Optical and Thermal-Transport Properties of an Inhomogeneous d-Wave Superconductor

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We calculate transport properties of disordered 2D d-wave superconductors from solutions of the Bogoliubov–de Gennes equations, and show that weak localization effects give rise to a finite-frequency peak in the optical conductivity similar to that observed in experiments on disordered cuprates. At low energies, order parameter inhomogeneities induce linear and quadratic temperature dependencies in microwave and thermal conductivities respectively, and appear to drive the system towards a quasiparticle insulating phase.

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Introduction.—The study of disorder in high-T_c superconductors (HTSC) remains an engaging topic for at least two reasons: first, it is apparent that significant disorder—perhaps originating with charge-donor impurities—is present in nearly all HTSC samples and, second, the controlled doping of substitutional impurities is a powerful means of studying the electronic state. Transport experiments on the cuprates at low T have given us information on the quasiparticle lifetime in the disordered superconductor and indicated the existence of a strong, near-unitarity-limit scattering potentials associated with impurities in the CuO_2 plane. The simplest BCS-quasiparticle theories have been successful at describing qualitative features of transport experiments, but fail to explain many of the details. This is the principal motivation for the current work addressing transport properties of dirty d-wave superconductors. The approach taken here is to model the paired state as an inhomogeneous superfluid via the Bogoliubov–de Gennes (BdG) equations. We focus most of our attention on optimally doped superconductors at low temperatures, where inelastic processes freeze out [1] and mean-field theory is most applicable.

It is well known that HTSC are strongly affected by disorder because of the d-wave symmetry of the pair order parameter Δ_{ij} (i and j are site indices of the paired electrons). In a pure sample, the density of states (DOS) $\rho(\omega)$ is gapless and vanishes as $|\omega|$ at the Fermi energy (taken to be 0 here). A single strong-scattering impurity produces a pair of subgap resonances at $\pm\omega_0$ ($\omega_0 < \Delta_{\max}$, where $\Delta_{\max}$ is the DOS peak associated with the gap edge in tunneling experiments). When a finite concentration n_i of impurities with impurity potential U is present, the isolated resonances are split, and they broaden into an "impurity band" centered at the Fermi energy. The energy scale γ of the impurity band, below which $\rho(E)$ crosses over from linear ($|E| > \gamma$) to constant ($|E| < \gamma$), is determined by n_i and U. These essential features are captured in the widely used self-consistent T-matrix approximation (SCTMA) for impurity scattering [2]. The SCTMA is a perturbative scheme which is useful for treating pointlike scatterers. It correctly incorporates the physics associated with strong-scattering potentials, but ignores correlation effects between impurities (i.e., localization effects), as well as the local response of the superfluid to the impurities. In the SCTMA, γ is also the quasiparticle scattering rate in the impurity band.

While the SCTMA-based notion of an impurity band appears to be fairly consistent with the observed thermodynamic properties of the optimally doped cuprates [3], the simplest theory based on this picture disagrees with transport experiments. Notably, the low-temperature behavior of both the thermal and microwave conductivities in several systems disagree with the simple prediction, $\sigma,\ \kappa/T \sim T^2$ [4]. For example, the low-temperature microwave conductivity in $YBa_2Cu_3O_{7-\delta}$ appears to vary roughly linearly with temperature, $\sigma \sim T$ [5]. In addition, the optical conductivity of disordered cuprates is observed to have a maximum at a disorder-dependent frequency of order 100 cm^{-1} [6]; this feature is also not found in the simple SCTMA analysis [7]. Finally, the SCTMA predicts the universality of residual transport coefficients, i.e., limiting values of κ/T and σ as $T \rightarrow 0$ which depend only weakly on disorder [8]. While this has been confirmed in thermal conductivity measurements on $YBa_2Cu_3O_{7-\delta}$ [9] and $Bi_2Sr_2CaCu_2O_8$ [10], there are other systems where universality is not seen [11]. We show below that some of these discrepancies can be understood within a BCS framework by going beyond the SCTMA.

