Unified Scaling Theory of the Electron Box for Arbitrary Tunneling Strength

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Electron tunneling leads to screening of the charge of small islands. The effect is strongest near degeneracy points of the charging energy. In order to describe the low energy physics of strong tunneling we introduce a *two-stage* scaling theory. In this unified theory several contradicting earlier descriptions find a natural interpretation. Nonperturbative expressions are derived for the energy levels, decay rates, and charge of the island. The strong renormalization of the effective capacitance of the junction is confirmed by Monte Carlo simulations.

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Charging effects in small capacitance tunnel junctions have attracted much interest because of the promising applications and the challenging theoretical questions they pose [1–3]. The simplest device to study these effects is the single electron box (SEB), a metallic island connected via a capacitor and a tunnel junction to a voltage source [4]. The essence of single electron effects is expressed by the energy scale $E_C = e^2/2C$ associated with the capacitance of the island. For capacitances in the range $C \sim 1$ fF, charging effects are pronounced at temperatures $T < E_C \sim 1$ K. The properties of a SEB can be continuously tuned by an external voltage, which induces a polarization charge Q_x at the junction. For weak tunneling the energy spectrum is a set of parabolas $E(Q_x - ne)$ with $E(Q) \equiv Q^2/2C$, and n is the number of excess electrons in the island.

Tunneling introduces quantum fluctuations of the charge in the island. They are prominent near the degeneracy points at $Q_x \approx (n + 1/2)e$ and/or for strong tunneling. The strength of tunneling is characterized by the dimensionless conductance $\alpha_0 \equiv \hbar/2\pi e^2 R_t$. Strong tunneling leads to nonperturbative effects such as screening of the island charge even at $T = 0$ and to a renormalization of the energies. Some of these effects may have been observed in recent experiments [5]. However, despite extensive theoretical studies, several published results in the nonperturbative regime [6–10] are in mutual disagreement. In this paper we develop a unified, self-consistent, nonperturbative description, aimed at settling the discrepancies.

The SEB is described by the tunneling Hamiltonian, supplemented by the charging energy $E(Q_x - ne)$. We consider here a metallic junction with a large number of channels N. Integrating out the electronic degrees of freedom we obtain an effective action in the phase representation [2,6], which in the limit $N \to \infty$ is valid for arbitrary tunneling conductance

$$\mathcal{Z}(Q_x) = \sum_{m=-\infty}^{\infty} e^{2\pi i m Q_x/e} \int_{-\infty}^{\infty} d\varphi_0 \times \int_{\varphi_0}^{\varphi_0+2\pi m} \mathcal{D}\varphi(\tau) \exp\left\{ -\int_0^\beta d\tau \frac{1}{4E_C}\left(\frac{d\varphi}{d\tau}\right)^2 + \int_0^\beta d\tau \int_0^\beta d\tau' \, \alpha(\tau - \tau') \cos[\varphi(\tau) - \varphi(\tau')] \right\}. \quad (1)$$

The summation over the winding number m and the periodic dependence on φ of the "cosine" tunneling term reflect the fact that the charge in the island, which is the variable canonically conjugate to the phase φ, is discrete. The Fourier transform of the tunneling kernel is $\alpha(\omega_n) = -\pi\alpha_0|\omega_n|$, up to a high energy cutoff $\omega_c \sim E_C = 1/\tau_c$.

Weak tunneling.— In the regime $\alpha_0 < 1$ a representation dual to (1) in terms of charges is more useful [2,6]

$$\mathcal{Z} = \sum_{k=-\infty}^{\infty} \int_{Q_x+ke}^{Q_x+ke} \mathcal{D}Q(\tau) \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\beta d\tau_1 \cdots d\tau_n' \, \alpha(\tau_1 - \tau_1') \cdots \alpha(\tau_n - \tau_n') e^{-\int_0^\beta d\tau \, E(Q(\tau))}. \quad (2)$$

