PAPER

Scaling theory for Mott–Hubbard transitions-II: quantum criticality of the doped Mott insulator

Anirban Mukherjee and Siddhartha Lal

Department of Physical Sciences, Indian Institute of Science Education and Research-Kolkata, W.B. 741246, India

E-mail: slal@iiserkol.ac.in

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Abstract

We present a $T = 0$K renormalization group (RG) phase diagram for the hole-doped 2D Hubbard model on the square lattice. The RG method employed is nonperturbative in treating quantum fluctuations of the single-particle occupation number via the unitarily decoupling of one electronic state at every RG step. As a result, the RG phase diagram possesses the quantum fluctuation energy scale ($\omega$) as one of its axes. Using effective Hamiltonians and wavefunctions for the low-energy many-body eigenstates for the doped Mott liquid obtained from the stable fixed point of the RG flows, we demonstrate the collapse of the pseudogap for charge excitations (Mottness) at a quantum critical point (QCP) possessing a nodal non-Fermi liquid with superconducting fluctuations, and spin-pseudogapping near the antinodes. The QCP is characterised using both thermodynamic and quantum information-theoretic measures. d-wave superconducting order is shown to arise from this quantum critical state of matter. The pseudogap phase possesses a variety of fluctuations that lead to several symmetry-broken phases at low-energies. Benchmarking of the ground state energy per particle and the double-occupancy fraction obtained from a finite-size scaling analysis against existing numerical results yields excellent agreement. We present detailed insight into the $T = 0$ origin of several experimentally observed findings in the cuprates, including Homes law and Planckian dissipation. We also establish that the heirarchy of temperature scales for the pseudogap ($T_{PG}$), onset temperature for pairing ($T_{onc}$), formation of the Mott liquid ($T_{ML}$) and superconductivity ($T_{C}$) obtained from our analysis is quantitatively consistent with that observed experimentally for some members of the cuprates. Our results offer insight on the ubiquitous origin of superconductivity in doped Mott insulating states, and pave the way towards a systematic search for higher superconducting transition temperatures in such systems.

1. Introduction

The study of transitions in strongly correlated electronic insulators, tuned by varying either the bandwidth or the filling, has a venerable history [1]. The prototypical system in such studies is the correlation-induced Mott insulator, with a ground state in which the repulsion-induced localization of charge degrees of freedom takes place at a filling commensurate with the lattice (typically half-filling for the 2D square lattice). The nature of the bandwidth-tuned Mott transition at $T = 0$, from a gapless metallic to a gapped insulating state at a fixed filling, has long been debated and forms the basis of an accompanying work [2]. Here, we focus on the case of the Mott transition driven by tuning the filling. Upon doping with holes, for instance, the physics behind charge localization competes strongly with hopping-induced electronic delocalization. This competition has been studied extensively within the realms of the 2D Hubbard model...
on the square lattice with a finite chemical potential away from 1/2-filling. A large number of numerical methods have been brought to bear on this problem. These include, for instance, quantum Monte Carlo simulations at finite-temperature [3–12], density matrix renormalization group [13–15], dynamical cluster approximation [16–20], cluster DMFT (CDMFT) [21–27] and the variational cluster approximation VCA [28, 29]. Together with several others, these techniques suggest a rich and detailed temperature-doping phase diagram that includes numerous phases including the antiferromagnetic Mott insulator, d-wave superconductivity, the pseudogap (or nodal–antinodal dichotomy) arising from electronic differentiation, non-Fermi liquid, stripes etc [7, 8, 16–27, 30–44]. These findings are, by and large, in keeping with the experimental phenomenology of the doped cuprate Mott insulators (see [45] for a recent review). A significant drawback remains, however, in the fact that detailed resolution of the low-energy neighbourhood of the Fermi surface is not available from these theoretical methods. Unfortunately, this leaves several critical questions unanswered on the nature and origins of the Fermi surface (FS) are gapped, and whose origin and role remain unknown [62]). The mystery of the strange metal and the pseudogap have also been reported within the FRG scheme [54–57]. While the method is non-perturbative in principle, numerical implementations of the FRG have typically needed truncations at finite orders in the loop expansion. Thus, despite much success, the FRG is limited thus far to studying weak-to-intermediate values of $U/t$.

The theoretical effort towards understanding the physics of the hole-doped 2D Hubbard model is given prominence by the experimentally rich phenomenology of the cuprate doped Mott insulators (see [45] for a recent review). It is widely believed that the physics of the cuprates is associated with that of (almost) decoupled Cu–O planes in which the doped holes (or electrons) pair into a d-wave superconducting state. Indeed, a very recent experimental study [58] has shown that the phase diagram of the cuprate system can be obtained with both qualitative, as well as quantitative, accuracy from a monolayer crystal of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ containing only two Cu–O planes. This presents strong evidence that the phase diagram encapsulates the $T = 0$ symmetry-broken phases of a single Cu–O plane that is stabilised at finite temperatures by weak inter-layer tunnelling [59] (and would have otherwise been forbidden by the Mermin–Wagner–Hohenberg theorem). An overarching understanding, however, of the mechanisms responsible for the observed complex phenomenology remains elusive. The challenges here include understanding a non-Fermi liquid (NFL) metallic phase with a striking resistivity that varies linearly with temperature [60, 61]. Another enduring puzzle involves the pseudogap (PG): a phase in which parts of the Fermi surface (FS) are gapped, and whose origin and role remain unknown [62]). The mystery of the pseudogap is reinforced by conflicting experimental findings, some of which suggest that it is the origin of the observed superconductivity in the form of pre-formed Cooper pairs, while others report fluctuations of various orders that are inimical to superconductivity [45]. Much debate has also ensued over the existence of a quantum critical point (QCP) lying hidden within the superconducting dome [63, 64]. That these phases are reached experimentally by exiting the Mott insulating state suggest that their origins lie therein [65], highlighting the need for understanding the Mott transition in generality.

In this work, we extend the unitary RG formalism developed in reference [2] for treating the case of the hole-doped 2D Hubbard model. This method is inspired by the strong-disorder RG approaches adopted by Dasgupta et al [66], Fisher [67], Rademaker–Ortuno [68] and You et al [69] and continuous unitary transformation (CUT) RG formalism [70–73]. An important advantage of our unitary RG formalism is that it allows for the analytic computation of non-perturbative RG equations of all 2-, 4-, and 6-point vertices, i.e., that have contributions from all loops resummed into closed-form expressions. We have also recently used this RG technique to obtain a zero temperature phase diagram for the Kagome spin-1/2 XXZ antiferromagnet at non-zero magnetic field [74]. In section 3, we review the RG formalism and some major results from reference [2]. In section 4, unveiling the presence of a quantum critical point (QCP) reached at a critical doping. We also present results in this section for the numerical benchmarking of the doped Mott liquid against results obtained from references [75–77], as well as provided analytical results that explain a large body of experimental phenomenology observed in the hole doped cuprates. The latter includes, for instance, a detailed analysis of the origin of Hones law [78] and Planckian dissipation [61]. We then
present results in section 5 for the presence of symmetry-broken states of matter (including superconductivity) in the RG analysis, and compare once more the results obtained with the well-known phenomenology of the cuprates. Finally, we conclude our presentation in section 6 by a detailed discussion of the relevance of our work to the cuprates, and by presenting future perspectives. Further details of the derivations of various RG relations are presented in several appendices.

2. Summary of main results

- **Hole-doping the Mott liquid & Mottness collapse:** we obtain from the RG an effective Hamiltonian and ground state wavefunction of the hole-doped symmetry-preserved Mott liquid, and demonstrate that it possesses signatures of topological order. The ground state energy \( E_g \) for the doped Mott liquid is obtained from a finite-size scaling analysis, and benchmarks very well with existing numerical results for the range of \( 2 \leq U/t \leq 12 \). Unambiguous signatures of a quantum critical point (QCP) are observed in thermodynamic [e.g. the ground state energy \( E_g \), hole-fraction \( (n_h) \), number compressibility \( (\kappa) \)] as well as quantum-information theoretic quantities [e.g. fidelity of the ground state wavefunction \( F \) and fidelity susceptibility \( (\chi_f) \)]. The abrupt collapse of the many-body gap along the nodal directions shows that the QCP cannot be described within the Landau paradigm of phase transitions. The QCP is observed to arise from the collapse of the pseudogap for charge fluctuations (Mottness \([79, 80]\)) as the chemical potential is tuned. The pseudogaps for spin and charge fluctuations are seen to host a variety of spin, charge and pairing fluctuations, which lead to the formation of several symmetry-broken phases at lower energiescales. Additional evidence is presented in video S4 (http://stacks.iop.org/NJP/22/063008/mmmedia). Codes used in the benchmarking have been made available electronically \([81]\).

- **Theory for the Mottness collapse QCP:** the theory for the QCP and its conical-shaped neighbourhood in phase diagram figure 2 reveal Cooper pairing along the AN stretches of the FS at high quantum fluctuation energiescales \([82, 83]\), together with gapless MFL regions along the nodal stretches. This reveals a universal relation between the superfluid stiffness and the onset scale for superconducting fluctuations, and is observed to be the \( T = 0 \) origin of Homes law. Additional evidence is presented in videos S2 and S3.

- **The correlated Fermi liquid and emergent symmetry broken orders:** A detailed \( T = 0 \) analysis of the correlated Fermi liquid and various symmetry broken phases of the doped Mott liquid offer considerable insight into their origins [e.g. the d-wave SC phase is observed to be tied to the \( k \)-space structure of the QCP]. Qualitative comparisons of our findings with known experimental observations on the cuprates are found to be favourable, prompting the extension of our analyses to finite temperatures. Additional evidence is presented in videos S5 and S6. Additionally, using values of \( t \) and \( U \) obtained from first-principles calculations, we estimate some typical temperature scales from our formalism for the cuprate Mott insulating materials HBCO and LCO, finding reasonable upper bounds for, e.g., the superconducting \( T_C \).

3. Unitary renormalization group formalism

In this section we briefly describe the unitary RG formalism formulated in \([2]\), the resulting RG equations, and by presenting the Hamiltonian obtained for the parent metal phase of the Mott insulating phase in the 1/2-filled Hubbard model. Later sections will be devoted to adapting the technique for studying the 2D Hubbard model on the square lattice with a chemical potential away from 1/2-filling. To begin with, we present the Hamiltonian of the 2D Hubbard model

\[
\hat{H} = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}\sigma} - \mu_{\text{eff}}) \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + U_0 \sum_{\mathbf{r}} \hat{\tau}_{\mathbf{r}\uparrow} \hat{\tau}_{\mathbf{r}\downarrow},
\]

where \( \hat{c}_{\mathbf{k}\sigma}^\dagger / \hat{c}_{\mathbf{k}\sigma} \) is the electron creation/annihilation operator with wave-vector \( \mathbf{k} \) and spin \( \sigma \), \( \hat{\tau}_{\mathbf{r}\sigma} = \hat{n}_{\mathbf{r}\sigma} - \frac{1}{2} \), \( \hat{n}_{\mathbf{r}\sigma} = \hat{c}_{\mathbf{r}\sigma}^\dagger \hat{c}_{\mathbf{r}\sigma} \) is the number operator at lattice site \( \mathbf{r} = j_1 \hat{x} + j_2 \hat{y} \), and \( \epsilon_{\mathbf{k}\sigma} \) is the bare dispersion. The effective chemical potential, \( \mu_{\text{eff}} = \mu - \frac{U_0}{2} \). The dispersion for the square lattice is \( \epsilon_{\mathbf{k}\sigma} = -2t(\cos k_x + \cos k_y) \). In this work, we will study doping-driven quantum phase transitions seen by tuning the effective electric field in the holon–doublon subspace, \( \Delta \mu_{\text{eff}} = -\frac{2\Delta E}{2} \).

Initial steps involve setting up the labelling scheme for the states in energy-momentum space with reference to the non-interacting Fermi surface (F) wave-vectors \( \mathbf{k}_F \). We mark the states in terms of unit vectors normal to \( F \) (i.e., \( \mathbf{e}_x = \frac{\nabla F}{\left|\nabla F\right|} \)) and lying at a distance \( \Lambda \) from \( F \): \( \mathbf{r} = \mathbf{k}_F + \Lambda \mathbf{e}_x \) (see figure 1). States are thus ordered in terms of distances \( \Lambda_N > .. > \Lambda_j > \Lambda_{j-1} > .. > 0 \), where \( \Lambda_N \) lies near the Brillouin zone.
(BZ) edge and the smallest $\Lambda$ is proximate to the Fermi surface. Following this construction, the electronic states are labelled equivalently as $[j,l] \equiv [k_{\Lambda}l] (l = \{\delta, (\sigma = \uparrow, \downarrow)\})$. By employing unitary transformations iteratively, the RG disentangles electronic states in shells, starting from near the BZ edge and scaling towards $E_F$. Thus, at step $j$, all the states on the curve labelled by $\Lambda_j$ are disentangled via a unitary rotation $U_j$. The resulting Hamiltonian $H_{j-1} = U_j H_j U_j^\dagger$ is off-diagonal only for states with $\Lambda < \Lambda_j$.

