} & E_{22} & \cdots & E_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ E_{N1} & \cdots & \cdots & E_{NN} \end{pmatrix},$$ \hspace{1cm} (87)

and the matrix $C_N$ is defined in equation (6). The tunneling action in equation (81) can be rewritten as
Grand canonical partition function of a serial metallic island system

\[ S_T[\vec{\varphi}(\tau)] = -\int_0^{\beta E_C} d\tau \int_0^{\beta E_C} d\tau' \alpha(\tau - \tau') \left\{ g_{1S} \cos[\varphi_1(\tau) - \varphi_1(\tau')] \ight. \\
\left. + \sum_{I=2}^N g_{II-1} \cos[(\varphi_{I-1}(\tau) - \varphi_{I-1}(\tau')) - (\varphi_I(\tau) - \varphi_I(\tau'))] \\
+ g_{DN} \cos(\varphi_N(\tau) - \varphi_N(\tau')) \right\} , \tag{88} \]

with the tunneling kernel

\[ \alpha(\tau - \tau') = \frac{1}{4(\beta E_c)^2 \sin^2 \left( \frac{\pi}{\beta E_c}(\tau - \tau') \right)} . \tag{89} \]

### 3.2. Winding numbers

The partition function in equation (82) is expressed as the sum over paths with different boundary conditions. Instead of evaluating each path integral separately up to a certain cutoff and adding them up. In numerical calculations, it is more convenient to make the transformation

\[ \varphi_I(\tau) = \xi_I(\tau) + \nu_{k_I} \tau, \tag{90} \]

where \( \nu_{k_I} = \frac{2\pi k_I}{\beta E_c} \) with all periodic paths obey the condition,

\[ \xi_I(0) = \xi_I(\beta E_c). \tag{91} \]

Using this transformation, one can rewrite the partition function in equation (82) in a suitable form as

\[ Z[\vec{\xi}, \vec{k}] = N_{sys} \prod_{I=1}^N \left[ \sum_{k_I=-\infty}^{\infty} \int_{\xi_I(0)}^{\xi_I(\beta E_c)} D[\xi_I(\tau)] e^{-S_{\text{eff}}[\vec{\xi}, \vec{k}]} \right] , \tag{92} \]

where the effective action can be expressed in terms of the winding numbers as

\[ S_{\text{eff}}[\vec{\xi}, \vec{k}] = S_C[\vec{\xi}, \vec{k}] + S_T[\vec{\xi}, \vec{k}] . \tag{93} \]

The Coulomb action in equation (86) can be rewritten as

\[ S_C[\vec{\xi}, \vec{k}] = \int_{\xi(0)}^{\xi(\beta E_c)} d\tau \frac{1}{4} \vec{\xi}^T E_N \vec{\xi} + \frac{4\pi^2}{\beta E_c} \vec{k}^T E_N \vec{k} + 2\pi i (\vec{n}_d^T \cdot \vec{k}) , \tag{94} \]

where \( \vec{\xi}(\tau) = (\xi_1(\tau), \ldots, \xi_N(\tau))^T \) with given winding numbers, \( \vec{k} = (k_1, \ldots, k_N)^T \). The tunneling action in equation (88) can be rewritten as

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3.3. Average electron number

In this section, we apply the partition and the effective action in equations (92)–(95) to calculate average electron numbers in the serial island system. The total electron number of the serial island system may be defined as

$$\langle n_{\text{Total}} \rangle = \sum_{I=1}^{N} \langle n_I \rangle,$$

where $\langle n_T \rangle$ denotes the total average electron number of the system and $\langle n_I \rangle$ denotes the average electron number of the island $I$. Analogous to the definition of charge fluctuations in the single electron box [14, 15], the average electron number on island $I$ can be expressed as

$$\langle n_I \rangle = n_{0I} + \frac{1}{2\beta E_C} \left( \partial \ln Z / \partial n_{0I} \right).$$

By inserting the partition function in equation (92) into (97), we can express the average electron number on islands into three cases, i.e.

$$\langle n_1 \rangle = n_{01} - \frac{4\pi i}{\beta E_C} (\langle E_{11} k_1 \rangle + \langle E_{12} k_2 \rangle),$$

$$\langle n_I \rangle = n_{0I} - \frac{4\pi i}{\beta E_C} (\langle E_I k_I \rangle + \langle E_{I-1} k_{I-1} \rangle + \langle E_{I+1} k_{I+1} \rangle),$$

and

$$\langle n_N \rangle = n_{0N} - \frac{4\pi i}{\beta E_C} (\langle E_N k_N \rangle + \langle E_{N-1} k_{N-1} \rangle),$$

for the first, intermediate, and last island, respectively. The coefficients in equations (98)–(100) are elements of the matrix obtained in equation (87). The expectation value of the winding numbers $\langle k \rangle$ in equations (98)–(100) is defined as
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\[ \langle k_I \rangle = \prod_{I=1}^{N} \left[ \sum_{k_I = -\infty}^{\infty} \int_{\xi_I(0)}^{\xi_I(\beta E_C)} D[\xi_I(\tau)] \right] k_I e^{-S_{\text{eff}}[\vec{\xi}, \vec{k}]} \]

where the effective action is obtained in equations (93)–(95). In analytical calculation, one cannot obtain an exact solution of the expectation value of the winding number in equation (101), because it is a non-Gaussian integral. However, by quantum Monte Carlo calculation, one can evaluate the expectation value of the winding number and the average electron number of the island system, as an example in the following section. Moreover, in the Monte Carlo calculation of the expectation value in equation (101), the fermionic sign problem [13] would arise from the imaginary part of the Coulomb action in equation (94). To reduce the influence of the fermionic sign problem, one can apply the idea in [27] to perform the quantum Monte Carlo simulation.