Tunneling at times τ_i changes the charge in discrete steps, $Q(\tau) = Q_x + ke + e\sum_i[\Theta(\tau - \tau_i) - \Theta(\tau - \tau_i')]$. We study the vicinity of the degeneracy point $\delta = |Q_x - e/2| \ll e$, where the gap between the energy of the two lowest states is small, $2\Delta(Q_x) = E(e/2 + \delta) - E(e/2 - \delta) \ll E_C$. This allows us to truncate the Hilbert space to two states. The bare propagator for the upper (lower) level takes the form $\mathcal{G}_\pm(\tau) = \exp[-|\tau|E(e/2 \pm \delta)]$, and in lowest order the partition function is $\mathcal{Z}^{(0)} = \sum_\pm \mathcal{G}_\pm(\beta)$. Tunneling events are described by the $\alpha(\tau)$ term visualized in Fig. 1. A first order perturbative analysis yields in leading logarithmic order

$$\mathcal{Z}^{(1)} \approx e^{-E_C\tau/4}\{e^{\Delta_0\tau}[1 + \alpha_0(\Delta_0\tau + 1)\ln(\tau_c/\bar{\tau})] + e^{-\Delta_0\tau}[1 + \alpha_0(-\Delta_0\tau + 1)\ln(\tau_c/\bar{\tau})]\}. \quad (3)$$

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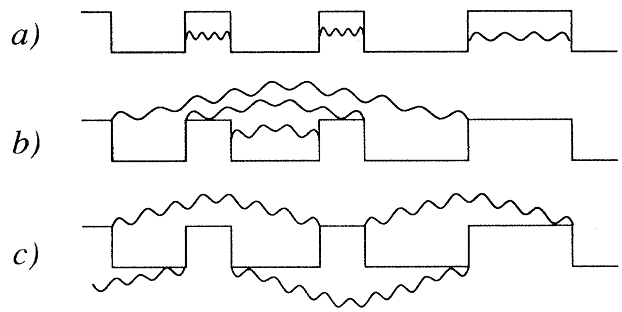

FIG. 1. Typical diagrams contributing to Z in the two-level system approximation: (a) repeated bumps, (b) rainbows, and (c) crossing diagrams.

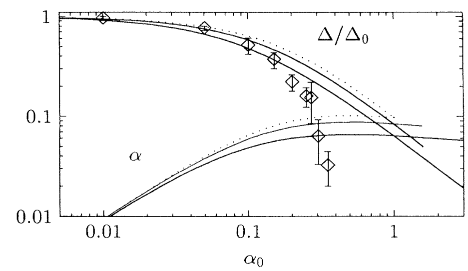

FIG. 2. The effective gap Δ and tunneling strength α obtained by integrating the scaling equations for different initial values ($\Delta_0/E_C = 0.005, 0.025, 0.05$), compared with the values inferred from the Monte Carlo study (diamonds).

Here $1/\bar{\tau} = \max[1/\tau, \Delta_0, T]$ acts as a low frequency cutoff and regularizes the infrared singularities. Constants of $\mathcal{O}(1)$, depending on details of the high frequency cutoff procedure, are ignored.

Higher order terms, shown in Fig. 1, can be classified as rainbows, repeated bumps, or crossing diagrams. Because of phase space restrictions crossing diagrams yield lower powers of logarithms than the first two types. We discard this class, i.e., we work in the "Noncrossing approximation." Since we use standard renormalization group techniques to treat the infrared singularities of the higher order terms [11], we sketch the derivation only (see also [12]). As the high frequency cutoff is gradually lowered, close pairs of instantons with separation in the range $(\tau_c, \tau_c + \delta\tau_c)$ are integrated out, and their effect is absorbed in renormalized parameters. The elimination of close pairs belonging to either class of diagrams requires a modification of the gap, as can be seen from Eq. (3). Rainbow diagrams further modify α, while repeated bumps introduce a wave-function renormalization factor Z.

