Microscopic model for a strongly correlated superconducting single-electron transistor

Enrico Perfetto and Michele Cini*

Dipartimento di Fisica, Universita' di Roma Tor Vergata, Via della Ricerca Scientifica, 1-00133 Roma, Italy, INFN-Laboratori Nazionali di Frascati, Via E.Fermi 40, 00044 Frascati, Italy

and Istituto Nazionale per la Fisica della Materia

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We model a Superconducting Single-Electron Transistor operating by repulsive interactions. The device consists of a ring of Hubbard clusters, placed between electrodes and capacitively coupled to a gate potential. In each cluster, a pair of electrons at appropriate filling feels a weak effective interaction which leads to pairing in part of the parameter space. Thus, the system can host many bound pairs, with correlation induced binding. When the charging energy exceeds the pairing energy, single-electron tunneling prevails; in the opposite regime, we predict the Coulomb blockade pattern of two-electron tunneling. This suggests that in tunneling experiments repulsion-induced pairs may behave in a similar way as phonon-induced ones.

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I. INTRODUCTION

In recent years, a variety of transport experiments have been reported in molecular size systems, such as quantum dots and nanotubes, as a contribution to the current boost towards of the progress in nanoscale technology. From the theoretical side, circuits of several kinds have been modeled,¹ and in applied electronics the Single-Electron Transistors² are among the most important devices. These are realized by connecting a nanoscopic conducting island to metallic leads and to a gate voltage. The energy gaps existing between states with a different number of particles allow us to fix the number of electrons in the island very sharply; as a consequence single electrons can tunnel to or from the conductor. Even more appealing situations arise when the above scenario is complicated by electron-electron interactions, as in the case of a Superconducting-Single Electron Transistor (S-SET).

A S-SET is a mesoscopic device obtained by linking capacitively a superconducting grain to two normal leads and to a gate electrode as well.³ The latter allows one to control the number N of electrons on the grain by tuning the gate voltage *Vg*. Such a system has been studied both experimentally⁴ and theoretically⁵⁻⁷ in great detail during the past years. In a normal island the parity of *N* oscillates between even and odd values, by varying V_g ; conversely in a superconducting island *N* is always even because of the paired nature of the ground state. Therefore the S-SET transport properties in the linear regime are governed by Andreev reflection under the critical temperature T_c of the central island, while above T_c single electron tunneling prevails. This leads to well pronounced Coulomb blockade peaks of the conductance $G = \partial I/\partial V|_{V=0}$ as a function of the gate voltage. In particular the parity-controlled tunneling produces $2e/C_o$ periodic peaks in the pair-tunneling regime, in contrast with the e/C_g periodicity of the normal system (here C_g is the capacity of the gate electrode). This behavior is well reproduced by models $5\frac{5}{7}$ using a gate controlled BCS Hamiltonian H_{BCS} ; the connection to free electron leads employs a tunneling Hamiltonian, usually treated by second-order perturbation theory.

In the present article we propose a model for a S-SET with a strongly correlated, repulsive Hubbard-like model instead of H_{BCS} as the "superconducting" grain Hamiltonian. That is, we look for a superconducting response entirely driven by the electronic correlations rather than by the phonon-mediated effective attraction. The occurrence of twoelectron tunneling in non BCS systems was observed by Ashoori *et al.*⁸ in a 1 μ m GaAs tunnel capacitor. Purely electronic mechanisms were proposed to explain this behavior and the GaAs quantum dot models ranged from a semiclassical description⁹ to a Hubbard model framework.¹⁰ Unlike the systems considered by Refs. 9 and 10, in our *gedankenexperiment*, like in a S-SET, the tunneling current is due to many bound pairs hosted by the device in a wide range of gate potentials.

The plane of the paper is the following. In the next section we introduce the microscopic model that we are going to study. Section III is devoted to determine some important properties of the strongly correlated central island. We show that the electronic correlations provide a nontrivial characteristic energy which can be compared with the electrostatic charging energy in order to distinguish between a *normal* regime and a *superconducting* one. In particular in these two regimes the parity of the number of particles in the ground state oscillates exactly like in a S-SET. In Sec. IV we explicitly calculate the conductance as a function of the gate voltage by using a master equation approach.¹¹ It is found that the linear response of our strongly correlated device shows Coulomb blockade pattern. A normal behavior is observed in the noncorrelated and in the very strongly correlated regimes; while in the intermediate case, the spacing between the conductance peaks doubles. Finally the conclusions are drawn in Sec. V.

