

Scaling of the Quasiparticle Spectrum for d -wave Superconductors

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In finite magnetic field H , the excitation spectrum of the low energy quasiparticles in a two-dimensional d -wave superconductor exhibits a scaling with respect to $H^{1/2}$. This property can be used to calculate scaling relations for various physical quantities at low temperature T , such as the finite magnetic field specific heat, quasiparticle magnetic susceptibility, optical conductivity tensor, and thermal conductivity tensor. These predictions are compatible with existing experimental data. Most notably, the measured thermal Hall coefficient κ_{xy} in YBCO is found to scale as $\kappa_{xy} \sim T^2 F(\alpha T/H^{1/2})$ for $T \lesssim 30$ K in agreement with our predictions. [S0031-9007(97)02477-0]

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The scientific community has been slowly coming to a consensus that the high T_c superconductors have a d -wave order parameter [1]. One of the major differences between these and conventional superconductors is that d -wave superconductors have gapless low energy excitations in certain directions in k space, whereas s -wave superconductors are gapped. As a result, the low temperature behavior in the d -wave case can be quite different from that of conventional superconducting materials. Thus, in order to properly interpret experiments on these novel materials (and eventually develop a microscopic theory), we must have a clear understanding of the physics associated with a d -wave order parameter. In this work, we attempt to elucidate some of this physics by deriving scaling relations obeyed by the quasiparticle energies and eigenfunctions. Using these relations, we are then able to deduce scaling properties of a number of important physical quantities.

We begin our analysis with the Bogolubov [2] equations, $\mathcal{H}\psi = \epsilon\psi$ where $\psi = (u, v)$ is a Nambu 2-spinor whose components are the particlelike and holelike part of the quasiparticle wave function, respectively. Here,

$$\mathcal{H} = \begin{pmatrix} h + V - E_F & \hat{\Delta} \\ \hat{\Delta}^* & -h^* - V + E_F \end{pmatrix} \quad (1)$$

with E_F the Fermi energy, and h the kinetic part of the effective single particle Hamiltonian, and $V(\mathbf{r})$ is the effective disorder potential. As a model system we choose to work with the effective one-particle Hamiltonian $h = \frac{(\mathbf{p}-\mathbf{A})^2}{2m}$ with m the electron effective mass. Although this neglects any direct Hartree or exchange pieces of the interaction, such pieces are thought to be relatively unimportant except in renormalizing m and V . (In this Letter we have set the charge of the electron e , the speed of light c , and Planck's constant \hbar all to unity.)

In Eq. (1), $\hat{\Delta}$ is the gap operator for spin singlet superconductivity defined as $\hat{\Delta}g(\mathbf{r}) = \int d\mathbf{r}' \Delta(\mathbf{r}, \mathbf{r}')g(\mathbf{r}')$ for any $g(\mathbf{r})$, where $\Delta(\mathbf{r}, \mathbf{r}') = -v(\mathbf{r} - \mathbf{r}')\langle\psi_1(\mathbf{r})\psi_1(\mathbf{r}')\rangle$ with v the interelectron interaction. If we rewrite $\Delta(\mathbf{r}, \mathbf{r}')$ in terms of center of mass coordinate $\mathbf{R} = \frac{\mathbf{r}+\mathbf{r}'}{2}$ and rela-

tive coordinate $\mathbf{x} = \mathbf{r} - \mathbf{r}'$, then Fourier transform with respect to \mathbf{x} , we can write the gap function as $\Delta(\mathbf{R}, \mathbf{k})$.

In this work we consider a two-dimensional d -wave superconductor. It is believed that this accurately represents the high T_c materials. We choose to consider a gap function with pure d_{xy} symmetry rather than $d_{x^2-y^2}$ for notational simplicity. The final results for $d_{x^2-y^2}$ are identical. The gap function is written as $\Delta(\mathbf{R}, \mathbf{k}) = \Delta_{d_{xy}}(\mathbf{R})k_x k_y / (k_F)^2$. Shifting back to the coordinates \mathbf{r} and \mathbf{r}' , then integrating by parts, the gap operator can be re-expressed as $\hat{\Delta} = \frac{1}{p_F} \{p_x, \{p_y, \Delta_{d_{xy}}(\mathbf{r})\}\}$, where p_x and p_y are the components of the momentum operator, p_F is the Fermi momentum, and the brackets represent the symmetrization, $\{a, b\} = \frac{1}{2}(ab + ba)$. The function $\Delta_{d_{xy}}$ is the d -wave order parameter used in Ginzburg-Landau theory [3]. We can then consider calculating $\Delta_{d_{xy}}$ in an inhomogeneous system by using a Ginzburg-Landau approach, then using $\Delta_{d_{xy}}$ in Eq. (1) to find the quasiparticle spectrum. We note that this approach is not fully self-consistent in the sense that we will not use the derived quasiparticle states to then recalculate the gap function.

