Use of a Generalized Thouless Energy in Describing Transport Properties of Josephson Junctions

J. K. Freericks, A. N. Tahvildar-Zadeh, and B. K. Nikolić

***Abstract*—The concept of a Thouless energy, introduced originally in the context of Anderson localization (as the inverse diffusion time through a finite-size disordered conductor), has turned out to be an essential energy scale for understanding proximity-induced superconductivity in a normal metal connected to a superconductor; in particular, it has had significant success in the quasiclassical description of phenomena in superconductor-normal-metal-superconductor Josephson junctions. We generalize the concept of a Thouless energy to include transport through strongly correlated insulators, and show how it provides a unified description of transport and indicates how the quasiclassical picture breaks down as we turn on electron-electron correlations in the normal metal layer of a Josephson junction to tune it through the Mott metal-insulator transition.**

***Index Terms*—Josephson junction, metal-insulator transition, Thouless energy, transport.**

I. Introduction

In the 1970s, Thouless and collaborators formulated a characteristic energy scale of finite-size disordered conductors when they applied scaling theory to the Anderson localization problem [1], [2]. Remarkably, even though the Thouless energy ($E_{\rm Th} = \hbar/\tau_c$) governs much of the quantum phenomena in disordered metals, it is expressed in terms of the classical diffusion time $\tau_c = L^2/\mathcal{D}$ for an electron to pass through a diffusive conductor of size L, which is described by a diffusion constant $\mathcal{D}$. Similarly, it is described by the time of flight $\tau_c = L/v_F$, with v_F the Fermi velocity, for an electron in a ballistic conductor of size L. In recent years, studies of mesoscopic superconductivity have pointed out the prominent role played by $E_{\rm Th}$ in understanding the proximity effect in normal metals coupled to a superconductor [3]. In particular, the concept of a characteristic single-particle energy scale $E_{\rm Th}$, which is the counterpart to the superconducting energy gap (set by many-body interactions), has found wide application in the description of equilibrium and nonequilibrium phenomena in (long) superconductor-normal-metal-superconductor junctions [4], [5].

If a Josephson junction is constructed out of a sandwich of a superconductor (S)—barrier (B)—superconductor and the barrier thickness L is less than the dephasing length L_ϕ (which is determined ultimately by inelastic scattering processes, and can be as long as a micron or more), then quantum-mechanical coherence effects can take place on long length scales when the energy of the particles is close to the Fermi energy. In particular, in cases where the Thouless energy is much smaller than the superconducting gap, then quasiparticles with energies less than $E_{\rm Th}$ can propagate in a phase-coherent fashion through the device, and it is the Thouless energy, not the superconducting gap Δ that determines the transport through the junction. In SNS junctions (with N denoting a normal metal barrier), the Thouless energy governs the transport when the junction is long [4], [5].

The question then arises, is it possible to construct an analogue of the Thouless energy for diffusive (or ballistic) metals that determines the transport properties of a Josephson junction when the barrier is made out of a strongly correlated insulating material? The answer is yes, and we now describe how to do this. But first we must introduce some notation related to normal-state transport in Josephson junctions.

The quantum unit of resistance is $R_Q = h/2e^2$. The dimensionless resistance of a junction (in the normal state) r_N then satisfies [2], [6]

$$r_N = \frac{R_N}{R_Q} = \frac{1}{2\pi E_{\rm Th}\Delta_E^{-1}}, \tag{1}$$

where R_N is the normal state resistance of the junction and Δ_E^{-1} is the inverse level spacing of the junction (not to be confused with the superconducting energy gap). In finite, disordered systems, one can calculate all the quantum mechanical energy levels and their average spacings to estimate Δ_E. Another way to proceed, though, is to use thermodynamic quantities, since the volume Ω multiplied by the density of states (DOS) at the Fermi energy E_F can be identified with the inverse level spacing

$$\Delta_E^{-1} = \Omega N(E_F). \tag{2}$$

This approach works fine for metals, which have a nonzero DOS at the Fermi energy, but it is problematic for insulators, which have vanishing DOS within the insulating gap region. We propose to generalize (2) in a straightforward way, by recognizing that it can be written in a uniform fashion via [7]

$$\Delta_E^{-1}(T) = \Omega \int d\omega N(\omega)\left[-\frac{df(\omega)}{d\omega}\right], \tag{3}$$

where $f(\omega) = 1/[1+\exp(\{\omega-\mu\}/T)]$ is the Fermi-Dirac distribution function with μ being the chemical potential and T the temperature. Note that at low temperature, the derivative of the Fermi-Dirac distribution function approaches a delta function, and (3) reduces to (2) since the chemical potential approaches

Manuscript received October 4, 2004. This work was supported by ONR Grant N00014-99-1-0328. Computer time was provided by the Arctic Region Supercomputer Center and the Mississippi Region Supercomputer Center (ERDC).
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Digital Object Identifier 10.1109/TASC.2005.850107

E_F as $T \to 0$. However, in an insulator the integral has strong temperature dependence, so this generalization of the inverse level spacing depends strongly on temperature.

