 Finite-temperature charge dynamics and the melting of the Mott insulator

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The Mott insulator is the quintessential strongly correlated electronic state. A full understanding of the coupled charge and spin dynamics of the Mott-insulating state is thought to be the key to a range of phenomena in ultracold atoms and condensed matter, including high-Tc superconductivity. Here we extend the slave-fermion (holon-doublon) description of the two-dimensional Mott insulator to finite temperatures. We benchmark its predictions against state-of-the-art quantum Monte Carlo simulations, finding quantitative agreement. Qualitatively, the short-ranged spin fluctuations at any finite temperatures are sufficient to induce holon-doublon bound states, and renormalize the charge sector to form the Hubbard bands. The Mott gap is understood as the charge (holon-doublon) gap renormalized downwards by these spin fluctuations. With increasing temperature, the Mott gap closes while the charge gap remains finite, causing a pseudogap regime to appear naturally during the process of melting the Mott insulator.

The Mott insulator1 and its associated metal-insulator transition (MIT)2,3 have been recognized since the foundational work of Mott and Peierls4 as phenomena generic to strongly correlated electron systems. The discovery of high-Tc superconductivity in a class of quasi-two-dimensional (quasi-2D) doped Mott insulators5 triggered an enduring experimental and theoretical quest to understand the many anomalous properties of the cuprates, including the strange metal, the pseudogap6–8 and indeed the superconductivity itself, in a complete and correct description of the Mott insulator.

In Mott’s original proposal,2 the insulating state arises due to the strong on-site Coulomb interaction, U, and has no explicit relation to symmetry-breaking, which usually takes the form of magnetic order. Hubbard9 obtained the incoherent upper and lower Hubbard bands and considered the interaction-driven MIT, while Brinkman and Rice associated the MIT with the divergence of the quasiparticle mass.10 Although these results are the cornerstone of our understanding of the Mott insulator, they do not take into account the spin fluctuations and their influence on the charge dynamics. In experiment, most Mott insulators possess antiferromagnetic (AFM) long-range order at low temperatures.3 However, in 2D this is forbidden at T > 0 by the Mermin-Wagner theorem and the low-energy physics is dominated by short-ranged spin fluctuations.11–16 For any finite U, charge fluctuations are also important, because they create empty sites (holons) and doubly-occupied sites (doublons), whose tendency to form bound states has been proposed as the key to the high-energy physics of the Mott insulator.17–24 Clearly a full description requires a proper account of both spin and charge fluctuations.25 While progress has been made in this direction through the development and application of a wide variety of sophisticated numerical methods,26 a physical understanding remains far from complete.

In this study we use a holon-doublon formulation to provide such insight. We perform analytical slave-fermion calculations and compare these with quantum Monte Carlo (QMC) simulations to verify their quantitative accuracy. Qualitatively, this approach is capable of treating both the low- (spin) and high-energy (charge) degrees of freedom in a consistent way, thereby capturing their interplay. We show that long-ranged AFM order is not required, because short-ranged spin fluctuations induce holon-doublon bound states, and further that they renormalize the charge sector to produce a Mott gap that is smaller than the charge (holon-doublon) gap. This reconstruction of the electronic states produces a quasiparticle, the “generalized spin polaron,” at the Hubbard-band edges, while most of the composite states lie higher in energy and their thermal evolution explains the origin of the pseudogap regime in the Mott insulator.

Analysis

Our slave-fermion analysis is performed within the self-consistent Born approximation (SCBA, see Methods).24 Our QMC simulations deploy the most modern versions (see Methods) of standard techniques27–29 and the dynamical information is obtained by stochastic analytic continuation (SAC).30,31 The formation of holon-doublon bound states establishes the charge sector, with a charge gap on the scale of U, and its convolution with the spin sector constructs the lower and upper Hubbard bands. The Mott gap is understood as the holon-doublon gap less the energy of the spin fluctuations, and the contrast dependence of these scales on temperature causes a
At any finite temperature, only short-range fluctuations are present and these are well described by the two-operator condensation $\sum_{i,\delta,\sigma}(s_{i,\bar{\delta},\sigma}s_{i+\delta,\sigma}) \neq 0$ (while $\langle s_{i,\sigma}^\dagger \rangle = 0$). We comment that in a very recent study of the Hubbard model at finite doping,34,35 which also uses an Ansatz with fermionic charge degrees of freedom, this short-range-correlated spin state is described by an SU(2) gauge theory with no orientational order but a finite Higgs (amplitude) field.

Following the slave-boson mean-field theory of the AFM Heisenberg model,36 we replace $\sum_{\sigma}(\sigma s_{i,\bar{\sigma}}s_{i+\delta,\bar{\sigma}})$ by its mean value, which decouples the second line of Eq. (2), and calculate the holon and doublon Green functions at the level of the SCBA. A more complete description is provided in Sec. S1 of the Supplementary Information (SI). For a quantitative benchmarking of the static and dynamic SCBA results, we compare these with numerical data obtained by QMC and SAC, the technical details of which are summarized in Sec. S2 of the SI. For consistency we apply both methods at a system size of 16×16.

