

Specific heat of underdoped cuprates: Resonating valence bond description versus Fermi arcs

J. P. F. LeBlanc,^{1,*} E. J. Nicol,¹ and J. P. Carbotte²

¹*Department of Physics, University of Guelph, Guelph, Ontario, Canada N1G 2W1*

²*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4L8*

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A recent microscopic model of the pseudogap state, based on the resonating valence bond (RVB) spin liquid, has provided a simple ansatz for the electronic self-energy in which a gap forms on the antiferromagnetic Brillouin zone as the limit of a Mott insulator is approached in the underdoped regime. Here, the ansatz is employed to calculate the electronic specific heat when a superconducting gap is also included. We find qualitative agreement with all experimental observations in the underdoped regime of the cuprates. We explore the relationship of the theory to two other purely phenomenological approaches, the nodal liquid and the Fermi arc model, and provide justification for their use on experimental data in light of this microscopic RVB theory.

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Simplified models, such as BCS theory, which ignore much of the complicated details associated with actual metals, have had an enormous impact on our understanding of the superconducting state. A generalization of BCS to include the d -wave symmetry of the superconducting gap in the cuprates has taken us a long way in understanding the overdoped and optimally doped part of their phase diagram. However, it has failed so far to provide even a first qualitative picture of the observed properties as the Mott transition is approached in the underdoped regime. Some additional essential element is still missing, which has been widely recognized as associated with the opening of a pseudogap, although the exact nature of the phenomenon remains unknown. Recently, Yang, Rice, and Zhang¹ (YRZ) provided a simple model for the self-energy in the pseudogap phase from which the coherent part of the electronic Green's function can be constructed. The work is based on results for a resonating valence bond spin liquid and contains a gap which is formed on the antiferromagnetic Brillouin zone (AFBZ) as the doping is reduced and the transition to a correlation-induced Mott insulating state is approached from the metallic side. Since its appearance in 2006, the model has had considerable success in understanding some aspects of Raman² and optical properties³ of the underdoped cuprates and has also been applied to angle-resolved photoemission (ARPES) data.⁴

In view of these developments, it is very important to test the YRZ model on other data. In this Rapid Communication, we consider the electronic specific heat, which has long been known to show anomalous properties⁵⁻⁷ not describable within simple BCS theory. Lacking the existence of a well-developed and accepted microscopic theoretical framework, Loram *et al.*⁵⁻⁷ included a depression of the electronic density of states (DOS) near the Fermi energy to analyze their early specific-heat work. More recently, a similar analysis applied to optical data^{8,9} has also yielded new insights, including clarification of temperature-dependent Fermi arcs. More sophisticated, but still purely phenomenological, approaches to the pseudogap phase have appeared, including the idea of a nodal liquid¹⁰ and of temperature-dependent Fermi arcs.¹⁰⁻¹⁴ In these models, the pseudogap exhibits d -wave symmetry and forms on the Fermi surface. At high temperatures only the antinodal region is gapped while the

remaining ungapped arc length about the nodal direction is proportional to temperature. The limit of a nodal liquid is when the pseudogap is taken to form over the entire Fermi surface.^{10,14} In comparison to these models, the YRZ approach is profoundly different in that the pseudogap forms on the AFBZ. After presenting our results, we will provide an analysis of how YRZ relates to both the nodal liquid and Fermi arc model.

There are many other theoretical approaches to the pseudogap phase, for example, preformed pairs, existing below an onset temperature, T^* , with phase coherence taking hold only at the lower superconducting T_c . These preformed pairs arise either from a homogeneous state^{15,16} or from including inhomogeneities on the nanoscale.¹⁷ There are also extensions of BCS theory which include the formation of finite momentum pairs that persist above T_c .¹⁸ Another class of theories involves competing orders, such as d -density waves,¹⁹ which set in at T^* and can coexist with superconducting order below T_c .