II. THE MODEL

Let us consider the grand-canonical Hamiltonian,

$$
\mathcal{H} - \mu \hat{N}_{tot} = H_{\text{device}} + H_{\text{leads}} + H_T. \tag{1}
$$

Here H_{device} is an extended Hubbard model of the central island coupled capacitively to a gate voltage V_g ; H_{leads} de-

FIG. 1. (a): Scheme of the strongly correlated S-SET. The device consists of Λ Hubbard clusters arranged in a ring and linked symmetrically to one another. (b) A pictorial representation of H_{α} and H_T .

scribes the left and right reservoirs, supposed to be identical free electron gases for simplicity; H_T is the tunneling Hamiltonian, that connects the central device to the leads; μ is the chemical potential and \hat{N}_{tot} is the total number of particles operator. The carriers are electrons, of charge −*e*,*e*.0. Let us examine these three terms in detail. As in previous work, 12 the central island consists in a ring of Λ identical 5-site centered-square Hubbard clusters, denoted by the index α ; see Figs. 1(a) and 1(b). Each cluster is described by the Hamiltonian

$$
H_{\alpha} = \sum_{\sigma,i=1}^{4} t(p_{\alpha,0\sigma}^{\dagger}p_{\alpha,i\sigma} + \text{h.c.}) + U \sum_{i=0}^{4} \hat{n}_{\alpha,i\uparrow} \hat{n}_{\alpha,i\downarrow}, \tag{2}
$$

with the creation operators on the α -th cluster $p^{\dagger}_{\alpha,0\sigma}$ for the central site, and $p^{\dagger}_{\alpha,i\sigma}$, $i=1,\ldots,4$ for the remaining 4 sites; $\hat{n}_{\alpha,i\sigma} = p^{\dagger}_{\alpha,i\sigma} p_{\alpha,i\sigma}$, and σ is a spin index.

In the device, each cluster α is linked to the two nearest neighbors ones (denoted by $\alpha+1$ and $\alpha-1$) by the hopping Hamiltonian H_{τ} [see Fig. 1(a)] whereby a particle in the *i*-th site of the α -th cluster can hop towards the *i*-th site of the $\beta = \alpha \pm 1$ -th clusters:

$$
H_{\tau} = \tau \sum_{\alpha=1}^{\Lambda} \sum_{\beta=\alpha \pm 1} \sum_{\sigma,i=1}^{4} (p^{\dagger}_{\alpha,i\sigma} p^{\dagger}_{\beta,i\sigma} + \text{h.c.}). \tag{3}
$$

 H_{device} also contains an electrostatic charging energy term due to an effective capacitance *C* of the central island. Finally the island is connected capacitively to the gate which is at a potential V_g [see Fig. 1(b)]. Therefore we have

$$
H_{\text{device}} = \sum_{\alpha=1}^{\Lambda} H_{\alpha} + H_{\tau} + \frac{(\hat{N}e)^2}{2C} - e(V_g - \mu)\hat{N},\tag{4}
$$

where \hat{N} is total number of particles operator in the central device. We remark that the capacitive term is essentially long-ranged and accounts for the monopole contribution to the charging energy, while the *U* terms depend on the way the charges are distributed in the island. In all electrostatic terms \hat{N} should be referred to an average population corresponding to a neutral situation; but, actually, any shift *N*

FIG. 2. Δ (in eV) as a function of *U/t*. The maximum binding occurs at *U* \sim 5*t* where $\Delta \approx$ -0.042*t*. For *U*>34*t*, Δ becomes positive and pairing disappears.

 $\rightarrow \hat{N} - \langle \hat{N} \rangle$ would produce a constant and a linear term in \hat{N} that just modifies μ .

