Superconductor-insulator quantum phase transition in a single Josephson junction

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The superconductor-to-insulator quantum phase transition in resistively shunted Josephson junctions is investigated by means of path-integral Monte Carlo simulations. Our numerical technique allows to directly access the regime of the Josephson-to-charging energy ratios E_J/E_C of order one. Our results unambiguously support an earlier theoretical conjecture, based on renormalization-group calculations, that at $T \to 0$ the dissipative phase transition occurs at a universal value of the shunt resistance $R_S = h/4e^2$ for all values E_J/E_C. On the other hand, finite-temperature effects are shown to turn this phase transition into a crossover, whose position depends significantly on E_J/E_C, as well as on the dissipation strength and temperature. The latter effect needs to be taken into account in order to reconcile earlier theoretical predictions with recent experimental results.

I. INTRODUCTION

Mesoscopic Josephson junctions are well known to exhibit a variety of intriguing phenomena which are of primary importance both from a fundamental point of view, as well as for various applications including quantum-state engineering with electronic devices. Among these are macroscopic quantum tunneling with dissipation,[1] Coulomb blockade,[2–4] macroscopic quantum coherence, and dissipative quantum phase transitions.[3] Recent progress in nanolithographic techniques allows one to routinely fabricate ultrasmall tunnel junctions with capacitances C as low as $10^{-15}-10^{-16}$ F, and to perform detailed experimental studies of various features related to the above phenomena.

In the course of these studies it was realized—both theoretically and experimentally—that the observed properties of the system may crucially depend on the nature of the effective electromagnetic environment coupled to a mesoscopic junction. One of the most remarkable consequences of this dependence for Josephson junctions (JJ's) is the quantum ($T=0$) superconductor-to-insulator phase transition (SIT) driven by dissipation. The latter is controlled, e.g., by the magnitude of the ohmic shunt resistance R_S of the external leads. This quantum phase transition was predicted by Schmid[5] and subsequently studied in Refs. 6–8 (see also Refs. 3 and 9 for an extensive review of this and later theoretical activity). Thus, at low temperatures the supercurrent in mesoscopic JJ's can be maintained only provided that quantum fluctuations of the Josephson phase are suppressed by dissipation. If dissipation is not strong enough, quantum fluctuations wash out the Josephson effect and no supercurrent can flow across the system. Alternatively, one can interpret this SIT as a destruction of the Coulomb blockade for Cooper pairs by quantum fluctuations of the charge in an external resistor R_S. Experimentally this quantum dissipative phase transition for single resistively shunted JJ's was studied in Refs. 10–13. The results of these experiments are qualitatively consistent with the above physical picture.

Similar experimental studies have been also performed

for JJ arrays and chains.[14–16] In these cases an interplay between short- and long-range quantum fluctuations of the superconducting phase in the presence of dissipation yields a nontrivial low-temperature phase diagram.[17–19] A quantum dissipative phase transition was also discussed in the case of ultrathin homogeneous superconducting wires.[20,21]

It is worth pointing out that the above physical picture is not restricted to superconducting systems only. For instance, it is well known that the problem of a quantum resistively shunted JJ is equivalent to that of a quantum particle diffusing in a periodic potential coupled to a dissipative environment. In this case, the phase transition from diffusion to localization occurs upon increasing the coupling strength to a dissipative Caldeira-Leggett bath.[5–9] A formally identical Lagrangian also describes tunneling of electrons in a Luttinger liquid, see, e.g., Ref. 9. Similar physics was discussed for normal-metallic conductors.[22] Thus, even though below we will specifically address the case of a resistively shunted JJ, our results can also be applied in other physical situations.