**Results**

Figure 1 shows the $U$-dependence of the average double-site occupancy, $D = \frac{1}{N} \sum_{ij} \langle n_{i\uparrow}n_{j\downarrow} \rangle$, at a temperature $T = 0.125$. $D$ reflects the extent of charge fluctuations, which are finite for any non-infinite $U$ and nonzero $T$ due to quantum and thermal fluctuations. $D$ is suppressed as $U$ increases, and we find excellent (percent-level) agreement of SCBA and QMC. Also shown in Fig. 1 are the results of a dynamic cluster approximation (DCA), which are extrapolated to the thermodynamic limit,26 and thus confirm not only the SCBA and QMC results but also the degree to which they are representative of the infinite system. In the inset of Fig. 1 we show the $T$-dependence of $D$ computed for a fixed $U = 6$. The weak dip in $D(T)$ has been the subject of extensive debate,37–41 because this sensitive feature depends strongly on the method used. Our slave-fermion approach provides a straightforward understanding of possible nonmonotonic behaviour in terms of the competition between a weakening spin-fluctuation-induced holon-doublon stabilization energy and strengthening thermal fluctuations.
In the slave-fermion framework, the electron Green function, $G(k, i\omega_n)$, is the convolution of the charge (holon-doublon) and spin propagators. A detailed derivation is presented in Sec. S3 of the SI. Its calculation gives direct access to the electron spectral function, $A(k, \omega) = -\frac{1}{\pi} \text{Im} G^R(k, \omega + i\delta)$, and the density of states (d.o.s.), $\rho(\omega) = \frac{1}{N} \sum_k A(k, \omega)$. Figure 2a shows the SCBA and QMC d.o.s. for $U = 8$ at temperatures $T = 0.125$ and 0.25. Three features are evident immediately. (i) Despite the absence of AFM order, $\rho(\omega)$ shows a clear single-particle gap, the Mott gap ($\Delta_{\text{Mott}}$), separating the lower and upper Hubbard bands. $\Delta_{\text{Mott}}$, marking a region of very strongly suppressed d.o.s., survives at temperatures in excess of $T = 0.25$, although its decrease signals a gradual “melting” of the Mott insulator as $T$ increases. (ii) The sharp low-energy peak at the Hubbard-band edge indicates the existence of a well-defined quasiparticle as a consequence of mutual charge and spin renormalization. Following the discussion of a hole moving in an ordered AFM,42–44 we name this feature a “generalized spin polaron” and find that it is well-defined at low temperature but loses coherence (as thermal fluctuations exceed spin fluctuations) towards $T = 0.25$. (iii) At $T = 0.125$, $\rho(\omega)$ shows an obvious peak-dip-hump structure above the Mott gap, a much-debated feature that was not captured in early QMC simulations45 but is clearly reproduced here by both SCBA and QMC.

Figures 2b and 2c show respectively the SCBA and QMC spectral functions, $A(k, \omega)$, across the Brillouin zone for $U = 8$. The results are again quantitatively similar in line shapes and positions, albeit with differences in peak intensities and a small but systematic discrepancy in gaps. The larger gaps calculated by SCBA may reflect an overestimation of the effects of short-range spin fluctuations at intermediate values of $T$.

Interpretation

Extensive calculations of the type illustrated in Figs. 1 and 2 verify that the SCBA results are completely consistent with QMC over the full range of intermediate $U$ and $T$. Thus it is safe to conclude that the holon-doublon formulation and SCBA treatment do incorporate correctly the interactions and mutual renormalization between the charge and spin fluctuations. Hence the qualitative physics underlying the key features of the Mott insulator, including the quasiparticle dynamics, Mott gap and pseudogap, can finally be uncovered.

To separate the charge and spin contributions in the slave-fermion framework, the binding energy of the holon-doublon bound state can be extracted from the charge Green function by the Eliashberg parameterization46,47 (Sec. S3 of the SI). The self-energy of the charge, or holon-doublon, Green function is a $2 \times 2$ matrix,

$$
\Sigma(k, i\omega_n) = i\omega_n [1 - Z(k, i\omega_n)] I + \chi(k, i\omega_n) \sigma_3 + \phi_1(k, i\omega_n) \sigma_1 + \phi_2(k, i\omega_n) \sigma_2
$$

where $\sigma_i$ ($i = 1, 2, 3$) are Pauli matrices, $I$ the identity matrix, $Z(k, i\omega_n)$ the renormalization factor, $\chi(k, i\omega_n)$ contains the corrections to the dispersion and the binding is contained in the off-diagonal terms, $\phi_1(k, i\omega_n)$ and $\phi_2(k, i\omega_n)$. The dispersion relation, $E_k$, of the holon-doublon collective mode is obtained from the poles of the Green function and the holon-doublon gap is twice its minimum value, $\Delta_{\text{bd}} = 2 \min |E_k|$. The value of $\Delta_{\text{bd}}$ obtained in this way is shown by the dashed green lines in Fig. 2a, which clearly lie inside the peak in the SCBA $\rho(\omega)$ but outside its innermost tails. $\Delta_{\text{bd}}$ defines the high energy scale of the Mott insulator and its origin in holon-doublon binding gives it a temperature-dependence analogous to the BCS superconducting gap.

The Mott gap, $\Delta_{\text{Mott}}$, on the other hand, is the single-particle gap and is smaller than $\Delta_{\text{bd}}$ due to the renormalization of the charge sector by the spin degrees of freedom.
FIG. 3. Mott physics: electron reconstruction, melting of the insulator and origin of the pseudogap. a. Schematic representation of how the Mott-insulating state of electrons, with gap $\Delta_{\text{Mott}} \approx \Delta_{\text{bd}} - 2\Omega(T)$, is formed from the convolution of charge degrees of freedom (holons and doublons) with spin (particle-hole) fluctuations, whose characteristic “band” width is $\Omega(T)$. b. $\rho(\omega)$ in the gap region over the full range of temperatures, computed from SCBA with $U = 6$ and $\delta = 0.1$, and normalized to a peak height of 1. c. Temperature-dependence of the charge ($\Delta_{\text{bd}}$, green) and Mott ($\Delta_{\text{Mott}}$, red) gaps for the Hubbard model with $U = 6$, estimated from the SCBA $\rho(\omega)$. Red squares indicate the lower bound on $\Delta_{\text{Mott}}$. The red star and circle mark respectively the lower and upper bounds on the temperature, $T_{c}^{\text{Mott}}$, at which $\Delta_{\text{Mott}}(T)$ vanishes. The dashed red line indicates an extrapolation based on our lower-bound values.

freedom. This is evident in the electronic d.o.s.,

$$
\rho(\omega) = \sum_{\mathbf{q}} a(\omega, \mathbf{q}) \int_{-\infty}^{\infty} \! d\varepsilon \rho_{\text{bd}}^{1}(\mathbf{q}, \varepsilon) \delta(\omega + \Omega_{\mathbf{q}} - \varepsilon) + \sum_{\mathbf{q}} b(\omega, \mathbf{q}) \int_{-\infty}^{\infty} \! d\varepsilon \rho_{\text{bd}}^{2}(\mathbf{q}, \varepsilon) \delta(\omega - \Omega_{\mathbf{q}} - \varepsilon),
$$

where $\rho_{\text{bd}}^{1}(\mathbf{q}, \varepsilon)$ and $\rho_{\text{bd}}^{2}(\mathbf{q}, \varepsilon)$ are the holon-doublon d.o.s., $a(\omega, \mathbf{q})$ and $b(\omega, \mathbf{q})$ are momentum-dependent prefactors containing the Fermi and Bose distribution functions and $\Omega_{\mathbf{q}}$ is the spectral function of the spin fluctuations. An analysis is presented in Sec. S4 of the SI. The $\delta$-function in Eq. (4) specifies how the lower and upper Hubbard bands, and hence the electronic d.o.s. and spectral function, are produced from holon-doublon bound states dressed by the emission and absorption of low-energy spin fluctuations.