Approach.—The BdG equations will be solved at two levels of approximation. Like the SCTMA, non-self-consistent (NSC) solutions assume that Δ_{ij} is homogeneous, but, unlike the SCTMA, NSC solutions incorporate quantum coherence (i.e., localization) effects associated with scattering from multiple impurities exactly. Self-consistent (SC) BdG solutions involve a further step in which the nonlinear response of Δ_{ij} to the local disorder potential is determined. In both cases, the BdG equations are solved on a tight-binding lattice with $N = 1600$ sites and up to 50 disorder configurations. In matrix form, the mean-field Hamiltonian is

$$\mathcal{H} = \sum_{ij} \Phi_i^\dagger \begin{bmatrix} t_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -t_{ij}^* \end{bmatrix} \Phi_j , \tag{1}$$

with $\Phi_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow})$. The subscripts i and j refer to site indices, and $t_{ij} = -t\delta_{\langle i,j\rangle} + (U_i - \mu)\delta_{i,j}$, with $\delta_{\langle i,j\rangle} = 1$ for nearest neighbor sites and 0 otherwise. All energies in this work are measured in units of t, and the lattice constant is $a = 1$. The bond order parameter is $\Delta_{ij} = -V\langle c_{j\downarrow}c_{i\uparrow}\rangle$ with V the nearest neighbor pairing interaction. The pure d-wave superconducting state occurs in the disorder-free limit and is related to the bond order parameters by $\Delta_{ij} = \frac{1}{2}\Delta_0[(-1)^{x_{ij}} - (-1)^{y_{ij}}]$ with (x_{ij}, y_{ij}) connecting sites i and j, and where Δ_0 is the homogeneous d-wave amplitude. Spatial fluctuations arise naturally when one solves Δ_{ij} self-consistently in the presence of a disorder potential. For this work $V = 3.28$, making $\Delta_0 = 0.8$ which is a factor of $\sim$4 larger than the realistic case. The eigenstates are found using standard linear algebra routines to diagonalize Eq. (1). The quasiparticle DOS is $\rho(\omega) = N^{-1}\langle\sum_n \delta(\omega - E_n)\rangle$, where E_n are the eigenenergies for a given impurity configuration and $\langle\cdots\rangle$ represents configuration averaging.

The complex conductivity is

$$\sigma(\omega, T) = \left\langle \frac{e^2\hbar}{i\omega\pi N}\sum_{n,n'}|\hat{\gamma}^0_{nn'}|^2 \frac{f(E_n) - f(E_{n'})}{\hbar\omega^+ - E_n + E_{n'}}\right\rangle, \tag{2}$$

where $\hat{\gamma}^\alpha_{nm} \equiv \langle n|(p_x/m) \otimes \tau^\alpha|m\rangle$ is the matrix element of the velocity between eigenstates n and m, τ^α ($\alpha = 0,\ldots,3$) is the Pauli matrix in particle-hole space, and $\omega^+ = \omega + i0^+$. We use a binning procedure to evaluate the real part of $\sigma(\omega, T)$. Note that expression (2) is not manifestly gauge invariant, but we do not expect this to be a problem since the collective response of the one-component charged order parameter occurs at the plasma frequency.

For numerical reasons, we are restricted to evaluating $\sigma(\omega, T)$ in the "gapless regime," $\gamma \gtrsim T$, which has been studied in intentionally damaged samples of $YBa_2Cu_3O_{7-\delta}$ [6,12]. In this regime, the SCTMA predicts [4] that the real part of the conductivity is $\sigma_{\rm SCTMA}\ (\omega \to 0, T) = \sigma_{00} + \alpha(T/\gamma)^2$ and $\sigma_{\rm SCTMA}(\omega, 0) = \sigma_{00} + \alpha'(\omega/\gamma)^2$, with a universal value for the residual conductivity: $\sigma_{00} = e^2 v_F/(\pi^2\hbar v_\Delta)$. In this expression, v_F is the Fermi velocity and $v_\Delta = |\nabla_k \Delta_k|$ is the quasiparticle velocity component parallel to the Fermi surface. Both impurity vertex corrections and Fermi-liquid corrections renormalize σ_{00} in an approximation [13], where s-wave scattering is generalized to include anisotropic components, but where weak localization corrections and order parameter inhomogeneities are neglected. In this scheme the thermal conductivity is not renormalized [13], $\kappa(T)/T = \kappa_{00} + a(T/\gamma)^2$, with universal value $\kappa_{00} = \frac{1}{3}k_B^2(v_F^2 + v_\Delta^2)/v_F v_\Delta$ which survives this class of perturbative corrections.