For a homogeneous system there are gapless nodes on the Fermi surface at the points $\mathbf{p} = (\pm p_F, 0)$ and $\mathbf{p} = (0, \pm p_F)$ where $\hat{\Delta}$ vanishes. To study the low lying excitations near these points, we linearize the Hamiltonian. As an example, we consider linearizing around the point $\mathbf{p} = (p_F, 0)$. We write $\psi = e^{ik_F x} \tilde{\psi}$ such that we can recast the Bogolubov equations as $(\tilde{\mathcal{H}}_0 + \tilde{\mathcal{H}}_1)\tilde{\psi} = \epsilon\tilde{\psi}$ where $\tilde{\mathcal{H}}_0$ is the leading linearized term

$$\tilde{\mathcal{H}}_0 = \begin{pmatrix} v_F(p_x - A_x) + V & \frac{1}{p_F} \{p_y, \Delta_{d_{xy}}(\mathbf{r})\} \\ \frac{1}{p_F} \{p_y, \Delta_{d_{xy}}^*(\mathbf{r})\} & v_F(-p_x - A_x) - V \end{pmatrix} \quad (2)$$

and $\tilde{\mathcal{H}}_1$ is the remaining piece

$$\tilde{\mathcal{H}}_1 = \begin{pmatrix} h & \hat{\Delta} \\ \hat{\Delta}^* & -h^* \end{pmatrix}, \quad (3)$$

where $v_F = p_F/m$ is the Fermi velocity.

For sufficiently small energy excitations, $\tilde{\mathcal{H}}_0$ is much greater than $\tilde{\mathcal{H}}_1$, and it will be a reasonable approximation to neglect $\tilde{\mathcal{H}}_1$. To determine when this is a good approximation, we consider the homogeneous case of $\Delta_{d_{xy}}$ a real constant with $\mathbf{A} = 0$, and $V = 0$. We then find that $\tilde{\mathcal{H}}_0$ is just the Dirac Hamiltonian for massless fermions in two dimensions, and thus has a conical linear spectrum of quasiparticles with $\epsilon_{\mathbf{p}} = \pm \sqrt{(v_F p_x)^2 + (\Delta_{d_{xy}} p_y / p_F)^2}$. Note that the conical spectrum is highly anisotropic since $v_F \gg \Delta_{d_{xy}} / p_F$. For excitations at temperature T , the typical momenta are $p_x \sim T / v_F$ and $p_y \sim T p_F / \Delta_{d_{xy}}$. The largest term in $\tilde{\mathcal{H}}_1$ is then the term $p_y^2 / (2m)$ which would be on order $E_F (T / \Delta_{d_{xy}})^2$. For YBCO and BSCCO, photoemission spectroscopy [4] indicates that $E_F \approx 3000$ K, and $\Delta_{d_{xy}} \approx 300$ K. We also note that the Fermi surface is not circular, but is somewhat flattened at the nodes (more squarelike with rounded corners). This means we should really use an effective mass m_y in the $p_y^2 / (2m)$ term of $\tilde{\mathcal{H}}_1$ which lowers the energy scale of $\tilde{\mathcal{H}}_1$ by another factor of perhaps two or three. Thus, we estimate that $\tilde{\mathcal{H}}_1 / \tilde{\mathcal{H}}_0 \approx T / (100 \text{ K})$, so that the condition $\tilde{\mathcal{H}}_0 \gg \tilde{\mathcal{H}}_1$ may be well satisfied at temperatures as high as 20 K.