Our strategy here is to invert the conventional logic, and not think of the resistance as the ratio of the level spacing to the Thouless energy, but rather think of the Thouless energy as an energy scale extracted from the resistance and the inverse level spacing of the barrier. The key requirement for this heuristic approach is the ability to compute (or measure) the two-probe resistance of a finite thickness of a strongly correlated material that is sandwiched between two ballistic semi-infinite leads [7], [8]. Hence we define the (temperature-dependent) Thouless energy to be

$$E_{\rm Th}(T) = \frac{\hbar}{2e^2 R_N(T) AL \int d\omega N_B(\omega)\left[-\frac{df(\omega)}{d\omega}\right]}, \quad (4)$$

where A is the cross-sectional area of the device, and L is the thickness of the scattering region. Equation (4) provides an operational definition of the Thouless energy that can be directly measured for a device by measuring the dependence of the normal-state resistance on temperature, and evaluating the relevant integral using the bulk DOS for the material that is employed as the barrier. This procedure is not normally carried out by experimentalists, but we think it can be quite helpful in understanding properties of the Josephson junction and of the normal state transport. Note that (4) not only agrees with all of the conventional definitions of the Thouless energy for diffusive and ballistic systems, but also provides a unifying picture that treats both known cases with the same expression and can also treat insulators. In this sense, we do not need to determine the type of transport before employing (4), instead, we can determine the Thouless energy directly from a measurement of the resistance.

II. Numerical Analysis

Our work will focus on numerical simulations of multilayered nanostructures that represent the Josephson junction. We stack infinite two-dimensional planes in the z-direction. The planes to the left are made of a ballistic superconductor, as are those to the right. In the middle, we have the planes of the barrier, which we describe by a Falicov-Kimball (FK) [9] model, which can be thought of as noninteracting band electrons that interact with charge scattering centers with a strength U^{FK}. Such a system can be realized by a binary alloy, that has the same hopping integral between different species, but a different site energy (the difference equals U^{FK}). The Falicov Kimball model has a metal insulator transition as a function of U^{FK}, which allows us to tune the metallicity of the barrier from a ballistic metal to a Mott insulator. We choose to have on average one scattering center for every other site in the barrier planes, hence it corresponds to a 50%-50% binary alloy system. In the insulating phase, the properties don't depend too strongly on the details of the insulator, so our model will be able to provide generic results for many systems. Note that we have chosen to match the chemical potentials in the superconductor and in the barrier, so there is no charge rearrangement at the interfaces, and no Schottky-like barriers.

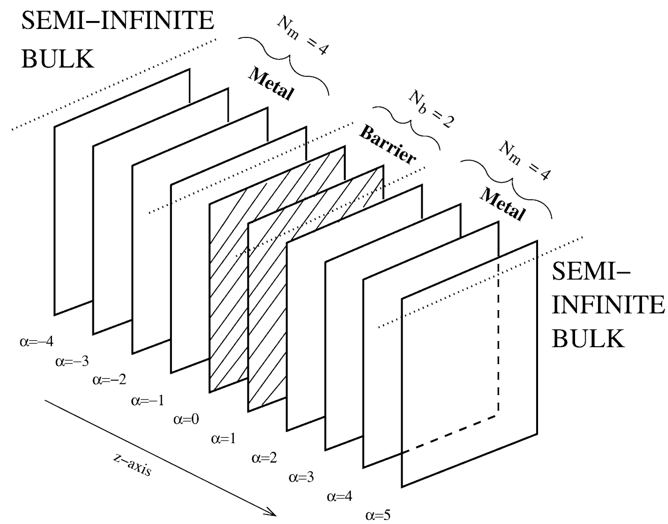

Fig. 1. Schematic of the multilayered nanostructure representing the Josephson junction. The metal planes of the lead are superconducting, while the barrier planes are described by the Falicov-Kimball model. In our calculations we actually use 30 metallic lead planes on the right and the left of the barrier before connecting them to their respective semi-infinite leads.