In the YRZ model, both the superconducting gap, Δ_{sc} , and the pseudogap, Δ_{pg} , have a d -wave k -space dependence described by: $\Delta_{sc} = \frac{\Delta_{sc}^0}{2}(\cos k_x a - \cos k_y a)$ and $\Delta_{pg} = \frac{\Delta_{pg}^0}{2}(\cos k_x a - \cos k_y a)$, with a the lattice constant. For a doping x , the YRZ model is described by a propagator,

$$G(\mathbf{k}, \omega, x) = \sum_{\alpha=\pm} W_k^\alpha / [\omega - E_k^\alpha - \Delta_{sc}^\alpha / (\omega + E_k^\alpha)], \quad (1)$$

where $E_k^\pm = \frac{\xi_k - \xi_k^0}{2} \pm E_k$, $E_k = \sqrt{\tilde{\xi}_k^2 + \Delta_{pg}^2}$, $\tilde{\xi}_k = (\xi_k + \xi_k^0)/2$, and $W_k^\pm = \frac{g(x)}{2}(1 \pm \frac{\tilde{\xi}_k}{E_k})$, where $g(x)$ weights the coherent part.⁴ The energy dispersion $\xi_k = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a - 2t''(\cos 2k_x a + \cos 2k_y a) - \mu_p$ includes hopping out to third nearest neighbor, while $\xi_k^0 = -2t(\cos k_x a + \cos k_y a)$ is the first nearest-neighbor term, which determines the placement of the pseudogap off the Fermi surface, coinciding with the AFBZ boundary. These energy dispersions contain doping-dependent coefficients: $t(x) = g_t(x)t_0 + 3g_s(x)J\chi/8$, $t'(x) = g_t(x)t'_0$, and $t''(x) = g_t(x)t''_0$, where $g_t(x) = 2x/(1+x)$ and $g_s(x) = 4/(1+x)^2$ are the Gutzwiller factors. The dispersion here uses μ_p as an effective chemical potential or Fermi level at $T=0$, determined by

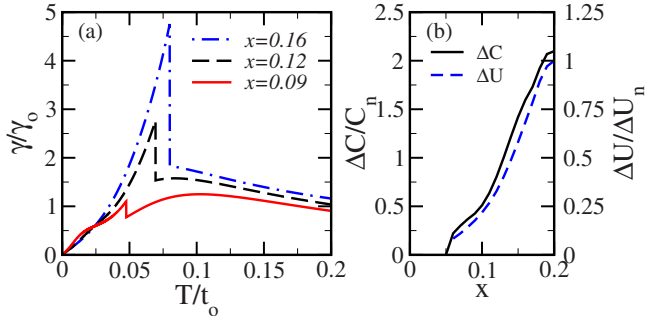


FIG. 1. (Color online) (a) Plot of γ/γ_0 vs T/t_0 for the YRZ model with $x=0.16$, 0.12 , and 0.09 . (b) Plot of normalized jump, $\Delta C/C_n = \Delta C/\gamma(T_c)T_c$, and normalized internal energy, $\Delta U/\Delta U_n$ as functions of doping, x .

the Luttinger sum rule. Values of other parameters in the dispersion were taken from Ref. 1 to be: $t'/t_0 = -0.3$, $t''/t_0 = 0.2$, $J/t_0 = 1/3$, and $\chi = 0.338$; while the optimal superconducting gap Δ_{sc}^0 was chosen to give an effective optimal T_c around 90 K for a ratio of $2\Delta_{sc}^0(T=0)/k_B T_c = 6$,²⁰ for units of $t_0 = 0.1$ eV, where $\Delta_{sc}^0(T)$ is the gap amplitude given in BCS theory at temperature, T .

From the YRZ propagator of Eq. (1), one can extract the YRZ spectral function and see that there are four energy branches, given by the energies, $\pm E_{sc}^\alpha$, where $E_{sc}^\alpha = \sqrt{(E_k^\alpha)^2 + \Delta_{sc}^2}$. One can straightforwardly calculate the specific heat, $C(T)$, from the entropy, S , given at temperature, T , by the standard formula summed over the four energy branches, which reduces to

$$S = -2k_B \sum_{\alpha=\pm} \sum_k W_k^\alpha \{ f(E_{sc}^\alpha) \ln[f(E_{sc}^\alpha)] + f(-E_{sc}^\alpha) \ln[f(-E_{sc}^\alpha)] \}, \quad (2)$$

where f is the Fermi function and k_B , the Boltzmann constant. The temperature dependence enters through both f and the temperature-dependent superconducting gap.

The electronic specific-heat gamma, denoted by $\gamma(T) = C(T)/T$, is a constant, $\gamma(T) = \frac{2\pi^2}{3} k_B^2 N(0)$, in the noninteracting case, with $N(0)$, the electronic density of states at the Fermi level. $\gamma(T)$ is presented in Fig. 1, for several doping values, normalized by the constant $\gamma_0 = \frac{2\pi^2}{3} k_B^2 N(0, x=0.16)$. These results are based on the generic phase diagram, illustrated by Fig. 2(a), which is slightly modified from that previously used by YRZ, with optimal doping now at $x=0.16$. This is more relevant for comparison with the specific-heat data of Loram *et al.*⁵⁻⁷ Other phase diagrams based on the analysis of a large database have also appeared in the literature,^{21,22} in which the pseudogap line ends near the upper edge of the superconducting dome, rather than at $x=0.2$. Since, in this work, we are only interested in making a qualitative comparison with experiment, we have made no attempt to alter other basic parameters of the pseudogap state introduced in the original paper of YRZ (Ref. 1) in order to improve quantitative agreement with experimental data.