We now apply a magnetic field H perpendicular to the plane of the sample to create a vortex lattice such that the phase of $\Delta_{d_{xy}}$ twists by 2π as we go around each vortex. Since the screening length is very long, we can assume H is homogeneous. The distance between vortices is proportional to the magnetic length $l_H \sim H^{-1/2}$. We now claim that for $T \ll T_c$ and $H \ll H_{c2}$, to a very good approximation, the Hamiltonian $\tilde{\mathcal{H}}_0$ has a simple scaling form that we write (in a slight abuse of notation) as $\tilde{\mathcal{H}}_0^H(\mathbf{r}) = [H/H_0]^{1/2} \tilde{\mathcal{H}}_0^{H_0}(\mathbf{r}[H/H_0]^{1/2})$. In other words, if we can find the eigenvectors $\tilde{\psi}_n^{H_0}(\mathbf{r})$ and eigenenergies $\epsilon_n^{H_0}$ of the Hamiltonian $\tilde{\mathcal{H}}_0$ in field H_0 , then the eigenenergies and eigenvectors in field H can be written as

$$\tilde{\psi}_n^H(\mathbf{r}) = \tilde{\psi}_n^{H_0}(\mathbf{r}[H/H_0]^{1/2}), \quad (4)$$

$$\epsilon_n^H = [H/H_0]^{1/2} \epsilon_n^{H_0}. \quad (5)$$

The first of these equations is the statement that the functional form of the eigenvector scales as the vortex lattice, whereas the second is a reflection of the Hamiltonian being linear in momentum. To show that these scaling properties hold, we consider each term in $\tilde{\mathcal{H}}_0$ individually. It is easy to show that the vector potential in field H can be written in a scaling form $\mathbf{A}_H(\mathbf{r}) = [H/H_0]^{1/2} \mathbf{A}_{H_0}(\mathbf{r}[H/H_0]^{1/2})$. Similarly, \mathbf{p} must scale as the inverse of the magnetic length l_H so $\mathbf{p}^H = [H/H_0]^{1/2} \mathbf{p}^{H_0}$. Thus we need only examine $\Delta_{d_{xy}}$ and V .

We first consider the scaling of $\Delta_{d_{xy}}$. In order to have the desired scaling of $\tilde{\mathcal{H}}_0$, we must have $\Delta_{d_{xy}}^H(\mathbf{r}) = \Delta_{d_{xy}}^{H_0}(\mathbf{r}[H/H_0]^{1/2})$. This is simply the statement that, like the wave function $\tilde{\psi}$, the functional dependence of $\Delta_{d_{xy}}$

on position scales with the vortex lattice. For $H \ll H_{c2}$ the vortex cores are very small and far apart so we are not concerned with the behavior of the order parameter in the vicinity of these cores. Away from the cores, the amplitude of the order parameter is fixed, and the scaling of the remaining phase degree of freedom is then an obvious result of Ginzburg-Landau theory.

We now turn to consider the disorder term V . For Gaussian delta-function correlated disorder such that $\langle V \rangle = 0$, and $\langle V(\mathbf{r})V(\mathbf{r}') \rangle = V_0 \delta(\mathbf{r} - \mathbf{r}')$, the disorder does not define a length scale so that given a realization of disorder $V(\mathbf{r})$, another configuration $V'(\mathbf{r}) = [H/H_0]^{1/2} V(\mathbf{r}[H/H_0]^{1/2})$ is equally likely. In other words, the disorder term (in an ensemble average) has the proper scaling properties to preserve Eqs. (4) and (5). However, in perturbation theory, disorder leads to a logarithmic divergence which is cut off by the band width. When such a cutoff and scattering between low energy nodes is accounted for, disorder produces a nonzero density of states [7] at zero energy which breaks the scaling. The energy scale below which the scaling is expected to fail, however, is exponentially small in the inverse of the disorder strength. Thus, for weak disorder, the scaling should hold at temperatures high compared to this exponentially small scale. For more general types of disorder with a nonzero correlation length, the temperature scale below which scaling is broken can become somewhat larger. We also note that since there is no Anderson's theorem [2] for d -wave superconductors, disorder will reduce the overall value of the gap and thereby reduce the maximum temperature at which the condition $\tilde{\mathcal{H}}_0 \gg \tilde{\mathcal{H}}_1$ is satisfied.

As with adding a magnetic field to free electrons, the free k states are no longer good eigenstates for the system, but in a semiclassical approximation the particle can be thought of as having dynamics in both k space and real space. Thus, the particle equally samples each direction of the anisotropic Dirac cone and the effective velocity becomes the geometric average of the two Fermi velocities v_F and $\Delta_{d_{xy}} / p_F$. It is then convenient to define $\alpha^{-1} = \sqrt{\Delta_{d_{xy}} / m}$, which is this average velocity.