Figure 3a provides a schematic illustration of the excitation of an electron in a Mott insulator. The lower and upper bands in the charge sector (red) are the holon-doublon d.o.s. and have gap $\Delta_{\text{bd}}$. In the spin sector (blue), low-energy excitations of particle-hole nature exist over a bandwidth of $\Omega$, but only those on an energy scale $\Omega(T)$, which is governed by the temperature, are activated. The electronic degrees of freedom (purple) are reconstructed as the convolution of the two sectors and hence their excitations are characterized by a gap $\Delta_{\text{Mott}}(T) \approx \Delta_{\text{bd}}(T) - 2\Omega(T)$. In contrast to band insulators, where the gap is largely independent of temperature, the Mott gap is the consequence of temperature-dependent correlation effects. As $T$ increases, $\Delta_{\text{Mott}}$ should be driven downwards both by the decrease in $\Delta_{\text{bd}}(T)$ and by the increase of the effective spin-fluctuation scale, $\Omega(T)$.

Unlike $\Delta_{\text{bd}}(T)$, the accurate extraction of $\Delta_{\text{Mott}}(T)$ from the electron Green function is complicated due to the lack of a single-particle dispersion relation analogous to that for the holons and doublons. We estimate the Mott gap from our numerical (SCBA) solution for the electron d.o.s., $\rho(\omega, T)$ shown in Fig. 3b, by a procedure of assuming an effective gap and modelling its “filling.” The finite d.o.s. at small $\omega$ is a consequence of two effects, the (finite-size) broadening $\delta$ and thermal activation over a $T$-dependent gap $[\Delta_{\text{Mott}}(T)]$. Because the former is governed by a Lorentzian function and the latter by the (exponential) activation barrier, as detailed in Sec. S5 of the SI, the process is dominated by $\delta$ and we neglect the direct effects of $T$; this approximation therefore provides a lower bound for $\Delta_{\text{Mott}}(T)$. The problem of finding the Mott gap, meaning the gap in the reconstructed (spin-charge-recombined) spectrum at any given $T$, is thus reduced to a deconvolution removing the broadening effect of $\delta$. This we execute by a linear regression method, as explained in detail in Sec. S5 of the SI, and our results for $U = 6$ are shown by the red line and squares in Fig. 3c.

A qualitatively different approach to estimating the vanishing of $\Delta_{\text{Mott}}(T)$ is provided by noting the presence of a small peak in $\rho(\omega, T)$ at $\omega = 0$ when $T$ exceeds a certain value (Figs. 3b and S4). This quasiparticle peak can be taken as indicating that the lower and upper Hubbard bands have overlapped, to the extent that their convolution exceeds the other broadening effects, and thus it provides an effective upper bound on the temperature at which $\Delta_{\text{Mott}}$ vanishes. Clearly the single-particle gap decreases faster than the charge gap, going continuously to zero at a temperature, which we denote $T_{c}^{\text{Mott}}$, well below $T_{c}^{\text{bd}}$. Even at low temperatures, the difference between $\Delta_{\text{bd}}$ and $\Delta_{\text{Mott}}$ grows linearly with temperature, as anticipated above (Fig. 3c). This difference in the $T$-dependences of the two gaps is another crucial feature of
the distinctive low-energy physics intrinsic to the Mott insulator. While the QMC results differ from SCBA in quantitative details, the qualitative picture of the two gaps remains robust.

A further piece of essential physics concerns the energy scales of the spin fluctuations and gap renormalization. Energies in the spin sector are controlled by the AFM coupling, $J$, and the relevant temperatures for a finite (two-spin) magnetic correlation parameter are a fraction of this, as shown on the horizontal axis of Fig. 3c. However, the charge sector has energies of order $U$, and the renormalization, $\Omega(T)$ of the holon-doublon gap, $\Delta_{bd}(T)$, is a fraction of this (from Fig. 3c one might estimate $\Omega(T) \approx 5T \approx UT$). This remarkable “leverage effect,” by which the low-energy spin processes bring about high shifts of energy in the charge processes, lies at the heart of the mixing of energy scales in the Mott insulator.

The $\omega = 0$ axis of Fig. 3c can be interpreted as a finite-temperature phase diagram for the Hubbard model (1). $\Delta_{Mott}(T)$ implies that the region to the left of the red line is fully gapped, not only for bound holons and doublons but also for electrons, and this is the Mott insulator. As $T$ is increased, the melting of the Mott insulator is revealed as a two-step process. At $T^{bs}_{crit}$, the optimal electronic states created by spin-charge reconstruction, which lie in the tails of the Hubbard bands (Fig. 2a), have touched, creating the peak at $\omega = 0$ in $\rho(\omega)$ (Fig. 2b). However, $\Delta_{bd}(T)$ remains finite and most of the electronic states remain gapped; the consequent suppression of the d.o.s. around the Fermi level makes this a pseudogap regime. As $T$ approaches $T^{bd}_{c}$, the pseudogap fills in with low-lying electronic states, and only above $T^{bd}_{c}$ does the closing of the charge gap push the system into the metallic regime. This pseudogap behaviour or enduring small spectral weight inside the holon-doublon gap, is observed consistently in many numerical studies of the Hubbard model, including our QMC simulations (shown in Secs. S2 and S5 of the SI). Here we find that the slave-fermion framework captures this phenomenon, whose origin lies in the leveraged effect of the short-ranged spin fluctuations.

Discussion

To place our results in context, all slave-particle decompositions involve an uncontrolled assumption, which can only be justified post facto. For this we have used QMC simulations to benchmark our results, and the comparison reveals that the holon-doublon approach does an excellent job of representing the relevant degrees of freedom and of capturing all the important aspects of their interactions. In addition, any mean-field treatment is subject to the weakness that the local constraint can be enforced only on average, and thus the results are critically dependent on how well the essential physics of the system is captured at lowest order. Again our calculations demonstrate that the holon-doublon framework passes this test with distinction, for all values of $U > 2t$ (Fig. 1) and temperatures $T \lesssim 0.5J$. Unlike some approaches, our study is general in that the finite-$T$ response contains no problems induced by the potential pathologies of its perfectly nested noninteracting band.