According to the existing theoretical picture,[3,9] at $T=0$ quantum localization of the Josephson phase should occur as the shunt resistance becomes equal to the quantum resistance unit, $R_S = R_q = \pi\hbar/2e^2 \simeq 6.5$ $k\Omega$, *independently* of the strength of the Josephson coupling E_J. In the limit of small Josephson energies (as compared to the effective charging energy of the junction, $E_C = e^2/2C$) this conclusion can be justified within a perturbative renormalization-group analysis. Such an analysis can then be extended to the limit of large $E_J \gg E_C$ by means of a duality transformation between the phase and the charge.[3,9] Since in both limits one obtains an E_J-independent phase boundary at $R_S = R_q$, it is reasonable to *conjecture* that its position remains unchanged for all values E_J/E_C including the regime of experimental interest $E_J \sim E_C$.

Although this conjecture can further be supported by a number of qualitative arguments, as well as by the existence of a self-duality point,[5,9] the structure of the phase diagram for moderate values E_J/E_C still needs to be rigorously verified. Moreover, the results of recent experiments[12,13] could

be interpreted as *contradicting* the above conjecture. In these works, the samples with sufficiently large $E_J/E_C \gtrsim 7 \div 8$ were found to be superconducting even for shunt resistances R_S substantially higher than R_q. This observation could suggest that the true phase boundary should depend not only on the amount of dissipation in the system, but also on the ratio E_J/E_C. A similar conclusion could be reached from the results reported in Refs. 10 and 15.

All these developments motivated us to perform an additional theoretical investigation of the dissipative phase transition in a single resistively shunted superconducting junction, at moderate values of the Josephson coupling energy $E_J \sim E_C$. Since in this range there exists no small parameter in the problem, it can hardly be rigorously investigated by analytical methods. Therefore, in this paper we analyze the problem numerically by means of path-integral (PI) Monte Carlo (MC) simulations. This method allows us to quantitatively study the effect of quantum fluctuations of the Josephson phase, depending on the dissipation parameter $\alpha = R_q/R_S$ and the ratio E_J/E_C in the interesting parameter range.

Our main conclusions can be summarized as follows: (i) Our detailed MC analysis unambiguously supports an earlier conjecture that in the zero-temperature limit the superconductor-to-insulator phase transition always occurs at the dimensionless dissipation strength $\alpha = 1$, independently of the ratio E_J/E_C, (ii) at nonzero temperatures this phase transition is substituted by a *crossover*, whose position depends on the ratio E_J/E_C, as well as on temperature T and dissipation strength α, and (iii) at $T \to 0$ this crossover line approaches the phase-transition line $\alpha = 1$. These observations allow to fully reconcile the existing theoretical picture of the dissipative phase transition in a single resistively shunted JJ with the experimental results.[12,13]

II. QUANTUM DISSIPATIVE PHASE TRANSITION

We proceed within the standard path-integral formulation of the problem outlined in Ref. 3. The grand partition function of the system "JJ+shunt" can be expressed as a path integral over the Josephson phase ϕ,

$$Z \sim \int \mathcal{D}\phi \exp(-S[\phi]/\hbar), \qquad (1)$$

where S is the effective action

$$S[\phi] = \int_0^\beta \left[\frac{\hbar^2}{16E_C} \left(\frac{d\phi}{d\tau} \right)^2 - E_J \cos\phi(\tau) \right]$$

$$\times d\tau + \frac{\alpha\hbar}{8\beta^2} \int_0^\beta d\tau \int_0^\beta d\tau' \frac{[\phi(\tau) - \phi(\tau')]^2}{\sin^2[\pi(\tau - \tau')/\beta]} \quad (2)$$

and $\beta \equiv \hbar/k_B T$. The first and second terms in $S[\phi]$ account, respectively, for the charging and Josephson contributions. The third—nonlocal in time—term describes dissipation produced by an ohmic resistor. An additional dissipative contribution to the action, due to tunneling quasiparticles, is usually negligibly small in the interesting limit of energies

and/or temperatures well below the superconducting gap. Hence, in what follows this contribution will be ignored for the sake of simplicity.