The disentanglement of an entire curve at distance $\Lambda_j$ is represented via a product of unitary rotations $U_j = \prod_{c \in \{l,\sigma = \uparrow, \downarrow\}} U_{j(c)}$, where $U_{j(c)}$ disentangles one state $k_{\Lambda_j}l\sigma$ on the curve $\Lambda_j$. The form of $U_{j(c)}$ is $\frac{1}{\sqrt{2}} [1 + \eta(c) - \eta(c)]$ where $n = (j,l)$ and $\eta(c)$ & $\eta(c)$ are electron–hole transition operators

$$\eta(c) = \frac{1}{\tilde{\omega}(c) - \tilde{\omega}(m)} Tr_n[\tilde{\omega}(m) (1 - n)](1 - n) Tr_n(c_n^\dagger H(m) c_n).$$

Here, $m = (j,l+1)$ and $\eta(c)$, $\eta(c)$ fulfill the algebra $\{\eta(c), \eta(c)\} = 1$, $\{\eta(c), \eta(c)\} = 1 - 2\tilde{n}(c)$, $\tilde{\omega}(m)$ is a quantum fluctuation operator whose eigenvalues $\omega$ allow us to probe different parts of the many-body spectrum. The formalism obtains a hierarchy of RG flow-equations for various $n$-particle interaction vertices. In this work, we have studied only the 1-particle self-energy, as well as 2- and 3-particle scattering vertices. From the stable fixed-point solutions of these vertex-RG flow-equations, we obtain effective Hamiltonians. Further, from the unitary RG evolution of the Hamiltonian $H_{j-1} = U_j H_j U_j^\dagger$, we can extract the spin-/charge-type forward scattering $(V_{i,j}^{(i)})$, backscattering $(K_{i,j}^{(i)})$, tangential scattering $(L^{(i)})$ and the three-particle vertex $(R_{i,j}^{(i)})$ RG equations as follows [2]

$$\Delta V_{i,j}^{(i)} = \pm \frac{p_{\pm}(V_{i,j}^{(i)})^2}{[G_{j}^{(i)}]^{-1} - V_{i,j}^{(i)}}$$

$$\Delta K_{i,j}^{(i)} = \pm \frac{p_{\pm}(K_{i,j}^{(i)})^2}{[G_{j}^{(i)}]^{-1} - K_{i,j}^{(i)}}$$

$$\Delta L^{(i)} = \frac{\hat{K}_{i,j}^{(i)}}{\omega + \hat{\epsilon}_{i,j}^{\dagger}} - \frac{\hat{V}_{i,j}^{(i)}}{\omega + \hat{\delta}_{i,j}^{\dagger}}$$

$$\Delta R_{i,j}^{(i)} = \frac{\hat{V}_{i,j}^{(i)}}{\omega + \hat{\epsilon}_{i,j}^{\dagger}} \frac{\hat{K}_{i,j}^{(i)}}{\omega + \hat{\delta}_{i,j}^{\dagger}} + \frac{\hat{K}_{i,j}^{(i)}}{\omega + \hat{\epsilon}_{i,j}^{\dagger}} \frac{\hat{V}_{i,j}^{(i)}}{\omega + \hat{\delta}_{i,j}^{\dagger}} - \frac{[G_{j}^{(i)}]^{-1} + 1}{\frac{1}{8} R_{i,j}^{(i)}}.$$
where $p$ is chosen so as to maximise $G^{(0)}_{ij}$. Additionally, from the RG equation (3), we obtain an RG invariant $C = [pK_{ij}^{(0)}]^{-1} + [(1 - p)K_{ij}^{(0)}]^{-1}$.

We can now present the effective theory for the parent metallic phase of the Mott insulating phase in the 2D Hubbard model. At large fluctuation scales $\frac{W}{\tilde{t}} - \omega > \frac{W}{2}$, the effective Hamiltonian for the parent metallic state is found to be [2]

$$H_1 = \sum_{ij} \epsilon_{ij} n_{ij} + \sum_{ij,\tilde{\sigma}} R^a_{ij} a^\dagger_{ij,\tilde{\sigma}} (1 - n_{ij,\tilde{\sigma}}),$$

where $R^a_{ij} = \tilde{\omega} - 2^{-1}(\epsilon_{ij} + \epsilon_{\tilde{\sigma}})$. Here $\Lambda^\dagger_\sigma$ is the momentum scale below which the Fermi liquid is absent, and $\tilde{\omega} = \max_{ij} 2^{-1}(\epsilon_{ij} + \epsilon_{\tilde{\sigma}})$ is the renormalized fluctuation scale determined from the fixed point of the RG for forward scattering. The ground state for the metallic phase is given by

$$|\Psi_{\text{gappless}}\rangle = \prod_{\Lambda^\sigma} \prod_{\Lambda^\sigma'} |1_{\Lambda^\dagger 1_{-\Lambda^\dagger .0 - \Lambda^\dagger .}}\rangle .$$

By incorporating the three-particle vertices in the one-particle self-energy, we obtain the renormalized self-energy and quasiparticle residue (2) as

$$\Sigma(\tilde{\omega}) = \tilde{\omega}_1 \ln \left| \frac{N(\tilde{\omega}, \Lambda^\dagger .)}{\tilde{\omega}_3} \right|, \quad Z(\tilde{\omega}) = \left( 2 - \ln \left| \frac{\tilde{\omega}_1}{N(\tilde{\omega}, \Lambda^\dagger .)} \right| \right)^{-1},$$

where $\tilde{\omega}_1 = N(\tilde{\omega}, \Lambda^\dagger .) (\tilde{\omega} - \frac{1}{2} \epsilon_{\Lambda^\dagger .})$, and $N(\Lambda^\dagger ., \tilde{\omega})$ is the total number of states within the window $\Lambda^\dagger$ along the direction $\tilde{\omega}$ normal to the FS. Thus, the imaginary part of the self-energy (and therefore the inverse lifetime) has the form $\Sigma^\imath = \tilde{\omega}_1 = \tilde{\omega}_3$. Altogether, this reproduces the marginal Fermi liquid phenomenology proposed for the strange metal phase of the cuprates [84].

### 4. Mottness collapse and quantum criticality with hole-doping

We present the RG phase diagram for the 2D Hubbard model with doping away from 1/2-filling in figure 2. This phase diagram results from longitudinal and tangential scattering RG equations (equations (3) and (4)) upon including effects of doping $\Delta \mu_{\text{eff}} \neq 0$ and Cooper pair scattering processes across the Fermi surface. Upon doping the Mott insulator via an effective chemical potential, we observe a marginal Fermi liquid (marginal Fermi liquid model in figure 2) in the energy scale $\frac{W}{\tilde{t}} - \omega < W$. This phase is analytically continued from that observed at 1/2-filling case ($\Delta \mu_{\text{eff}} = 0$) with a 2e−1h dispersion contained in the Hamiltonian equation (7). On lowering the energy scale, the marginal Fermi liquid undergoes once again a Lifshitz transition into the pseudogap phase (marginal Fermi liquid phase of the cuprates). The onset energy scale for spin fluctuations that gap the AN is $\omega > \omega_{\text{PG}} \equiv \omega_{\text{PG}}$. Further lowering the energy scale gaps the charge fluctuations at the AN, i.e., creates a charge pseudogap at AN. The energy scale for the gap of charge fluctuations at the AN (dotted red line in figure 2) is delayed, falling linearly with increasing doping: $\omega > \omega_{\text{PG}} = -\Delta \mu_{\text{eff}}$. Upon yet lowering the energy scale for fluctuations causes the exit from the pseudogap via a second Lifshitz transition into a Mott liquid state (solid blue region). The Mott liquid insulator comprises the following region in the phase diagram (figure 2, video S4): $(\frac{W}{\tilde{t}} - \omega < 1.2\tilde{t})$ with $\Delta \mu_{\text{eff}} > -2.8\tilde{t}$ and $(\frac{W}{\tilde{t}} - \omega < 2\Delta \mu_{\text{eff}})$ with $\Delta \mu_{\text{eff}} < -2.8\tilde{t}$ and $\Delta \mu_{\text{eff}} = -2\tilde{t}$.

The variation of spin charge hybridization parameter $p$ (see section 3) with doping $\Delta \mu_{\text{eff}}$ leads to a separation of the charge gap-dominated and spin gap-dominated parts of the pseudogap within the phase diagram figure 2, such that the boundary of the charge gap-dominated pseudogap (dotted red line in figure 2) is observed to fall with increasing doping straight into a quantum critical point (QCP) at $\omega_{\text{QCP}} = W/2 = -\Delta \mu_{\text{eff}}$. This is called the collapse of Mottness [79, 80]. The QCP is associated with point-like Fermi surfaces at the four nodal points, and spin-gapping that increases monotonically from near the nodes to the antinodes (figure 3(b), videos S2 and S3). The resulting nodal metal supports a 2e−1h dispersion that is analytically continued from $\frac{W}{\tilde{t}} - \omega = W$ at $\Delta \mu_{\text{eff}} = 0$ down to $\frac{W}{\tilde{t}} - \omega = 0$, and given by $\epsilon_{\text{QCP}} = -\sqrt{2\tilde{t}A}$. This linear dispersion signals the Lorentz invariance emergent precisely at the QCP. Thus, the $U(1)$ symmetry of the charge fluctuations is promoted to SU(2) at the QCP due to the emergent particle-hole symmetry of the gapless nodal Dirac electrons. Indeed, these findings for the QCP are in striking agreement with the works of Phillips and co-workers [85].

For $\omega > \omega_{\text{PG}}$, to the left of the QCP, lies the Mott liquid discussed earlier. For $\omega > \omega^\dagger = -2\Delta \mu_{\text{eff}}$, to the right of the QCP, lies a correlated Fermi liquid (CFL) arising from RG relevant tangential scattering.
Figure 2. RG phase diagram with hole doping showing quantum critical point (QCP) at $-\Delta \mu_{\text{eff}} = 4 = \omega$ and its wedge extending to higher energies. All phases (NFL, PG, ML, correlated Fermi liquid (CFL), PG–CFL and QCP-wedge) and related energy scales are shown in the colour bars, and discussed in detail in the text. Dashed line shows highest energy scale for superconducting fluctuations. Insets: N, AN and FS-averaged spectral function $[A(E)]$ for the QCP and gapless CFL (grey region: $\omega = 3.2$, $\Delta \mu_{\text{eff}} = -7.5$).

Figure 3. (a) Resistivity ($\rho$) vs $4 - \omega$ for various $\Delta \mu_{\text{eff}}$, showing passage from NFL into (blue) ML, (green) the QCP and (red) PG–CFL. (b) Map of $A(E)$ at the QCP.

4.1. Low energy eigenstates of the doped Mott liquid and the QCP

From the RG equation (3) at finite $\Delta \mu_{\text{eff}}$, we obtain the relation between the fixed point spin and charge backscattering coupling

$$K^* (\omega, \Delta \mu_{\text{eff}}) = \frac{\bar{U}_0 (1 - p) K^*_c (\omega, \Delta \mu_{\text{eff}})}{K^*_c (\omega, \Delta \mu_{\text{eff}}) - \bar{U}_0 p},$$

where the parameter $p$ is determined upon maximizing the Green’s function equation (6). For instance, within the Mott liquid phase with $W/2 - \omega = 0$, $p = 0$ for $2.9 > -\Delta \mu_{\text{eff}} > 0$, $p = 1$ for $W/2 > -\Delta \mu_{\text{eff}} > 2.9$. For these two cases, $K^*_c (\omega, \Delta \mu_{\text{eff}}) = K^*_c (\omega, \Delta \mu_{\text{eff}}) = \bar{U}_0$, such that the fixed point Hamiltonian is given by

$$H^* (\Delta \mu_{\text{eff}}) = \sum_i U_0 \left( A_{i,3} \cdot A_{i,3} - S_{3,3} \cdot S_{3,3} \right) + \Delta \mu_{\text{eff}} \sum_i A_i^0.$$
The pseudospins are defined as,

$$A_{+\beta} = \sum_{A \in \Lambda} A_{\alpha \beta}, S_{+\beta} = \sum_{A \in \Lambda} S_{\alpha \beta}, A_{\alpha \beta} = f^{\dagger}_{A,\beta} \frac{\sigma}{2} f_{A,\beta}, S_{\alpha \beta} = f^{\dagger}_{A,\beta} \frac{\sigma}{2} f_{A,\beta}. \quad (12)$$

Here, $f^{\dagger}_{A,\beta} = \left[ c^{\dagger}_{A,\beta \sigma} c_{A,\beta \sigma * \sigma} \right]$ and $f_{A,\beta} = \left[ c_{A,\beta \sigma} c^{\dagger}_{A,\beta \sigma * \sigma} \right]$ are the spinorial representation for a pair of fermions. The low-lying eigenstates and eigenenergies of the doped Mott liquid is given by

$$|\Psi_i\rangle = \prod_{\alpha} |A_{+\alpha} = A_{-\alpha} = N^+_\alpha, A = n, A^z = n, S_{\alpha \beta} = 0\rangle, \quad (13)$$

$$E(n) = \sum_{\alpha} E_0 \left[ n(n+1) - 2N^+_\alpha (N^+_{\alpha} + 1) \right] + \Delta \mu_{\text{eff}} n. \quad (14)$$

This many body wavefunction can be seen as resulting out of the doping the ground state wavefunction for the Mott liquid at half filling ($\Delta \mu_{\text{eff}} = 0$) with $n$ holes, where $n$ is bounded $0 \leq n \leq 2N^+_{\text{h}}$ from angular momentum algebra. These low lying states have been obtained by respecting the attractive nature of the spin pseudospin interactions and the repulsive nature of the charge pseudospin interactions. The ground state energy $E_{\text{g}}(\Delta \mu_{\text{eff}})$ can then be obtained from a numerical search of the lowest eigenvalue of the energy function $E(n)$ equation (14). From this, we can obtain the hole-doping fraction $f_\text{h} = \frac{n^*}{N^+_\text{h}}$. We conducted a test of these results by comparing the ground state energy obtained for $U = 8t$ and at a hole-doping fraction of $f_\text{h} = 0.125$ (i.e., 12.5% hole doping) against that obtained from various other numerical methods as given in reference [75]. Figure 4(a) shows a finite-size scaling plot of $E_{\text{g}}(\Delta \mu_{\text{eff}})$ per particle at 12.5% hole doping and system sizes (i.e, number of sites) varying between 32 × 32 to 32768 × 32768. The value of $E_{\text{g}}(\Delta \mu_{\text{eff}})$ per particle in the thermodynamic limit from this analysis appears to be converging towards $-0.776$ (in units of the hopping amplitude $t$), and compares well with the range of $-0.74 > (E_{\text{g}}/\text{perparticle}) > -0.77$ obtained from reference [75, 76]. We also point the reader to further benchmarking exercises presented in appendix B with $U/t = 2, 4, 6, 10$ at 12.5% doping. Once more, we find excellent agreement with the results obtained from the numerical methods employed in references [75–77], offering confidence on the effective Hamiltonian and ground state wavefunction derived for the doped Mott liquid.

