

Phase diagram of quantum capacitive junctions.

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Mesoscopic capacitances, in the quantum regime, are described as a quantum rotor coupled to a dissipative bath. We analyze the phase diagram of this model, as function of the capacitance, the coupling to the bath (that is, the conductance of the device), and the decay of the correlation functions in the bath, i. e., the strength of the many body effects within the leads. By combining Monte-Carlo and analytical techniques, we present the full phase diagram. The similarities and differences with other models of quantum junctions are discussed.

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Quantum dissipative systems [1–3] are models for mesoscopic electronic devices. They consist of one, or more, tunnel junctions between normal or superconducting electrodes. Quantum effects are associated to the dynamics of a collective variable which describes the overall phase of the electronic wavefunction. For the case of superconducting systems, this variable is the phase of the order parameter [4]. A collective variable, conjugate to the total charge, can be defined for normal junctions as well [6,7]. The magnitude of the quantum fluctuations is governed by the capacitances in the device.

Standard models describe these systems in terms of a few collective variables. In the simplest case, these variables are the phase mentioned previously, and its conjugate variable, the charge. The influence of the remaining, microscopic, degrees of freedom is taken into account by means of effective transport coefficients (viscosity, conductance) which couple the collective variable to a reservoir, described in terms of harmonic oscillators. Two generic models have been analyzed within this framework: i) The Caldeira-Leggett model [1] which describes the dynamics of a junction where the quantization of charge is unimportant, and ii) The quantum rotor [6,8], in which only quantized charge transfer processes take place. The first model has been extensively studied. A generalization of it, the Schmid model [9], also describes junctions between Luttinger liquids [10].

In the following, we will study in detail the second of these models. We consider a system made of gapless components, in which quantum (charging) effects are important. We do not include, in the description of the environment, processes which destroy the charge quantization in the device, such as an external electromagnetic field. We consider the effective action:

$$S_{\text{eff}} = \frac{\hbar}{2E_C} \int \dot{\theta}^2 d\tau + \alpha \tau_c^{2g-2} \int d\tau \int d\tau' \frac{1 - \cos(\theta_\tau - \theta_{\tau'})}{(\tau - \tau')^{2g}} \quad (1)$$

The model has four parameters: i) a short time cut-

off, τ_c , ii) the charging energy, $E_C = (e^2/C)^{-1}$, where C is the capacitance of the device, iii) a dimensionless coupling, $\alpha \sim \hbar/(e^2 R)$, where R is the resistance, and iv) the exponent g . The case of $g = 1$ corresponds to a quantum capacitance between two normal metals. $g \neq 1$ implies the existence of strong many body effects in the electrodes. They may arise because of shake-up and exciton effects [11] induced by electrons as they tunnel, closely related to the Mahan-Nozières-de Dominicis [12] processes in X-ray photoemission. An alternative way of inducing a value of $g \neq 1$ is when the electrodes are one dimensional Luttinger liquids, a situation which can be realized experimentally [13].

The model given in (1), has been studied extensively by a variety of methods. A standard perturbative renormalization group analysis can be performed when $\alpha \gg 1$ and $g \sim 1$ [14]. The scaling shows the existence of a phase transition along a critical line, $\alpha_c \propto (1 - g_c)^{-1}$.

The case $g = 1$ has also been analyzed analytically [15–17], and numerically [18,19]. The system shows a crossover from a high α regime, dominated by small amplitude oscillations (spin waves), to a disordered phase for small values of α . The possibility of a sharp transition, instead of a crossover, has also been postulated [16,18,19]. Because of the periodicity in the variable θ , different sectors, characterized by the conjugate variable to θ , can be defined. The edge of the Brillouin Zone generated in this way can be mapped onto a dissipative two level system [6,20], and solved. When $E_C = 0$, the rotor loses its dynamics. In terms of the environment, implicit in (1), we can define an effective Schmid model, with a non linear potential acting on the position closest to the rotor (see below).

The model is also related to the “quantum rotor” problem, introduced in the study of monopole induced proton decay in grand unified field theories [21]. This model can be solved exactly, in the limit $E_C \tau_c \rightarrow 0$, (see [21] and also [22]). As will be discussed later, this model is equivalent to eq. (1) for $\alpha = N$ and $g = 1$, where N is the number of fermion flavors coupled to the rotor.