The Hamiltonian is then [9]

$$\hat{\mathcal{H}} = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U_i \left(c^\dagger_{i\uparrow} c_{i\uparrow} - \frac{1}{2}\right)\left(c^\dagger_{i\downarrow} c_{i\downarrow} - \frac{1}{2}\right) + \sum_{i\sigma} U_i^{\rm FK} c^\dagger_{i\sigma} c_{i\sigma}\left(w_i - \frac{1}{2}\right). \quad (5)$$

The lattice sites are those of a simple cubic lattice (with lattice constant a), and we choose the nearest-neighbor hopping to be the same within the planes and between the planes; we also choose the hopping to be the same in the superconductor as in the barrier (see Fig. 1). This hopping energy will be used as our energy scale. The superconductor is described by an attractive Hubbard model [10] (with interaction strength $U = -2t$) in mean field theory, which is equivalent to a BCS superconductor, but with the energy cutoff determined by the band structure rather than the phonon frequency. The superconducting transition temperature is $T_c = 0.112$ and the superconducting gap at zero temperature is $\Delta = 0.198$ [11], [12]. The barrier planes are described by the Falicov-Kimball model, with an average concentration of scattering centers $\langle w_i \rangle$ equal to 1/2, and the classical variable w_i is one when an A atom is at site i and zero when a B atom is at site i. The Hubbard interaction is chosen to vanish in the barrier region.

Our calculations use an inhomogeneous version of dynamical mean field theory in both the normal [13] and the superconducting [11], [12] states to calculate R_N and I_c (the critical current of the Josephson junction). The details of this computational scheme are given elsewhere [11], [12]; this technique is a self-consistent recursive Green's function approach that becomes exact as the coordination number of the lattice increases to infinity—it is expected to be quite accurate in three dimensions.

In the bulk, the FK model has a metal-insulator transition on a cubic lattice when $U^{FK} \approx 4.9$. The transition is continuous, so the mean free path decreases from $\ell \approx 2.3a$ when $U^{FK} = 2$,

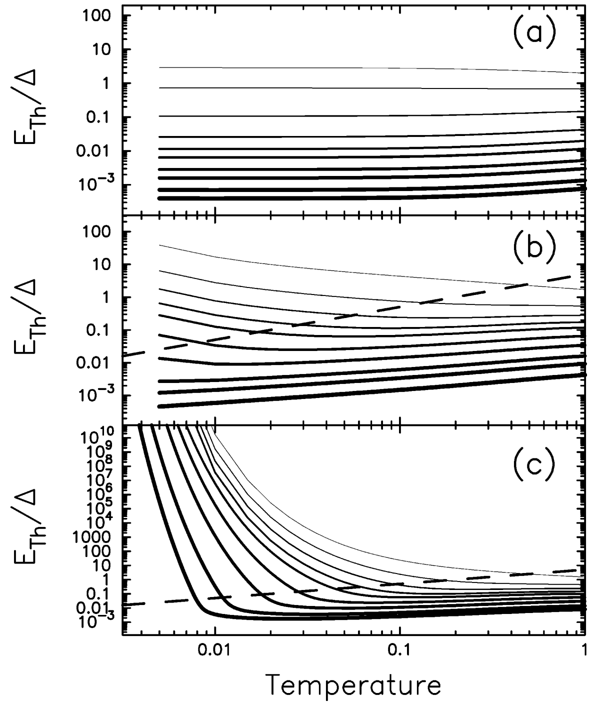

Fig. 2. Thouless energy (in units of the superconducting gap) versus temperature for (a) $U^{FK} = 4$, (b) $U^{FK} = 5$, and (c) $U^{FK} = 6$. The different curves correspond to different thicknesses the barrier; from top to bottom they are: panel (a) $L/a = 1, 2, 5$, 10, 15, 20, 30, 40, 60, and 80; panel (b) $L/a = 1$, 2, 3, 4, 5, 7, 10, 15, 20, 30; and in panel (c) $L/a = 1$, 2, 3, 4, 5, 7, 10, 15, and 20. Note how the temperature dependence increases as the barrier becomes more insulating. The dashed line in the bottom two panels is the line $E_{\mathrm{Th}} = T$.