Experimentally, despite the intensive interest in cuprate materials and Mott physics, detailed studies of undoped Mott insulators are complicated by the fact that neither angle-resolved photoemission spectroscopy (ARPES) nor scanning tunnelling spectroscopy (STS) can obtain a signal from a well-gapped insulator at low $T$. Extensive ARPES studies of insulating cuprates have mapped the spectral function (Figs. 2b and 2c) to observe the Mott gap and the strongly renormalized noninteracting band, but lack the resolution and temperature-sensitivity to address details such as the filling and closing of the Mott gap. STS measures the local d.o.s. (Fig. 2a) and recent studies have observed the Mott gap and its persistence to finite temperatures, albeit in systems that are already lightly hole-doped (which we note is the next challenge for the slave-fermion description). Very recently, AFM order has been observed in a system of ultracold $^6$Li atoms on an optical lattice, which also realizes an undoped Hubbard model at finite temperatures. Given the finite nature (of order 100 atoms) of these systems, both our SCBA and QMC techniques are perfectly suited for calculations and quantitative comparison with this type of experiment.

In summary, we have shown by analytical SCBA calculations and unbiased QMC simulations that the slave-fermion (holon-doublon) description of the Hubbard model contains all the essential physics of the Mott insulator. Thus we obtain complete insight into the underlying physical processes, which emerge from the interplay of high-energy holon-doublon binding and low-energy, short-ranged spin fluctuations. The latter induce the former, even in the absence of long-range AFM order, and on this basis the lower and upper Hubbard (electronic) bands are formed from spin-renormalized holon-doublon states. The reconstructed bands contain a well-defined “generalized spin polaron” quasiparticle, and the renormalization introduces a strong energetic leverage effect. The Mott gap is naturally smaller than the charge gap and closes first as temperature increases. Because this process involves only a small fraction of the spin-polaron states, the regime below the closing of the charge gap provides a natural explanation of the pseudogap phenomenon. Thus our analytical and numerical results provide a unified understanding of the dynamics and melting of the undoped Mott insulator and form the basis for an investigation of the doped case.

Methods

The self-consistent Born approximation to the motion of a holon or a doublon in an antiferromagnetic environment is equivalent to neglecting any distortion of the spin configuration caused by the presence of the charged entity. Formally, the approximation is made by neglecting Feynman diagrams with crossing propagators, which is similar to considering only retraceable paths. The approximation preserves the coupling between the holon or doublon and the spin excitations, which is responsible for
the coherent peak in the spectral function.

Our finite-temperature QMC simulation code is based on the Quantum Electron Simulation Toolbox (QUEST), which is a FORTRAN 90/95 package containing modern algorithms, such as delayed updating, and integrating the latest BLAS/LAPACK numerical kernels. QUEST has integrated several legacy codes by modularizing their computational components for ease of maintenance and programme interfacing. The current version may be accessed at https://code.google.com/archive/p/quest-qmc/.

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Author contributions

SCBA coding and calculations were performed by X.-J.H. with assistance from J.C., H.-D.X., R.-Z.H. and H.-J.L. QMC coding and calculations were performed by C.C. and Z.Y.M. Data refinement and fitting were performed by X.-J.H., C.C. and Z.Y.M. The theoretical framework was conceived by T.X. and B.N. The figures were prepared by X.-J.H., C.C., B.N., Z.Y.M. and T.X.

Additional information

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Competing Financial Interests

The authors declare no competing financial interests.
Supplementary Information for “Finite-temperature charge dynamics and the melting of the Mott insulator”

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S1. SLAVE-FERMION FORMALISM FOR $T > 0$

In our previous work, we applied the holon-doublon slave-fermion decomposition at $T=0$. The spin degrees of freedom are represented by bosonic operators, $s_i$, and we take them to be governed by the Heisenberg model, following the treatment of Arovas and Auerbach. At $T=0$, the long-ranged antiferromagnetic (AFM) order of the system is captured by the condensation of a single operator, $\langle s_i \rangle \neq 0$, and the remaining active bosonic degrees of freedom represent the AFM fluctuations. At any finite temperature, only short-ranged AFM fluctuations are present and this is represented at the mean-field level by two-operator condensation of the form $\sum_\sigma (s_{i,\sigma} s_{i+\delta,\sigma}) \neq 0$ on the bonds connecting all sites $i$ to their nearest neighbours ($\delta=(\pm a,0)$ and $(0,\pm a)$, where $a$ is the lattice constant). By introducing the bond operator

$$Q_{i,\delta} = s_{i,\uparrow} s_{i+\delta,\downarrow} - s_{i,\downarrow} s_{i+\delta,\uparrow},$$

one may reformulate the Heisenberg model as

$$H_S = -\frac{1}{2} J \sum_{i,\delta} (Q_{i,\delta}^\dagger Q_{i,\delta} - \frac{1}{4}).$$

Following Ref. 36, we take the mean-field parameter to be uniform and static,

$$Q = -\frac{1}{2} J \langle s_{i,\uparrow} s_{i+\delta,\downarrow} - s_{i,\downarrow} s_{i+\delta,\uparrow} \rangle,$$

for all $i$ and $\delta$, and we release the constraint on the slave-boson sector, $s_{i,\uparrow}^\dagger s_{i,\uparrow} + s_{i,\downarrow}^\dagger s_{i,\downarrow} = 1$, replacing it by the constraint $d_i^\dagger d_i + e_i^\dagger e_i + \sum_{\sigma} s_{i,\sigma}^\dagger s_{i,\sigma} = 1$ appropriate to the full slave-fermion problem. The constraint acts to provide an additional and self-consistent coupling of the spin and charge degrees of freedom. In principle, the corresponding two-operator expectation value $P = \langle s_{i,\uparrow}^\dagger s_{i+\delta,\uparrow} + s_{i,\downarrow}^\dagger s_{i+\delta,\downarrow} \rangle$ is also finite in the coupled problem, but we find from the three-parameter mean-field solution that its value is sufficiently small, at all temperatures, for its neglect to be fully justified in the treatment to follow.