Both leads are free electron gases with chemical potentials μ_{γ} , $\gamma=l$, *r*; hence

$$
H_{\text{leads}} = \sum_{\gamma=l,r} \sum_{k,\sigma} (\varepsilon_k - \mu_\gamma) c_{k,\gamma,\sigma}^\dagger c_{k,\gamma,\sigma}, \tag{5}
$$

with $\mu = \mu_l = \mu_r - eV$,¹⁶ where *V* is the bias.

Finally the tunneling Hamiltonian is taken to be

$$
H_T = \sum_{\eta,k,\sigma} \left[T^{(l)}(c_{k,l,\sigma}^{\dagger} f_{1,\eta\sigma} + \text{h.c.}) + T^{(r)}(c_{k,r,\sigma}^{\dagger} f_{[\Lambda/2],\eta\sigma} + \text{h.c.}) \right],\tag{6}
$$

where the $f^{\dagger}_{\alpha,\eta\sigma}$ are eigen-operators of the noninteracting term of $H_{\alpha}^{a, \gamma} \Sigma_{i\sigma} f(p_{\alpha,0\sigma}^{\dagger}p_{\alpha,i\sigma} + p_{\alpha,i\sigma}^{\dagger}p_{\alpha,0\sigma}) = \Sigma_{\eta,\sigma} \epsilon_{\eta} f_{\alpha,\eta\sigma}^{\dagger} f_{\alpha,\eta\sigma}$ We observe that the tunnel junctions connect two opposite clusters to the leads; namely the $\alpha=1$ cluster is linked to the left electrode and the $\alpha = [\Lambda/2]$ cluster to the right lead (here $[x]$ means the integer part of *x*); see Fig. 1(a). Note also that $T^{(\gamma)}$ is independent of η ; in other terms we are using "white" wires, that is, leads that do not filter electrons according to the square symmetry of electronic states in each cluster. This is a simple way to ensure the 3D nature of the leads, which is essential to allow Andreev reflection.

In the next section we draw some relevant properties of H_{device} which mimic the behavior of H_{BCS} despite the presence of strong electronic correlations.

III. PROPERTIES OF THE CENTRAL ISLAND

In order to understand the physics of the device that we propose, it is useful to focus first on properties of H_{α} , referred to as a single 5-site cluster. The Hamiltonian H_{α} is a prototype example of electronic pairing from repulsion; this is signaled by the property $\Delta < 0$, where $\Delta = \varepsilon(4) + \varepsilon(2)$ $-2\varepsilon(3)$ and $\varepsilon(m)$ is the ground state energy with *m* electrons. There is pairing at $m=4$ for $U/t < 34$, the minimum value is Δ = -50 meV at *t*=1 eV and *U* ~ 5 eV and the binding energy is $|\Delta|$ (see Fig. 2). The mechanism has been investigated elsewhere, $13,14$, and need not concern us here; we just say that broadly speaking it is a lattice counterpart of the Kohn-Luttinger mechanism.¹⁵

When a negative Δ occurs, its competition with e^2 / C determines the parity of the number N_{gs} of electrons in the

ground state of H_{device} for small values of the inter-cluster hopping τ .

Here we are interested in the behavior of the device at low temperatures $kT \ll |\Delta|$. Up to $o(\tau)$ and $o(\tau^2)$ corrections, the ground state energy $E(N)$ of the central device with a fixed even or odd number of particles N is

$$
E_N = \begin{cases} \Lambda \varepsilon(2) + (N - 2\Lambda)I_P + \left(\frac{N}{2} - \Lambda\right)\Delta + \frac{(Ne)^2}{2C} - e(V_g - \mu)N, & \text{for even } N;\\ \Lambda \varepsilon(2) + (N - 2\Lambda)I_P + \left(\frac{N}{2} - \Lambda - \frac{1}{2}\right)\Delta + \frac{(Ne)^2}{2C} - e(V_g - \mu)N, & \text{for odd } N,\end{cases}
$$
(7)

where $I_P = \varepsilon(3) - \varepsilon(2)$. Since one bound pair exists at $m=4$ electrons in the 5-site cluster, the first bound pair in the Λ -cluster system appears at $N=2\Lambda+2$ electrons. From Eq. (7), it follows that in the range $2\Lambda \le N \le 4\Lambda$, N_{gs} is always even if the pair binding energy overcomes the charging energy. We call the situation when $|\Delta| > e^2 / C$ the *superconducting* regime. Otherwise the system is *normal* and any *N* is lowest in a range of V_g . In Fig. 3 we plot the ground state energy of H_{device} as a function of V_g in both regimes, for τ $=0$. It also relevant to focus on the critical values of V_g where ground states of different N_{gs} cross. We define $(\Delta V_g)_n$ as the spacing between the critical values in the normal regime and $(\Delta V_g)_{sc}$ such a spacing in the superconducting regime; it holds that