We will study the action in eq. (1) by means of a numerical Monte-Carlo procedure, supplemented by analytical methods, and by comparing to the extensive literature mentioned above. The dynamics of the collective variable θ , arises from its interaction with the microscopic degrees of freedom of the environment. Instead of studying numerically a 1D system with long range interactions, we analyze a 2D model with short range interactions. The environment is modeled by a 2D X-Y system, with couplings $J_x = J_\tau = J_B$, where the subscripts x and τ stand for the space and the imaginary time dimensions. The planar spins are defined at the nodes of a square lattice, with periodic boundary conditions. We assign to each spin an angle, $\phi_{x,\tau}$. In order for the environment to show algebraic correlations, we have $J_B > J_c \approx 1.12$. For $J_B \gg J_c$, a standard spin wave analysis gives:

$$\langle \cos(\phi_{x,\tau} - \phi_{x,\tau'}) \rangle \propto \frac{1}{(\tau - \tau')^{\frac{J_c}{4J_B}}} \quad (2)$$

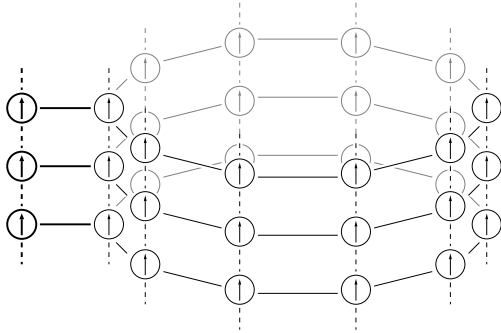


FIG. 1. Sketch of the model analyzed numerically in the text.

The rotor is defined as an additional 1D X-Y model which is coupled to the environment in the way shown in fig. (1). It introduces two parameters, J_R and J_D . The first one determines the correlation length of the rotor when decoupled of the bath, and the second gives the magnitude of the interaction with the environment. In terms of the action (1), $J_R \propto E_C^{-1}$, and, approximately, $J_D^2 \propto \alpha$. The rotor is described in terms of the angle θ . We couple it to the nearest column of environment spins by a term:

$$S_{coupling} = J_D \sum_{\tau} \cos(\theta_{\tau} - n\phi_{x_0,\tau}) \quad (3)$$

where n is an integer defined to facilitate the tuning of the parameter g in (1).

By integrating out the environment degrees of freedom, we obtain an effective action, which, at long imaginary times, behaves like (1). The periodicity of the variables

in our discrete model constrains the effective interactions between the θ_{τ} 's to be also periodic. The existence of algebraic decay in the environment (2), determines a similar decay for the effective retarded interactions of the rotor. An exact mapping of the parameters J_B, J_R, J_D into τ_c, α, g can only be done numerically. A reasonable approximation can be obtained by integrating out the environment using second order perturbation theory, and reexponentiating the result. Then, as mentioned earlier, $\alpha \sim J_D^2$. Finally, using the spin wave result (2), we find $2g = (n^2 J_c)/(4J_B)$. Note that, as $J_B > J_c \approx 1.12$, the only way of achieving values of $2g > 0.3$ is to make $n > 1$ (we will mostly take $n = 4$).

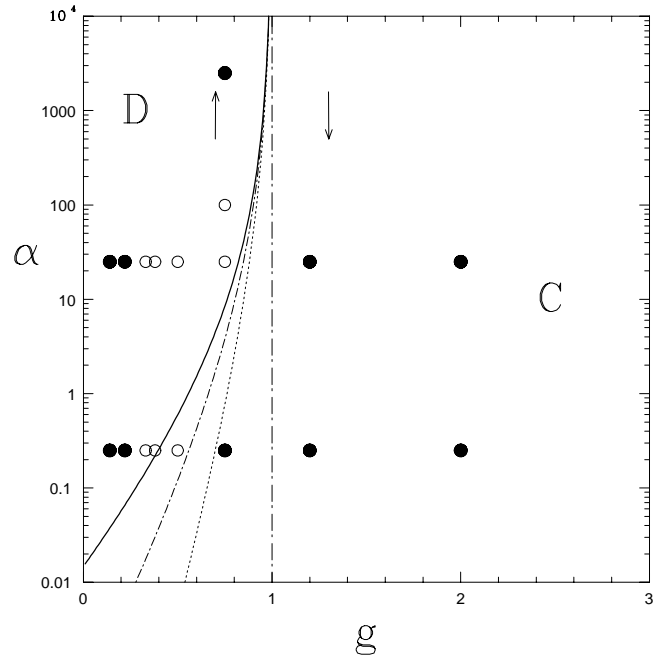


FIG. 2. Phase diagram of the model. Circles are points analyzed by Monte-Carlo ($E_C = 0.4$, in units of the cutoff). The full circles denote cases when an unambiguous characterization of the correlation functions can be made. The lines denote the prediction of the critical line from the variational spin wave analysis discussed in the text. Full line, $E_C = 0.4$. Broken line, $E_C = 0.2$. Dashed line, $E_C = 0.05$. Arrows in the top part give the flow of the RG scaling equations for $\alpha \gg 1$ and $g \sim 1$. The two phases that we find are denoted C (capacitive) and D (dissipative).