The mean-field Hamiltonian can be expressed as

$$H_S = \sum_k \begin{pmatrix} \frac{\lambda}{z Q \eta_k} s_{k,\uparrow} \cr \frac{\lambda}{z Q \eta_k} s_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} z Q \eta_k \cr \lambda \end{pmatrix} \begin{pmatrix} s_{k,\uparrow} \cr s_{-k,\downarrow} \end{pmatrix}$$

$$+ \frac{N z Q^2}{J} - 2\lambda N + \lambda \sum_i (d_i^\dagger d_i + e_i^\dagger e_i),$$

where $z=4$ is the coordination number and $\eta_k = \frac{1}{2} i (\sin k_x + \sin k_y)$. The Bogoliubov transformation

$$\begin{pmatrix} s_{k,\uparrow} \cr s_{-k,\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} \alpha_k \cr \beta_k \end{pmatrix}$$

with

$$|u_k|^2 = \frac{1}{2} + \frac{\lambda}{2\Omega_k}, \quad |v_k|^2 = \frac{\lambda}{2\Omega_k} - \frac{1}{2},$$

$$u_k v_k = -\frac{z Q \eta_k}{2 \Omega_k}, \quad \Omega_k = \sqrt{\lambda^2 - 4 Q^2 (\sin k_x + \sin k_y)^2}$$

diagonalizes the Hamiltonian to yield the form

$$H_S = \sum_k \Omega_k \alpha_k^\dagger \alpha_k + \sum_k \Omega_k \beta_k^\dagger \beta_k + \sum_k \Omega_k$$

$$+ \lambda \sum_i (d_i^\dagger d_i + e_i^\dagger e_i) + \frac{N z Q^2}{J} - 2 N \lambda, \quad (S6)$$

where $\lambda$ is the Lagrange multiplier associated with the constraint. The mean-field equations for any temperature, $T$, are given by

$$\frac{J}{N} \sum_k \frac{z (\sin k_x + \sin k_y)^2}{\Omega_k} \left( n_k + \frac{1}{2} \right) = 1$$

$$\frac{1}{N} \sum_k \frac{\lambda}{\Omega_k} \left( n_k + \frac{1}{2} \right) = 1 - \frac{1}{2} \sum_i (d_i^\dagger d_i + e_i^\dagger e_i),$$

where $n_k = 1/(e^{\Omega_k/T} - 1)$ is the Bose distribution function. Self-consistent solution of these equations yields temperature-dependent mean-field parameters, $\lambda(T)$ and $Q(T)$, whose effect is to increase the excitation gap of the effective spin dispersion relation of the thermally disordered magnetic system. It is important to note that the gap in the spin spectrum remains significantly smaller than $T$ at all relevant temperatures.

To combine the spin degrees of freedom with the charge, the mean-field solution for the Heisenberg model is substituted into Eq. (2) of the main text. The most important term is the replacement of $(s_{i,\uparrow} s_{i+\delta,\uparrow} - s_{i,\downarrow} s_{i+\delta,\downarrow})$ in the quadratic decoupling of the second line by its mean value, $2 Q/J$. Together with the third line, this term forms an effective unperturbed Hamiltonian for the charge dynamics, while the remaining terms describe interactions. With this separation, Eq. (2) can be expressed as

$$H = \sum_k \psi_k^\dagger \xi_k \psi_k + \sum_{k,q,l} \psi_k^\dagger M(k,q,l) \psi_{k-q+l}.$$
where \( \psi^\dagger_{\mathbf{k}} = (d^\dagger_{\mathbf{k} \downarrow}, e_{\mathbf{k}}) \) is the Nambu spinor for the charge degrees of freedom,

\[
\tilde{\varepsilon}_{\mathbf{k}} = \begin{pmatrix}
U/2 & 2t z Q \eta_{\mathbf{k}} / J \\
-2t z Q \eta_{\mathbf{k}} / J & -U/2
\end{pmatrix},
\]

(S10)

and

\[
M(\mathbf{k}, \mathbf{q}, \mathbf{l}) = -\frac{t z}{N} \sum_\sigma \left( \gamma_{\mathbf{k}+\mathbf{l}} \ 0 \\
\gamma_{\mathbf{k}-\mathbf{q}} \ 0
\right) s^\dagger_{\mathbf{q},\sigma} s_{\mathbf{k},\sigma},
\]

(S11)

where \( \gamma_{\mathbf{k}} = \frac{1}{4}(\cos k_x + \cos k_y) \). The first term of Eq. (S9) describes the charge dynamics in the absence of spin renormalization, with holon-doublon binding appearing in the off-diagonal part of the matrix. The second term incorporates all the interactions between the charge and spin degrees of freedom, which in contrast to the \( T = 0 \) case contains two spin bosons and requires a sum over three free momenta.

We define the full charge, or holon-doublon, Matsubara Green function as

\[
F(\mathbf{k}, \tau) = -\langle T_\tau \psi_\mathbf{k}(\tau) \psi^\dagger_{\mathbf{k}}(0) \rangle
\]

(S12)

and calculate this within the self-consistent Born approximation (SCBA). The corresponding Feynman diagrams, shown in Fig. S1, are the bare term, \( F(0) \), and the first loop, in which the magnon Green function is also a 2 \( \times \) 2 matrix,

\[
D(\mathbf{k}, \tau) = -\left( \frac{\langle T_\tau s_{\mathbf{k},\uparrow}(\tau) s^\dagger_{\mathbf{k},\uparrow}(0) \rangle \langle T_\tau s^\dagger_{-\mathbf{k},\downarrow}(\tau) s_{-\mathbf{k},\downarrow}(0) \rangle}{\langle T_\tau s^\dagger_{\mathbf{k},\downarrow}(\tau) s_{-\mathbf{k},\downarrow}(0) \rangle \langle T_\tau s_{\mathbf{k},\uparrow}(\tau) s^\dagger_{-\mathbf{k},\uparrow}(0) \rangle} \right).
\]

At this level we obtain the self-consistent Dyson equation for the Matsubara Green function of the charge sector,

\[
F(\mathbf{k}, i \omega_n) = \frac{1}{i \omega_n - \tilde{\varepsilon}_{\mathbf{k}} - \Sigma(\mathbf{k}, i \omega_n)},
\]

where the retarded Green function is obtained by the analytic continuation \( i \omega_n \to \omega + i \delta \). This \( \delta \) term denotes a broadening of the peaks in the spectral response and is set to \( \delta = 0.1 \) throughout our calculations: a smaller value would be of little physical meaning because of the finite size of the system. As noted in the main text, all SCBA calculations are performed on a 16 \( \times \) 16 lattice for the purposes of comparison with Quantum Monte Carlo (QMC) results (Sec. S2).