3.4. Two-island system

In this section, we focus on the two-metallic island system [18, 28] and calculate average electron numbers of the system by the Monte Carlo method. Limbach et al [18] reported the experimental results of two-metallic island systems, usually called the single electron-pump (the SEP), which can be represented by the circuit diagram in figure 2. This arrangement is biased by the voltage difference \( V_D - V_S \) denoted by \( V_{DS} \). Two gate voltages can tune the electrostatic potentials on two islands, i.e. \( V_{g1} \) and \( V_{g2} \), which couple directly to the islands by the capacitance \( C_{g1} \) and \( C_{g2} \). The experimentally unavoidable stray capacitors are represented by \( C_{2L} \) and \( C_{1R} \). We conclude this experiment with table 1 containing all parameters that one needs to simulate the average electron number of the SEP.

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Table 1. Parameters of the SEP [28]. A dimensionless conductance of the individual tunneling junction is defined as $g_j = G_j/G_K$, where $j \in \{1S, 21, D2\}$, $G_K = e^2/h$, and $G_{cl}^2$ stands for the high-temperature conductance of the SEP. The charging energy $E_C$ defined as in equation (84) is equal to 0.184 meV.

| Parameters | $C_S$ | $C_1$ | $C_D$ | $C_{g1}$ | $C_{1R}$ | $C_{2L}$ | $g_{1S}$ | $g_{21}$ | $g_{21}$ | $G_{cl}^2$ |
|------------|-------|-------|-------|----------|----------|----------|----------|----------|----------|-----------|
| Values     | 181   | 173   | 236   | 50.5     | 18.0     | 21.5     | 58.6     | 0.52     | 1.32     | 0.83      | 10.0      |
| Units      | (aF)  | (aF)  | (aF)  | (aF)     | (aF)     | (aF)     | —        | —        | —        | (μS)      |

From the definition of the total average electron number in equation (96), we can rewrite the total average electron number for the two-island system as

$$\langle n_{\text{Total}} \rangle = \langle n_1 \rangle + \langle n_2 \rangle,$$

(102)

where the average electron number of the first and second island can be obtained by

$$\langle n_1 \rangle = n_{01} - \frac{4\pi i}{\beta E_C} (E_{11}\langle k_1 \rangle + E_{12}\langle k_2 \rangle),$$

(103)

and

$$\langle n_2 \rangle = n_{02} - \frac{4\pi i}{\beta E_C} (E_{22}\langle k_2 \rangle + E_{21}\langle k_1 \rangle),$$

(104)

where the induced charges on the first and second islands are generally denoted by $n_{01} = (C_S V_S + C_1 V_1 + C_{g1} V_{g1} + C_{2L} V_{g2})/e$, and $n_{02} = (C_1 V_1 + C_D V_D + C_{g2} V_{g2} + C_{1R} V_{g1})/e$, respectively. The expectation value of the winding number $\langle k_I \rangle$ of the two-island system is expressed as

$$\langle k_I \rangle = \sum_{k_1, k_2} \frac{\xi_{1}(\beta E_C)}{\xi_{1}(0)} \frac{\xi_{2}(\beta E_C)}{\xi_{2}(0)} \int D[\xi_1(\tau)] \int D[\xi_2(\tau)] k_I e^{-S_{\text{eff}}[\vec{\xi}, \vec{k}]}$$

(105)

where the effective action reads

$$S_{\text{eff}}[\vec{\xi}, \vec{k}] = S_C[\vec{\xi}, \vec{k}] + S_T[\vec{\xi}, \vec{k}],$$

(106)

and the Coulomb action

$$S_C[\vec{\xi}, \vec{k}] = \int_{(0)}^{\xi_{1}(\beta E_C)} d\tau \frac{1}{4} \vec{\xi}^T \mathbb{E}_C \vec{\xi} + \frac{4\pi^2}{\beta E_C} \vec{k}^T \mathbb{E}_2 \vec{k} + 2\pi i (\vec{n}_g^T \cdot \vec{k}),$$

(107)

where $\vec{\xi} = (\xi_1, \xi_2)^T$, $\vec{k} = (k_1, k_2)^T$, and $\vec{n}_g^T = (n_{01}, n_{02})$. For the two-island system, the matrix in equation (87) is reduced to be

$$\mathbb{E}_2 = \frac{2E_C}{e^2} C_2 \equiv \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix},$$