A plot of $E_{\text{g}}$ as a function of $f_\text{h}$ (figure 4(b)) clearly shows cusp-like behaviour at $f_\text{h} = 0.25$, signalling a quantum critical point (QCP). The discontinuity in the first derivative is also seen in a plot of $E_{\text{g}}$ vs $-\Delta \mu_{\text{eff}}$ (inset of figure 4(b)), as well as a plot of $f_\text{h}$ vs $-\Delta \mu_{\text{eff}}$ (figure 5(a)). The step-like discontinuity observed in $f_\text{h}$ at $-\Delta \mu_{\text{eff}} \approx 7.2$ indicates the topological reconstruction of a fully connected Fermi surface as the spin pseudogapped parts of the FS vanish at this value of the chemical potential. This is reinforced by a plot of the number compressibility $\kappa$ with the chemical potential $\Delta \mu_{\text{eff}}$ in the inset of figure 5(a): the first spike indicates the appearance of point-like nodal FS at the QCP, while the second denotes the reconstruction of a fully connected FS. Our observation of $f_\text{h} \sim -\Delta \mu_{\text{eff}}$ and a constant $\kappa$ for the hole-doped Mott liquid is not consistent with the relation $f_\text{h} \sim \sqrt{\Delta \mu_{\text{eff}}}$, $\kappa \sim (\Delta \mu_{\text{eff}})^{-1/2}$ observed, for instance, in reference [86].
Figure 5. (a) Variation of hole doping $f_h$ with chemical potential $\Delta \mu_{\text{eff}}$ for lattice size $1024 \times 1024$. Inset: number compressibility $\kappa$ as a function of chemical potential $\Delta \mu_{\text{eff}}$. Spikes in $\kappa$ are visible at $-\Delta \mu_{\text{eff}} = 4$ and at $-\Delta \mu_{\text{eff}} \sim 7.2t$. (b) Variation of the energy gap $\Delta E$ per particle of the doped Mott liquid along the nodal direction with the chemical potential $\Delta \mu_{\text{eff}}$.

Figure 6. Variation of the Double occupancy $D$ of the doped Mott liquid with the hole fraction $f_h$. The plot shows a steady decline of $D$ as $f_h$ is increased towards the QCP.

sector in the present work, we have not taken into account such shifts in the Fermi energy here. Further detailed investigations will be needed to overcome this limitation, and will be dealt with in a future work.

In order to understand better the nature of the QCP, we present a plot of the energy gap $\Delta E$ per particle along the nodal direction in the doped Mott liquid with varying $-\Delta \mu_{\text{eff}}$ in figure 5(b). The plot shows that $\Delta E$ per particle rises steadily from a value of 0.002 and saturates at 0.004 well before the QCP is approached from the underdoped side. This saturated value of $\Delta E$ appears to be robust very close to the QCP, and collapses abruptly to 0 at the QCP. This signals the nucleation of gapless nodal Fermi points precisely at the QCP, and corresponds to a topology change in the Luttinger surface of zeros for the gapped Mott liquid. The QCP is an example of a Lifshitz transition driven by electronic correlations [26]. We can also compute the doublon occupancy from the hole-doping fraction $f_h$, $D = D_0(1 - f_h)$, where $D_0$ is the doublon fraction at half-filling. This is shown in figure 6, and shows a steady decline in the doublon occupancy of the doped Mott liquid from half-filling till the QCP. We also note that the value of 0.045 is obtained for the doublon occupancy $D$ at a hole doping of 12.5%, and compares well with the range $0.04 < D < 0.045$ obtained from various numerics in reference [75].

The eigenenergies for the gapped parts of the FS at and across the QCP $-W \leq \Delta \mu_{\text{eff}} \leq -\frac{W}{2}$ can be similarly obtained from the fixed point Hamiltonians at $\omega = \frac{W}{2}$ (equation (19)). For the gapless regions, the lowest excitations appear near zero energy. Taken together, this allows for a determination of the ground state energy ($E_g$) and hole-doping fraction ($f_h$) as a function of chemical potential $\Delta \mu_{\text{eff}}$ for a range of chemical potential that crosses the QCP. The results are shown in figures 4(b) and 5(a). Specifically, we find that $E_g$ rises steadily with $\Delta \mu_{\text{eff}}$ from its value at the QCP to zero as the chemical potential leads to the reconstruction of a fully connected FS (inset of figure 4(b)). Interestingly, $f_h$ is seen to attain a plateau upon increasing $\Delta \mu_{\text{eff}}$ away from the QCP, transitioning abruptly at the FS reconstruction. These findings are consistent with results obtained from the dynamical cluster quantum Monte Carlo method applied to the 2D Hubbard model with doping away from 1/2-filling [19, 87], and unveil the mechanism responsible for the experimentally observed topological reconstruction of the Fermi surface near critical doping [88–90]. We will further discuss these results below, as we study the interplay of spin, charge, Cooper and tangential...
scattering processes in the vicinity of the QCP. The codes used for the numerical computations of the ground state energy and hole fraction shown here are made available electronically [81].

4.2. Signature of QCP in ground state fidelity susceptibility with doping

The fidelity of many-body ground state wavefunctions, computed as an overlap between wavefunctions obtained by tuning a parameter, has emerged recently as a candidate for tracking quantum phase transitions (QPT) [91, 92]. In this section, we will use fidelity to observe signatures of the QCP seen above. Fidelity is computed here from the overlap between ground states at $\omega = 0$ obtained for infinitesimal variation ($\epsilon > 0$) of the effective chemical potential $\Delta_{\text{eff}}$

$$F(\Delta_{\text{eff}}, \epsilon) = |\langle \Psi_g(\Delta_{\text{eff}}) | \Psi_g(\Delta_{\text{eff}} - \epsilon) \rangle|.$$ 

The value of $\omega = W/2$ represents the quantum fluctuation scale proximate to the Fermi surface of the tight binding model. Therefore, varying $\Delta_{\text{eff}}$ while holding $\omega = W/2$ fixed allows us to explore the fidelity of the many body ground state wavefunctions across the quantum critical point. The ground state wavefunctions for $\Delta_{\text{eff}} > -\frac{W}{2}$ can be represented purely in terms of pseudospins (equation (13)), in which the quantum number $n(\Delta_{\text{eff}})$ is determined by minimizing the energy density equation (14). For $-\Delta_{\text{eff}} < -\frac{W}{2}$, the fidelity is obtained as $F(\Delta_{\text{eff}}, \epsilon) = \delta_{n(\Delta_{\text{eff}}), n(\Delta_{\text{eff}} - \epsilon)}$.

However, for $-\Delta_{\text{eff}} > W/2$, a gapless node formed at $N = (\pi/2, \pi/2)$ stretches subsequently into an arc in momentum space. The gapped states in the AN regions can still be described in terms of the pseudospin wavefunctions equation (13), whereas the gapless regions are described by separable eigenstates of the Hamiltonian equation (7) in the occupation number basis of $|\mathbf{k}\sigma\rangle$. Thus, the ground states describing the journey across the QCP can, using equations (8) and (13), be written as $|\Psi_g(\Delta_{\text{eff}})\rangle = |\Psi_{\text{gapped}}\rangle|\Psi_{\text{gapped}}\rangle$. From here, the overlap between neighbouring ground states for $-\Delta_{\text{eff}} > W/2$ axis is obtained as

$$\langle \Psi_g(\Delta_{\text{eff}}) | \Psi_g(\Delta_{\text{eff}} - \epsilon) \rangle = \left( \frac{2N^*}{n(\Delta_{\text{eff}} - \epsilon) + N^*} \right)^{-\lambda(\Delta_{\text{eff}}, \epsilon)},$$

where $\lambda(\Delta_{\text{eff}}, \epsilon)$ is the increment of the gapless stretch and $2N^*$ is the number of electronic states transformed into $N^*$ bound pairs in the momentum-space window.

Plots figures 7(a) and (b) show the variations of $\log(F(\Delta_{\text{eff}}, \epsilon))$ and fidelity susceptibility ($\chi_F(\Delta_{\text{eff}}) = d^2 \log(F(\Delta_{\text{eff}}))/d\Delta_{\text{eff}}^2$) with $-\Delta_{\text{eff}}$ respectively in the neighbourhood of the QCP at $-\Delta_{\text{eff}} \approx 4$. Note that, in order to avoid the log singularities in the numerical evaluation of $F(\Delta_{\text{eff}}) = 0$, we have added a lower cutoff of $10^{-15}$. Precisely at the QCP ($-\Delta_{\text{eff}} \approx 4$), $\log F$ falls suddenly to zero as the nodal points become gapless, and $\chi_F$ shows a large sudden variation. This indicates that an increase in the gapless region from nodal point to arc forces the many-body wavefunction through a cascade of orthogonality catastrophes. The fidelity then rises $F \to 1$ with increasing $\Delta_{\text{eff}}$, indicating the recreation of a connected Fermi surface.

4.3. Theory for the vicinity of the QCP

Doping via an effective chemical potential $\Delta_{\text{eff}} = -\Delta_{\text{bk}}$ generates a doublon–holon imbalance via a field-like term for the charge pseudospins $-\Delta_{\text{eff}}(A^+_{x-s} + A^+_{x+s})$. This lowers the global SU(2) charge symmetry to U(1). Doublon–holon imbalance at lower values competes with the umklapp scattering term $\langle A^+_{x-s}A^+_{x+s} + \text{h.c.} \rangle$ and finally dominates over it at larger values. On the other hand, this uniform field favours spin-backscattering of different finite $p$ pair momentum Anderson pseudospins $|\mathbf{c}_{\mathbf{k}}\rangle^{\uparrow} = |\mathbf{p} - \mathbf{k}\sigma\rangle$.

Indeed, there exists a direct equivalence between $p$ pair momentum (centered about $p = 0$) spin-backscattering terms and the electron hole pseudospin scattering terms,

$$\sum_{p,k,l} K_{\alpha\beta}^p c^\dagger_{p,k\sigma} c^\dagger_{p-k\sigma} c_{p',k'\sigma}^l c_{p-k',l}^\dagger = -\sum_{a,b} K_{\alpha\beta}^a S_{a\sigma} S_{b\sigma} + \text{h.c.}.$$ 

Here $\alpha = \{p, s, \delta\}$ is a set comprising of pair momentum ($p$), $s$ normal to FS and $\delta$ i.e. is the momentum shift from a pair of states $|\mathbf{k}\rangle_{\Lambda\Lambda'}, |\mathbf{k}_{-\mathbf{A}(T)}\rangle$ chosen symmetrically about the nodal points, $\mathbf{k} = \mathbf{k}_{\Lambda\Lambda'}, \mathbf{k}' = \mathbf{k}_{\Lambda'\Lambda}$ are momentum state involved in the scattering where $\Lambda' = \Lambda - 2\Lambda + \delta$, $\Lambda'$ is the momentum space width around FS obtained from the fixed point of the spin backscattering RG equation equation (3). In the equivalent pseudospin description $S_{a\sigma} = f^\dagger_{a\sigma} f_{a\sigma}$ where $f^\dagger_{a\sigma} = (c^\dagger_{k\sigma} c^\dagger_{k'\sigma})$ and $a = (\mathbf{k}, \mathbf{k}', b = (\mathbf{p} - \mathbf{k}, \mathbf{p} - \mathbf{k}')$.

In accounting for all possible pair-scattering processes in the vicinity of the QCP, we include the contribution of Cooper and tangential scattering channels equation (4) in the spin-backscattering RG
equation \((\Delta K_{\Delta}^{(2)})\) equation (3)

\[
\Delta K_{\Delta}^{(2)} = -\frac{(1 - p)(K_{\Delta}^{(2)})^2}{\epsilon_j} + \frac{(K_{\Delta}^{(2)})^2}{\omega} - \frac{\epsilon_j}{\Lambda_{\Delta}^{(2)}} - \frac{\Delta \mu_{\Delta\text{eff}}}{\omega + \epsilon_{\text{avg}}} - \frac{N_{\Delta}^2(L_{\Delta}^{(2)})^2}{\alpha}
\]

where \(\epsilon_j = \epsilon_{k_A} + \epsilon_{p - k_A}\) is the pair kinetic energy, \(\Delta \mu_{\Delta\text{eff}} = \Delta \mu_{\text{eff}} - \Delta \mu_{\text{eff}}^*\) is the effective chemical potential for the marginal Fermi liquid centered around the node, and renormalized by the fluctuation scale \(\omega_{\Delta}\). Note that, once again, we have \(\Lambda_1 = \Lambda_0 \exp(-j)\) and \(\Lambda_{j+1} = \Lambda_0 \exp(-(j - 1))\), such that \(\Lambda \log \Lambda_0 = 1\). \(\epsilon_j = \epsilon_{k_A} + \epsilon_{p - k_A}\) and \(\Lambda_{j+1} = \Lambda_1 - 2\Lambda + \delta\) is the longitudinal momentum of the electronic state comprising the electron hole pair. In the above RG equation, the spin-charge hybridized backscattering strength (with Cooper channel contribution) is given by \(K_{\Delta}^{(2)} = p K_{\Delta}^{(1)} + (1 - p)K_{\Delta}\), \(K_{\Delta}^{(1)}\) being the vertex strength for finite momentum Umklapp scattering pairs. The negative sign of the first and third terms in the above RG equation originates from the interchangeing of electron and hole creation operators. The second term contains contributions to spin-backscattering from the Cooper channel due to Cooper pairs with zero and non-zero pair-momentum. The third term accounts for the influence of tangential scattering on the spin-backscattering.

