The physical properties of hole-doped cuprate high-temperature superconductors are strongly influenced, over a wide range of temperature and doping, by a depletion in the electronic density of states known as the pseudogap. In momentum-space it is manifest as a gapping of the large hole-like Fermi surface near the antinodal regions of the Brillouin zone, at \((\pm \pi, 0)\) and \((0, \pm \pi)\), leaving behind ungapped “Fermi arcs” [1]. The origin of the pseudogap remains a mystery second only to that of superconductivity itself. A key question is whether the pseudogap closes at a temperature \(T^*\). The absence of a specific heat anomaly, together with persistent entropy losses up to 300 K, have long suggested that the pseudogap does not vanish at \(T^*\). However, amid a growing body of evidence from other techniques pointing to the contrary we revisit this question. Here we investigate if, by adding a temperature dependence to the pseudogap energy and quasiparticle lifetime in the resonating-valence-bond spin-liquid model of Yang, Rice and Zhang, we can close the pseudogap quietly in the specific heat.

Abstract – The physical properties of hole-doped cuprate high-temperature superconductors are heavily influenced by an energy gap known as the pseudogap whose origin remains a mystery second only to that of superconductivity itself. A key question is whether the pseudogap closes at a temperature \(T^*\). The absence of a specific heat anomaly, together with persistent entropy losses up to 300 K, have long suggested that the pseudogap does not vanish at \(T^*\). However, amid a growing body of evidence from other techniques pointing to the contrary we revisit this question. Here we investigate if, by adding a temperature dependence to the pseudogap energy and quasiparticle lifetime in the resonating-valence-bond spin-liquid model of Yang, Rice and Zhang, we can close the pseudogap quietly in the specific heat.

The physical properties of hole-doped cuprate high-temperature superconductors are strongly influenced, over a wide range of temperature and doping, by a depletion in the electronic density of states known as the pseudogap. In momentum-space it is manifest as a gapping of the large hole-like Fermi surface near the antinodal regions of the Brillouin zone, at \((\pm \pi, 0)\) and \((0, \pm \pi)\), leaving behind ungapped “Fermi arcs” [1]. The origin of the pseudogap remains a mystery second only to that of superconductivity itself, and it is widely hoped that by investigating the former we might uncover valuable insights for understanding the latter. A key question is whether the pseudogap closes at a temperature \(T^*\). In recent years, evidence has been building that suggests that it does. These include abrupt changes in the Kerr Effect [2], time-resolved reflectivity [3], as well as the direct observation of a reconstruction of the antinodal electronic structure by angle-resolved photoemission spectroscopy [3,4] (ARPES). In this work, we aim to reconcile those results with thermodynamic measurements, in particular the electronic entropy and specific heat, which have long suggested that the pseudogap is temperature independent [5-8].

By way of introduction, the electronic entropy is defined as \(S(T) = -2k_B \int f_w(E,T)N(E)dE \) [9], where \(N(E)\) is the density of states, and \(f_w(E,T)\) is a “Fermi window” which expands with temperature and is related to the Fermi distribution function \(f\) by \(f \ln f + (1 - f)\ln(1 - f)\). Put simply, \(S(T)\) is a count of the thermally active states. The electronic specific heat coefficient is given by the temperature derivative of the entropy, \(\gamma(T) = \partial S(T)/\partial T\).

Three apparently universal observations have been made from high-resolution differential specific heat studies on a variety of hole-doped cuprates [5–8,10]. These are: i) a loss of entropy in low to slightly overdoped samples, that persists right up to the highest temperatures measured. The entropy decreases at a rate of about 1 \(k_B\) per doped hole; ii) a collapse in the magnitude of the specific heat jump, \(\Delta\gamma\), at \(T_c\) below a critical doping of 0.19 holes/Cu; and iii) a smooth downturn in the normal-state electronic specific heat with no specific heat jump at \(T^*\). These features were originally modeled by Loram in terms of a temperature-independent non–states-conserving V-shaped gap, pinned to the Fermi level \((E_F)\) of a flat density of states. The gap widens with reducing doping [8]. In contrast to the superconducting gap, where the low-energy states are pushed just above the gap edge, it is surmised in this model that the pseudogap redistributes those states to much higher energies. In this scenario \(T^*\) represents an energy scale where thermal fluctuations become comparable in magnitude to the size of the pseudogap, rather than a phase transition temperature. If one tries to fill in such a pseudogap with temperature, thereby simulating expanding Fermi arcs [1,11], problems arise. Firstly, the lost entropy is eventually recovered, contradicting i). Secondly, a kink in the entropy appears at \(T^*\) together with a corresponding jump in the heat capacity [12], contradicting iii). And finally, we might expect a double-peak structure to appear in the
superconducting anomaly near critical doping, where $T^*$ is less than $T_c$, altering the doping dependence of $\Delta \gamma(T_c)$ compared to ii). But perhaps this just means that this model is incomplete, and if so, what are we missing?