FIG. 3. E_N − E_8 , where E_N is the ground state energy of H_{device} , versus *Vg*, for several numbers *N* of particles. (a) In the *superconducting* regime; (b) in the *normal* regime. Solid lines are used for even *N* and dotted lines for odd *N*. In the insets we plot the grandcanonical averages of \hat{N} in H_{device} . We used $\Lambda = 4$, $t = 1$ eV, $\tau = 0$, $kT = 0.001$ eV, $C = 50$ e/V; with this choice $e^2 / C = 0.02$ eV. In (a) *U*=5 eV $(\Delta = -0.043 \text{ eV})$ and in (b) *U*=0.2 eV $(\Delta = -0.0008 \text{ eV})$. V_g is in V, E_N is in eV.

$$
(\Delta V_g)_n = \frac{e}{C} + \frac{\Delta}{e},
$$

$$
(\Delta V_g)_{sc} = \frac{2e}{C}.
$$
 (8)

The charge fluctuations in the superconducting regime as a function of the gate voltage are about double spaced with respect to the normal regime, that is the typical condition experimentally realized in a S-SET.⁴

We can also visualize the previous results by plotting the gran-canonical average of the number of particles in the isolated central device as a function of V_g . We use the standard definition

$$
\langle N \rangle = \frac{1}{Z} \text{Tr} [\hat{N} e^{-(H_{\text{device}} - \mu \hat{N})/k} \mathbf{I}], \tag{9}
$$

where *Z*=Tr[$e^{-(H_{\text{device}} - \mu \hat{N})/kT}$]; Tr is dominated by the low energy states of H_{device} with $\tau=0$. In Fig. 4(a) one can observe the so called Cooper staircase, characteristic of the superconducting regime.

Below, for computational convenience, we assume that $\tau \ll |\Delta|$ and deal with H_{τ} perturbatively.¹² So, the critical values of V_g where level crossing occurs are spread into intervals of width $o(\tau)$ in the normal regime and $o(\tau^2)$ in the superconducting regime. Anyway the qualitative behavior is still close to Figs. 3 and 4.

IV. CALCULATION OF THE LINEAR CONDUCTANCE

Next, we consider the effects of small bias voltage *V* applied between leads, i.e., the linear conductance $G \equiv \partial I/\partial V$ for $V \rightarrow 0$, versus the gate voltage V_{φ} . In the present article, we follow the approach proposed by Beenakker¹¹ and get the formula for the conductance from a master equation. We take $T^{(l)}$, $T^{(r)} \ll kT$, $|\Delta|$ in order to provide that *(i)* the parity of the ground state is stable with respect to thermal effects, (*ii*) the elementary tunnel processes between the leads and the central devices involve a few particles at a time and the broadening of the levels of H_{device} due to the presence of the leads is smaller than the thermal one. As discussed by Beenakker, $¹¹$ </sup> these limitations characterize the Coulomb blockade regime.

In the normal regime single-electron tunneling dominates. The theory works very much like in Ref. 11 and we calculate the first-order transmission rates,

FIG. 4. $\langle N \rangle$ versus V_g . (a) In the *superconducting* regime; (b) in the *normal* regime. The parameters are the same as in Fig. 3. V_g is in V.