MC simulations with this effective action have been carried out by standard discretization of the quantum paths into N imaginary-time slices.[23] In order to maintain the accuracy of the calculation, as the temperature is lowered, the Trotter number N has been increased proportionally to the imaginary time β. In our simulations we have taken $N = 4\beta E_C/\hbar$. This choice was proven to be sufficient in order to reach the necessary convergence of the calculated quantities: Repeating the calculations for some data points with larger N did not change our results. We have employed Metropolis sampling to carry out PI MC simulations at temperatures down to $k_B T = E_C/125$. A simulation run consists of successive MC steps, and all path coordinates are updated in each step. For each set of parameters $(\alpha, E_J/E_C, T)$, we generated 5×10^5 quantum paths for the calculation of ensemble-averaged values. More details on this kind of MC simulation can be found elsewhere.[24]

In order to quantify the quantum delocalization of the phase we consider the mean-square fluctuations of the quantum paths

$$\langle (\delta\phi)^2 \rangle = \langle (\phi(\tau) - \bar\phi)^2 \rangle, \qquad (3)$$

where $\bar\phi = \beta^{-1} \int_0^\beta \phi(\tau) d\tau$ is the mean value of the phase for a given path. The quantity (3) was calculated by means of PI MC simulations with the aid of Eqs. (1) and (2).

In Fig. 1(a) we present $\langle (\delta\phi)^2 \rangle$ as a function of α for $E_J/E_C = 2$. Different symbols correspond to different temperatures; from top to bottom: $k_B T/E_C = 0.02, 0.05$, and 0.11. One observes that the phase delocalization increases as the temperature is lowered. At $\alpha = 1$ one also observes a change of the slope in the data points. This change becomes more and more pronounced as the temperature is lowered, indicating the expected tendency to a vertical line at $\alpha < 1$ and $T \to 0$. Unfortunately the noise in the calculated values increases as T is reduced, especially for $\alpha < 1$, where one expects an insulating regime (ϕ delocalized). For $\alpha > 1$, however, the quantum paths obtained in the MC simulations are merely confined to a single potential well, and the phase ϕ is localized (superconducting regime). A similar picture is found for all other values of E_J/E_C at which our simulations have been performed. The results obtained for $E_J/E_C = 0.75$ are presented in Fig. 1(b) for comparison. In agreement with intuitive expectations, one finds that the phase fluctuations increase with decreasing ratio E_J/E_C. However, the phase-transition point $\alpha = 1$ remains insensitive to this ratio in all cases.

In Fig. 2 we show the average mean-square displacement $\langle (\delta\phi)^2 \rangle$ versus α for several values of the ratio E_J/E_C at a low temperature as compared to the charging energy $k_B T = 0.02 E_C$. Values of E_J/E_C increase from top to bottom: 0.2, 0.5, 1, and 2. As expected, for a given dissipation strength α, the phase becomes "more localized" as the ratio E_J/E_C increases, since the effective potential barrier for the phase increases as well. Figure 2 also demonstrates that stronger suppression of the phase fluctuations $\langle (\delta\phi)^2 \rangle$ is al-
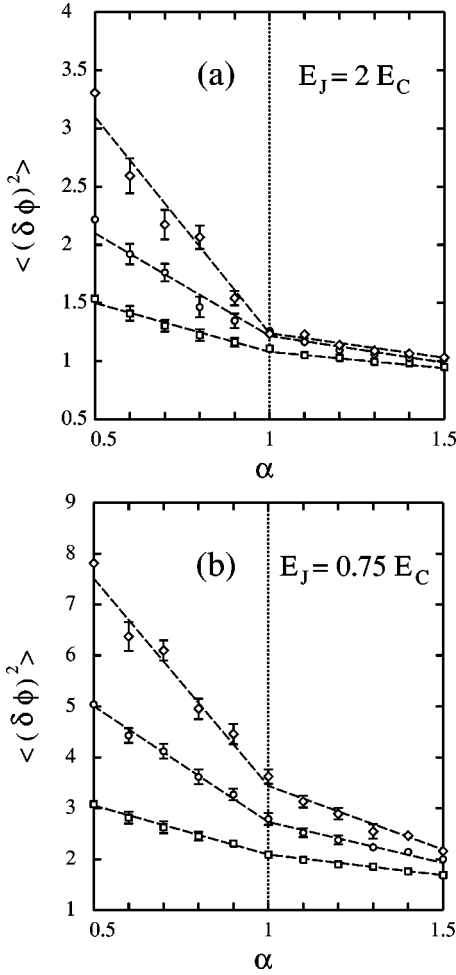
FIG. 1. Mean-square displacement $\langle(\delta\phi)^2\rangle$ as a function of the dissipation strength α for (a) $E_J = 2E_C$ and (b) $E_J = 0.75E_C$ at three different temperatures: Squares, $k_BT = 0.11E_C$; circles, $k_BT = 0.05E_C$; diamonds, $k_BT = 0.02E_C$.