On either side of the QCP, spin-backscattering with \(p = 0\) pair-momentum is suppressed by tangential scattering (\(\omega > \omega_1\)) and \(\pi\)-momentum \(e\hbar\) pair-backscattering (\(\omega > \omega_{\Delta}\)) processes, leading to the establishing of the CFL and Mott liquid phases respectively. Remarkably, right above the QCP (i.e. \(\omega_{\Delta} < \omega < \omega_1\)), we observe that the antinodal spin gap (composed of \(p = 0\) pair-momentum Cooper pairs) carries the highest spectral weight. This can be seen from the smallest magnitude of the inverse Green function for \(p = 0\) pair-momentum: \(G_{p=0}^{-1}(\omega, p) = (\omega - (\epsilon_{k_A} + \epsilon_{p - k_A})/2)\). We also note that for \(\Delta \mu_{\Delta\text{eff}} = 0\), only the first term has leading contribution in the above RG equation, thus analytically continuing to the \(\Delta \mu_{\Delta\text{eff}} = 0\) (i.e. 1/2-filled) case (equation (3)).

The fixed point Hamiltonian obtained by investigating the RG relation equation (18) for the gapped parts and the 2e–1hole RG relation for the gapless parts of the FS (equation (3))

\[
H' = \sum_{\Lambda,\delta=\Delta,\Lambda_0} \sum_{\alpha,\beta} R_{\alpha\beta}^{\delta} h_{\delta,\alpha} h_{\delta,\beta} (1 - \hat{n}_{\delta,\alpha}) + \sum_{i=1}^{N} K_{\alpha,\beta}^{\delta} A_{\alpha,\beta} \cdot A_{\alpha,\beta} + \sum_{j=1}^{\delta_0} K_{\alpha,\beta}^{(2)} (B_{\alpha} \hat{B}_{\beta}^* + \text{h.c.})
\]

\[
- \sum_{i=1}^{\delta_0} K_{\alpha,\beta}^{(2)} S_{\alpha,\beta}^{\delta_0} + \sum_{\delta,\delta'} \sum_{\Lambda} L_{\alpha,\beta}^{\delta,\alpha,\beta,\Lambda} h_{\delta,\alpha} h_{\delta',\beta} + \sum_{\delta,\delta'} \sum_{\Lambda} \epsilon_{\alpha,\beta} h_{\delta,\alpha} + \sum_{\delta,\delta'} (\Delta \mu_{\Delta\text{eff}} B_{\alpha}^* + \Delta \mu_{\Delta\text{eff}}^* A_{\alpha}^*)
\]

where the charge (A) fluctuation pseudospins has been defined earlier, and the generalized Cooper pairs/Anderson pseudospins are given by \(B_{\Lambda} = f_{\Lambda} \frac{\epsilon}{\delta} f_{\Lambda}^{*} = (c_{\Lambda}^d \epsilon_{p - k})\) and indices \(c = (k, p - k)\), \(d = (k', p - k')\) label these pseudospins. The momentum vectors in terms of \(\Lambda, \delta\) are \(\mathbf{k} = k_{\Lambda,\delta}, \mathbf{k}' = k_{\Lambda',\delta'}\) and \(\delta = \delta (\omega, \Delta \mu_{\Delta\text{eff}})\) is the normal vector up to which gapless part stretches. \(\Lambda'' = -\Lambda + \delta\) is the normal distance at which the partner electronic state of 2-electron 1-hole composite is placed. \(\rho = \{\delta, \delta\}\) is a set comprising of offset momentum \(\delta\) and normal \(\delta\). The set \(\alpha\) and indices \(a\) and \(b\) are as defined earlier. The \(p = 0\) pair-momentum Cooper pair pseudospin scattering terms can, as discussed earlier, be recast in terms of the electron–hole pseudospins \(-S_{\alpha,\beta}^{\delta} S_{\alpha,\beta}^{\delta} + \text{h.c.} = (B_{\alpha}^* \hat{B}_{\beta}^* + \text{h.c.})\). This confirms that even as we study a model of repulsive electronic correlations, the effective attractive nature of spin pseudospin backscattering is responsible for the formation of preformed Cooper pairs in the gapped
antinodal regions of the FS [65, 82]. Thus, the first term in equation (19) corresponds to the 2e–1h nodal marginal Fermi liquid metal. The second and third terms govern the gapping mechanisms of the Fermi surface by charge and Anderson pseudospins respectively. The fourth term is associated with tangential scattering in the gapless stretches of the FS, while the fifth term (proportional to $B_{\pm\lambda}^f$) reflects the doublon–holon disparity with hole doping.

The Hamiltonian $H^f(\omega, \Delta \mu_{\text{eff}})$ naturally encompasses the doped Mott liquid Hamiltonian with insulating ground states in the region $0 > -\Delta \mu_{\text{eff}} > -\Delta \mu_{\text{eff}}^c$ and $\omega = \frac{\mu}{\Delta}$. This can be seen as follows: $R_{\delta f}^I = 0$ for all $\delta, L_{\gamma}^f = 0$ from equations (3) and (4). Then the resonant pairs with $\delta = 0$ interacting via scattering vertex dominates over all others equation (18). Further, the z-component of the total Cooper-pair pseudospin is equal to the z-component of the total charge pseudospin: $\sum_{\lambda,\delta} B_{\lambda f}^z = \sum_{\lambda,\delta} A_{\lambda f}^z$. This leads to the Hamiltonian for the insulating Mott liquid equation (11) centered about the QCP ($B_{\pm\lambda}^f = \sum_{\lambda,\delta} B_{\pm\lambda}^f$)

$$H^f(\omega, \Delta \mu_{\text{eff}}) = \sum_{\lambda,\delta} U_{\lambda,\delta} (A_{\lambda,\delta} \cdot A_{\lambda,\delta} - S_{\lambda,\delta} \cdot S_{\lambda,\delta}) + \sum_{\lambda} \Delta \mu_{\text{eff}} A_{\lambda f}^z + \Delta \mu_{\text{eff}} B_{\pm\lambda}^f. \tag{20}$$

The existence of competing gapping instabilities of some parts of the FS, as well as tangential scattering of Landau quasiparticles and preformed Cooper pairs between the gapless nodal regions and the gapped antinodes signals a drastic change in the nature of many-particle entanglement across the QCP [80]. This can be seen simply from the nature of the state of the nodal points on the FS. The QCP at optimal doping is associated with a sudden appearance of the nodal marginal Fermi liquid’s excitations which can be written in terms of a separable state, while on either side the state at the node is strongly entangled through longitudinal and tangential scattering in the Mott liquid (underdoped) and CFL (overdoped) phases respectively. Thus, the nodal state is an eigenstate of the Mott liquid Hamiltonian (involving the charge pseudospins $A$) upon undoping away from the QCP as discussed above, and possesses Landau quasiparticles with $0 < Z_1 < 1$ upon overdoping away from the QCP. Finally, the nodal excitations precisely at the QCP show $Z_1 \rightarrow 0$ and $Z_3 \rightarrow 1$. The phase precisely above the QCP contains preformed Cooper pairs in spin–gapped antinodal regions coupling with the MFL’s excitations in the gapless nodal stretches, extending into the entire conical region lying above the QCP in the phase diagram shown in figure 2. This feature of the phase diagram is reminiscent of the quantum critical cone typically observed at finite temperatures above a QCP, but with temperature (i.e., the energy scale for thermal fluctuations) here replaced by $\omega$ (the scale for the quantum fluctuations). We will turn to a discussion of this in the next subsection. We end this subsection with an interesting observation on the variation of critical doping for the QCP ($f^*_{0h}$) against the Hubbard repulsion $U$ (shown in figure 8). The plot shows that the value of critical doping lowers with increasing $U_0$: $f_{0h}^* = 74\%$ for $U_0 = 2t$, while $f_{0h}^* = 16.4\%$ for $U = 12t$. We stress that we have computed $f_{0h}^*$ only for those values of $U_0/t$ at which we have benchmarked our ground state energy against other numerical methods (see appendix B). We have also checked that the qualitative feature of the phase diagram presented in figure 2 for $U_0/t = 8$ remains unchanged for $2 \leq U_0/t \leq 12$. We also note that for this entire range, the QCP always appears at a fixed chemical potential independent of $U_0$: $\Delta \mu_{\text{eff}} = -\frac{\mu}{2}$. The variation of $f_{0h}^*$ with $U/t$ certainly deserves further investigation.

4.4. $T = 0$ origin of Homes law: Planckian dissipation and preformed Cooper pairs

The V-shaped region bounded by the lines $\omega_{\text{PG}} < \omega < \omega^f$ in the phase diagram figure 2 has a simpler fixed point Hamiltonian compared to equation (19) owing to the RG irrelevance of charge backscattering and

![Figure 8](image_url)
tangential scattering terms

\[ H_t = \sum_{\Lambda, \rho} R_{\rho} \hat{n}_{\Lambda, \rho} \hat{n}_{\Lambda, \rho} (1 - \hat{n}_{\Lambda, \rho}) + \sum_{\alpha} \frac{K_{\alpha}}{2} (B_{\alpha}^+ B_{\alpha} + \text{h.c.}) + \sum_{k \in \mathcal{N}} \hat{c}_k \hat{n}_k + \Delta \mu_{\text{eff}} B_s^+ . \] (21)

The set \( \rho, \alpha \) has been defined earlier, here \( \alpha \) is restricted to the sets \( \alpha = \{ p = 0, \delta, \delta \} \). The second term then describes the zero momentum Cooper pair scattering processes. We will now focus our attention on the physics of the AN and N points on the FS. The nodal points are important as the QCP is realized with four nodal gapless MFL metals. On the other hand, the antinodes possess the highest spin gap (figure 3(b)); the highest single-particle spectral weight (due to the van Hove singularities of the electronic dispersion) are converted to that of Cooper pairs at the antinodes.

The spin-backscattering RG equations for the N and AN points at fluctuation scales \( (\omega, \Delta \mu_{\text{eff}}) \) and \( (\omega = 0, \Delta \mu_{\text{eff}} = \Delta \mu_{\text{eff}}^s) \) within the 'V' shaped region in the vicinity of the QCP are given by

\[ \Delta K_{\alpha_1}^{(j)} = \frac{-p \epsilon_{\Lambda \delta_{\text{AN}}}^j}{\omega_c - p \epsilon_{\Lambda \delta_{\text{AN}}}^j - (1 - p) \epsilon_{\Lambda \delta_{\text{AN}}} - \frac{K_{\alpha_1}^{(j)}}{4}} + \frac{(K_{\alpha_1 \delta_{\text{AN}}}^{(j)})^2}{\omega_c - \epsilon_{\Lambda \delta_{\text{AN}}} - |\Delta \mu_{\text{eff}}| - \frac{K_{\alpha_1}^{(j)}}{4}} \]

\[ \Delta K_{\alpha_2}^{(j)} = \left( \frac{-K_{\alpha_2}^{(j)} \epsilon_{\Lambda \delta_{\text{AN}}}^j}{W - \frac{t}{2} (\epsilon_{\Lambda \delta_{\text{AN}}} - \epsilon_{\Lambda \delta_{\text{AN}}} + \epsilon_{\Lambda \delta_{\text{AN}}} - \epsilon_{\Lambda \delta_{\text{AN}}}) - \frac{K_{\alpha_2}^{(j)}}{4}} + \frac{(K_{\alpha_2 \delta_{\text{AN}}}^{(j)})^2}{W - \frac{t}{2} (\epsilon_{\Lambda \delta_{\text{AN}}} - \epsilon_{\Lambda \delta_{\text{AN}}} - \epsilon_{\Lambda \delta_{\text{AN}}}) - \frac{K_{\alpha_2}^{(j)}}{4}} \right) = 0 \] (22)

where \( \alpha_1 = \{ p = 0, \delta_{\text{AN}} \}, \alpha_2 = \{ p = 0, \delta_{\text{AN}} \} \) and \( \Lambda_1 = \Lambda_0 \exp(-j) \) and \( \Lambda_1 = \Lambda_0 \exp(-(j - 1)) \), such that \( \Delta \log \Lambda_{\mathcal{N}}^1 = 1 \). From the second of these RG relations, we find that the Cooper instability is marginal along the nodal directions. This results from the fact that the Cooper pair and e–h pair along \( \delta \equiv N \) has the same dispersion energy: \( (\epsilon_{\Lambda \delta_{\text{AN}}} + \epsilon_{\Lambda \delta_{\text{AN}}} - \epsilon_{\Lambda \delta_{\text{AN}}} - \epsilon_{\Lambda \delta_{\text{AN}}}) \approx \omega_{\text{FN}} \Lambda_{\mathcal{N}} \). This then leads to the exact cancellation of the two terms in the RG relation for \( \Delta K_{\alpha_2}^{(j)} \). This leads to protection of the gapless nodal points from gapping via a Cooper instability. Therefore, the nodal Hamiltonian precisely at the QCP is composed of 2e–1h degrees of freedom described by the above Hamiltonian (equation (21)), but with \( K_{\alpha_1}^{(j)}(\omega, \Delta \mu_{\text{eff}}, \delta) = 0 \) and \( B_{\Lambda \delta}^j = 0 \).

\[ H_{\text{QCP}}^{\text{sc}}(\omega, \Delta \mu_{\text{eff}}^s) = \sum_{\Lambda, \delta} R_{\Lambda \delta} \hat{n}_{\Lambda, \delta} \hat{n}_{\Lambda, \delta} (1 - \hat{n}_{\Lambda, \delta}) + \sum_{k \in \mathcal{N}} (\epsilon_k - \Delta \mu_{\text{eff}}^s) \hat{c}_k \hat{n}_k . \] (23)

The nodal liquid state described here possesses 2e–1h composite excitations of the MFL with a gapless Dirac dispersion, i.e., the dynamical exponent of the excitations is \( z = 1 \). Signatures of a nodal liquid state appear to have been observed in ARPES measurements carried out within the PG phase of the slightly underdoped cuprate Bi2212 above the superconducting dome [93], as well as in transport measurements [61]. The direct experimental evidence for the 2e–1h composite excitations is, however, desirable.