We have studied the model by Monte-Carlo [25]. Typical system sizes are $l_x = 20 - 40$ and $l_\tau = 100 - 200$. The number of configurations used is ~ 20000 . The samples, produced by the Metropolis algorithm, were not correlated (autocorrelation < 0.1). The cases analyzed are shown in fig. (2). The two phases depicted in this figure

are characterized by the rotor correlation functions:

$$G(\tau - \tau') = \langle \cos(\theta_\tau - \theta_{\tau'}) \rangle \quad (4)$$

This function shows two distinct regimes, as shown in fig. (3). For sufficiently large values of g , or low values of α , the correlation (4) decays exponentially, while, if g is small, it shows an algebraic dependence on $\tau - \tau'$.

The thick line shown in fig. (2) separates the two regimes. In terms of the original model, an algebraic decay in (4) implies dissipative behavior, although it needs not be ohmic. When (4) decays exponentially, the system behaves as a capacitor, with an effective capacitance proportional to the inverse correlation length [23].

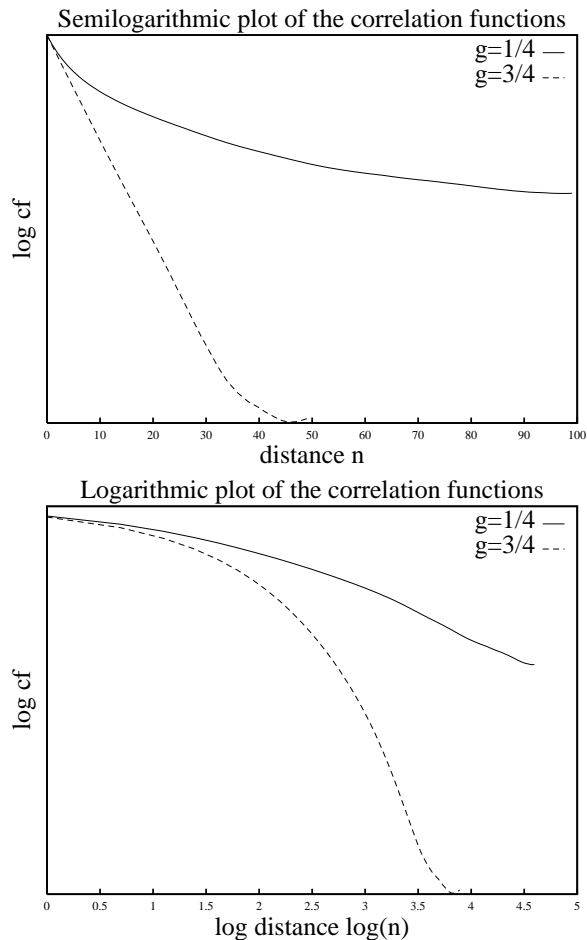


FIG. 3. Values of $\langle \cos(\tau - \tau') \rangle$ as function of $\tau - \tau'$. The two cases shown correspond to $g = 1/4$ and $\alpha \sim 0.27$ ($J_D/J_c = 0.5$), full line, and $g = 3/4$ and $\alpha \sim 0.27$, broken line.

We now study the phase diagram of the model by variational methods. The standard way is to employ the self consistent harmonic approximation (SCHA), which amounts to a spin wave approximation. The couplings of the model are replaced by quadratic interactions, whose

strength is then optimized. This scheme has already been applied to the action (1), for $g = 1$ [15], and at finite temperatures. For the related Schmid model, it reproduces correctly the phase diagram [24].

For that purpose, we use the hamiltonian formalism:

$$\mathcal{H} = E_C \frac{P^2}{2} + V [1 - \cos(\theta - \phi_0)] + \omega_c \sum_{n=0}^{\infty} \frac{p_n^2}{2} + \frac{v_s^2 (\phi_n - \phi_{n+1})^2}{2} \quad (5)$$

where $[\theta, P] = [\phi_n, p_n] = i$ and $\alpha \propto (V/\omega_c)^2$. For a decoupled chain ($V = 0$), we have $\lim_{t \rightarrow \infty} \langle [\phi_0(t) - \phi_0(0)]^2 \rangle = 1/(4\pi v_s) \log(\omega_c t)$, so that $2g = 1/(4\pi v_s)$. Note that, in this representation, the connexion of this model and the Schmid model in the limit $E_C \rightarrow 0$ is transparent.