ways obtained when the dissipation strength α increases for a given value of E_J/E_C. Again in all cases we observe that the change of the slope in the data points for $\langle(\delta\phi)^2\rangle$ occurs exactly at $\alpha = 1$, indicating the existence of the phase transition at this point.

Further information can be obtained by investigating the dependence of $\langle(\delta\phi)^2\rangle$ on temperature. As expected, in our simulations we observe that for all values of E_J/E_C and α, the quantum delocalization of ϕ increases as the temperature is lowered. In Fig. 3(a) we have plotted the temperature dependence of $\langle(\delta\phi)^2\rangle$ for $E_J/E_C = 2$. Different symbols represent several α values, which increase from top ($\alpha = 0$) to bottom ($\alpha = 1.2$). At low T ($E_C \gtrsim 10k_BT$), for all values of α one finds that $\langle(\delta\phi)^2\rangle$ follows a power-law dependence on temperature, as shown by the dashed lines in Fig. 3(a). In particular, in the dissipationless limit $\alpha = 0$, it is reasonable to expect the quantum paths to be in a diffusive regime, so that $\langle(\delta\phi)^2\rangle \propto \beta$. This is indeed confirmed by our calculations. In the presence of dissipation the phase diffusion slows down, as indicated by a decrease in the slope of the dashed lines in Fig. 3(a). From this plot we find $\langle(\delta\phi)^2\rangle \propto \beta^\gamma$, with an exponent γ smaller than unity for $\alpha > 0$. Again, the local-
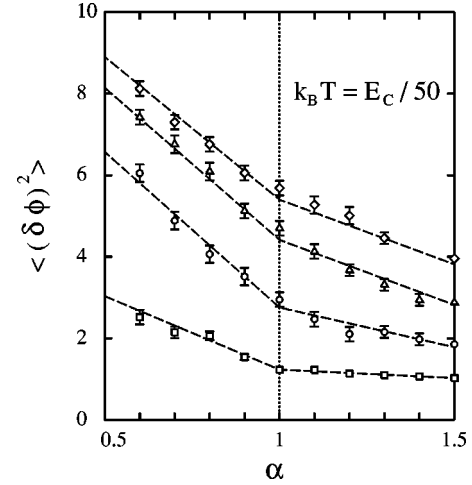

FIG. 2. Mean-square displacement $\langle(\delta\phi)^2\rangle$ as a function of the dissipation strength α for $k_BT = 0.02E_C$. Results are given for several values of the ratio E_J/E_C. From top to bottom: $E_J/E_C = 0.2$, 0.5, 1, and 2. Error bars, if not shown, are of the order of the symbol size.

ization phase transition at $\alpha = 1$ is clearly observable in Fig. 3(a), since essentially no diffusion of the phase takes place at $\alpha \gtrsim 1$ and sufficiently large β. Something similar occurs for other ratios E_J/E_C, as shown in Fig. 3(b) for $E_J/E_C = 0.75$. The main difference with the previous case is that the low-temperature regime $\langle(\delta\phi)^2\rangle \propto \beta^\gamma$ is reached at lower T ($E_C \gtrsim 30k_BT$).