At the AN points, however, the Cooper-channel scattering RG relation is relevant, with a final fixed point window \( (\Lambda_{\mathcal{N}}^* \Lambda_{\mathcal{N}}^* \Lambda_{\mathcal{N}}^* \Lambda_{\mathcal{N}}^*) \) determined from the criterion

\[ \omega_{\text{sc, onset}} = |\Delta \mu_{\text{eff}} - \Delta \mu_{\text{eff}}^s| - \frac{1}{2} (\epsilon_{\Lambda_{\mathcal{N}}^* \Lambda_{\mathcal{N}}^* \Lambda_{\mathcal{N}}^* \Lambda_{\mathcal{N}}^*) = \frac{K_{\alpha_1 \alpha_2}^{(j)}}{4} . \] (24)

The frequency scale \( \omega_{\text{sc, onset}} \) lying above the QCP in the phase diagram figure 2 at which superconducting fluctuations are able to condense into preformed pairs is a function of \( \Delta \mu_{\text{eff}} \). A non-zero spectral weight for Cooper pairs along the AN direction at optimal doping \( \rho = \Lambda_{\mathcal{N}}^* \omega_{\text{sc, onset}}, \Delta \mu_{\text{eff}} = \Delta \mu_{\text{eff}}^s \) is then obtained from equation (24) for \( \omega_{\text{sc, onset}} \rightarrow 0^+ \). Therefore, the fluctuation scale \( \omega_{\text{sc, onset}} \) is largest at optimal doping \( \Delta \mu_{\text{eff}} = \Delta \mu_{\text{eff}}^s \) and falls away from optimality. This explains the dashed line in figure 2 displaying the onset of a gapped state at the AN regions involving the formation of Cooper pairs. We stress that this state comprises of a fixed number of Cooper pairs, and therefore lacks the off-diagonal long-ranged order (ODLRO) associated with phase stiffness characteristic of superconductivity. Thus, such a state should display large superconducting phase fluctuations. Indeed, signatures of large superconducting phase fluctuations at temperatures much higher than the superconducting \( T_c \) have been observed in careful Nernst effect measurements on the cuprates [94]. Remarkably, the experiments reveal a 'dome' associated with the onset of phase fluctuations enveloping the dome of true d-wave superconductivity, similar to that observed in the RG phase diagram figure 2.

We have just established that the net spectral weight of the spin gapped regions around the AN is converted into that for preformed Cooper pairs within the low energy subspace (equation (12)) in the
vicinity of the QCP. Further, the nodal marginal Fermi liquid at the QCP can be shown to adiabatically continue to the region lying outside the gapped parts of the FS, and described by Hamiltonian equation (7). This marginal Fermi liquid metal has earlier been shown to follow the Planckian dissipation law (section 3). Indeed, Planckian dissipation has received experimental confirmation as the origin of the linear-in-$T$ resistivity in several members of the cuprate family of materials recently [61]. Thus, the coexistence of preformed pairs at the AN alongwith a Planckian dissipator at the N calls for an investigation of the experimentally observed Homes law [78]. This is an empirical relation between the normal state Drude conductivity $\sigma(T_C)$, the superconducting critical temperature $T_C$ and the superfluid weight $\rho_s$ observed for the d-wave superconductivity in the cuprates: $A\sigma_{DC}(T_C)T_C = \rho_s$, where $A$ is a universal constant. We search for the $T = 0$ origin of this relation in the theory of the state residing within the conical-shaped part of the phase diagram lying above the QCP. Thus, we first compute the antinodal (AN) superfluid weight from the Fertel–Glover–Tinkham (FGT) sum rule

$$\int_0^{\omega_{\text{onset}}} d\tilde{\omega} \text{Re}[\sigma_{n\lambda\text{AN}}(\tilde{\omega}) - \sigma_{s\lambda\text{AN}}(\tilde{\omega})] = \frac{\pi}{2} \rho_s,$$

(25)

where $\sigma_{n\lambda\text{AN}}(\tilde{\omega})$ is the normal state conductivity for the marginal Fermi liquid metal present initially at the AN before the instability. On the other hand, $\sigma_{s\lambda\text{AN}}(\tilde{\omega})$ is the conductivity of the many-body state that contains preformed Cooper pairs, and we have labelled $\tilde{\omega} = \frac{\omega}{\Lambda} - \omega$. We then decompose the integral over $\tilde{\omega}$ into one over $0 < \tilde{\omega} < \omega_{\text{onset}}$ and another over $\omega_{\text{onset}} < \tilde{\omega} < \infty$

$$\int_0^{\omega_{\text{ons}}(\tilde{\omega}_{\text{onset}})} d\tilde{\omega} \text{Re}[\sigma_{n\lambda\text{AN}}(\tilde{\omega}) - \sigma_{s\lambda\text{AN}}(\tilde{\omega})] = \int_0^{\omega_{\text{ons}}(\tilde{\omega})} d\tilde{\omega} \text{Re}[\sigma_{n\lambda\text{AN}}(\tilde{\omega}) - \sigma_{s\lambda\text{AN}}(\tilde{\omega})]$$

$$+ \int_{\omega_{\text{ons}}(\tilde{\omega})}^{\infty} d\tilde{\omega} \text{Re}[\sigma_{n\lambda\text{AN}}(\tilde{\omega}) - \sigma_{s\lambda\text{AN}}(\tilde{\omega})].$$

(26)

The second integral vanishes because the integrated spectral weight of the $2e–1h$ continuum in the normal and gapped state of preformed Cooper pairs is equal. Further, in the first integral, there is no contribution from $\sigma_{s\lambda\text{AN}}(\tilde{\omega})$ as the $2e–1h$ degrees of freedom are not present within the momentum space window along $s_{\text{AN}}$ ($-\Lambda_{\text{AN}}^*, \Lambda_{\text{AN}}^*$). For $\tilde{\omega} < \omega_{\text{ons}}$, denoting the antinodal conductivity as $\sigma_{n\lambda\text{AN}}(\tilde{\omega}_{\text{ons}}) = \sigma_{s\lambda\text{AN}}(\tilde{\omega})$, the FGT sum rule amounts to

$$\int_0^{\omega_{\text{ons}}(\tilde{\omega}_{\text{ons}})} d\tilde{\omega} \text{Re}[\sigma_{n\lambda\text{AN}}(\tilde{\omega}_{\text{ons}})] = \omega_{\text{ons}}(\tilde{\omega}_{\text{ons}}) \sigma_{n\lambda\text{AN}}(\tilde{\omega}_{\text{ons}}) = \frac{e^2 \Lambda_{\text{AN}}^*(\Delta_{\mu\text{eff}})}{m} = \frac{\pi}{2} \rho_s,$$

(27)

where we have used the relation $n = \Lambda_{\text{AN}}^*(\Delta_{\mu\text{eff}})/2\pi$ for the state number density $n$ in the Drude relation for the conductivity. Using the Planckian dissipation law section 3, along with the FGT relation for the superfluid weight given above, we obtain a relation analogous to Homes law for the onset scale for superconducting fluctuations at the antinodes ($T_{\text{ons}} = h\omega_{\text{ons}}(\tilde{\omega}_{\text{ons}})/k_B$)

$$\rho_s(\Delta_{\mu\text{eff}}, 0) = \frac{4k_B}{h} \sigma_{n\lambda\text{AN}}(T_{\text{ons}}) T_{\text{ons}}(\Delta_{\mu\text{eff}}).$$

(28)

The frequency scale $\omega_{\text{ons}}(\tilde{\omega}_{\text{ons}})$ is itself obtained from 9, and by picking up the normal $\delta_1 = \left(1 - \frac{\Delta_{\mu\text{eff}}}{\sqrt{2}\pi}\right) \delta_{\text{AN}}$ in the vicinity of $\delta_{\text{AN}}$ to avoid the discontinuity at the antinodal van Hove singularities

$$\omega_{\text{ons}} = N(\delta_1, 0) \left(\frac{1}{2} \max(\epsilon_{\Lambda^* - \delta_1} + \epsilon_{-\Lambda^* - \delta_1}) - \frac{1}{2} \max(\epsilon_{\Lambda^{*\prime} - \delta_1} + \epsilon_{-\Lambda^{*\prime} - \delta_1})\right)$$

$$= N(\delta_1, 0) \left(\epsilon_{\Lambda^* - \delta_1} - \epsilon_{\Lambda^{*\prime} - \delta_1}\right).$$

(29)

From the geometry of the square Fermi surface the number of states within the gapped window along normal $\delta$ is determined to be $N^*(\delta_1, 0) = \Lambda_{\mu\text{eff}}^* N \left(\frac{1}{\sqrt{2}} - \frac{\delta_1}{\sqrt{2}}\right).$ In the above equation $\Lambda^*$, $\Lambda^{*\prime}$ are determined from equation (5) respectively and $N^*(\delta_1, 0)$ is the total number of gapped states at $\omega = 0$. In keeping with our earlier discussion, $T_{\text{ons}}$ is largest at optimality (\Delta_{\mu\text{eff}}) and falls off with doping away from optimality on either side. In the next section, these fluctuations will be seen to interplay with the spin-gap in leading to d-wave superconductivity [87]. Further, we have shown in equation (A.13) (see appendix A for a detailed derivation) that the superconducting critical temperature $T_C$ is linearly related to $T_{\text{ons}}$ with a proportionality constant related to the extent of the pseudogap (seen in terms of the difference between the electronic dispersion at the antinodes and the nodes). In this way, we offer insight into the $T = 0$ origin of Homes law [78].
4.5. Mixed optical conductivity of the correlated Fermi liquid

The fluctuation scale \( \omega^* = \omega - \Delta_{\mu,\text{eff}}^* + W \text{sgn}(\Delta_{\mu,\text{eff}}) > 0 \) marks the boundary across which the tangential scattering processes become RG relevant (equation (4)). Starting from the QCP

\[
\omega^* = \omega - \Delta_{\mu,\text{eff}}^* = \Delta_{\mu,\text{eff}}^* + 1.
\]

As can be seen from the numerator of equation (4), a growing spectral weight gradually enhances the RG flow rate for tangential scattering processes. It is also important to note that on these gapless stretches, the effect of forward scattering is still RG relevant (equation (5)) leading to 2e–1h composite excitations of the marginal Fermi liquid. The tangential scattering processes, on the other hand, enhance the quasi-particle excitations of the Fermi liquid. The outcome of these competing tendencies is attributed to quantum critical scaling in the neighbourhood of a QCP at optimal doping.

The above equations for \( L^* \) and \( R_{\text{fl}}^* \) are satisfied within the windows \( \Lambda_{\sigma}^1 \) and \( \Lambda_{\sigma}^2 \) respectively. Near the QCP, \( \Lambda_{\sigma}^1 < \Lambda_{\sigma}^2 \) such that the MFL dominates over the FL within the gapless regions of the FS. Upon gradually increasing the doping away from the QCP leads to \( \Lambda_{\sigma}^1 > \Lambda_{\sigma}^2 \) such that the enhanced tangential scattering on the enlarged gapless stretches leads to the Fermi liquid quasiparticles dominating over the composite excitations of the MFL. The imaginary part of the single particle self-energy section 3 then allow us to obtain the inverse quasiparticle lifetime as a mixture of MFL and FL forms

\[
(\tau(\Delta_{\mu,\text{eff}}))^{-1} = \alpha(\Delta_{\mu,\text{eff}})\omega + \beta(\Delta_{\mu,\text{eff}})\omega^2,
\]

where the coefficients \( \alpha \) and \( \beta \) are functions of the chemical potential \( \Delta_{\mu,\text{eff}} \), and undergo a gradual evolution from QCP to the overdoped regions of the phase diagram. This gives rise to a mixed nature of the optical conductivity as a function of \( \Delta_{\mu,\text{eff}} \). This appears to be consistent with the observations of van der Marel et al [95], where a form of the optical conductivity that departs from the expected MFL form was attributed to quantum critical scaling in the neighbourhood of a QCP at optimal doping.