Results.—Typical results for $\rho(\omega)$ near unitarity—defined by $\omega_0 \ll \gamma$ and corresponding to $U \approx 10$ and $U \approx 5$ in the NSC and SC calculations, respectively—are shown in Fig. 1. NSC calculations agree semiquantitatively with SCTMA calculations except below an exponentially small energy [14]. The SC result, by contrast, shows a large disorder-induced suppression of the DOS relative to the SCTMA plateau. As discussed elsewhere [14] the "disorder-induced pseudogap" (DIP) at the Fermi energy appears to be a generic feature of SC BdG solutions and has an energy scale related to ω_0 but which grows with increasing n_i. We stress that, for typical planar Cu substituents in HTSC, this is an energy scale which is comparable to those explored in transport experiments.

Figure 1 shows the basic low-T result for the conductivity with strong-scattering impurities. $\sigma_{\rm SCTMA}(\omega)$ is approximately Drude-like for $\omega > \gamma$, but saturates at the universal value [7,8] σ_{00} for $\omega < \gamma$. Numerical solutions of the BdG equations deviate significantly from this with $\sigma(\omega < \gamma)$ linear in frequency, and rising to a peak at $\omega \approx \gamma$. This is true for both $\sigma_{\rm SC}$ and $\sigma_{\rm NSC}$ (the SC and NSC BdG conductivities, respectively), and is therefore the result of weak localization corrections to the SCTMA result [15]. Indeed, Fig. 1(c) shows that $\delta\sigma(\omega) \equiv \sigma_{\rm NSC}(\omega) - \sigma_{\rm SCTMA}(\omega)$ satisfies a scaling relation, $\delta\sigma(\omega)/\sigma_{00} = F(\omega/\gamma)$, which is similar to the weak localization scaling relation for dirty 2D metals. In contrast, $\sigma_{\rm SC}(\omega)$ does not display a simple scaling relation, as we discuss below. At this point, we simply remark that $\sigma_{\rm SC}(\omega)$ always has less finite ω spectral weight than $\sigma_{\rm SCTMA}(\omega)$ for the same value of U [as illustrated in Fig. 1(a)], with the lost weight appearing in the superfluid response [16].

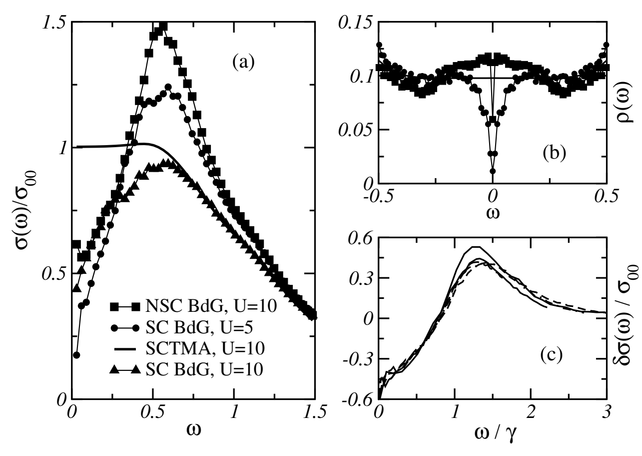

FIG. 1. Finite frequency conductivity for $\mu = 1.2$, $T = 0$, and $\Delta = 0.8$ (i.e., $v_F/v_\Delta = 2.5$). (a) Curves are for self-consistently determined order parameter (SC BdG), homogeneous order parameter (NSC BdG) and SCTMA with $n_i = 0.04$. (b) Density of states for NSC BdG and SCTMA with $U = 10$, and SC BdG with $U = 5$ (unitarity limit). The gap edge for the tunneling density of states is $\Delta_{\max} \approx 1$; the SCTMA impurity bandwidth is $\gamma \approx 0.45$. (c) Scaling of the NSC BdG conductivity for $U = 10$ and $n_i = 0.02$, 0.04, 0.06, 0.08, and 0.14. Corresponding γ are $\gamma = 0.29$, 0.43, 0.55, 0.67, and 0.91. A small deviation arises for $n_i = 0.02$ from finite size effects.