Comparison of Fig. 1(a) with the experimental results of Loram *et al.* (Ref. 5 and Fig. 4, for example) shows that our theoretical results capture all essential qualitative features

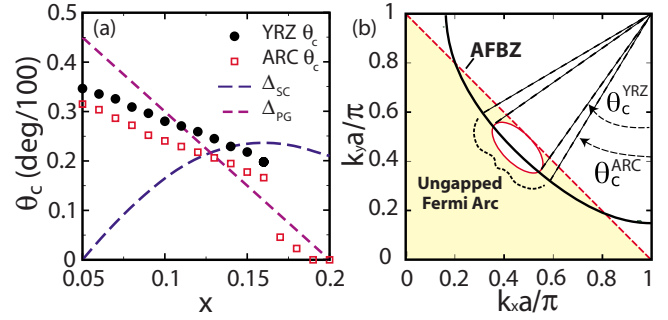


FIG. 2. (Color online) (a) The phase diagram via the magnitudes of the gaps $\Delta_{sc}^0(x)/t_0 = 0.24(1 - 82.6(x - 0.16)^2)$ and $\Delta_{pg}^0(x)/t_0 = 0.6(1 - x/0.2)$. Also, the values of the critical angles, θ_c^{ARC} and θ_c^{YRZ} vs x . (b) One quadrant in k space identifying the critical angles where pseudogap exists. The ellipse is a Luttinger pocket from the YRZ theory for $x=0.05$.

observed. First, as one proceeds toward the underdoped regime, there is a significant decrease in $\gamma(T)$, as T_c is approached from above. This reflects an effective decrease in the DOS around the Fermi energy in the normal pseudogapped state. Second, the jump at T_c is greatly reduced with increased pseudogap. In Fig. 1(b), we summarize the doping dependence of the normalized jump, $\Delta C/\gamma(T_c)T_c$, as well as the normalized condensation energy, $\Delta U/\Delta U_n$ at $T=0$, derived from our entropy calculations. Recall that the internal energy, U , is related to the specific heat by $dU/dT = C(T)$ and ultimately to the entropy. The condensation energy ΔU is defined as the difference between U in the superconducting state, and its value in the normal state at $T=0$. This is given by $\Delta U = \int_0^{T_c} (S_{normal} - S_{sc}) dT$. ΔU_n is the condensation energy when the pseudogap is set to zero in both the normal and superconducting states.

Both normalized quantities, the jump and the condensation energy, are seen to drop precipitously with decreasing x due to the increase in pseudogap, which is not part of any pure BCS formulation, in which both quantities would be constant for all doping. Our findings agree qualitatively with the data of Loram *et al.*⁵⁻⁷ It is clear that the model of YRZ has captured an additional essential element of the physics of the underdoped cuprates not present in standard BCS models. Note that our values of $\Delta C/\gamma(T_c)T_c$ are larger than experiments indicate and that this is mainly due to our use of a large gap ratio of 6, on the order of that indicated by scanning tunnel microscope (STM).²⁰ However, a smaller value would give better quantitative agreement, indicating that the STM data may not reflect the bulk.

Next, we make connection with the nodal liquid and the Fermi arc approaches. For both cases, we assume that the pseudogap is located on the usual large Fermi surface [shown as the solid black curve in Fig. 2(b)]. This corresponds to replacing the AFBZ energy ξ_k^0 of the YRZ model by the energy ξ_k . In this limit, the expression of Eq. (2) reduces to the standard BCS expression, with the square of the superconducting gap replaced by the sum of the square of superconducting and pseudogap. For the Fermi arc model we apply an additional constraint that the pseudogap is nonzero only in an arc located around the antinodal direction such that

$$\Delta_{\text{pg}}^{\text{ARC}}(\mathbf{k}) = \begin{cases} \frac{\Delta_{\text{pg}}^0}{2} (\cos k_x a - \cos k_y a), & (\theta < \theta_c^{\text{ARC}}) \\ \frac{\Delta_{\text{pg}}^0}{2} (\cos k_x a - \cos k_y a), & (\theta > \frac{\pi}{2} - \theta_c^{\text{ARC}}) \end{cases} \quad (3)$$