(108)
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with the capacitance matrix

$$C_2 = \begin{pmatrix} C_{\Sigma 1} & -C_1 \\ -C_1 & C_{\Sigma 2} \end{pmatrix},$$

where $C_{\Sigma 1} = C_5 + C_1 + C_{g1} + C_{2L}$ and $C_{\Sigma 1} = C_1 + C_D + C_{g2} + C_{1R}$. The tunneling action of the two-island system reads

$$S_T[\vec{\xi}, \vec{k}] = -\int_{\xi(0)}^{\xi(\beta E_c)} d\tau \int_{\xi(0)}^{\xi(\beta E_c)} d\tau' \alpha(\tau - \tau') \left\{ g_{1S} \cos[\xi_1(\tau) - \xi_1(\tau')] + \nu_{k_1} k_1 \right\}$$

$$+ g_{21} \cos[(\xi_1(\tau) - \xi_2(\tau')) - (\xi_2(\tau) - \xi_2(\tau')) + (\nu_{k_1} - \nu_{k_2})(\tau - \tau')]$$

$$+ g_{D2} \cos[\xi_2(\tau) - \xi_2(\tau') + \nu_{k_2} k_2] \right\}.$$  \hspace{1cm} (110)

Using the parameters in table 1, we have calculated the average electron numbers in equations (102)–(104) by the quantum Monte Carlo method. Figures 3(a) and (b) show that the average electron number on the first and second islands are step functions of two dimensionless gate voltage variables. For the condition $V_{DS} = 0$, when two gate voltages are increased, the total average electron rises. This situation is well known as the Coulomb staircase and the essential behavior of a single-electron box [14, 15]. The total average electron number of the system is also the Coulomb staircase shown in figure 3(c). In this case, therefore, the single-electron pump behaves like a single-electron box consisting of two coupling islands. Then, electrons can propagate between the two islands, controlling with the two gates.

Furthermore, we found that the projection of the total average electron number on the dimensionless gate voltage plane shows hexagonal domains as in figure 3(d). The average electron numbers on each island take a fixed value indicated by the numbers in the hexagonal domains. Let us consider the triple point in the black circle, shown in figure 3(d), where three adjacent states can be occupied. Circling the triple point counter-clockwise corresponds to the sequence $(1, 1) \rightarrow (2, 1) \rightarrow (1, 2)$, which describes an electron that can transfer from left to right. Therefore, in the presence of $V_{DS}$, current can flow through the two islands from the source lead to the drain lead by applying the gate voltages corresponding to the position of the triple point in the $(n_{01}, n_{02})$ plane. According to the experimental results, the maximum conductance peaks of the SEP occurred near the triple points [18].

To verify the hexagonal domains, we have calculated the charge stability diagram of the two-island system by the method in [24], which is called the traditional stability diagram. This stability diagram was calculated by concerning only the charging energy of the system, in which the degeneracy lines between the stable charge regions depend on two dimensionless gate voltages parameters, as shown by the doted lines in figure 3(d). We emphasize that the tunneling effect and temperature dependence were neglected in calculating the traditional stability diagram [24]. As a result, we found that the doted lines overlap the borders of the hexagonal domains for low temperatures. In other words, it showed that we could construct the stability diagram of the two-island system using the average electron numbers, including the tunneling effect, which is then called the quantum stability diagram. Since single-electron transport in the island systems includes
Figure 3. The average electron numbers of the first, second, and two islands are shown in (a)–(c), respectively, were calculated by the quantum Monte Carlo method for $\beta E_C = 20.0$, and the corresponding temperature $T = 0.1$ K. The projection of the total average electron number on the dimensionless gate voltage plane $(n_{01}, n_{02})$ shows that the hexagonal domains mark regions indicated by the electron state $(n_1, n_2)$.

the tunneling process, the quantum stability diagram could become a powerful tool to study the island systems beyond the classical picture.

4. Conclusions

In this paper, we have calculated the grand canonical partition function of the serial metallic island system by the imaginary-time path integral formalism. By the large
channel approximation, the partition function as a path integral over phase fields with a path probability given the effective action functional. Furthermore, we have proposed calculating average electron numbers of the metallic island system and rewritten them in suitable forms for the quantum Monte Carlo simulation. For the demonstration, we have calculated the average electron numbers for the SEP. The results show that the average electron numbers increase with the two gate voltage variables as a step function. Therefore, the single-electron pump behaved like the single-electron box consisting of two coupling islands, wherein electrons can propagate between the two islands, controlling by the two gates. In addition, we have proposed the method to construct the stability diagram for a finite temperature, including the tunneling effect, by a projection image of the total average electron number on the dimensionless gate voltage variables plane. As a result, the stability diagram could describe the occurrence of the Coulomb blockade regions in agreement with the traditional stability diagram, in the limit of low temperature. Finally, we anticipate that the partition function will be helpful as a starting point for a further theoretical investigation into the serial island system. It would also be interesting to use the approaches described in this paper to describe single-electron device’s experiments.

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