5. Symmetry breaking orders and superconductivity

In this section, we perform analysis of symmetry-broken phases for the Hubbard model upon doping away from 1/2-filling. As before, this involves a renormalization group analysis in the background of symmetry breaking fields: staggered chemical potential \( \sum_{ij}(-1)^{ij}n_i \) (for the \( \pi \), \( \pi \) charge density wave), staggered magnetic field \( \sum_{ij}(-1)^{ij}S_i^z \) (for the \( \pi \), \( \pi \) spin density wave), the spin-nematic order field \( Q_{\pi,\pi} = \langle r_1 - r_2 \rangle S_i^z S_j^z \), and finally a U(1) symmetry-breaking field \( \sum_{ikc} c_i^k \bar{c}_{\pi,k} \) for superconductivity. The corresponding RG equations are given in appendix A. The full RG phase diagram away from 1/2-filling, and with \( \pi \), \( \pi \) CDW, \( \pi \), \( \pi \) SDW, spin-nematic and d-wave superconducting broken symmetry orders, is shown in figure 9. The effective Hamiltonians and gap functions familiar for these symmetry broken states of matter are easily obtained from the dominant symmetry breaking coupling at the RG fixed point. Results for symmetry-broken orders at finite-temperature can then be obtained via standard mean-field methods. Below, we confine ourselves to a discussion of the findings shown in the phase diagram figure 9.

We find the \( \pi \), \( \pi \) SDW Neel antiferromagnet for energies \( 4 - \omega \geq 4 - \omega_{\text{ins}} = 1.2 \) and doping \( 0 \geq \Delta_{\mu,\text{eff}} \geq -1.75 \) (deep underdoping), and the \( \pi \), \( \pi \) CDW for energies \( 4 - \omega \geq 0.8 \) and doping \( -3.05 \geq \Delta_{\mu,\text{eff}} \geq -4 \) (moderately underdoped). A d-wave superconducting dome is found to extend between a doping range of \( -1.5 \geq \Delta_{\mu,\text{eff}} \geq -6 \) and has an optimal gap scale \( \Delta_{\text{sc}} \) at the critical doping \( \Delta_{\mu,\text{eff}} = -4 \) corresponding to the QCP. We have already presented earlier our finding for the variation of the superfluid density \( \rho_s \) with chemical potential, with a discussion on why \( \rho_s \) is maximal at optimal doping. In keeping with this, the highest \( \Delta_{\text{sc}} \) arises from a maximal density of bound Cooper pairs in the gapped regions of the Fermi surface interplaying with the critical fluctuations of the gapless regions for a chemical potential tuned to the QCP [96] (see green curve in figure 13(b)). The optimal quantum fluctuation energy scale for the onset of superconductivity is the kinetic energy of a pair of electrons from diametrically opposite nodal points on the FS: \( W/2 - \omega_{\text{sc}} = W/2 - 2\epsilon_{\Lambda^*}^{\text{node}} \), where \( \Lambda^*/\Lambda_0 \) is the
Figure 9. RG phase diagram for 2D Hubbard model with doping and \((\pi, \pi)\) CDW (green), \((\pi, \pi)\) SDW (red) and d-wave superconducting (SC) orders (yellow) included. \(K^*/U_0\) in the white-deep blue colourbar represents the ratio of renormalized coupling to bare coupling symmetry unbroken PG and ML states. Gap scales for various symmetry broken phases are shown in the colour bars. Origin of superconductivity from spin-PG nodal NFL with superconducting fluctuations is described in text. The SC 'dome' is centered about the QCP (optimality) and falls away on either side due to competition with insulating orders (underdoped) and gapless CFL (overdoped). The solid black line indicates the chemical potential dependent energy scale for the onset of nematic fluctuations, while the thin dashed line denotes the onset of superconducting fluctuations.

Figure 10. Figures (a) and (b) represents resistivity with (green) and without any form of symmetry breaking (blue), and inverse superfluid stiffness \((\sigma_{-1}^{-1})\), yellow) at various dopings. (a) \(\Delta\mu_{\text{eff}} = -1.75\) passage from PG to ML (blue), from PG to SC through spin-gap dominated ML. Inset: peak in spin susceptibility within SC region \(\Delta\mu_{\text{eff}} = -1.75\). (b) \(\Delta\mu_{\text{eff}} = -5.5\) passage from NFL to PG-CFL (blue), from NFL to SC through PG-CFL (green).

dimensionless spectral weight for the marginal nodal electronic quasiparticles obtained from the RG. Deep in the underdoped regime \((-1.5 \geq \Delta\mu_{\text{eff}} \geq -1.75\)), a coexistence of \((\pi, \pi)\) SDW and d-wave superconducting orders appears likely [97] (see inset of figure 10(a)). Similarly, within the lightly underdoped region, a coexistence of \((\pi, \pi)\) CDW and d-wave SC orders appears likely (see inset of figure 11(b)).

As a clear demonstration of the d-wave nature of the superconducting order parameter, we show in figure 12 the variation of the superconducting (SC) gap from maximum at one antinode (AN1 = (0, \(\pi\))) to a node at the nodal point \(k_x, k_y = (\pm \pi/2, \pm \pi/2)\) and finally maximizing again at (AN2 = (\(\pi\), 0)). The three curves are made at the brink of entry into SC dome from underdoping (blue), optimal (green) doping, and overdoping (red) sides. At optimality, the connected Fermi surface becomes an arc with lowering quantum fluctuation scale \(4 - \omega\) and collapses to a point on entering the superconducting dome. The journey from above the superconducting dome to the final entry into superconducting dome at optimal doping can be seen from the variation of the gap from antinodes to the nodes in figure 13(a).

The experiments in reference ([96]) appear to show that optimal superconductivity is associated with the largest Fermi surface volume at the brink of entering SC dome as optimality is approached from the underdoped side. We find evidence for this, as shown in figure 13(b). The graph for the mildly underdoped
Figures (a) and (b) show resistivity ($\rho$) with (green) and without any form of symmetry-breaking (blue), and inverse superfluid stiffness ($\sigma_{sc}^{-1}$, yellow) at various dopings. (a) $\Delta\mu_{eff} = -4$: passage from PG to ML (blue), from PG to SC through charge-gap dominated ML. Inset: peak in charge susceptibility within SC region. (b) $\Delta\mu_{eff} = -3.25$: passage from NFL with connected FS to spin-PG nodal NFL at QCP (blue), from NFL to SC through spin-PG nodal NFL (green).

Figure 12. Gap $\Delta_{sc}(\theta)$ vs the angular coordinate $\theta$ for chemical potential and $4 - \omega$ values given by $\mu_{eff} = -2.5, 4 - \omega_{c1} = 0.8$ (red curve) in the underdoped regime. At optimal doping $\Delta\mu_{eff} = -4.0, 4 - \omega_{c2} = 1.2$ (green curve). At overdoping $\Delta\mu_{eff} = -5.5, 4 - \omega_{c3} = 0.5$ (blue curve).

regime ($-2\Delta\mu_{eff} < W$) shows that a smaller Fermi pocket with high concentrations of holons and low concentration of bound spinon pairs undergoes a superconducting d-wave transition where the Fermi volume shrinks to a point. In the optimally doped regime ($-2\Delta\mu_{eff} \sim W$) on the brink of transitioning into the superconducting dome, we observe a larger gapless Fermi pocket with a peak in the concentration of Cooper pairs (in the gapped parts of the Fermi surface) and an intermediate concentration of holons. On the brink of entering the dome at overdoping ($-2\Delta\mu_{eff} > W$), we find a reduction in the Cooper pair density at the neighbourhood of the antinodes coinciding with a lowering hole concentration on a fully connected Fermi surface. This shows that optimality arises from an interplay of a peak in the density of Cooper pairs in the gapped parts of the Fermi surface (as well as the superfluid density $\rho_s$) and the critical fluctuations associated with a quantum critical Fermi surface (arising from the QCP). The dome-like structure of $T_C$ is observed to be inherited from the similar structure of $T_{on}$ (as discussed earlier; also see appendix A), and offers an explanation for the quadratic dependence of $T_C$ on the hole-doping concentration commonly observed in the cuprates [98].

We now establish the origin of the nodal structure of d-wave superconducting order as the QCP at $\mu_{eff} = -4$. We have shown above that the nodal points support a gapless NFL metal, as the irrelevance of all gapping mechanisms at the nodes arise from the topological signature of the doublon propagator. Thus, the onset of superconductivity at critical doping takes place in the backdrop of this protection for the nodal gapless states. We have also seen that the spin-gap at optimal doping has d-wave structure, but without a sign change across the nodes. The $U(1)$ phase rotation symmetry breaking RG calculation presented in appendix A further reveals that the nodal points act as domain walls for the growth of the superconducting

![Figure 11](image1.png)

![Figure 12](image2.png)
Figure 13. (a) Gap $\Delta(\theta)$ vs the angular coordinate $\theta$ along the $\Delta_{\mu_{\text{eff}}} = -4.0$ optimal doping axis for different values of $4 - \omega_{SC}$ lying above the dome. The different curves have been staggered for purposes of clarity. The gap $\Delta(\theta)$ vs the angular coordinate upon just entering the superconducting dome is given by the black curve. (b) Left vertical axis: blue curve represents the gapless arc length of the Fermi surface at the brink of the superconducting transition for six different $\omega_{cric}$ and $-2\Delta_{\mu_{\text{eff}}}$ values i.e., $(2.922, 6.5), (2.869, 7.0), (2.837, 7.5), (2.827, 8.0), (2.839, 8.5)$, and $(2.87, 9.0)$. Right vertical axis: at those same values, the green curve represents the Cooper pair density in the gapped regions in the neighbourhood of the antinodes, and the red curve represents the holon densities in the gapless parts neighbouring the nodes.

Figure 14. Figures (a)–(d) show the full momentum space resolved spectral function $A(k\Lambda)$, where the black curves show extent of SC fluctuations around Fermi surface. (a) To the right of SC dome (CFL). (b) Within d-wave SC dome, with nodal NFL. (c) To the left of SC dome (ML). (d) Vertically above SC dome at optimal doping.

order upon scaling down to low energies: the RG-integrated superconducting order parameter 
\[
\langle c_{\Lambda}^\dagger c_{\Lambda} \rangle = -\langle c_{\Lambda}^\dagger c_{\Lambda} \rangle \propto e^{i\gamma_{s,node}},
\]
where the relative phase $\gamma_{s,node} = -i \ln(\text{sgn}[2(\epsilon_{\Lambda} - \epsilon_{\Lambda_{\text{node}}})])$ and $2(\epsilon_{\Lambda} - \epsilon_{\Lambda_{\text{node}}})$ is the energy scale for a Cooper pair (with respect to the nodes). The alternation of sign in this energy scale is, thus, the alternation in sign of the pairing order parameter.

The suppression of d-wave superconductivity is clearly observed in the presence of the CDW order (figure 5(a)), while the charge-gap dominated Mott liquid (dark blue region in figure 5(a)) leads to further suppression of superconductivity. These results obtained are in consonance with the finding of two distinct antinodal energy-gap scales in recent ARPES and STM experiments carried out on the PG phase of the cuprate La-Bi2201 [99], one of which appears to be linked with the onset of superconductivity and the other with charge ordering. The black curve in the RG phase diagram corresponds to the onset of spin-nematic fluctuations, and appears to be confined within a range of chemical potential $-1.4 \geq \Delta_{\mu_{\text{eff}}} \geq -4$ associated with moderate to light underdoping. The highest scale (in $4 - \omega$) for the onset of spin-nematic fluctuations lies well within the pseudogapped part of the phase diagram, in broad agreement with recent experimental findings in the cuprates [100–104]. For $-4 \geq \Delta_{\mu_{\text{eff}}} \geq -6$, the competition between the nodal NFL metal, the spin-pseudogapped parts of the FS and the tangential scattering leads to the reconstruction of the FS. This is apparent in the suppression of superconducting fluctuations (dashed line in figure 5) beyond critical doping and shows how competition with the CFL suppresses d-wave superconductivity. Variations of the resistivity ($\rho$) and inverse superfluid stiffness ($\frac{1}{\sigma_{SC}}$) upon tuning $\omega$ towards the QCP is shown in figures 11(a) and (b) (see also videos S5 and S6). Maps of the single-particle spectral function $A(E)$ within and in the neighbourhood of the d-wave SC phase are also presented in figures 14(a)–(d). These results are in excellent agreement with several transport and spectroscopy measurements made in various parts of the cuprates phase diagram [45, 62, 63, 88–90, 93, 94, 99–104].

Finally, we close this section by computing numerical values for some of the temperature scales, e.g., $T_{\text{ons}}$ (the onset of the formation of pre-formed Cooper pairs at the gapped antinodal regions) and $T_{\text{ML}}$ (the
scale at which the entire FS is gapped during the formation of the Mott liquid), for the materials HgBa$_2$CuO$_4$ and La$_2$CuO$_4$ by using the values for the parameters of the effective one-band Hubbard model found in reference [105]. First, in the limit of large system size $N \to \infty$, using the formula for $\bar{\omega}_{\text{ons}}^c$ (equations (29) and (5)), we obtain

$$\bar{\omega}_{\text{ons}}^c \leq \omega_{\text{PG}} = \frac{\Lambda^{**}N^2}{8\pi \sqrt{2}} \frac{16\pi^2}{N^2} = \sqrt{2t\pi\Lambda^{**}} = \sqrt{2t\pi} \arcsin \left( \frac{\bar{\omega}}{2t} \right) = 0.067t,$$  

(33)

where $\bar{\omega} \approx \omega_{\text{PG}} = 0.034t$ as given earlier. Then, using the values of the hopping parameter $t$ for HgBa$_2$CuO$_4$ and La$_2$CuO$_4$ with $t \approx -0.461, -0.482$eV [105], we find the onset temperature scale of pair formation $T_{\text{ons}}$ is bounded (on the upper side) by the pseudogap temperature $T_{\text{PG}}$ are given by $T_{\text{PG}} = 0.067t \times 11.605K = 358K$ and $374K$ for HBCO and LCO respectively. This is in fair agreement with experimental estimates of $T_{\text{PG}} \sim 200–300K$ for most of the cuprates [106]. That the onset temperature scale for pairing $T_{\text{ons}}$ is less than $T_{\text{PG}}$ is consistent with the findings from Nernst measurements of reference [94].