Neglecting disorder, $\Delta_{d_{xy}}$ and \mathbf{A} can both be considered to be periodic functions with the periodicity of the vortex lattice [6]. Due to this periodicity, the eigenstates can be divided into Brillouin zones with one band of excitations per zone. The first zone should then have a maximum k vector of approximately $|\mathbf{k}_{\max}| \approx l_H^{-1}$, with l_H the magnetic length. The number of different zones with momentum less than some k is roughly $(k/k_{\max})^2$. The typical energy scale of an excitation of wavevector k is then $k\alpha^{-1}$. Thus, the typical energy E_n of the n th band is given roughly by $E_n \sim \sqrt{n} k_{\max}$ or $E_n^2 \approx n\alpha^{-2}H$. Finally, it will be useful to define the dimensionless parameter $x = \alpha T / H^{1/2}$ which is roughly the number squared of bands that are considerably occupied at temperature T . For YBCO, $\alpha \approx 0.05 \text{ T}^{1/2} / \text{K}$.

Using the above described scaling laws, we can extract a number of important statements about physical quantities. As a first example we examine the specific heat. We write the energy as

$$U = \sum_n \epsilon_n^H f(\epsilon_n^H/T) = [H/H_0]^{1/2} \sum_n \epsilon_n^{H_0} f(\epsilon_n^{H_0}[H/H_0]^{1/2}/T), \quad (6)$$

where f is the Fermi function. The volume ν of the system here scales as $l_H^2 \sim 1/H$ so that $\nu = \nu_0[H_0/H]$. Thus, the energy density can be written as $U/\nu = H^{3/2}F_U(\alpha T/H^{1/2})$ where F_U is some scaling function that we can write down in terms of eigenenergies, but cannot evaluate without fully diagonalizing $\tilde{\mathcal{H}}_0$. Here we have used the fact that the sum in Eq. (6) is only a function of the dimensionless quantity $x = \alpha T/H^{1/2}$. Recall that $T \ll T_c$ so that the magnitude of the gap does not change much with T . Differentiating to obtain the electronic specific heat per unit volume, we find

$$C_v = TH^{1/2}F_C(\alpha T/H^{1/2}), \quad (7)$$

where F_C is again some unknown scaling function. Note that Eq. (7) does not include contributions to the specific heat from electrons in the vortex cores. These contributions, however, are thought to be small [10].

Experimental measurements of electronic specific heat are quite difficult being that there are many nonelectronic contributions such as phonons. The easiest way to experimentally test Eq. (7) is to compare the specific heat in magnetic field perpendicular to the c axis to that in field parallel to the c axis. Assuming isotropic magnetic field dependence of all other contributions to the specific heat (including Schottky anomaly), the difference in these specific heats should also follow Eq. (7). This is indeed found to be true in the data of Ref. [8], but for the data of Ref. [9] the scaling form holds well only at high fields.

A semiclassical approximation by Volovik [10], as well as later work of Won and Maki [11], predicts the low temperature form $C_v \sim T\sqrt{H}$ (equivalent to F_C being a constant for small argument). This term in the electronic specific heat has been measured by several groups [12]. Kopnin and Volovik [13] also calculated the form of the scaling function F_C at large argument, with a crossover between the two forms predicted for $T/H^{1/2} \approx \nu_F$, which is roughly the same scale as our predicted crossover scale $T/H^{1/2} \approx \alpha^{-1} \approx \nu_F \sqrt{\Delta_{d_{xy}}}/E_F \approx 20 \text{ K}/T^{1/2}$.

Similar to the discussion above, the free energy density, $F/\nu = (U - TS)/\nu$ with $S = \sum_n [f_n \ln f_n + (1 - f_n) \ln(1 - f_n)]$ and $f_n = f(\epsilon_n/T)$, can be written in the scaling form $F/\nu = H^{3/2}F_F(T/H^{1/2})$. We then conclude that the quasiparticle magnetic susceptibility per unit volume [11] scales as $\chi = d^2(F/\nu)/dM^2 = \frac{1}{T}F_\chi(\alpha T/H^{1/2})$ with F_χ an unknown scaling function. Since there is no crossing of states through the Fermi level as we change magnetic field, we do not predict any

de Haas-van Alphen oscillations. However, there may be oscillatory contributions to the susceptibility from the condensed fraction and the normal vortex cores that we do not consider here [14].