The first order scaling equations are

$$\frac{d(\Delta/\omega_c)}{d\ln\omega_c} = (2\alpha Z^2 - 1)\frac{\Delta}{\omega_c}, \quad \frac{d(2\alpha Z^2)}{d\ln\omega_c} = (2\alpha Z^2)^2. \tag{4}$$

They can be readily integrated down to a low energy scale ω_c:

$$\alpha(\omega_c) = \alpha_0\left[1 + 2\alpha_0\ln\left(\frac{E_C}{\omega_c}\right)\right]^{-1}, \quad \Delta(\omega_c) = \Delta_0\left[1 + 2\alpha_0\ln\left(\frac{E_C}{\omega_c}\right)\right]^{-1}. \tag{5}$$

At $T = 0$ the renormalized gap (RG) provides the low energy cutoff, and the scaling stops at $\omega_c = \Delta(\omega_c)$. Then Eq. (5) becomes a self-consistent equation for Δ. At finite temperature the RG has to be stopped at $\omega_c = \max[\Delta, T]$, the energy scale where infrared singularities in the perturbation expansion disappear. Typical solutions are shown in Fig. 2.

Strong coupling.— For $\alpha_0 \gg 1$, a renormalization group analysis has been performed in Refs. [6,13,14]. While the discreteness of the charge was not accounted for in that approach, the overall conclusions can be carried over. The scaling equations are obtained in a $1/\alpha$ expansion with leading terms

$$\frac{d(E_C/\omega_c)}{d\ln\omega_c} = \left(\frac{1}{\tilde{\alpha}} - 1\right)E_C/\omega_c, \quad \frac{d(1/\tilde{\alpha})}{d\ln\omega_c} = -1/\tilde{\alpha}^2, \tag{6}$$

where $\tilde{\alpha} = 2\pi^2\alpha$. In this approach, the overall bandwidth E_C is rescaled, in contrast to the weak-coupling regime where the gap Δ is rescaled. But it is safe to assume that both scale proportional to each other. Clearly α decreases in the strong-coupling regime. This allows us to develop a unified picture, which is the central thesis of our work: in the case of strong tunneling we apply a *two-step scaling procedure*. As the energy scale ω_c decreases from ω_{c0}, first $\tilde{\alpha}$ decays according to Eq. (6) from its large initial value $\tilde{\alpha}_0$ to $\tilde{\alpha}(\omega_c) = \tilde{\alpha}_0[1 - (1/\tilde{\alpha}_0)\ln(\omega_{c0}/\omega_c)] \sim 1$. The bandwidth also decreases to a value $E_C^* \approx E_C^0\exp(-\tilde{\alpha}_0)$, and the cutoff reaches $\omega_c \sim E_C^*$. From there on we use the weak-coupling scaling governed by Eq. (4) with initial cutoff $\omega_c \approx E_C^*$, initial bandwidth $\Delta_0\exp(-\tilde{\alpha}_0)$, and $\alpha_0 \approx 1/2\pi^2$. The final result for the gap for strong bare coupling is

$$\Delta(\omega_c) = \Delta_0 e^{-\tilde{\alpha}_0}[1 + \pi^{-2}\ln(E_C^0 e^{-\tilde{\alpha}_0}/\omega_c)]^{-1}. \tag{7}$$

To substantiate our results we performed a Monte Carlo (MC) analysis of the problem, starting from the phase representation (1). The ground state energy is extracted by finite size scaling (the size of the MC lattice is $L \propto \beta E_C$) and the effective bandwidth from the curvature of the lower part of the band. Details are described elsewhere [12]. The results are displayed in Figs. 2 and 3. The agreement with the scaling theory is quite satisfactory, providing a strong, independent support for our unified scaling theory.