$$
\Gamma_{q_{N-1},i_N}^{(\gamma)} = \frac{2\pi}{\hbar} T^{(\gamma)^2} \left| \sum_{\eta,\sigma} \langle q_{N-1} | f_{\alpha,\eta\sigma} | i_N \rangle \right|^2, \tag{10}
$$

from the i_{N-1} -th state of the central device with N particles (denoted $|i_N\rangle$) to the q_{N-1} -th state of the central device with *N*−1 particles $(|q_{N-1}\rangle)$ via tunneling to the left *(l)* or right *(r)* lead. Remember that $\alpha=1$ for $\gamma=l$ and $\alpha=[\Lambda/2]$ for $\gamma=r$. In the actual calculations below, we obtain $|i_N\rangle$ in second-order perturbation theory in H_r ; we mix the degenerate groundstate multiplets of energy E_N of H_{device} , which determine the low-energy properties of the system. By first-order perturbation theory in H_T , one gets the familiar formula

$$
G^{(I)} = \frac{\rho e^2}{KT} \sum_{N=2\Lambda+1}^{4\Lambda} \sum_{i_N, q_{N-1}} \frac{\Gamma_{q_{N-1}, i_N}^{(r)} \Gamma_{q_{N-1}, i_N}^{(l)}}{\Gamma_{q_{N-1}, i_N}^{(r)} + \Gamma_{q_{N-1}, i_N}^{(l)}} \times P^{(0)}(i_N) [1 - f(E_{i_N} - E_{q_{N-1}})]. \tag{11}
$$

Here, $P^{(0)}(i_N)$ is the Boltzmann equilibrium probability for occupying the eigenstate $|i_N\rangle$ with energy E_{i_N} ; *f* is the Fermi distribution function, and ρ is the density of states at the Fermi level in both leads. Each term in Eq. (11) depends on *V_g* through the statistical factor $P^{(0)}(i_N)[1 - f(E_{i_N} - E_{q_{N-1}})]$ and produces the well known Coulomb blockade behavior.^{11,17} The linear conductance is highly suppressed unless the gate voltage is fine tuned at $E_{i_N} \sim E_{q_{N-1}} - \mu$, where sharp peaks of $G^{(1)}$ occur. The second-order contribution in H_T depends on $o(T^{\gamma})^4$) rates which are negligible with respect to the $o([T^{\gamma}]^2)$ Γ coefficients; therefore we can safely avoid working out the second-order current in this regime.

When $|\Delta| > e^2 / C$, only even *N* have an important weight in the appropriate range of V_g [see Fig. 3(a)]; therefore the resonance condition $E_{i_N} = E_{j_{N-1}} - \mu$ never holds and the firstorder conductance $G^{(1)}$ is highly suppressed for any value of *Vg*. In this *pair tunneling regime*, accordingly, we must go on calculating the conductance up to second-order in H_T .⁵⁻⁷ Three-body, four-body transitions and so on can be disregarded, however, as $\overline{T}^{(l)}$ and $\overline{T}^{(r)}$ are both small compared to the charging energy. Since electrons can get paired in the device but not in the leads, we may think of the second-order processes in terms of Andreev reflections. First, one of the two electrons tunnels from one lead to the device (which is in the $|m_{N-2}\rangle$ state) and forms a virtual excited state. Then the second one tunnels into the device and form a bound pair $(|i_N\rangle)$ state).

In principle in second-order, one should also take into account the *cotunneling* processes,¹⁸ which leave the population of the central island unchanged. Such processes provide a current away from the resonances. Anyway, as long as our device is in the small bias and low temperature regime, the cotunneling current is found to be negligible, as in the case of Ref. 6. Therefore the *sequential tunneling* m_{N-2} $\rightarrow i_N$ is the major transport mechanism, and it is possible only at the two-electron degeneracy points. The full derivation of the solution of the detailed balance equations¹¹ will be presented elsewhere. Setting

$$
G_0^{(\text{II})} = \frac{128\pi e^2 \rho^2}{\Delta^2 \hbar} \frac{T^{(l)^4} T^{(r)^4}}{T^{(l)^4} + T^{(r)^4}},
$$
(12)

one gets for the conductance

$$
\frac{G^{(\text{II})}}{G_0^{(\text{II})}} = \sum_{N=2\Lambda+2}^{4\Lambda,\text{even}} \sum_{i_N, m_{N-2}} \Xi_{i_N, m_{N-2}} e^{(E_{i_N} - E_{m_{N-2}} - 2\mu)/2kT}
$$

$$
\times P^{(0)}(i_N) \frac{(E_{i_N} - E_{m_{N-2}} - 2\mu)/2kT}{\sinh[(E_{i_N} - E_{m_{N-2}} - 2\mu)/2kT]}.
$$
(13)