We now turn to consider electrical and thermal transport properties. We first define [15] the charge velocity operator $\mathbf{v}^{(1)} \equiv i[\tilde{\mathcal{H}}, \mathbf{r}\sigma_z]$ and the thermal velocity operator $\mathbf{v}^{(2)} \equiv i[\tilde{\mathcal{H}}, \{\tilde{\mathcal{H}}, \mathbf{r}\}]$. Operating on a state $\psi = e^{ik_F x} \tilde{\psi}$ near the node at $(p_F, 0)$, we find

$$\mathbf{v}^{(1)} e^{ik_F x} \tilde{\psi} = e^{ik_F x} [\tilde{\mathcal{H}}_0, \mathbf{r}\sigma_z] \tilde{\psi} + \text{smaller terms}, \quad (8)$$

$$\mathbf{v}^{(2)} e^{ik_F x} \tilde{\psi} = e^{ik_F x} [\tilde{\mathcal{H}}_0, \{\tilde{\mathcal{H}}_0, \mathbf{r}\}] \tilde{\psi} + \text{smaller terms}, \quad (9)$$

where the smaller terms are typically smaller by order $\tilde{\mathcal{H}}_1/\tilde{\mathcal{H}}_0$. It is then easy to see from this form that the operator $\mathbf{v}^{(2)}$ scales as $H^{1/2}$ whereas $\mathbf{v}^{(1)}$ scales as H^0 .

We now use the Kubo formula to write the generalized response function at frequency ω as [15]

$$L_{ij}^{ab} = \frac{T}{\nu} \sum_{nm} \frac{\langle n | \mathbf{v}_i^{(a)} | m \rangle \langle m | \mathbf{v}_j^{(b)} | n \rangle f(\epsilon_n/T, \epsilon_m/T)}{(\epsilon_n - \epsilon_m - \omega - i0^+)(\epsilon_n - \epsilon_m + i0^+)}$$

where f is the thermal occupation factor, ν is the volume of the system, the indices i and j take the values \hat{x} and \hat{y} , and the indices a and b take the values 1 and 2 (for charge and heat transport, respectively). Noting that the volume of the system scales as H^{-1} and the energies all scale as $H^{1/2}$, we immediately obtain the two parameter scaling law $L_{ij}^{ab} \sim T^{a+b-1} F_{ij}^{ab}(\alpha T/H^{1/2}, \alpha \omega/H^{1/2})$, where F_{ij}^{ab} is again some scaling function that we will not evaluate. The real part of the optical conductivity tensor is defined as $\text{Re}[\sigma_{ij}] = \frac{1}{T} \text{Re}[L_{ij}^{11}]$ which immediately yields a two parameter scaling law for the optical conductivity.

$$\text{Re}[\sigma_{ij}] \sim F_{ij}^{11}(\alpha T/H^{1/2}, \alpha \omega/H^{1/2}). \quad (10)$$

It should be noted that in this Kubo formula calculation the response of the superfluid fraction has been neglected. This then does not include, for example, the response of the system due to the motion of vortices [16].

We now turn our attention to the dc ($\omega = 0$) thermal conductivity tensor κ , defined as the matrix that relates the heat current \mathbf{j}_q to the temperature gradient via $\mathbf{j}_q = \kappa \nabla T$. We note that experimentally, a large part of the diagonal components of this tensor is due to phonon transport of heat. However, the Hall (off diagonal) component of this tensor should be completely electronic in origin [17]. Note, that when calculating κ , one must usually take into account the effect of the thermoelectric coefficient L^{12} . However, here we can neglect that contribution, since there is never any voltage in the superconducting state. Thus, we have $\kappa_{ij} = \frac{1}{T^2} L_{ij}^{22}$, and we obtain the naive scaling law $\kappa_{ij} \sim TF_{ij}^{22}(\alpha T/H^{1/2})$. Although this is indeed the correct scaling form for the (electronic part of the) diagonal component of the tensor, it is not correct for the Hall component. It can, in fact,

be shown that the scaling function F_{xy}^{22} here is precisely zero due to the particle-hole symmetry inherent in the linearized Hamiltonian $\tilde{\mathcal{H}}_0$. This result is very easy to understand. Imposing a heat source on one side of the system excites many particles and holes. Both particles and holes diffuse in the direction of the heat sink. In a magnetic field, the particles curve one way and the holes curve the other way. Thus, when there is particle-hole symmetry, there is no net Hall transport of heat.