The MC method gives poor results for the gap Δ close to the band edges. The reason is that different terms in the winding number summation enter with oscillating phase factors $\exp(2\pi i m Q_x/e)$. For states close to the bottom of the band, $Q_x \approx 0$, these oscillations are slow,

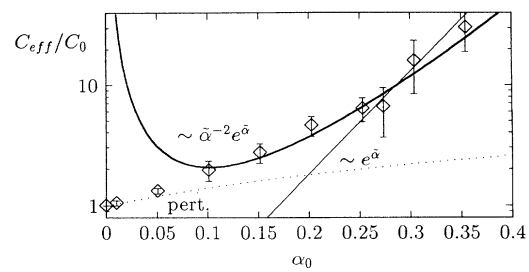

FIG. 3. Monte Carlo results (diamonds) for the effective capacitance in the weak and the (nonperturbative) intermediate tunneling regime. Comparison is made with the results from perturbation theory, from Ref. [8] and from [13].

but near degeneracy points they are fast. At the band edges the normalized partition function is small, $\mathcal{Z}(Q_x \sim e/2) \sim \exp[-\beta(E_C - \Delta)] \ll 1$. Thus, MC has to extract a small number from the sum of many large terms with oscillating phases, making the result extremely sensitive to approximations.

Several previous studies have dealt with this problem. Panyukov and Zaikin [8] considered strong coupling by an instanton technique in the phase representation. They find a renormalized bandwidth $E_C^* \sim E_C\tilde{\alpha}^2\exp(-\tilde{\alpha})$, which agrees with the results of large-α scaling, as well as with our MC data down to remarkably low α, as shown in Fig. 3. They further conclude that the ground state energy *completely flattens* in a wide interval around degeneracy points $Q_x = (n + 1/2)e$. This conclusion differs from ours; we argue that it arises due to insufficient accuracy of the instanton technique close to the band edge: (i) Similarly as in the MC simulation terms with oscillating phase factors $\exp(2\pi i m Q_x/e)$ are summed in Eq. (1). Thus innocent looking approximations can profoundly alter the result near band edges. (ii) The technique used in Ref. [8] is unusual in the sense that the action is independent not only of the location but also of the width of the instantons; thus instantons of all lengths contribute with similar weight. In order to test the validity of the dilute instanton approximation we calculated the average width $\langle\sigma\rangle_N$ of an instanton in an N-instanton configuration. Following Ref. [8] we first separate the zero energy modes (location and inverse width of the instantons) in the partition function $\mathcal{Z}(N)$ and then integrate the remaining fluctuation determinant to obtain the renormalized action of the independent instantons. This yields the width

$$\langle\sigma_i\rangle = \frac{1}{\mathcal{Z}(N)}\int\prod_j^N d\tau_j\int\prod_j^N d\sigma_j\;\sigma_i N![4TE_C^*\cos(2\pi Q_x)] = \frac{\beta}{2N+1}, \tag{8}$$

where the integration is constrained to nonoverlapping instanton configurations [8]. Clearly the gas of N instantons is *never* dilute. Furthermore, we find that instanton–anti-instanton pairs attract each other with a potential $S(i,j) = -16\alpha\sigma_i\sigma_j/[(\sigma_i+\sigma_j)^2 + (\tau_i - \tau_j)^2]$, while like instantons do not interact. Then close pairs of instantons are favored, further enhancing the deviations from a dilute, noninteracting instanton gas. Recalling that close to the band edges extreme accuracy is required, we conclude that the flattening of the band at the edges, predicted in Ref. [8], is an artifact of the approximation.

The strong-coupling case has also been treated by a straight-line approximation [10]. We decompose $\varphi(\tau) = \varphi_0 + 2\pi m\tau/\beta + \delta\varphi(\tau)$ and expand the action (1)

$$S_m(\delta\varphi) = T\sum_{\nu>0}\left[\frac{\omega_\nu^2}{4E_C} + \frac{\tilde{\alpha}_0}{2\pi}(|\omega_\nu - \omega_m| + |\omega_\nu + \omega_m| - 2|\omega_m|)\right]|\delta\varphi_\nu|^2. \tag{9}$$

The modes with $|\omega_\nu| < |\omega_m|$ are soft, with an energy independent of $\tilde{\alpha}_0$. The fluctuation determinant is

$$\frac{\det(m)}{\det(0)} = a^{-m}m!\prod_{\nu=1}^m\frac{1}{1+\nu/a}\prod_{\nu=m+1}^\infty\left[1 - \frac{m}{\nu(1+\nu/a)}\right], \tag{10}$$

where $a \equiv 2E_C\tilde{\alpha}_0/\pi^2 T$. In the limit $a \gg 1$ the partition function becomes

$$\mathcal{Z}(Q_x) \approx \frac{a^m}{m!}e^{-\tilde{\alpha}_0|m|}e^{i2\pi m Q_x/e}. \tag{11}$$