In the following we will investigate the effects of a tight-binding density of states, thermal lifetime broadening, and the combination of these with a Fermi surface reconstruction model for the pseudogap given by the resonating valence bond spin liquid ansatz of Yang, Rice and Zhang (YRZ) [13]. Detailed descriptions of the YRZ model have been published several times [13–15], but for completeness we briefly list the equations used in this work. In the normal state the coherent part of the electron Green’s function is given by

$$G(k, \omega, x) = \frac{g_t(x)}{\omega - \xi_k - E^g_0(k)},$$

where $\xi_k = -2t(t)(\cos k_x + \cos k_y) - 4t'(t) \cos k_x \cos k_y - 2t''(t)(\cos 2k_x + \cos 2k_y) - \mu_p(x)$ is the tight-binding energy-momentum dispersion, $E^g_0(k) = [E^0_0(x)/2](\cos k_x - \cos k_y)$ is the pseudogap. The chemical potential $\mu_p(x)$ is chosen according to the Luttinger sum rule. The doping-dependent coefficients are given by $t(x) = g_t(x)t_0 + (3/8)g_s(x)J\chi$, $t'(x) = g_t(x)t'_0$ 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 bare parameters $t'/t_0 = -0.3$, $t''/t_0 = 0.2$, $J/t_0 = 1/3$ and $\chi = 0.338$ are the same as used previously [13]. Equation (1) can be re-written as

$$G(k, \omega, x) = \sum_{\alpha = \pm} \frac{g_t(x)W^\alpha_k(x)}{\omega - E^\alpha_0(k)},$$

where the energy-momentum dispersion is reconstructed by the pseudogap into upper and lower branches

$$E^\pm_k = \frac{1}{2}(\xi_k - \xi_k^0) \pm \sqrt{\left(\frac{\xi_k + \xi_k^0}{2}\right)^2 + E^2_0(k)},$$

that are weighted by

$$W^\pm_k = \frac{1}{2} \left[1 \pm \frac{(\xi_k + \xi_k^0)/2}{\sqrt{[(\xi_k + \xi_k^0)/2]^2 + E^2_0(k)}}\right].$$

In the superconducting state there are four energy branches $\pm E^\pm_k = \pm \sqrt{(E^0_k)^2 + \Delta^2_k}$, where $\alpha = \pm$ and $\Delta_k = [\Delta_0(x)/2](\cos k_x - \cos k_y)$ is the superconducting gap. The density of states (DOS), from which the entropy and heat capacity can be calculated, is given by

$$N(\omega) = \sum_{\alpha = \pm,k} g_t(x)W^\alpha_k(u^\alpha_k)^2 \delta(\omega - E^\alpha_k) + (v^\alpha_k)^2 \delta(\omega - E^\alpha_k),$$

where $(u^0_k)^2 = 0.5(1 + E^0_k/E^g_0)$ and $(v^0_k)^2 = 0.5(1 - E^0_k/E^g_0)$ are the Bogoliubov weights.

The reason for choosing this model is because it successfully describes experimental data from a wide range of techniques [16], including the specific heat [17,18]. However, the previous works did not consider a temperature-dependent pseudogap term. In fig. 1 we plot the calculated energy-momentum dispersion in the superconducting state along cuts in the $k_y$-direction near the antinodes for $x = 0.12$, both with, and without $(E_0 = 0)$ the pseudogap. The results reproduce the ARPES-derived dispersions measured below and above $T^*$, respectively [3,4], providing compelling evidence for the closure of the pseudogap at $T^*$. Key details are reproduced such as the separation between the momentum of the minimum binding energy of the dispersion $k_G$ from the Fermi momentum $k_F$, a signature of non–particle-hole symmetric order [4]. Moreover, we can identify the flat dispersion of the shoulder feature observed in ARPES energy dispersion curves [3] as belonging to the Bogoliubov dispersion arising from the upper YRZ band, $-\sqrt{(E^+_k)^2 + \Delta^2_k}$.

![Diagram](image-url)
Closing the pseudogap quietly

Fig. 2: (Color online) Density of states for \( x = 0.20 \) and 0.14 in the case of: (a) a rigid shift of the Fermi level and no lifetime broadening; (b) the addition of thermal lifetime broadening terms \( \pi k_B T \) and \( 2 \pi k_B T \), respectively; and (c) a YRZ-like reconstruction. The corresponding electronic entropies are shown in plots (d) to (f). Plot (f) includes experimental data for \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) [6] and the calculated curves include the thermal broadening terms. The two fits to the \( x = 0.14 \) data correspond to the two pseudogap temperature dependences of \( E_g(T) \).