Further, we find $T_{\text{ML}} \approx \frac{N}{t_{\text{ons}} \omega_{\text{PG}}} = 119K$ and $124K$ for HBCO and LCO respectively. Recalling the relation between $T_{\text{ML}}$ and the superconducting transition temperature $T_C$ obtained in equation (A.14), we see that the upper bound for $T_C$ is provided by $T_{\text{ML}}$. An upper bound of around 120K for the $T_C$ is reasonable for the experimentally known $T_C$ of 40K for LCO and 90K for HBCO. Importantly, $T_C$ is also found to be bounded (on the upper side) by $T_{\text{ons}}$ (see equation (A.13)), it appears plausible to search for mechanisms that can raise $T_C$ further towards $T_{\text{ons}}$. We will further discuss this point briefly in the concluding section.

6. Conclusions and perspectives

There are several interesting consequences of our RG analysis of the hole-doped 2D Hubbard model on the square lattice, and we now discuss each of these in turn. First, we wish to stress that the simplicity of the Hubbard Hamiltonian (i.e., possessing effectively only two parameters, $U/t$ and $\mu/t$) offers the possibility that several of our results are of likely importance for the broad understanding of the phenomenology of filling-driven Mott transitions in a variety of strongly correlated electronic systems with strong electronic differentiation arising from the tight binding dispersion [1]. Equally importantly, given the recent experimental demonstration in reference [58] of the encapsulation the entire cuprate phase diagram from experiments on a monolayer crystal of Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ containing only two Cu–O planes, we believe that our study is of importance in learning the physical mechanisms responsible for the complexity of the phase diagram. Indeed, the striking similarities between the RG phase diagram presented in figure 5 with the well-known experimental phase diagram of the cuprates [45] (with the quantum fluctuation axis $\omega$ in the former replaced by temperature in the latter) suggest that we have taken strides in meeting our goal.

In the RG phase diagram figure 2, the collapse of the pseudogap for charge excitations (Mottness) upon hole doping is seen to lead to a QCP lying between Mott liquid and correlated Fermi liquid phases. The QCP involves a drastic change in the nature of the ground state as well as the many-body spectrum: the underdoped side of the QCP is a gapped and hole-doped Mott liquid, while the overdoped side involves the collapse of Mottness as the mechanism for the formation of hole pairs. Upon including the possibility of phase stiffness within the RG, we find the existence of a dome of d-wave superconductivity that surrounds the QCP. Remarkably, even as the superconducting phase shields the QCP, it possesses properties of that criticality (e.g., gapless nodes, gap with d-wave symmetry). In this way, we find that the pseudogap is both friend and foe to the emergent superconductivity: the underdoped
Mottness-related pseudogap contains fluctuations that can nucleate various orders (SDW, CDW and spin-nematicity) imimical to superconducting order, its collapse unveils the spin-pseudogapped state of matter that finally leads to a state with pre-formed Cooper pairs (and eventually phase stiffness and the ODLRO pertaining to superconductivity).

We can now address the striking qualitative agreement of RG phase diagram figure 5 with the experimentally obtained temperature versus doping phase diagram for the cuprates [45]. We believe that this arises from the fact that the RG unveils an entire hierarchy of energy scales on the quantum fluctuation axis $\omega$ related to the metallic, pseudogap, Mott liquid and symmetry broken phases. Further, at various points in this work, we have shown analytic relations between these $T=0$ energy scales and equivalent temperature scales at which these phases can be observed. Importantly, we have also established that the hierarchy of temperature scales for the pseudogap ($T_{\text{PG}}$), onset temperature for pairing ($T_{\text{onset}}$), formation of the Mott liquid ($T_{\text{ML}}$) and superconductivity ($T_{\text{C}}$) obtained from our analysis is quantitatively consistent with that observed experimentally for some members of the cuprates.

The effective Hamiltonians and low-energy wavefunctions obtained for the fixed points of the RG formalism has afforded considerable insight into the nature of the Mott liquid at half-filling, as well as with hole doping. This is evidenced by the remarkable consistency between the numbers obtained for the ground state energy per site and double occupancy fraction with those obtained from various numerical methods in reference [75–77]. This benchmarking gives us confidence in the nature of the Mott liquid state as well as in the quantum phase transition that it undergoes upon doping. The effective Hamiltonians have also enabled an understanding of the essence of various universal features of the large body of experimental results obtained for the cuprates, e.g., Homes law, Planckian dissipation and the T-linear resistivity of the normal state, the mixed nature of the optical conductivity at overdoping, optimality with doping and the dome-like structure of the superconducting phase etc. In seeking further comparisons with the extensive body of experimental data available for the cuprates, it appears plausible to carry out a numerical simulation of these effective Hamiltonians at finite temperature. We leave this for a future work.

Even as these results offer considerable evidence that the strong correlation physics of the one-band Hubbard model at, and away from, 1/2-filling is pertinent to the physics of high-temperature superconductivity [107], they also open several new directions for further investigation. Foremost among these lies the search for answers to questions on what makes certain members of the cuprate family special in the search for higher superconducting $T_{\text{C}}$, as well as what could enable a raise in $T_{\text{C}}$. In reaching some conclusions on the former, the results obtained from recent DFT + downfolding study of Hirayama et al [105] on $\text{La}_2\text{CuO}_4$ and $\text{HgBa}_2\text{CuO}_4$ offer some insight. This study appears to conclude that the latter member of the cuprate family has a higher $T_{\text{C}}$ than the former as it is better described by an effective one-band Hubbard model in two dimensions, whereas the former is likely to have a larger hybridisation with a second dispersive band (arising from the Cu $3d_{x^2−y^2}$ orbital) near the putative Fermi surface. It appears quite plausible that such hybridisation will be harmful to the physics of the Mott liquid and resulting emergent superconductivity we find from our studies, and can be studied in future. This suggests that materials that afford the isolation of Cu–O planes described by an effective 2D one-band Hubbard model are more likely to offer a higher superconducting $T_{\text{C}}$, and is consistent with the recent findings of high-temperature superconductivity from a monolayer crystal of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ [58].

In seeking answers to the question on how to further raise the superconducting $T_{\text{C}}$, it is important to make an increasingly realistic model pertinent to the cuprates. Thus, one should first investigate the role played by next-nearest neighbour hopping within the Cu–O plane. Our results predict, for instance, that shortening the extent of the pseudogap will likely enhance the optimal quantum fluctuation energy scale for the onset of d-wave superconducting order. This can be achieved, for instance, by tuning the curvature of the Fermi surface via next-nearest neighbour hopping [108]. Similarly, a study of the effects of an inter-plane electron hopping element appears relevant, as the presence of other Cu–O planes is observed in some members of the cuprates (e.g., $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ (Bi2223) [109], $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$ (Hg1223) [110] and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (Y123) [111] as being important in leading to higher $T_{\text{C}}$ upon the application of pressure. Our findings are also likely to be pertinent to the ubiquitous presence of superconductivity in several other forms of strongly correlated quantum matter, e.g., the heavy-fermion systems, where there exist proposals for how the collapse of Mottness can lead to superconductivity [112]. For instance, as a particle-hole transformation on one of the sublattices of the 2D square lattices connects between the repulsive and attractive Hubbard models ([113]), we believe that our results are also significant in understanding the physics of the latter. Finally, given that we now have wavefunctions available for the ground and low-lying excited states of the doped Mott liquid, a direction worth pursuing is to understand the nature of many-body entanglement in this system. Given the effort presently invested in such investigations, any progress in this direction will likely help usher new ways in which to think about the many-particle physics of strongly correlated electronic systems.
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Appendix A. RG equation of the symmetry breaking orders

In the doped Mott liquid Hamiltonian (equation (20)), we include \((\pi, \pi)\) charge density wave, \((\pi, \pi)\) spin density wave symmetry-breaking fields together with the Hamiltonian for the 1-e and 2e–1h composites (equation (7))

\[
\hat{H} = \sum_{s, j} \Delta A_{s, j} + \sum_{s, j} \Delta S_{s, j} + \sum_{s, j} \epsilon_{s, j} \Delta \mu_{\text{eff}} \left( \hat{n}_{s, j} - \frac{1}{2} \right) + \sum_{s, j} \hat{b}_{s, j} \hat{a}_{s, j} (1 - \hat{n}_{s, j}) + \sum_{s, j} \hat{U}_{s, j} \hat{S}_{s, j},
\]

where \(A_{s, j}\) and \(S_{s, j}\) are the \(x\)-components of the charge and spin pseudospins respectively given by equation (12). We now perform a second level of the RG calculation for the symmetry-breaking instabilities by block-diagonalizing in the eigenbasis of the single-particle piece of the Hamiltonian equation (A1)

\[
\hat{H}_1 = \sum_{s, j} \epsilon_{s, j} \hat{A}_{s, j} + \hat{S}_{s, j} = \hat{H}_1.
\]

The RG equations for the CDW and SDW instabilities are given by

\[
\frac{\Delta K_{\epsilon/\lambda\sigma}}{\Delta \log \Lambda} = \frac{K_{\epsilon/\lambda\sigma}^2}{\omega - \tilde{\epsilon}_{\epsilon/\lambda\sigma} - \frac{1}{4}K_{\epsilon/\lambda\sigma}}.
\]

The fixed point values of the CDW and SDW gaps can be obtained from the fixed points reached by solving the RG equations

\[
\omega - \tilde{\epsilon}_{\epsilon/\lambda\sigma} - \frac{1}{4}K_{\epsilon/\lambda\sigma}^2 = 0 \rightarrow \Delta_{\ast} = \frac{1}{2} \sum_{j} K_{j}^2 \langle S_{s, j}^z \rangle, \quad \Delta_{\ast} = \frac{1}{2} \sum_{j} K_{j}^2 \langle S_{s, j}^z \rangle.
\]

Finally, in order to achieve the phase stiffness and ODLRO associated with superconductivity, we add a \(U(1)\) symmetry-breaking field to the Hamiltonian equation (19) \(\hat{H}_{SB} = \sum_{\lambda, j} \Delta \mu_{\text{eff}} \hat{S}_{s, j}^\lambda\), where \(\Delta \mu_{\text{eff}} = \hat{c}_{s, j}^\lambda \hat{c}_{s, j}^\lambda \) is defined in equation (12). By performing the block-diagonalization in the rotated single-particle basis (i.e., similar to equation (A2)), leads to a modified RG equation (equation (19)) for the superconducting fluctuation terms in equation (19)

\[
\Delta K_{\epsilon/\lambda\sigma\lambda} \left( \delta \right) = \frac{-\left( 1 - p \right) \left( K_{\epsilon/\lambda\sigma\lambda} \left( \delta \right) \right)^2}{\omega - \frac{1}{2} \sqrt{\Delta_{\ast}^2 + \left( \epsilon_{s, j} + \epsilon_{\cdot, \cdot, \cdot} \right) \left( \Delta \mu_{\text{eff}} - \Delta \mu_{\text{eff}}^\lambda \right)} + 2 \left( \hat{S}_{s, j}^\lambda \right)^2} - \frac{\left( 1 - p \right) \left( \epsilon_{s, j} - \epsilon_{\cdot, \cdot, \cdot} \right) - \frac{K_{\epsilon/\lambda\sigma\lambda}^2 \left( \delta \right)}{4}}{\omega - \frac{1}{2} \sqrt{\Delta_{\ast}^2 + \left( \epsilon_{s, j} + \epsilon_{\cdot, \cdot, \cdot} \right) \left( \Delta \mu_{\text{eff}} - \Delta \mu_{\text{eff}}^\lambda \right)} + 2 \left( \hat{S}_{s, j}^\lambda \right)^2} - \frac{\left( 1 - p \right) \left( \epsilon_{s, j} - \epsilon_{\cdot, \cdot, \cdot} \right) - \frac{K_{\epsilon/\lambda\sigma\lambda}^2 \left( \delta \right)}{4}}{\omega + \text{sgn} \left( \Delta \mu_{\text{eff}} \right) W + \left( \epsilon_{s, j}^\lambda - \Delta \mu_{\text{eff}} \right) - L_0^\lambda \left( \delta \right)}
\]

(A.5)
where we have taken \( \Lambda_j = \Lambda_0 \exp(-j) \) and \( \Lambda_{j-1} = \Lambda_0 \exp(-(j - 1)) \), such that \( \Delta \log \Lambda_0 = 1 \). The RG equation at critical doping \( \Delta \mu_{\text{eff}} = \Delta \mu_{\text{eff}}^* \) is given by

\[
\Delta K_{0,0,j}(\delta) = -\frac{(K_{0,0,j}^{(i)}(\delta))^2}{\omega - \frac{1}{2} \sqrt{\Delta_{\omega}^2 + (\epsilon_{k_{j1}} + \epsilon_{-k_{j1}} + 2\Sigma(\delta))^2} - \frac{(1-p)K_{0,0,j}^{(i)}(\delta)}{4}}
\]

\[
\omega - \frac{1}{2} \sqrt{\Delta_{\omega}^2 + (\epsilon_{k_{j1}} + \epsilon_{-k_{j1}} + 2\Sigma(\delta))^2} - \frac{K_{0,0,j}^{(i)}(\delta)}{4}.
\]

(A.6)

In what follows, we show how this RG equation unveils the d-wave symmetry of the SC order. For \( \omega < \omega^* = 2^{-1} \max (\epsilon_{k_{j1}} + \epsilon_{-k_{j1}} + 2\Sigma(\delta))^2 = 4 \sin(\Lambda_0/\sqrt{2}) \) (the highest kinetic energy of pairwise states present along the nodes at a distance \( \Lambda_0 \)) in a momentum-space arc centered about the nodes, we find that the RG equation for superconducting fluctuations is RG irrelevant: \( \Delta K_{0,0,j} < 0 \), as \( \omega - \frac{1}{2} \sqrt{\Delta_{\omega}^2 + (\epsilon_{k_{j1}} + \epsilon_{-k_{j1}} + 2\Sigma(\delta))^2} < 0 \). On the other hand, the RG equation for superconducting fluctuations for all the other normal directions to the FS are RG relevant.