The proof [6] that the linearized Hamiltonian yields $\kappa_{xy} = 0$ is a little bit involved. The particle-hole symmetry is expressed mathematically by saying that given an eigenpair $\epsilon_n, \tilde{\psi}_n$ satisfying $\tilde{\psi}_n = \epsilon_n \tilde{\psi}_n$, it can be shown that there exists another eigenvector $\tilde{\psi}'_n = \sigma_y \tilde{\psi}_n^*$ with the same eigenvalue also satisfying $\tilde{\mathcal{H}}_0 \tilde{\psi}'_n = \epsilon_n \tilde{\psi}'_n$ where σ_y is the usual Pauli spin matrix. Using this symmetry and adding up the contributions to κ_{xy} from all four nodes on the Fermi surface, it can be shown that κ_{xy} vanishes. It should be noted that κ_{xy} remains zero even when we include the smaller terms from Eq. (9) (but σ_{xy} does not).

In order to find a nonzero κ_{xy} , we must break the particle-hole symmetry by including the contributions from $\tilde{\mathcal{H}}_1$. As mentioned above, at low T , we have $\tilde{\mathcal{H}}_1 \ll \tilde{\mathcal{H}}_0$ so that $\tilde{\mathcal{H}}_1$ can be treated perturbatively. Inclusion of this term then shifts the eigenenergies via $\epsilon_n \rightarrow \epsilon_n + \delta\epsilon_n$ and the eigenstates $|n\rangle \rightarrow |n\rangle + \delta|n\rangle$. Lowest order perturbation theory then yields

$$\delta\epsilon_n^H = \langle n^H | \tilde{\mathcal{H}}_1 | n^H \rangle$$

$$\delta|n^H\rangle = \sum_m \frac{|m^H\rangle \langle m^H | \tilde{\mathcal{H}}_1 | n^H \rangle}{\epsilon_n^H - \epsilon_m^H} = [H/H_0]^{1/2} \delta|n^{H_0}\rangle.$$

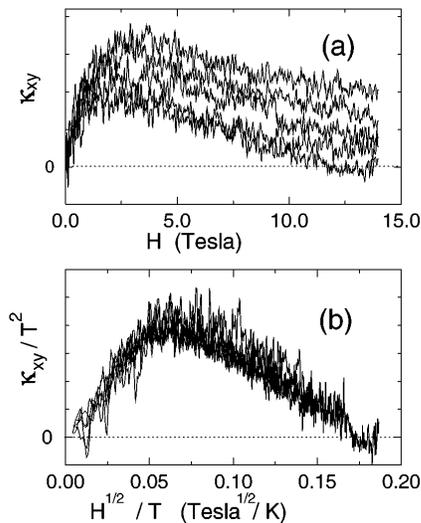


FIG. 1. Thermal Hall data from Ref. [18]. (a) Thermal Hall transport coefficient κ_{xy} plotted against external magnetic field H at temperatures (from bottom to top) 20, 22.5, 25, 27.5, and 30 K. For technical reasons data have not yet been taken below 20 K. (b) Collapse of these five curves according to the scaling law shown in Eq. (11). Note that the characteristic scale of $H^{1/2}/T$ is approximately $0.05 \text{ T}^{1/2}/\text{K}$.

Including these first-order corrections into the Kubo formula and expanding, we find these correction terms give a leading contribution to the thermal Hall conductivity that scales as

$$\kappa_{xy} \sim T^2 F_{\kappa_{xy}}(\alpha T/H^{1/2}) \quad (11)$$

with $F_{\kappa_{xy}}$ again some scaling function. As shown in Fig. 1, experimental results of Ref. [18] do indeed show this scaling form at temperatures below 30 K. (for technical reasons data have not yet been taken at temperatures below 20 K). The characteristic scale for features in the function $F_{\kappa_{xy}}$ (i.e., where the curve becomes nonlinear) is predicted to be $x \approx 1$ or $H^{1/2}/T \approx 0.05 \text{ T}^{1/2}/\text{K}$, which is in good agreement with experiment.

In conclusion, we have found that the scaling properties of the quasiparticle spectrum in d -wave superconductors provides a very general and powerful tool for analyzing various physical quantities.

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