We comment that, despite the simplicity of the AFM Heisenberg model, there is no exact solution for the \( S = 1/2 \) case on the square lattice. The study of the two-dimensional (2D) quantum AFM Heisenberg model is of great importance in its own right as a fundamental problem in quantum magnetism. To date, the most definitive analytical results for the low-temperature regime were obtained by two-loop renormalization-group calculations on the quantum nonlinear \( \sigma \) model (NL\( \sigma \)M). It has also been shown that spin fluctuations in the 2D Hubbard model at low temperature can be described by the quantum NL\( \sigma \)M for any value of the Coulomb repulsion, \( U \). The accuracy of these results notwithstanding, an integration of the NL\( \sigma \)M into the present framework is not straightforward, and we will show that the holon-doublon framework with mean-field decoupling is already sufficient to gain semi-quantitative accuracy.

S2. QUANTUM MONTE CARLO

We investigate the half-filled 2D Hubbard model by determinant QMC. The quartic term in Eq. (1) of the main text, \( U(n_{\mathbf{i},\uparrow} - \frac{1}{2})(n_{\mathbf{i},\downarrow} - \frac{1}{2}) \), is decoupled by Hubbard-Stratonovich transformation to a form quadratic in \( (n_{\mathbf{i},\uparrow} - n_{\mathbf{i},\downarrow}) = (c_{\mathbf{i},\uparrow} c^\dagger_{\mathbf{i},\uparrow} - c_{\mathbf{i},\downarrow} c^\dagger_{\mathbf{i},\downarrow}) \), which introduces an auxiliary Ising field on each lattice site. The QMC procedure obtains the partition function of the underlying Hamiltonian in a path-integral formulation in a space of dimension \( N = L \times L \) and an imaginary time \( \tau \) up to \( \beta = 1/T \). All of the physical observables are measured from the ensemble average over the space-time \( (N\beta) \) configurational weight of the auxiliary fields. As a consequence, the errors within the process are well controlled: specifically, the \((\Delta \tau)^2\) systematic error from the imaginary-time discretization, \( \Delta \tau = \beta/M \), is controlled by the extrapolation \( M \to \infty \) and the statistical error is controlled by the central-limit theorem (simply put, the larger the number of QMC measurements, the smaller the statistical error).

The QMC algorithm is based on Ref. 27 and has been refined by including global moves55 to improve ergodicity and delay updating of the fermion Green function, which increases the efficiency of the QMC sampling. Details concerning the QMC simulation code are provided in the Methods section. We have performed simulations for system sizes \( L = 4, 8, 10, 12, 14 \) and 16. The interaction, \( U \), is varied from 2 to 12 in units of the hopping strength, which is set to \( t = 1 \), and for each \( U \) we simulate temperatures from \( T = 0.0625 \) to 1 (inverse temperatures \( \beta = 16 \) down to 1).

The QMC simulations give direct access to the imaginary-time fermion Green function

\[
G_{\sigma}(\mathbf{k}, \tau) = -\frac{1}{N} \sum_{i,j} e^{i \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle c_{i\sigma}(\tau) c^\dagger_{j\sigma}(0) \rangle,
\]

(S14)

where \( i, j \in [1, N] \) are site labels, \( \tau \in [0, \beta] \) is the imaginary time, and \( \langle \ldots \rangle \) is the Monte Carlo expecta-
tion value. Concerning the spin index, $\sigma$, in the half-filled Hubbard model $G(k,\tau) = G_\uparrow(k,\tau) = G_\downarrow(k,\tau)$. While the slave-fermion treatment offers a specific calculation based on certain uncontrolled (but presumably justified) approximations, the quantity $G(k,\tau)$ obtained from QMC is exact on a finite-size system and has controlled errors.

To obtain real-frequency data, it is necessary to perform analytic continuation of the imaginary-time data. For this purpose we have employed stochastic analytic continuation (SAC),\textsuperscript{30,31} by which the spectral function, $A(k,\omega)$, is obtained from the Green function, $G(k,\tau)$, by a stochastic inverse Laplace transformation,

$$G(k,\tau) = \int d\omega \frac{e^{-\omega \tau}}{e^{-\beta \omega} + 1} A(k,\omega). \quad \text{(S15)}$$

The most recent implementation of the SAC method reproduces the spectral function using a large number of $\delta$-functions sampled at locations in a frequency continuum and collected in a histogram.\textsuperscript{33,56,57} From the spectral function it is straightforward to obtain the local density of states, $\rho(\omega)$, other static physical observables, such as the double occupancy, $D = \frac{1}{N} \sum_i (n_{i\uparrow} n_{i\downarrow})$, are also measured readily in QMC.

To access the single-particle gap, i.e. the Mott gap, $\Delta_{Mott}$, of the main text, one may attempt to read it directly from the gap in $\rho(\omega)$. From the robust exponential decay of $G_\uparrow(\tau)$ in imaginary time at lower temperatures, shown for $\beta = 8$ in Fig. S2a, the analytic continuation is straightforward and yields high-quality results for $\rho(\omega)$ (Fig. S2b). We find in this temperature regime that the density of states is well characterized by a single gap, $\Delta_{Mott} = 3.2(3)$. However, it becomes more difficult to extract an accurate value for the Mott gap as the temperature.

FIG. S2. QMC and analytic continuation: low temperatures. a, Imaginary-time Green function, $G_{\uparrow}(\tau) = \frac{1}{N} \sum_{k \in BZ} G_{\uparrow}(k,\tau)$, at $U = 8$ and $\beta = 8$ ($T = 0.125$) for $L = 4,\ldots,16$. The logarithmic y-axis makes clear that $L = 8$, 12 and 16 give the same slope in the imaginary-time decay, which ensures high-quality results on analytic continuation. b, Local density of states, $\rho(\omega)$, obtained from SAC of the imaginary-time Green function in panel a. Results in the gap region have clearly converged for $L = 8$, 12 and 16 at this temperature.