The SCHA hamiltonian is:

$$\mathcal{H}_{SCHA} = E_C \frac{P^2}{2} + E_K \frac{(\theta - \phi_0)^2}{2} + \mathcal{H}_{chain} \quad (6)$$

where \mathcal{H}_{chain} is the last part in eq. (5) and E_K is the variational parameter. We need to minimize $\langle SCHA | \mathcal{H} | SCHA \rangle$, where $|SCHA\rangle$ is the ground state of \mathcal{H}_{SCHA} . In the limit $E_K, E_C \ll \omega_c$, we have:

$$\langle SCHA | \mathcal{H} | SCHA \rangle = c \sqrt{E_C E_K} - V \left(\frac{\sqrt{E_C E_K}}{\omega_c} \right)^g e^{-\sqrt{\frac{E_C}{E_K}}} \quad (7)$$

where c is a numerical constant of order unity.

Eq. (7) admits solutions for $g < 1$ and, roughly, $\alpha > c/(1-g)(E_C/\omega_c)^{(2-2g)}$, where c is a numerical constant of order unity. The factor $(1-g)^{-1}$ has been inserted in order to interpolate correctly to the $\alpha \rightarrow \infty$, $g \rightarrow 1$ limit. This line is plotted in fig.(2).

The possibility of a description of the physics of the model in terms of only spin waves does not necessarily imply that other effects are irrelevant. Experience with related models, however, like the Schmid model [24], or the 1D quantum sine-Gordon gives some confidence on the reliability of the approach.

We now turn to the relation of our work to the problem of monopole induced baryon decay. The main issue addressed in this context has been the dynamics of the baryons which build up the environment. It is, however, possible, to derive an effective action for the rotor coordinate. The leading terms should be those given in(1). As the rotor is coupled to free fermions, $g = 1$. The analysis in the literature [21,22], initially neglects the periodicity in the rotor coordinate. It implies, in expression (1), the substitution of $1 - \cos(\theta_\tau - \theta_{\tau'})$ by $(\theta_\tau - \theta_{\tau'})^2/2$. In [21], the coupling (that is, the fermion charge) is included in the definition of E_C , and the value of α is simply N , the number of fermion channels coupled to the rotor. This

model reduces to the Caldeira-Leggett model of a quantum particle in a dissipative environment [1], which can be solved exactly. The rotor coordinate experiences a frictional force, in agreement with the results in [21].

The solutions obtained within this scheme describe the model in terms of low energy electron hole pairs (spin waves, in our language). Such a description exhausts the physics of the problem in the right side of the phase diagram in fig.(2). Thus, the validity of the scheme depends on the value of E_C/ω_c . It is assumed in [21,22] that $E_C/\omega_c \rightarrow 0$, so that a spin wave description is marginally correct for $g = 1$.

Note that a wavefunction which restores the symmetry of the model can be written by superposing $|SCHA\rangle$ and the solutions of $\mathcal{H}_n = \mathcal{H}_{SCHA} + 2\pi n E_K(\theta - \phi_0)$. Such state, $\sum_n e^{ikn}|SCHA_n\rangle$, has the same physical properties as $|SHA\rangle$, because $\langle SCHA_n|SCHA_{n'}\rangle = \delta_{n,n'}$.

It is interesting to speculate what would happen if E_c/ω_c is finite. Then, quantum fluctuations in the rotor coordinate would decouple it, at low energies, from the fermions. The rate of monopole induced baryon decay would not be of order unity, but would tend to zero as ω^2/E_C^2 [11].

Summarizing, we have studied the phase diagram of a model used to describe a variety of physical systems, such as Coulomb blockade in a normal metal junction, the single electron transistor or the quantum box. The generalization that we make in letting the parameter g in eq. (1) be different from 1 allows us to study other situations, like charging effects in Luttinger liquid junctions, or shake-up and excitonic processes in normal junctions.

We find a phase diagram with two regions: one in which charging effects dominate and the system behaves as a capacitor at low energies, and another in which the quantization of the charge is irrelevant, and the device shows a dissipative response. This phase diagram has been obtained by Monte-Carlo methods, and its consistency checked against alternative analytical approaches, such as the RG for $\alpha \gg 1$ and $g \sim 1$ and variational ansätze for $\alpha \ll 1$. The phase diagram shows interesting deviations from the well understood phase diagram of the Schmid model: i) there is no duality, and the separatrix is not vertical, ii) there is a dynamically generated scale below which gaplike features appear (in the insulating phase) and iii) the charge quantization explicitly imposed in eq. (1) reduces the the range of parameters for which the system shows dissipative behavior.

We have studied the ground state only, and we have not considered the influence of finite voltages, which are important in some situations, like the single electron transistor. We can anticipate, however, that gate or bias voltages will only be relevant for the phase shown to the right in fig. (2).

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