In the regime $E_C\tilde{\alpha}_0 e^{-\tilde{\alpha}_0} \ll T \ll E_C$ we can confine ourselves to the terms $m = 0, \pm 1$ to obtain a renormalized bandwidth $E_C^* = (4E_C\tilde{\alpha}_0/\pi^2)e^{-\tilde{\alpha}_0}$ in good agreement with previous results. However, at lower temperature higher order terms become relevant, and the summation over m yields a negative partition function. This breakdown of the approximation is expected since it coincides with the crossover temperature where according to the scaling analysis the effective α decreases below 1, invalidating the strong-coupling scheme.

A scaling analysis similar to the present one was performed in Ref. [6] with the same gap renormalization equation. But the possibility of wave function or α renormalization was not considered there. Hence the prediction of a phase transition at $\alpha_0 = 1/2$ between a finite gap and a zero gap region is incorrect. Equation (5) shows that the scaling of α removes the transition and replaces it by a strong crossover around $\alpha_0 \sim 1/2$.

Two studies addressed directly the weak-coupling regime, one performing a poor man's scaling analysis [7], and one solving a Dyson equation [9]. Our results agree with both in leading logarithmic approximation. Differences arise since we solve for the gap self-consistently, which becomes important around $\alpha_0 \sim 1$.

We proceed to determine experimentally observable quantities. The ground state expectation value of the voltage of the junction is $\langle V(Q_x)\rangle = dE_0(Q_x)/dQ_x$, giving rise to a sawtooth pattern for $\alpha = 0$ [4]. The flattening of the band around the degeneracy points claimed in Ref. [8]

would imply that in the vertical part of a sawtooth a new S shape would develop. In the light of the above analysis there is no support for the flattening and S shape. Since no reliable treatment of the gap is available in the large-α_0 regime, we can display in Fig. 4 only the results for $\alpha_0 < 1$. The logarithmic corrections of Eq. (5) modify the vertical part only weakly. However, there is a strong suppression of the amplitude of the sawtooth oscillations already at moderate values of α_0.

Tunneling also leads to a finite lifetime Γ^{-1} and a broadening of excited levels. We determine it using the method of Ref. [9]. The ground state energy is $E_0(Q_x) \approx E_C/4 - \Delta(Q_x)$ for $|Q_x| < e/2$. But for $|Q_x| > e/2$ the argument of the logarithm turns negative for $|Q_x| > e/2$. The imaginary part of the energy can be interpreted as a lifetime effect according to $\Gamma = \mathrm{Im}\{E(Q_x)\} \approx 4\pi\alpha_0\Delta_0/\{[1 + 2\alpha_0 \ln(E_c/\Delta_0)]^2 + (4\pi\alpha_0)^2\}$. As long as $\Gamma \ll \Delta$, the excited levels remain well defined. The most pronounced experimental consequence of nonzero Γ is a smearing of the conductance proportional to Γ/Δ around the onset of the Coulomb blockade [15].

At finite temperatures thermal fluctuations have to be considered. If $T \ll E_C$ and $\alpha_0 < 1$, the physics near the band edges still involves only the two lowest charge states. From Eq. (5) we find quantities of experimental interest, the gap at $Q_x = e/2$ and the slope of the normalized voltage at the junction $\frac{1}{2}\beta E_C/[1 + 2\alpha_0 \ln(\beta E_C)]^2$, consistent with results of Refs. [7,9,15,16].