In order to find the parameter γ, for each α we numerically evaluated the logarithmic derivative $d\ln\langle(\delta\phi)^2\rangle/d\ln\beta \equiv \gamma$. The values γ obtained in this way are shown in Fig. 4 as a function of α for $E_J/E_C = 2$. These results clearly indicate a linear dependence of γ on α of the form $\gamma = 1 - \alpha$. Thus, from our numerical analysis we can conclude that at sufficiently low temperatures and $\alpha < 1$ the phase diffusion is described by the formula

$$\langle(\delta\phi)^2\rangle \propto \beta^{1-\alpha}. \tag{4}$$

This dependence turns out to apply for all values E_J/E_C used in our simulations. From a linear fit to our data points in Fig. 4 we find the transition point at $\alpha = 1.02 \pm 0.04$.

The prefactor in Eq. (4) depends on both E_J and E_C. In the limit $E_J \gg E_C$, one can demonstrate with the aid of the instanton technique[3] that this prefactor is proportional to $\Delta^{1-\alpha}$, where

$$\Delta = 16\left(\frac{E_J E_C}{\pi}\right)^{1/2}\left(\frac{E_J}{2E_C}\right)^{1/4}\exp(-\sqrt{8E_J/E_C}) \tag{5}$$

is the bandwidth without dissipation. For $E_J \sim E_C$ this equation does not apply anymore, but the qualitative trend remains the same: For a given value of E_C the prefactor increases monotonously with decreasing E_J; cf. Figs. 3(a) and 3(b).

To conclude this part of our analysis we emphasize again that—even though we present here our numerical results for the energy ratios $E_J/E_C = 2$ and 0.75—similar behavior is observed for other values of the Josephson coupling energy.
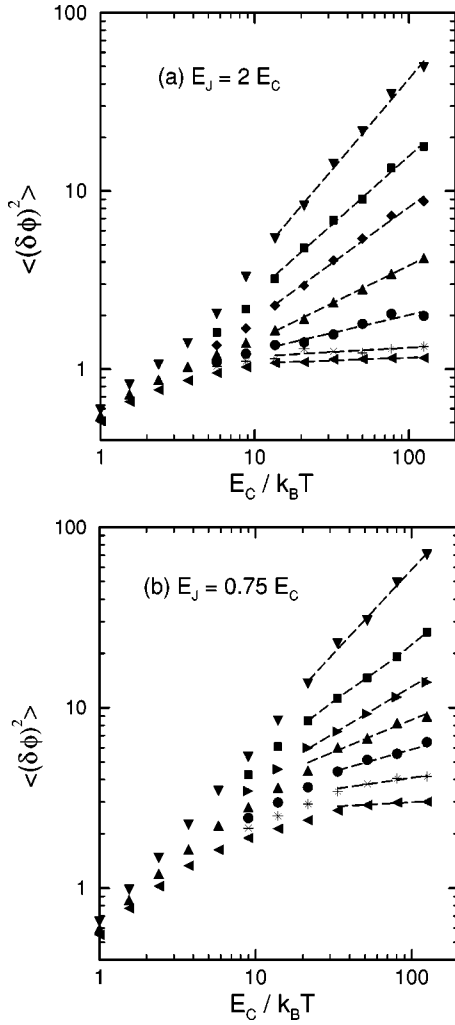
FIG. 4. Low-temperature exponent γ as a function of α for $E_J = 2E_C$. The dashed line is a linear fit to the data points.

FIG. 3. Temperature dependence of $\langle (\delta\phi)^2 \rangle$ for (a) $E_J = 2E_C$ and (b) $E_J = 0.75E_C$ at different values of α. From top to bottom: $\alpha = 0, 0.2, 0.4, 0.6, 0.8, 1$, and 1.2. Dashed lines indicate the low-temperature trend of the data points.