and $\Delta_{\text{pg}}^{\text{ARC}}=0$, otherwise. The angle $\theta=\arctan[(\pi-k_y)/(\pi-k_x)]$ is shown in Fig. 2(b). For our purposes, θ_c^{ARC} is a single fitting parameter, adjusted to give $\gamma_n(T=0)$ (n is for the normal pseudogapped state) equal to that of the YRZ model at the same doping. Additionally, we ignore any temperature dependence of the pseudogap magnitude below T_c as is suggested by Refs. 12 and 13 wherein they find that Raman data shows that there is little modification to the pseudogap below T_c . We further ignore complications of the disappearance of the pseudogap at some, relatively high, temperature T^* which is known to cause large specific-heat anomalies at T^* , which are not observed in experiment. In Fig. 2(a), the open red squares are the values of θ_c^{ARC} obtained from the fit to the specific heat using the construction of Fig. 2(b). In the YRZ model, the Luttinger pockets also form an ungapped region analogous to the Fermi arc model and it will be this region which is responsible for the specific heat. Consequently, for YRZ, we define θ_c^{YRZ} as the angle from (π, π) to the edge of the Luttinger pocket shown in Fig. 2(b) and plot this in Fig. 2(a) as a function of doping in comparison with θ_c^{ARC} . The arc model fits consistently show $\theta_c^{\text{ARC}} < \theta_c^{\text{YRZ}}$. This corresponds to the additional states (albeit with less quasiparticle weight^{3,4}) which are located along the AFBZ boundary in the YRZ model, which are absent in the arc model. One might imagine unravelling the Luttinger pocket onto the Fermi surface of the arc model for a conceptual picture of this comparison. Thus, we expect the arc model to capture much of the same features as the YRZ model for the specific heat. This contrasts to the nodal liquid case, which has the gap over the entire Fermi surface and no fitting parameters.

In the top two frames of Fig. 3, we compare superconducting (red dashed curve) and normal pseudogap (solid black curve) results for $\gamma(T)$ in the case $x=0.13$. Frame (a) is for YRZ, and frame (b) is for the nodal liquid. The shaded areas illustrate the entropy difference between these two states. The entropy readjustment is less for the nodal liquid and consequently the specific-heat jump at $T=T_c$ is reduced. These differences arise because the density of states at the Fermi surface, $N(0)$, is finite in the normal pseudogap state of the YRZ model while it is zero in the nodal liquid because the pseudogap exists over the entire Fermi surface, and thus, $\gamma_n(T \rightarrow 0) \rightarrow 0$ (n is for the normal pseudogapped state). A further comparison of these two cases is presented in Figs. 3(c) and 3(d), where we have chosen to compare directly the two normal states and the two superconducting states, respectively. The nodal liquid and YRZ agree well at large T , but deviate significantly for $T \lesssim 0.025t_0$, with the nodal liquid curve going to zero. The open red squares are results for the arc model with θ_c^{ARC} chosen to fit the value of $\gamma_n^{\text{YRZ}}(T=0)$. This results in a finite DOS at the Fermi level, for both the YRZ and arc models, which results in excellent agreement

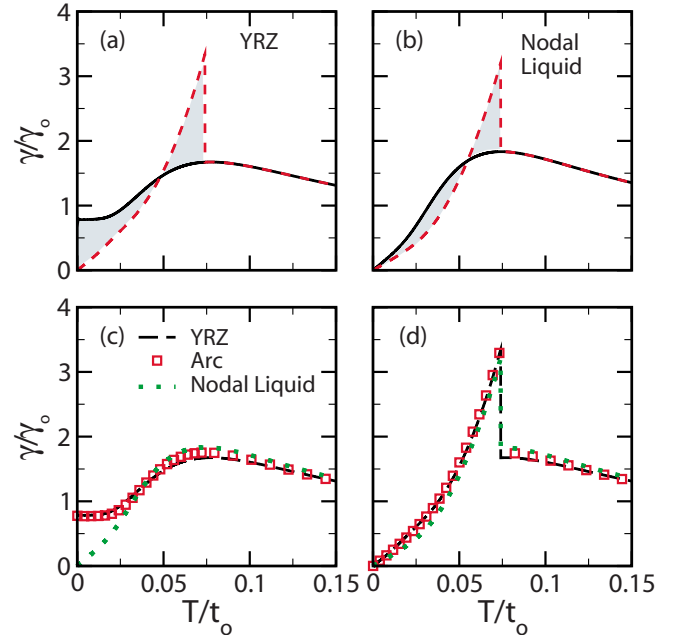


FIG. 3. (Color online) Plots of $\gamma(T)/\gamma_0$ comparing the superconducting state (red dashed) to the pseudogapped normal state (solid), with the areal displacement shaded: (a) YRZ model and (b) nodal liquid. The arc model fitted to YRZ for $x=0.13$ and compared to the nodal liquid: (c) pseudogapped normal state and (d) the superconducting state.