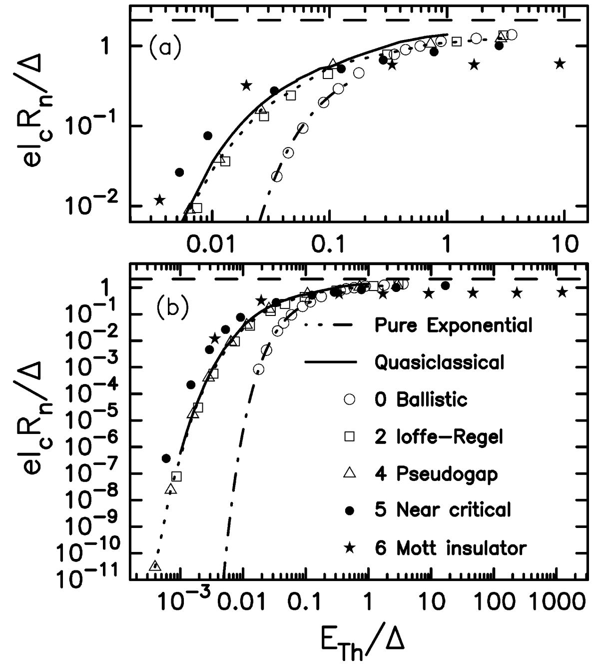

Fig. 3. Dependence of the figure of merit on the generalized Thouless energy in units of the superconducting gap. Five cases are included in the simulations: (i) a ballistic SNS junction ($U^{FK} = 0$); (ii) a diffusive SNS junction close to the Ioffe-Regel limit ($U^{FK} = 2$); (iii) a diffusive SNS junction well beyond the Ioffe-Regel limit ($U^{FK} = 4$); (iv) a Mott insulating barrier close to the critical value of U ($U^{FK} = 5$); and a (v) small-gap Mott insulator ($U^{FK} = 6$). The solid line is the quasiclassical approximation for diffusive SNS junctions, and the chain-dashed line is a simple exponential form, expected for a ballistic SNS junction. Panel (a) is a blow-up of the full plot shown in panel (b).

to $\ell \approx 0.24a$ when $U^{FK} = 4$, to $\ell \approx 0$ when $U^{FK} \approx 4.9$ (and $T = 0$). The Ioffe-Regel limit [14] is reached when the mean free path of the electrons approaches one lattice spacing, so that a Boltzmann equation approach is no longer applicable; in the FK model, it occurs around $U^{FK} = 2$, but the system remains metallic until $U^{FK} = 4.9$ where it has a transition to an insulator. While one would not expect a diffusive model for transport (with a Boltzmann equation) to hold for U^{FK} larger than about 2, we find no significant difference in the properties of the transport in this regime, with the exception of an anomalous temperature dependence of the resistivity as the metal-insulator transition is approached. In other words, the system behaves like a diffusive metal, but with a temperature dependent diffusion constant as the metal-insulator transition is approached.

We calculate the normal-state resistance of our Josephson junctions by using a Kubo formula [7], [8], [15], [16], for the conductivity matrix in real space, and employ Ohm's law (in the form $V = IR$) to extract the resistance from the real-space conductivity matrix. %(this approach requires us to use current conservation for the current %flowing from one plane to its neighboring plane). The normal-state resistance behaves as expected for these junctions [7]: in the metallic phase, we have an Ohmic scaling, with the resistance equal to a Sharvin contact resistance [17], [18] plus a contribution of $\rho_{dc}L$ coming from the "bulk" of the barrier, where ρ_{dc} is the bulk dc resistivity of the barrier. In an insulator, we find that at low temperature, or for thin barriers, the system transports current via tunneling, which has an exponential growth of the resistance with L. Once the junction is thick enough, or T is high enough, the transport is dominated by thermally excited quasiparticles, and it picks up an Ohmic scaling with the bulk resistivity (which is now strongly T dependent). The normal state resistance, and the density of states for the bulk barrier are all that we need to determine the Thouless energy. We plot this for three cases $U^{FK} = 4$, 5, and 6 in Fig. 2. The different curves correspond to different thicknesses of the barrier. Note how the Thouless energy has little temperature dependence in the anomalous metal ($U^{FK} = 4$), but it picks up stronger T dependence as we pass into the insulator, near the critical coupling $U^{FK} = 5$, and in a small-gap insulator $U^{FK} = 6$. In the (diffusive) metallic phase, we find E_{Th} scales like $1/L^2$ for thick junctions, as expected. In the insulating phases, it was found that the point where the temperature was equal to E_{Th} determined the approximate crossover from tunneling to incoherent transport [7]. Here we will examine what happens to a Josephson junction as a function of the Thouless energy.