The two-electron transition probability

$$
\Xi_{i_N,m_{N-2}} = \left| \sum_{l_{N-1}} \sum_{\alpha,\beta,\eta,\nu} \langle i_N | f_{\alpha,\eta}^\dagger | l_{N-1} \rangle \langle l_{N-1} | f_{\beta,\nu}^\dagger | m_{N-2} \rangle \right|^2
$$

takes into account the second-order process governing the Andreev reflection. Equation (13) predicts Coulomb blockade peaks for every V_g such that $E_{i_N} = E_{m_{N-2}} + 2\mu$, while the conductance is strongly suppressed elsewhere. Each peak has a correlation weight due to the coefficient $\Xi_{i_N,m_{N-2}}$, containing all the microscopic information on the correlated ground states of the central device.

For illustration, we numerically computed the conductance for a central device with Λ =4. In the superconducting regime, $G^{(II)}$ as a function of the gate voltage is shown in Fig. 5 for $t=1$ eV, $U=5$ eV, $\tau=0.0005$ eV, $kT=0.001$ eV, *C*=50 e/. Note that $\tau \ll |\Delta|$ =0.043 eV, and $|\Delta| > e^2 / C$ =0.02 eV. $G^{(II)}$ shows neat peaks, with spacing $(\Delta V_g)_{sc}$ $=2e/C=0.04$ V.

This superconductor-like behavior depends on the existence of pairing. As a countercheck, we calculate the linear conductance $G^{(I)}$ in the normal regime, when $\Delta=0$. We can

FIG. 5. Linear conductance $G^{(II)}$ as a function of V_o in the pairtunneling regime. We used Λ =4, $t=1$ eV, $U=5$ eV, $\tau=0.0005$, kT =0.001 eV, $C = 50$ e/V, $\mu = 0$. V_g is in V.

obtain this condition in two ways: namely in the noninteracting case when $U=0$ and in the very strongly correlated regime, when $U \approx 34$ eV, the other parameters remaining the same as in Fig. 5. $G^{(1)}$ is plotted in Fig. 6; since we are mainly interested in the period of the resonances, we use constant Γ 's and plot the results in arbitrary units. Indeed, for Δ =0 the period of the resonant peaks is *e*/*C* \approx 0.02 eV, i.e., a half of the period in the superconducting case.

V. SUMMARY AND CONCLUSIONS

We have shown that the Hamiltonian H models a S-SET in the linear regime. We pointed out that the repulsioninduced pairing occurring in H_{device} fixes a characteristic energy $|\Delta|$ which competes with the electrostatic charging energy e^2 /*C*. As in any S-SET, there is a *normal regime*, where $|\Delta| < e^2 / C$ and a *superconducting regime*, where $|\Delta| > e^2 / C$. In the first case the parity of the electron number in the ground state oscillates between even and odd values and the transport properties are governed by single-electron tunneling. Conversely in the superconducting regime the parity is always even and the major transport mechanism is the se-

FIG. 6. Linear conductance $G^{(1)}$ as a function of V_{ϱ} in the singleelectron-tunneling regime: (a) $U=0$; (b) $U=34$ eV. The other parameters are the same as in Fig. 5. V_g is in V.

quential tunneling of pairs. The explicit calculations have been performed for a ring of four 5-site clusters, but a general expression for the linear conductance is also derived.

Our results suggest a systematic way to produce a well controlled periodic two-electron pattern, even without any conventional superconductivity; an array of quantum dots similar to the one in Ref. 8 could be designed to this purpose.

Finally we underline that the model we propose is very flexible with respect (*i*) to the size and the shape of the Hubbard clusters; (*ii*) to the topology of the cluster array forming the central device. Indeed a wide variety of Hubbard clusters show the $\Delta < 0$ property at proper fillings, which is actually the key feature at the basis of our device; we could construct many alternative devices, based on graphs with different topologies, also in view of possible single-electronics applications to more complex circuits than a transistor.

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^{*}Electronic address: Michele.Cini@roma2.infn.it

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