In particular, we have performed detailed MC simulations also for $E_J/E_C = 0.25$ and 3, and found essentially the same behavior as the one discussed above. In all cases, from our numerical data we obtained unambiguous indications of the quantum localization phase transition at $\alpha = 1$.

III. EFFECT OF TEMPERATURE

Now let us see how the above physical picture is modified at nonzero T. Since any experiment is performed at a finite temperature, it is important to find out if the SIT can be observed under such conditions.

To begin with, we recall the argument[3] according to which superconductivity in Josephson junctions can be observed even for $\alpha < 1$, provided that the phase diffusion is slow enough, in the sense that the characteristic delocalization time τ_{del} for the phase ϕ exceeds the time of experiment. This situation can easily be achieved in the limit of very large $E_J \gg E_C$. In that case the time τ_{del} is exponentially large, and no delocalization effects can be detected in a real
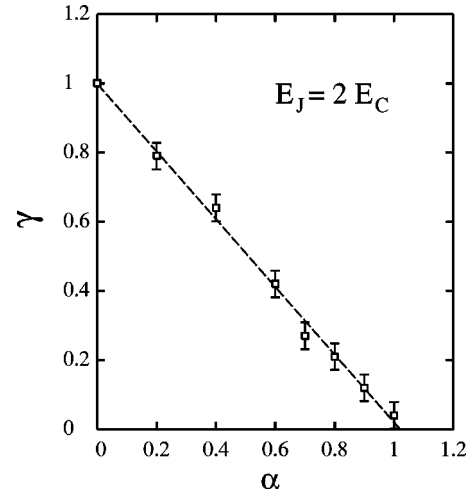
experiment. This argument imposes serious limitations on the observation of a SIT for sufficiently large values of E_J even at $T \to 0$. In Ref. 12 this argument was extended taking into account the accuracy of the voltage measurements. The authors[12] argued that for their experiment $1/\tau_{\text{del}}$ should be compared with the quantity eV_{min} rather than with the typical experimental time, where V_{min} is the minimum voltage detectable in the experiment. They also noticed that further limitations can occur due to temperature effects.

To explore the latter possibility we first notice that according to our result (4), at any nonzero temperature quantum fluctuations do not spread the phase ϕ to infinity even for $\alpha < 1$. The phase simply does not have "enough time" to diffuse, and $\langle (\delta\phi)^2 \rangle$ remains finite though increases with the inverse temperature β. Thus, at nonzero T and not very small E_J one might expect to observe a nonvanishing supercurrent even at small dissipation. This conclusion might appear paradoxical. One can argue that, if quantum fluctuations of the phase yield suppression of superconductivity already at $T = 0$ (and $\alpha < 1$), at nonzero temperatures this suppression can only increase further, because of an additional effect of thermal fluctuations.

In order to understand why this conclusion might not quite be correct, it is instructive to analyze the behavior of the (quasi-)charge variable[3] canonically conjugate to the Josephson phase ϕ. As discussed above, at $T = 0$ and $\alpha < 1$ the quasicharge is localized, i.e., Cooper pairs cannot tunnel across the junction due to the Coulomb blockade and, hence, the junction behaves as an insulator. At nonzero T this behavior persists as long as the temperature remains much smaller than the effective Coulomb gap for Cooper pairs. At $E_J \ll E_C$ this Coulomb gap is large ($\approx E_C$), while in the opposite limit $E_J \gg E_C$ it turns out to be exponentially small:[3]

$$\Delta_r = \Delta \left(\frac{\Delta}{\hbar \omega_p} \right)^{\alpha/(1-\alpha)}.$$ (6)