FIG. S3. QMC and analytic continuation: high temperatures. a, Imaginary-time Green function, $G_{\uparrow}(\tau) = \frac{1}{N} \sum_{k \in BZ} G_{\uparrow}(k,\tau)$, at $U = 8$ and $\beta = 4$ ($T = 0.25$) for $L = 4,\ldots,16$. Again the $L = 8$, 12 and 16 data provide converged values for the imaginary-time decay, but an exponential form is no longer clear. b, Local density of states, $\rho(\omega)$, obtained from SAC of the imaginary-time Green function in panel a. The gap no longer follows a single-exponential form, making it difficult to extract a reliable value of $\Delta_{Mott}$ at this temperature.
perature increases. Figure S3 shows $G_{ij}(\tau)$ and $\rho(\omega)$ at $U = 8$ for $\beta = 4$ ($T = 0.25$). Although the imaginary-time decay of $G_{ij}(\tau)$ has converged for $L = 8$, 12 and 16 (Fig. S3a), the finite-$T$ broadening that affects the Green function around $\tau = \beta/2$ makes the fit to an exponential decay less accurate. From $\rho(\omega)$ (Fig. S3b), it remains clear at a qualitative level that the spectrum has a gap, and that simulations for $L = 8$, 12 and 16 converge to the same curve, but it is no longer clear how to ascribe this behaviour to a specific value of $\Delta_{\text{Mott}}$. We discuss systematic ways of extracting lower and upper bounds on the Mott gap from $\rho(\omega)$ in Sec. S5.

### S3. CHARGE GREEN FUNCTION

Here we provide the derivation of the holon-doublon dispersion relation, $E_k$, used to define the gap, $\Delta_{\text{bd}}$, in the charge sector. To analyse the charge (holon-doublon) Green function of Eq. (S13), we begin by exploiting the fact that the Pauli matrices, $\sigma_i$ ($i = 1, 2, 3$), and the identity matrix, $I$, form a complete basis for all $2 \times 2$ matrices to reexpress Eq. (S10) as

$$\tilde{\varepsilon}_k = \frac{1}{2}U \sigma_3 - \zeta_k \sigma_2,$$

where $\zeta_k = 4tQ(\sin k_x + \sin k_y)/J$. For clarity we repeat here Eq. (3) of the main text for the self-energy in Eq. (S13),

$$\Sigma(k, i \omega_n) = i \omega_n [1 - Z(k, i \omega_n)] I + \chi(k, i \omega_n) \sigma_3 + \phi_1(k, i \omega_n) \sigma_1 + \phi_2(k, i \omega_n) \sigma_2,$$

in which $Z(k, i \omega_n)$ is the quasiparticle renormalization factor, $\chi(k, i \omega_n)$ contains the corrections to the dispersion, and the off-diagonal terms, $\phi_1(k, i \omega_n)$ and $\phi_2(k, i \omega_n)$ contain the effects of the binding interaction.\textsuperscript{46,47} Substituting Eq. (S17) into Eq. (S13) gives

$$F^{-1}(k, i \omega_n) = \begin{pmatrix} F_{11}(k, i \omega_n) & -F_{12}(k, i \omega_n) \\ -F_{12}^\dagger(k, i \omega_n) & F_{11}^\dagger(k, i \omega_n) \end{pmatrix},$$

in which

$$F_{11}(k, i \omega_n) = Z(k, i \omega_n) i \omega_n + [U/2 + \chi(k, i \omega_n)],$$

$$F_{12}(k, i \omega_n) = \phi_1(k, i \omega_n) i \phi_2(k, i \omega_n) - \zeta_k.$$  

By inversion of the matrix we obtain

$$F(k, i \omega_n) = \frac{1}{|\text{Det}F|} \begin{pmatrix} F_{11}^\dagger(k, i \omega_n) & F_{12}^\dagger(k, i \omega_n) \\ F_{12}(k, i \omega_n) & F_{11}(k, i \omega_n) \end{pmatrix},$$

where

$$|\text{Det}F| = Z^2(k, i \omega_n)(i \omega_n)^2 - [U/2 + \chi(k, i \omega_n)]^2 - \phi_1^2(k, i \omega_n) - \phi_2^2(k, i \omega_n) - \zeta_k^2,$$

and

$$R(k, \omega) = |\omega - E_k + i \Gamma(k, \omega)|$$

$$\times [\omega + E_k + i \Gamma(k, \omega)].$$

We have calculated the charge (holon-doublon) Green function, $F(k, \omega_n)$, numerically, which gives access to its component parts $Z(k, i \omega_n)$, $\chi(k, i \omega_n)$, $\phi_1(k, i \omega_n)$ and $\phi_2(k, i \omega_n)$. By reexpressing the denominator in the form given in Eq. (S21), we derive the effective holon-doublon quasiparticle dispersion, $E_k$, and the corresponding scattering rate, $\Gamma(k, \omega)$.\textsuperscript{58} As discussed in the main text, we define the holon-doublon gap as the minimum of $E_k$, i.e. $\Delta_{\text{bd}} = \min_k |E_k|$, and find that it occurs at $k = S = (\pi/2, \pi/2)$.

### S4. ELECTRON SPECTRAL FUNCTION

Here we provide the derivation of the expression for the electronic density of states given in Eq. (4) of the main text. The electron Green function, $G_{ij}^\sigma(\tau)$, can be expressed in the slave-fermion formulation as

$$G_{ij}^\sigma(\tau) = -(T_c c^\dagger_{i\sigma}(\tau) c^i_{\sigma}(0))$$

$$= -(T_c (s^F_\sigma(\tau)) d^i_{\sigma}(\tau) + \sigma_s^1(\tau) s^F_\sigma(\tau))$$

$$\times (d^i_{\sigma}(0) s^F_\sigma(0) + \sigma_s^1(0) e^i_{\sigma}(0))$$

$$\sim - (T_c d^i_{\sigma}(0)) \langle T_c s^F_\sigma(\tau) s^F_\sigma(0) \rangle$$

$$- (T_c e^i_{\sigma}(0)) \langle T_c s^F_\sigma(\tau) s^F_\sigma(0) \rangle$$

$$- \sigma_\tau (T_c d^i_{\sigma}(0)) \langle T_c s^F_\sigma(\tau) s^F_\sigma(0) \rangle$$

$$- \sigma_\tau (T_c e^i_{\sigma}(0)) \langle T_c s^F_\sigma(\tau) s^F_\sigma(0) \rangle,$$

if vertex corrections are neglected.\textsuperscript{59,60} In momentum space it is given by

$$G_{ij}(k, \omega_n)$$

$$= \frac{1}{N} \sum_q \left[ \int_{-\infty}^{\infty} ds \frac{U_q \mathcal{A}(k + q, \epsilon) U_q}{\omega_n + \Omega_q - \epsilon} [f(\epsilon) + n_q] ight.$$  