The finite-frequency conductivity peak exhibited in Fig. 1 is reminiscent of conductivity measurements in disordered HTSC [6]. Experimentally, the peak is also seen in the normal state $T > T_c$, generally at higher energies, whereas in our approximation it occurs at significantly lower energies, and is much less pronounced than in the superconducting state. It is clear that inelastic scattering is important in the normal state and needs to be incorporated in a complete explanation of the finite-frequency peak. Nevertheless, this is the simplest way of understanding this feature of the optical data, which has not been reproduced in any other approach to our knowledge.

The temperature dependence of the low-frequency conductivity is also of experimental interest. In Fig. 2 we have plotted $\sigma(\omega_1, T)$, where $\omega_1 = 0.0297$ is the lowest nonzero frequency, which is chosen since $\omega = 0$ suffers from finite size effects. The strong T dependence of $\sigma_{\rm NSC}(\omega_1, T)$ is similar to the SCTMA result. On the other hand, $\sigma_{\rm SC}(\omega_1, T)$ has a linear-T conductivity, reminiscent of most microwave conductivity experiments [5]. These results are generic for a wide range of U near unitarity. Figure 2 also shows the thermal conductivity

$$\kappa(T) = \frac{1}{2\pi\hbar T} \int dx\, x^2 \left(-\frac{\partial f}{\partial x}\right) \langle S_T(x) \rangle, \qquad (3)$$

where

$$S_T(x) = \frac{2\pi^2\hbar^2}{N} \sum_{n,n'} |\langle \hat{v}_g \rangle_{nn'}|^2 \delta(x - E_n)\delta(E_n - E_{n'}), \qquad (4)$$

where quasiparticle group velocity $\hat{v}_g = \hat{\gamma}^3 + \hat{v}_\Delta^x \otimes \tau^1$, and $\langle \hat{v}_\Delta^x \rangle_{ij} = (i/\hbar)(x_i - x_j)\Delta_{ij}$ in the site representation [17]. For a finite system, the δ functions in Eq. (4) are broadened to smooth the discreteness of the energy spectrum. It is apparent in Fig. 2 that the Wiedemann-Franz law $\kappa/\sigma T = L_0 \equiv k_B^2 \pi^2 / 3e^2$, which is already violated because of differences between the group and Fermi velocity, appears to also be violated at low T (at least in the NSC case) by weak localization corrections. For comparison, we show a similar calculation of the charge conductivity which becomes exact in the limit $\omega \ll T$,

$$\sigma(T) = \frac{e^2}{2\pi\hbar} \int dx \left(-\frac{\partial f(x)}{\partial x}\right) \langle S_\sigma(x) \rangle, \qquad (5)$$

where S_σ is identical to S_T with the replacement of $\hat{v}_g$ by $\hat{\gamma}^0$. From the figure, it is clear that Eq. (5) is in good agreement with $\sigma(\omega_1, T)$, and that both $\kappa(T)/T$ and $\sigma(T)$ exhibit a linear T dependence over a wide range of temperatures. The extent of the linear regime is discussed below. Linear power laws have been claimed in thermal conductivity measurements [10] (but other power laws have also been reported), and this work provides a potential mechanism. Conductivities with odd power laws in T are difficult to achieve in the SCTMA because all quantities in the gapless regime are analytic functions of ω. We note that quasilinear behavior over some intermediate temperature regime has been obtained in SCTMA approaches, by invoking a special combination of unitarity and weak scatterers [18], by fine-tuning scattering phase shifts [19], or by including order parameter fluctuations in a SCTMA-like approximation [20].

Finally, in Fig. 3 we study the dependence of $\sigma_{\rm SC}(\omega)$ on impurity concentration. As n_i is increased, the peak position in $\sigma_{\rm SC}$ increases, in qualitative agreement with the scaling of $\sigma_{\rm NSC}(\omega)$. The scaling of $\sigma_{\rm SC}(\omega)$ is not straightforward, however, since low-frequency spectral weight is depleted as n_i increases, in contrast to $\sigma_{\rm NSC}(\omega)$ which depends only weakly on n_i at low ω. The depletion is correlated with the growth of the DIP [shown in Fig. 3(b)], reminiscent of disordered interacting metals near the metal-insulator transition. For the model interaction chosen, we never observe a transition to a truly gapped state, and it is doubtful that a quasiparticle metal-insulator transition could be observed in real HTSC since superconductivity is destroyed in heavily damaged samples. However, the current work is strongly suggestive