Finally we turn to superconducting junctions and consider the effect of a Josephson coupling between the electrodes. In Ref. [6] a Kosterlitz-Thouless type transition was found for large E_J at $\alpha_0 = 1/4$. For small E_J and $Q_x = e/2$, a phase transition was claimed at $\alpha_0 = 1/2$, with the property that on the two sides of this critical value E_J scales either up or to zero. The strongest argument for this claim was a smooth connection between the two limits. However, as pointed out above, there is no phase transition at $E_J = 0$. Furthermore, we observe that all infrared processes are connected with the transfer of single electrons and not of Cooper pairs. Thus E_J does not renormalize for small α. The correct flow diagram is shown in Fig. 5.

In conclusion, we reinvestigated strong electron tunneling in ultrasmall normal and superconducting junctions and provided a unified picture by introducing a *two-stage scaling procedure*. In this framework discrepancies between previous works could be clarified. The exponential renormalization of the bandwidth has been firmly established. Measurable quantities such as the expectation value of the island charge and decay rates have been calculated as a function of the external parameters.

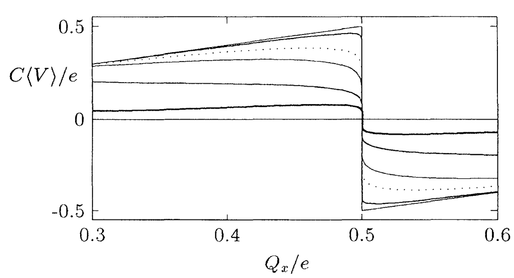

FIG. 4. The voltage at the junction close to the band edges for $\alpha_0 = 0.00, 0.01, 0.05, 0.1, 0.25, 0.5$ (from top to bottom).

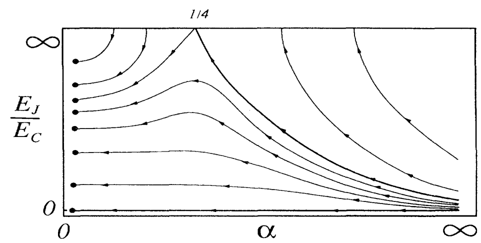

FIG. 5. The flow diagram in the E_J/E_C-α_0 plane for superconducting tunnel junctions.

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[1] D. Averin and K. K. Likharev, in *Mesoscopic Phenomena in Solids,* edited by B. L. Altshuler *et al.* (Elsevier, New York, 1991), p. 167.
[2] G. Schön and A. D. Zaikin, Phys. Rep. **198**, 238 (1990).
[3] See several articles in *Single Charge Tunneling,* edited by H. Grabert *et al.,* NATO ASI Ser. B, Vol. 294 (Plenum, New York, 1992).
[4] P. Lafarge *et al.,* Z. Phys. B **85**, 327 (1991); D. Esteve, in *Single Charge Tunneling* (Ref. [3]), Chap. 3.
[5] E. B. Foxman *et al.,* Phys. Rev. B **47**, 10 020 (1993).
[6] F. Guinea and G. Schön, Europhys. Lett. **1**, 585 (1986); J. Low Temp. Phys. **69**, 219 (1987).
[7] L. I. Glazman and K. A. Matveev, Sov. Phys. JETP **71**, 1031 (1990); K. A. Matveev, Sov. Phys. JETP **72**, 892 (1991).
[8] S. V. Panyukov and A. D. Zaikin, Phys. Rev. Lett. **67**, 3168 (1991).
[9] D. S. Golubev and A. D. Zaikin, Phys. Rev. B **50**, 8736 (1994).
[10] R. Fazio and G. Schön, Phys. Rev. B **43**, 5307 (1991).
[11] P. W. Anderson, G. Yuval, and D. R. Haman, Phys. Rev. B **1**, 4464 (1970).
[12] G. Falci, G. Schön, and G. T. Zimanyi, Physica (Amsterdam) **203B**, 409 (1994).
[13] J. M. Kosterlitz, Phys. Rev. Lett. **37**, 1577 (1976).
[14] S. A. Bulgadaev, JETP Lett. **45**, 622 (1987).
[15] H. Schoeller and G. Schön, Physica (Amsterdam) **203B**, 423 (1994); Phys. Rev. B **50**, 18 436 (1994).
[16] H. Grabert, Phys. Rev. B **50**, 17 364 (1994).