Here $\omega_p = \sqrt{8E_J E_C}/\hbar$ is the plasma frequency and Δ was defined in Eq. (5). If the temperature becomes higher than

the gap (6), $k_B T \gtrsim \Delta_r$, the Coulomb blockade for Cooper pairs (and, hence, the insulating behavior) is destroyed. This implies that the quasicharge Q gets strongly delocalized due to thermal effects. Because of the uncertainty relation

$$\delta Q \, \delta \phi \gtrsim e, \qquad (7)$$

delocalization of Q in turn restricts fluctuations of the canonically conjugate variable—the Josephson phase ϕ—and as a result of that the superconducting behavior can be partially restored. The same scenario can be reformulated in the phase space. One just needs to compare the typical inverse time during which the phase diffuses at a distance $\sim 2\pi$ with temperature. In the limit $E_J \gg E_C$ this inverse time $\hbar/\tau_{\rm del} \sim \Delta_r$, and we arrive exactly at the same condition $k_B T \sim \Delta_r$ for the crossover line between "insulating" and "superconducting" phases. Within logarithmic accuracy this crossover line agrees with the one found in Ref. 12.

Although the above consideration appears to be sufficient at high Josephson energies ($E_J \gg E_C$), no quantitative conclusion can yet be drawn for moderate couplings $E_J \sim E_C$. In order to study this parameter range one can apply a simple variational ansatz,[8] which leads to the self-consistency equations

$$D = E_J \exp(-\langle \phi^2 \rangle_{\rm tr}/2),$$

$$\langle \phi^2 \rangle_{\rm tr} = k_B T \sum_n \left[C(\omega_n/2e)^2 + \alpha |\omega_n|/2\pi + D \right]^{-1}, \qquad (8)$$

where $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies. At $T=0$ these equations have a nonzero solution for D (which corresponds to superconductivity) only at $\alpha>1$, whereas at nonzero temperature one can get a positive solution $D>0$ also for $\alpha<1$. By resolving these self-consistency equations at different T, one can qualitatively describe the above crossover for moderate values of E_J.

This crossover can be studied quantitatively by PI MC simulations, using the effective action given above in Eq. (2). With this purpose we have evaluated numerically the correlation function $\langle \phi(\tau)\phi(0) \rangle$ for different values of E_J/E_C, dissipation strength α, and temperature T. After Fourier transformation, this correlation function is directly related to the "Matsubara resistance" $\tilde{R}(\omega_n) = |\omega_n| \langle \phi\phi \rangle_{\omega_n}/4e^2$, which yields the system resistance after analytic continuation to real frequencies. This numerical analytic continuation is a separate complicated problem, which will not be discussed here. Fortunately, however, this procedure is not needed in order to establish the position of the crossover line.

Let us express the above correlation function in the form

$$|\omega_n| \langle \phi\phi \rangle_{\omega_n} = \frac{|\omega_n|}{C(\omega_n/2e)^2 + \alpha |\omega_n|/2\pi + \tilde{E}_J}, \qquad (9)$$

where $\tilde{E}_J$ is the effective (renormalized) Josephson coupling energy. It is easy to see that in the low-frequency limit the behavior of the correlation function (9) is totally different, depending on whether $\tilde{E}_J$ remains nonzero (superconductivity) or is fully suppressed by quantum fluctuations (insulat-
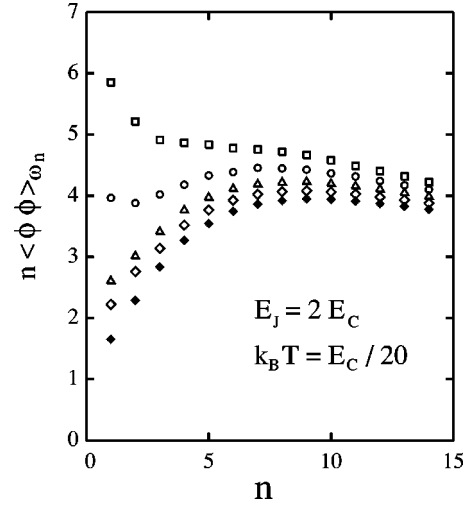