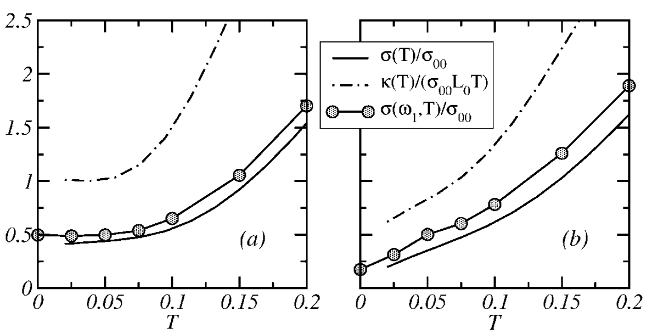

FIG. 2. T-dependent conductivity, normalized to σ_{00} for (a) NSC BdG and (b) SC BdG with $n_i = 0.06$, $U = 10$, $\mu = 1.2$, and $\Delta = 0.8$. $\omega_1 = 0.0297$ is the lowest nonzero frequency used in calculating σ with Eq. (2); $\kappa/(TL_0)$ and $\sigma(T)$ are evaluated using Eqs. (4) and (5).

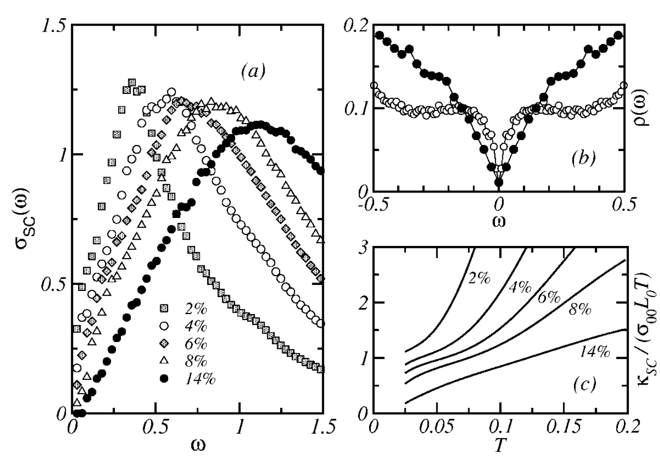

FIG. 3. Scaling of $\sigma_{\rm SC}(\omega)$ with n_i at $T = 0$. (a) $\sigma_{\rm SC}(\omega)$ for a range of n_i between 0.02 and 0.14, $U = 5$. (b) Density of states at $n_i = 0.04$ (open circles) and $n_i = 0.14$ (filled circles). (c) Thermal conductivity vs temperature for the same n_i, U.

that the physics of disordered cuprate superconductors is influenced by proximity to such a transition.

In Fig. 3(c), we plot the SC thermal conductivity for several impurity concentrations to illustrate the robustness of the (quasi-)linear-T regime. The regime is bounded by two disorder-dependent temperature scales; the upper crossover temperature is readily apparent up to $n_i = 0.08$, and is correlated with the weak localization scale γ, while the lower bound signals a downturn in κ/T which appears to scale with the DIP. For $n_i = 0.14$, there is no clear distinction between these scales. With current system sizes it is difficult to determine the lowest energy behavior. If one assumes that matrix elements of $\langle \hat{v}_g \rangle$ have only weak energy dependence near the Fermi surface, then we expect $S_T(x) \sim \rho(x)^2$ which is $\sim x^{2\alpha}$ near $x = 0$ ($\rho \sim x^\alpha$[14]) in the SC BdG calculations. For sufficiently small T, then, one anticipates a downturn with $\kappa/T \sim T^{2\alpha}$ below the DIP energy scale. It is clear that a strong suppression relative to the universal SCTMA result $\kappa(T) \rightarrow \kappa_{00}$ is to be expected.