In Fig. 3, we plot the figure-of-merit divided by the superconducting gap eI_cR_N/Δ versus the Thouless energy divided by the superconducting gap $E_{\mathrm{Th}}(T)/\Delta$ for a low temperature $T = 0.01 = T_c/11$. Five different cases are included: (i) a ballistic metal SNS junction $U^{FK} = 0$; (ii) a diffusive metal close to the Ioffe-Regel limit $U^{FK} = 2$; (iii) an anomalous metal close to the metal-insulator transition $U^{FK} = 4$ (the dotted line is a guide to the eye); (iv) an insulator close to the critical point of the metal-insulator transition $U^{FK} = 5$; and (v) a small gap correlated insulator $U^{FK} = 6$. In addition to the data that we calculated directly with our DMFT-based computer codes, we include two analytical expressions. The chain-dashed line is the prediction for a ballistic SNS junction, where the critical current decreases exponentially with thickness, and the resistance is just the Sharvin resistance, and is independent of L. The solid line is the prediction of the quasiclassical theory [4], [5], modified for finite temperature. We used the analytic result

$$eI_cR_N \approx \frac{32}{3+2\sqrt{2}}E_{\rm Th}\left[\frac{2\pi T}{E_{\rm Th}}\right]^{\frac{3}{2}} e^{-\sqrt{\frac{2\pi T}{E_{\rm Th}}}} \qquad (6)$$

for small $E_{\rm Th}$ and then joined it to the $T=0$ results for larger $E_{\rm Th}$.

The results in Fig. 3 are the main results of this work. They show that all diffusive metals, including those with mean free paths much less than a lattice spacing, obey the quasiclassical predictions. When the barrier is tuned through the metal-insulator transition (solid circles and stars), the results are still qualitatively similar to those of the quasiclassical approach, but the figure-of-merit is smaller for large $E_{\rm Th}$, and then crosses over (at about $E_{\rm Th} \approx 10\Delta$) and becomes larger for small $E_{\rm Th}$. Hence there is a weaker dependence on $E_{\rm Th}$ in the insulating cases, although the dependence is still quite a strong function of $E_{\rm Th}$ (recall Fig. 3 is a log-log plot). This is how the quasiclassical picture breaks down in a Josephson junction.

III. Conclusions

We have demonstrated that the concept of a Thouless energy can be generalized to strongly correlated metals and strongly correlated insulators. The generalization follows from the natural way to extract an energy scale from the resistance via the inverse level spacing, and has a strong temperature dependence for insulating barriers. The generalized form reduces to the well-known diffusive and ballistic limits of the Thouless energy when applied to diffusive or ballistic barriers (that can be described by a quasiclassical approach). We used the generalized Thouless energy to describe the superconducting properties of Josephson junctions, and learn where the quasiclassical approximation breaks down. First we found that the ballistic barriers have a simple dependence on the Thouless energy, since the resistance is independent of L, and the critical current depends exponentially on L, hence the figure of merit depends exponentially on $1/E_{\rm Th}$. Next we found that all diffusive metals, including metals that have a bulk resistivity that decreases as T increases (but remains finite at $T=0$), map onto the universal quasiclassical curve when we plot the figure of merit versus the Thouless energy. This shows that it is the Thouless energy that determines the critical current when it becomes an order of magnitude smaller than the superconducting gap. We find similar behavior for the correlated insulator barriers, but they no longer fit the universal form of the diffusive barriers. Instead, they pick up a weak dependence on the Thouless energy, even for $E_{\rm Th} > \Delta$, which suppresses the figure of merit below the quasiclassical prediction. When $E_{\rm Th}$ is reduced to about an order of magnitude smaller than Δ, the insulating barriers have a figure of merit higher than the quasiclassical prediction; we cannot tell if there is new universal behavior for the correlated insulators, or if the figure-of-merit simply increases with increasing barrier height.

We believe that analysis of Josephson junctions using the generalized Thouless energy may provide interesting insight into their properties. Since the normal state resistance does not depend strongly on T in the tunneling regime $E_{\rm Th} < T$, measurements can be made in the normal state that can be used to extract the Thouless energy and then be used to predict the value of I_cR_N for the Josephson junction (see Fig. 3). This analysis assumes that the junction has uniform barriers that are pinhole free. Because pinholes have a different T dependence to the resistance than uniform barriers, one might be able to use such an analysis as a high-temperature diagnostic for pinholes, but we have not yet been able to work out a definite scheme for how this can be done. We hope that this theoretical work will inspire additional experimental work into analyzing Josephson junctions with the generalized Thouless energy.

Acknowledgment

The authors acknowledge F. K. Wilhelm and T. T. Heikkilä for providing the results of the quasiclassical calculations and the useful discussion.

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