FIG. 5. Dependence of the "Matsubara resistance" $\tilde{R}(\omega_n) \propto |\omega_n| \langle \phi\phi \rangle_{\omega_n}$ on $n=\omega_n\beta/2\pi$, for $E_J/E_C=2$ and $k_B T=E_C/20$. Different symbols correspond to different values of the dissipation strength. From top to bottom: $\alpha = 0.6, 0.7, 0.8, 0.9,$ and 1.

ing regime). In the first case, for sufficiently low frequencies the function (9) should inevitably decrease with ω_n, while in the second case this function should increase and saturate at a finite value $2\pi/\alpha$ in the limit $\omega_n \to 0$. Thus, by studying the behavior of the function (9) it is possible to determine numerically from the PI MC simulations the position of the crossover line at different temperatures.

In Fig. 5 we present our MC results for the function $|n| \langle \phi\phi \rangle_{\omega_n}$ at $E_J=2E_C$, $k_B T=E_C/20$, and different values of α. One observes that for sufficiently small n this function increases with decreasing n for $\alpha=0.6$ (upper curve), saturates for $\alpha=0.7$, and decreases monotonously for $\alpha \geq 0.8$ (three lower curves). Thus, by studying the small-n behavior
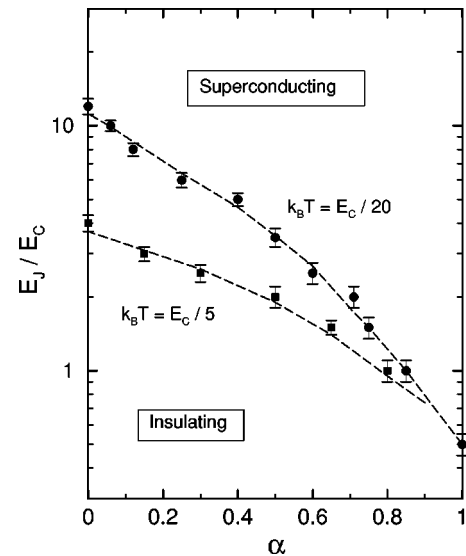

FIG. 6. Crossover lines between the insulating and superconducting regimes at two different temperatures, $k_B T=E_C/5$ (squares) and $k_B T=E_C/20$ (circles). Symbols are data points obtained from PI MC simulations. Dashed lines are guides to the eye.

of this function for different α values and E_J/E_C ratios, we arrive at the crossover line for the temperature $k_B T = E_C/20$. Other temperatures are treated analogously.

The resulting crossover lines are presented in Fig. 6 for two temperatures: $k_B T = E_C/5$ and $E_C/20$. In full agreement with the above qualitative considerations, one observes that the position of the superconductor-insulator crossover line is shifted towards larger values E_J/E_C as the temperature is lowered. The same trend is observed for all other temperatures used in our simulations. Combining these results with those discussed in the previous section, one arrives at the conclusion that the crossover line should approach the phase-transition line $\alpha = 1$ in the limit $T \to 0$. We would also like to point out that the position of the crossover line obtained within our MC analysis is fully consistent with that found experimentally in Refs. 12 and 13. It appears, therefore, that deviations from the theoretical prediction for the phase boundary $\alpha = 1$ observed in these experiments can be attributed to finite-temperature effects.[25]

In summary, the results of our MC simulations unambiguously demonstrate that the quantum ($T=0$) superconductor-insulator phase transition in resistively shunted Josephson junctions occurs at the value of the shunt resistance $R_S = R_q$, irrespective of the ratio E_J/E_C. For $\alpha < 1$, quantum diffusion of the Josephson phase ϕ yields a simple scaling dependence $\langle (\delta\phi)^2 \rangle \propto T^{\alpha-1}$. Finite-temperature effects turn the phase transition into a *crossover*, whose position depends on the ratio E_J/E_C, as well as on the dissipation strength α, and on temperature. Our results are fully consistent with recent experimental findings.[12,13]

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