Conclusions.—We have observed effects with two distinct physical origins in this work. First, there is a pronounced peak in $\sigma(\omega)$ at $\omega \approx \gamma$ arising from localization physics. This occurs whether or not the BdG equations are solved self-consistently and is consistent with the experimental fact that the peak is observed only in very disordered systems. Since $\gamma \sim \sqrt{n_i}$ for strong scatterers, our work suggests that a systematic study of samples with varying impurity concentrations will provide an experimental means to distinguish between the weak localization mechanism presented here and other proposed origins for the peak. Second, we have found that important physics associated with the correlated order parameter response to disorder arises at low energies. Perhaps the most striking result is the observation of linear-T power laws in the charge and thermal conductivities, as observed in some high-T_c systems. In addition, order parameter supression effects appear to eliminate the residual conductivities at asymptotically low temperatures expected on the basis of SCTMA and other treatments. We note that the current work assumes fairly disordered systems, and the extrapolation to the clean limit ($\gamma < T$) is not obvious. On the other hand, this is the first time that this additional source of off-diagonal scattering has been correctly accounted for in a transport theory, and there appears to be no reason, in principle, why these effects should also not be important in clean 2D systems and possibly even in higher dimensions. To compare directly with experiments, the effect of realistic Dirac cone anisotropies and inelastic scattering needs to be better understood. Work along these lines is in progress.

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[1] M. C. Nuss, P. M. Mankiewich, M. L. O'Malley, E. H. Westerwick, and P. B. Littlewood, Phys. Rev. Lett. **66**, 3305 (1991); D. B. Romero *et al.,* Phys. Rev. Lett. **68**, 1590 (1992); D. A. Bonn, D. C. Morgan, K. Zhang, R. Liang, D. J. Baar, and W. N. Hardy, J. Phys. Chem. Solids **54**, 1297 (1993).
[2] A. G. Yashenkin, W. A. Atkinson, I. V. Gornyi, P. J. Hirschfeld, and D. V. Khveshchenko, Phys. Rev. Lett. **86**, 5982 (2001), and references therein.
[3] D. J. Scalapino, Phys. Rep. **250**, 329 (1995).
[4] P. J. Hirschfeld, W. O. Putikka, and D. J. Scalapino, Phys. Rev. Lett. **71**, 3705 (1993); Phys. Rev. B **50**, 10 250 (1994).
[5] A. Hosseini, R. Harris, S. Kamal, P. Dosanjh, J. Preston, R. Liang, W. N. Hardy, and D. A. Bonn, Phys. Rev. B **60**, 1349 (1999).
[6] D. N. Basov *et al.,* Phys. Rev. B **49**, 12 165 (1994); D. N. Basov, B. Dabrowski, and T. Timusk, Phys. Rev. Lett. **81**, 2132 (1998).
[7] W. O. Putikka and P. J. Hirschfeld, Physica (Amsterdam) **194B–196B**, 1517 (1994).
[8] P. A. Lee, Phys. Rev. Lett. **71**, 1887 (1993).
[9] L. Taillefer, B. Lussier, R. Gagnon, K. Behnia, and H. Aubin, Phys. Rev. Lett. **79**, 483 (1997).
[10] S. Nakamae, K. Behnia, L. Balicas, F. Rullier-Albenque, H. Berger, and T. Tamegai, Phys. Rev. B **63**, 184509 (2001).
[11] N. E. Hussey, S. Nakamae, K. Behnia, H. Takagi, C. Urano, S. Adachi, and S. Tajima, Phys. Rev. Lett. **85**, 4140 (2000).
[12] K. Zhang, D. A. Bonn, R. Liang, D. J. Baar, and W. N. Hardy, Appl. Phys. Lett. **62**, 3019 (1993).
[13] A. C. Durst and P. A. Lee, Phys. Rev. B **62**, 1270 (2000).
[14] W. A. Atkinson, P. J. Hirschfeld, and A. H. MacDonald, Phys. Rev. Lett. **85**, 3922 (2000).
[15] L. P. Gorkov, A. Z. Larkin, and D. E. Khmelnitskii, JETP **30**, 248 (1979).
[16] A. Ghosal, M. Randeria, and N. Trivedi, Phys. Rev. B **63**, 20 505 (2001).
[17] Note that we have simply discretized the group velocity operator which gives the thermal current in the uniform case. Additional terms arise when deriving the thermal current in an inhomogeneous system which we have neglected here. A. Kampf (private communication).
[18] A. J. Berlinsky, D. A. Bonn, R. Harris, and C. Kallin, Phys. Rev. B **61**, 9088 (2000).
[19] S. Hensen, G. Müller, C. T. Rieck, and K. Scharnberg, Phys. Rev. B **56**, 6237 (1997).
[20] M. H. Hettler and P. J. Hirschfeld, Phys. Rev. B **59**, 9606 (1999).