Beyond \( \omega \gg \omega^* \), a gapless nodal stretch extends on both sides of the FS from \( k_{j1} \) to \( k_{j2} \). The fixed point Hamiltonian for \( \Delta \mu_{\text{eff}} = \Delta \mu_{\text{eff}}^* \) and for \( 2^{-1}W > \omega \gg \omega^* \) (with the initial \( \Delta_{\omega} = 0 \) is given by

\[
H_{\text{sc}}^* = \sum_{\Lambda,\delta=bj} \epsilon_{\Lambda,\delta} B_{\Lambda,\delta}^\dagger B_{\Lambda,\delta} + \sum_{p,j} B_{\Lambda,\delta}^\dagger \hat{n}_{j,p} h_{j,p} (1 - \hat{n}_{j,p}) + \sum_{p,j} \left( \sum_{\Lambda} \left( K_{0,0,j}(\delta) \right) (B_{-2\Lambda + A,j}^\dagger + B_{A,j}^\dagger) + \text{h.c.} \right)
\]

\[
+ \sum_{\Lambda} \left( K_{0,0,j}(\delta) (B_{-2\Lambda + A,j}^\dagger - B_{-2\Lambda + A,j}) \right) (B_{A,j}^\dagger - B_{A,j})
\]

(A.7)

where \( \Delta_{\omega}^*(\omega) = \sum \left( \sum_{\Lambda} \left( K_{0,0,j}(\delta) \right) (B_{-2\Lambda + A,j}^\dagger - B_{-2\Lambda + A,j}) \right) \) and \( K_{0,0,j}(\delta) = 4(\omega - \frac{1}{2} (\epsilon_{k_{j1}} + \epsilon_{-k_{j1}} + 2\Sigma(\delta))) \). Here, the first and second terms are the 1e and 2e–1h dispersions of the gapless nodal stretches respectively. The third and fourth terms denote the dispersion of the antinodal stretch residing outside and inside the emergent window respectively. The single-particle states residing outside the emergent window, i.e., \( \Lambda > \Lambda^* \), correspond to gapped marginal Fermi liquid quasiparticles with self energy given by equation (9). Finally, the fifth and sixth terms describe the effective \( U(1) \) symmetry-breaking mean-field and the (emergent Nambu–Goldstone) superconducting fluctuations respectively.

In this way, we obtain the self consistency equations for the superconducting order parameter (with d-wave symmetry) from the eigenstates of the symmetry-broken Hamiltonian lying within the emergent window

\[
\langle c_{A,\delta}^\dagger c_{A,\delta} \rangle = \frac{\Delta^2_{\omega}(\omega)}{\sqrt{\Delta^2_{\omega}(\omega) + (\epsilon_{A,j} + \Sigma(\delta))^2}}, \quad \langle c_{A,\delta}^\dagger c_{A,\delta} \rangle = \frac{\Delta^2_{\omega}(\omega)}{\sqrt{\Delta^2_{\omega}(\omega) + (\epsilon_{A,j} + \Sigma(\delta))^2}}
\]

(A.8)

and \( \langle c_{A,\delta}^\dagger c_{A,\delta} \rangle = 0 \). For minimizing the energy, we require \( \langle c_{A,\delta}^\dagger c_{A,\delta} \rangle = -\langle c_{A,\delta}^\dagger c_{A,\delta} \rangle \), such that \( K_{0,0,j}(\delta) (\langle c_{A,\delta}^\dagger c_{A,\delta} \rangle) (\langle c_{A,\delta}^\dagger c_{A,\delta} \rangle) < 0 \). The vanishing of the nodal order parameter \( \langle c_{A,\delta}^\dagger c_{A,\delta} \rangle \), along with the above displayed change of sign in the order parameter upon crossing the nodes, manifests in the d-wave nature of the superconductivity.

From the above analysis, we can now extract a temperature scale for the symmetry-broken d-wave superconductor using the relation between the quantum fluctuation scale \( \omega \) and temperature (2)) and the effective 1e self-energy of the states residing outside the emergent window. For this, we first expand the gapped dispersion energy about the one-particle gap \( \Delta_{\omega}^* \)

\[
\sqrt{\Delta^2_{\omega}(\omega) + (\epsilon_{A,j} + \Sigma(\delta))^2} = \Delta_{\omega}^* \sqrt{1 + \frac{(\epsilon_{A,j} + \Sigma(\delta))^2}{\Delta^2_{\omega}}} \approx \Delta_{\omega}^* \left( \frac{\epsilon_{A,j} + \Sigma(\delta)^2}{2\Delta_{\omega}^*} \right) \approx \frac{\epsilon_{A,j} + \Sigma(\delta)^2}{\Delta_{\omega}^*}.
\]

(A.9)
We thus obtain the renormalized self-energy along the nodal direction by choosing $\omega = \omega^*$ and using equation (9)

$$
\Sigma^{\omega^*}(\hat{s}) = \Delta_N^* = 4 \left( \omega^* - \epsilon_{\Lambda^* \beta} - \Sigma(\hat{s}) \right) f(\hat{s}, \omega^*) = 2\Delta_N^* \frac{f(\hat{s}, \omega^*)}{N^*(\hat{s}, \omega^*)} \ln \left| N^*(\hat{s}, \omega^*) \frac{\omega}{\omega^*} \right|,
$$

where $f(\hat{s}, \omega) = \sum_{i} \langle B_{\Lambda^* + \delta, \hat{s}} \rangle_x$ is the net spectral weight of the Cooper pairs along the normal $\hat{s}$ obtained from the self-consistency equations equation (A.8). In the above expression, we can determine $\Delta_N^*$ by following the steps leading to the derivation of equation (29)

$$
\Delta_N^* = \frac{N^*(\hat{s}_1, \omega^*)}{2} (\epsilon_{\Lambda_0 \beta} - \epsilon_{\Lambda^* \beta}).
$$

Here, $\Lambda^*$ is fixed point for equation (5). Using the relation between the quantum fluctuation scale $\omega$ and an equivalent temperature scale, we obtain the $T_C$ for the d-wave superconductivity as follows

$$
T_C = \frac{2\hbar}{k_B} \max \frac{\omega}{\sqrt{\lambda}} f(\hat{s}, \omega^*) = \frac{2\hbar}{k_B} (\epsilon_{\Lambda_0 \beta} - \epsilon_{\Lambda^* \beta}) f(\hat{s}_1, \omega^*),
$$

where $\hat{s}_1 = \hat{s}_{AN} \left( 1 - \frac{\Delta_p}{\sqrt{\lambda}} \right)$. The ratio of $T_C$ with onset scale of superconductivity $T_{ons}$ is then obtained as

$$
\frac{T_s}{T_{ons}} = 2 \frac{\epsilon_{\Lambda_0 \beta} - \epsilon_{\Lambda^* \beta}(\omega^*)_{\hat{s}_1}}{\epsilon_{\Lambda_0 \beta} - \epsilon_{\Lambda^* \beta}(0)} \frac{f(\hat{s}_1, \omega^*)}{N^*(\hat{s}_1, 0)}.
$$

For the Mott liquid, the temperature scale $T_{ML} = \frac{2N^*(\hat{s}_1, \omega^*)}{\sqrt{\lambda}} \left( \epsilon_{\Lambda_0 \beta} - \epsilon_{\Lambda^* \beta}(\omega^*)_{\hat{s}_1} \right)$ ([2]). As $\epsilon_{\Lambda_0 \beta} + \epsilon_{\Lambda_0 \beta} \simeq \epsilon_{\Lambda_0 \beta} = \epsilon_{\Lambda_0 \beta}(\hat{s}_{AN})$, we find $\omega_{ons} \approx \omega^*$, and we can write the ratio of $T_C$ and $T_{ML}$ as

$$
\frac{T_C}{T_{ML}} = 2 \frac{f(\hat{s}_1, \omega^*)}{N^*(\hat{s}_1, 0)}.
$$

Finally, the Hamiltonian that describes the inclusion of spin-nematic ordering for the spins is given by

$$
H_{nm} = Q(S_{nm}^{(i)})^2 + Q(S_{nm}^{(i)})^2 - 2Q(S_{nm}^{(i)})^2,
$$

where $S_{nm}^{(i)} = \sum_{x} S_i$, $i = (x,y,z)$ are the net spin angular-momentum operators along the x, y and z directions. The RG equation for spin-nematic ordering has the form

$$
\Delta Q_{ij} = \frac{Q_{ij}^2}{\omega - \frac{Q_{ij}}{4}} - \frac{P_i(K_{ij}^0)^2}{\omega - \epsilon_{p,q} - K_{ij}^0 - \frac{Q_{ij}}{4}},
$$

where the first term denotes the contribution from spin-nematic fluctuations, while the second term denotes the contributions from superconducting fluctuations that suppress nematicity.

**Appendix B. Benchmarking results for $2 \leq U/t \leq 12$**

In table B1, we present results for the ground state energy per site $E_g$ obtained from the RG fixed point theories for various values of $U/t$ at $f_h = 0$ and $f_h = 0.125$ hole doping (see main text for details of the method). The values in the third and fifth columns for $U/t = 2, 4, 6, 8, 12$ are obtained from several different numerical methods, as presented in LeBlanc et al [75] and Ehlers et al [76]. The ground state energy values for $U/t = 10$ are obtained from exact diagonalization studies [77] of a $4 \times 4$ Hubbard-cluster. The value in the fifth column for $U/t = 12$ and $f_h = 0.125$ (1/8 filling) is absent, as no values are available in the literature to compare against. We note that while the ground state energies shown in table B1 are typically either within the range found from various numerical methods or lie close to the range, the ground state energy value obtained for $U/t = 10$ and $f_h = 0.125$ is much lower than the range found the numerics of reference [75]. We do not understand the reason for this discrepancy at present. Further comparative and detailed investigations will be needed to resolve this discrepancy, and will be dealt with in a subsequent work.

Further, in figure B1, we present a plot of the ground state energy per site ($E_g$) obtained for $U/t = 8$ from the RG method for a k-space grid of size 1024 × 1024 (blue circles) and exact diagonalization (ED) on a 4 × 4 cluster (from data in reference [77]). The two approaches are in close agreement for small hole-doping ($f_h \lesssim 12.5\%$). However, while the RG unveils a QCP upon increasing doping, the ED calculations show a rounded-out minima. We have checked that the precisely the same QCP is attained at $U/t = 8$ from the RG for k-space grid sizes down to 256 × 256. This reveals the fact that while ED
Table B1. Ground state energy per site values obtained from the RG fixed points for $U/t = 2, 4, 6, 8, 10, 12$. The error bar for all data obtained from the RG is $O(10^{-4})$. Third and fifth columns for $U/t = 2, 4, 6, 8$ and 12 represent the range of values obtained for the ground state per site from several different numerical methods (presented in references [75–77]) for the half-filled ($f_h = 0$) and the doped ($f_h = 1/8$) Hubbard model respectively.

| $U_0/t$ | $E_g$ from RG $f_h = 0$ | $E_g$ from various numerical methods ($f_h = 0$) collated from [75, 77] | $E_g$ from RG at $f_h = 1/8$ | $E_g$ from other numerical methods ($f_h = 1/8$) collated from [75, 77] |
|---------|--------------------------|-----------------------------------------------------------------|--------------------------|-----------------------------------------------------------------|
| 2       | $-1.199$                 | $(-1.176)$–$(-1.116)$                                           | $-1.28$                  | $(-1.285)$–$(-1.267)$                                           |
| 4       | $-0.854$                 | $(-0.864)$–$(-0.85)$                                           | $-0.996$                 | $(-1.026)$–$(-1.0)$                                           |
| 6       | $-0.652$                 | $(-0.658)$–$(-0.651)$                                           | $-0.857$                 | $(-0.865)$–$(-0.829)$                                           |
| 8       | $-0.526$                 | $(-0.53)$–$(-0.51)$                                           | $-0.777$                 | $(-0.766)$–$(-0.709)$                                           |
| 10      | $-0.439$                 | $(-0.439)$                                           | $-0.733$                 | $-0.675$                                           |
| 12      | $-0.367$                 | $(-0.369)$–$(-0.362)$                                           | $-0.744$                 | —                                                             |

Figure B1. Plot of the ground state energy per site ($E_g$) obtained for $U/t = 8$ from the RG method for a $k$-space grid of size $1024 \times 1024$ (blue circles) and exact diagonalization (ED) on a $4 \times 4$ cluster (from data in reference [77]). The two approaches are in close agreement for small hole-doping ($f_h \leq 12.5\%$). However, while the RG reveals a QCP upon increasing doping, the ED calculations show a crossover behaviour expected for a small system.

Calculations show the crossover behaviour expected for a small system, the RG captures well the physics arising from divergent fluctuations of the doped Mott liquid near critical hole-doping $f_h^*$.

ORCID iDs

Siddhartha Lal https://orcid.org/0000-0002-5387-6044

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