over all temperatures. Similar results for the superconducting state are presented in Fig. 3(d). The agreement between YRZ and the arc model is excellent. Both show some slight deviations from the nodal liquid, but these deviations appear less important than in the normal pseudogapped state results of Fig. 3(c) where we find the low-temperature differences to be quite striking. However, it should be noticed that, in Fig. 3(d), the nodal liquid result (dotted) does fall below YRZ for all $T < T_c$, which results in substantial loss of area under these curves, indicating a smaller condensation energy of the superconducting state [shown in Fig. 4(a)]. It is clear from this comparison that placing the pseudogap on the Fermi

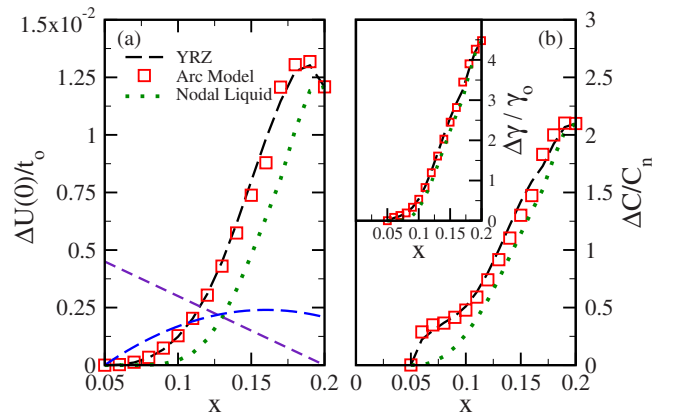


FIG. 4. (Color online) (a) Condensation energy, $\Delta U(0)/t_0$, vs x for all three models, overlaid with Δ_{sc}/t_0 and Δ_{pg}/t_0 from Fig. 2. (b) Plot of normalized jump vs x for all three models. Inset shows $\Delta\gamma(T_c)/\gamma_0$.

surface, rather than on the AFBZ, while at the same time cutting it off at θ_c^{ARC} reproduces well the YRZ results. For YRZ, there is no cut off, but rather the Luttinger contours move away from the gapped AFBZ boundary in the region of the nodes as is clear in Fig. 2(b).

Figure 4 provides further comparison of both the nodal liquid and Fermi arc models with the YRZ results, across the entire doping range. Figure 4(a) compares the condensation energy ΔU vs doping, x . There is excellent agreement between YRZ and the arc model, while the nodal liquid is consistently lower. Although the nodal liquid still captures the large decrease in condensation energy that is caused by the opening of the pseudogap, it overestimates the effect. The same remarks apply to Fig. 4(b) where $\Delta C/C_n$ is shown vs x . In the inset, we show the $\Delta\gamma(T_c)/\gamma_0$ for completeness.

In summary, we have found that the microscopic model of YRZ, based on the successful resonating valence bond spin liquid phase,^{23,24} which includes as its central essential element the formation of a pseudogap on the AFBZ in the underdoped region of the cuprate phase diagram, can account for all of the qualitative characteristics of the observed evolution of the specific heat as a function of doping. We have

also found that an arc model with pseudogap formation on the Fermi surface itself, but limited to a region around the antinodal direction resulting in an ungapped arc beyond θ_c in the nodal region, can adequately simulate the results obtained in YRZ theory. The basic reason for this fortunate circumstance is that, in YRZ, the Luttinger surfaces define pockets in the nodal direction around, but not directly on the antiferromagnetic Brillouin-zone boundary, which keeps the electrons in that nodal region from fully sampling the pseudogap on the AFBZ. We have shown that this effect can be well approximated by the ungapped Fermi arcs of the arc model. On the other hand, the nodal liquid idea with pseudogap over the entire Fermi surface accentuates the pseudogap effect as compared to YRZ. Nevertheless, such a model still has merit; because of its great simplicity, it can give straightforward insight into the qualitative behavior of the pseudogapped state.

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*leblanc@physics.uoguelph.ca

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