Since we wish to understand the effect of adding a temperature dependence to \( E_g \), from here onwards we fix the tight-binding coefficients to their values at \( x = 0.20 \) and neglect the \( g_t(x) \) prefactor in the equation for the density of states. (Normally the \( x \)-dependence of these terms, which narrow the bands but reduce the magnitude of the DOS, would complement rather than counteract the pseudogap.) To fit the experimental entropy data \( t_0 \) is set to 0.225 eV. Beginning for a moment without the pseudogap, the defining feature of the tight-binding DOS is the van Hove singularity (vHs) located just below \( E_F \) for \( x = 0.20 \) (see fig. 2(a)). Assuming a rigid shift of \( E_F \) away from the vHs with decreasing doping results in a persistent decrease in entropy, as shown in fig. 2(d). However at 300 K, the rate of decrease is only 0.33 \( k_B \)/hole compared with the observed 1 \( k_B \)/hole [8].

Lifetime broadening can also affect the high-temperature heat capacity, and hence the entropy, by smoothing features in the DOS [19]. From resistivity measurements [20] we infer a linear-in-temperature scattering rate (inverse lifetime) given by \( \Gamma = 0.01 t_0 + \beta k_B T \), with a slope \( \beta \) that increases with decreasing doping. The most computationally efficient way of incorporating this term is by convolving the DOS with the Lorentzian \( \Gamma/\pi \left( \omega - E \right)^2 + \Gamma^2 \). Figure 2(b) illustrates the thermally broadened vHs at 300 K for \( x = 0.20 \) and 0.14 with \( \beta = 1 \) and 2, respectively. The entropy decrease is now larger at 0.7 \( k_B \)/hole (fig. 2(e)), but it is still not enough, especially at low temperatures. This necessitates the incorporation of a pseudogap.

In fig. 2(c) we add a pseudogap for \( x = 0.14 \) by setting \( E_g^0 = 54 \text{ meV} \). Based on the ARPES results we initially assume that the pseudogap closes linearly with temperature according to \( E_g(T) = E_g^0 - 2k_B T \). The van Hove singularity and lifetime broadening effects are also included. The calculated entropy compares well with experimental data for \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) [6], shown in fig. 2(f), with the entropy decrease approaching the observed 1 \( k_B \)/hole. The low-temperature fit can be further improved by taking a more gradual initial \( T \)-dependence given by

\[
E_g(T) = E_g^0 \left[ 2 - 1/ \tanh \left( \frac{E_g^0 \ln 3}{4k_B T} \right) \right].
\]  

We now turn to the specific heat coefficient, \( \gamma \). Figure 3 shows \( \gamma(T) \) calculated for a 40 meV pseudogap which closes linearly with temperature in the presence of lifetime broadening \( \Gamma = 0.01 t_0 + k_B T \). Note the absence of a specific heat jump at \( T^* \).

Fig. 3: (Color online) Electronic specific heat for a YRZ-like pseudogap that closes as \( E_g = E_g^0 - 2k_B T \) in the presence of lifetime broadening \( \Gamma = 0.01 t_0 + k_B T \). Note the absence of a specific heat jump at \( T^* \).
we plot the doping dependence of the specific heat jump at $T_c$ assuming a parabolic superconducting gap doping dependence $\Delta(x) = 0.103t_0[1 - 82.6(x - 0.16)^2]$, and the YRZ pseudogap doping dependence $E_0^g(x) = 3t_0(0.2 - x)$ for $x \leq 0.2$. Here we take the closure of the pseudogap to lie at $x = 0.2$ in continuity with YRZ, however it has been extensively shown that this occurs at slightly lower doping $x = 0.19$ [21]. The pseudogap model reproduces the collapse of the specific heat jump as reported for example in refs. [10] and [8]. Note that here we have taken a doping-independent lifetime broadening, $\beta = 1$. Increasing $\beta$ with decreasing doping would increase the rate of collapse of $\Delta \gamma(T_c)$.

To conclude, the absence of a specific heat jump at $T^*$, together with persistent losses in entropy at high temperatures, has long been taken as evidence that the pseudogap does not close there. Driven by a growing body of evidence from other experimental probes pointing to the contrary we have explored this question. By adding a linear-in-temperature scattering rate to a YRZ-like reconstruction model, it is possible to close the pseudogap quietly in the specific heat. A similar result is expected for the antiferromagnetic Brillouin-zone-folding Fermi surface reconstruction model [22]. The entropy recovery expected from the closing gap is offset by scattering-induced broadening of the van Hove singularity. This scenario could be tested experimentally by searching for an ongoing divergence between neighbouring entropy curves above $T^*$.

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