$$+ \int_{-\infty}^{\infty} ds \frac{V_q \mathcal{A}(k + q, \epsilon) V_q}{\omega_n - \Omega_q - \epsilon} [1 - f(\epsilon) + n_q] \right],$$

with

$$U_q = \left( \frac{\nu_q}{\epsilon_q} \right)$$

$$V_q = \left( \frac{\nu_q}{\epsilon_q} \right),$$

whose components are given in Eq. (S6), and

$$\mathcal{A}(k + q, \epsilon) = - \frac{1}{\pi} \text{Im} F^R(k + q, \epsilon + i \delta)$$

$$= \begin{pmatrix} A_{11}(k + q, \epsilon) & A_{12}(k + q, \epsilon) \\ A_{21}(k + q, \epsilon) & A_{22}(k + q, \epsilon) \end{pmatrix},$$

which expresses the holon-doublon spectral function corresponding to the retarded charge Green function; $f(\epsilon)$ is the Fermi distribution function for holon-doublon quasiparticles and $n_q$ the Bose distribution for the spinons.
The corresponding electron spectral function is

\[
\tilde{A}_q(k, \omega) = -\frac{1}{\pi} \text{Im} G^R_\sigma(k, \omega) = \frac{1}{N} \sum_q \int_{-\infty}^{\infty} d\sigma U^d_{qA}(k+q, \varepsilon) U_q[f(\varepsilon) + n_q] \delta(\omega + \Omega_q - \varepsilon)
\]

\[
+ \frac{1}{N} \sum_q \int_{-\infty}^{\infty} d\varepsilon V^d_q A(k+q, \varepsilon) V_q[1-f(\varepsilon) + n_q] \delta(\omega - \Omega_q - \varepsilon),
\]

whence the electronic density of states is

\[
\rho(\omega) = \frac{1}{N} \sum_{k,\sigma} \rho_{\sigma}(k, \omega) = \sum_q a(\omega, q) \int_{-\infty}^{\infty} d\varepsilon \rho^{1d}_{hd}(q, \varepsilon) \delta(\omega + \Omega_q - \varepsilon)
\]

\[
+ \sum_q b(\omega, q) \int_{-\infty}^{\infty} d\varepsilon \rho^{2d}_{hd}(q, \varepsilon) \delta(\omega - \Omega_q - \varepsilon),
\]

in which

\[
\rho^{1d}_{hd}(q, \varepsilon) = U^d_{qA}(\varepsilon) U_q, \quad \rho^{2d}_{hd}(q, \varepsilon) = V^d_q A(q, \varepsilon) V_q.
\]

The quantities \(\rho^{1d}_{hd}(q, \varepsilon)\) and \(\rho^{2d}_{hd}(q, \varepsilon)\) contain the holon-doublon density of states, which is altered only quantitatively by the prefactors \(A(q, \varepsilon)\), while the holon-doublon gap remains unaffected. Its renormalization to the Mott gap is contained within the integrals over the two energy \(\delta\)-functions, \(\delta(\omega + \Omega_q - \varepsilon)\) and \(\delta(\omega - \Omega_q - \varepsilon)\), which approximate the convolution with the spin spectral function in the slave-fermion framework.

### S5. EXTRACTION OF THE MOTT GAP

Unlike the holon-doublon gap, it is difficult to extract the Mott gap from the electron Green function obtained in SCBA, as there is no analytical means of finding the poles in the self-energy. However, as noted in Sec. S2, it is even more difficult to read \(\Delta_{\text{Mott}}\) from QMC for temperatures in excess of approximately 0.15. Thus we revert to a detailed consideration of the densities of states, \(\rho(\omega, T)\), computed within the SCBA, in order to achieve reasonable estimates of \(\Delta_{\text{Mott}}(T)\). Here we describe the two types of analysis by which we obtain i) a lower bound on \(\Delta_{\text{Mott}}(T)\), using a quantitative fitting process which in essence neglects thermal fluctuations, and ii) an upper bound on the temperature, \(T^*_{\text{Mott}}\), at which \(\Delta_{\text{Mott}}(T) = 0\), based on a clear qualitative feature of \(\rho(\omega, T)\).

(i) Except at the highest temperatures, all of the d.o.s. functions we calculate by SCBA show the clear presence of a gap which, however, is partially filled. Factors contributing to this filling are the broadening, \(\delta\), which has a Lorentzian form (below), and the temperature, whose effects are exponentially activated. A qualitative indication of the differing nature of the two contributions can be obtained by comparing \(\rho(\omega, T)\) from SCBA, shown in Fig. 3b of the main text, with the results from QMC, shown in Fig. S4: \(\delta\) effects, which cause \(\rho(\omega)\) to become more “V-shaped” within the gap, are stronger in the SCBA data. However, we are constrained by finite-size effects not to reduce \(\delta\) in our calculations. Because the Lorentzian contribution is much stronger, we proceed by neglecting the thermal activation contribution. Nevertheless, the effect we aim to capture is that of additional states appearing within the low-temperature gap due to the reconstruction of the single-particle spectral function (from its spin and holon-doublon parts) at all higher temperatures.

The retarded Green function can be represented by

\[
G^R(\omega + i\delta) = \int_{-\infty}^{\infty} d\varepsilon \frac{\tilde{\rho}(\varepsilon)}{\omega - \varepsilon + i\delta},
\]

where \(\tilde{\rho}(\varepsilon)\), the intrinsic d.o.s., is expected to vanish below \(\Delta_{\text{Mott}}/2\). We need consider only the imaginary part of \(G^R(\omega + i\delta)\), which is the observed d.o.s.,

\[
\rho(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\varepsilon \frac{\delta}{(\omega - \varepsilon)^2 + \delta^2} \tilde{\rho}(\varepsilon).
\]

If \(\delta\) is infinitesimal, at \(T = 0\) and when the energy interval is continuous one has \(\tilde{\rho}(\omega) = \rho(\omega)\). In our calculations, however, \(\delta\) is finite and we have used an energy interval \(d\omega = 0.02\), on top of which we wish to demonstrate that the effects of finite temperatures on the spectral function are equivalent to those of a \(T\)-dependent effective Mott gap, \(\Delta_{\text{Mott}}(T)\).
The process of using each value of interval of the SCBA data is complicated by a lack of statistical errors, a more straightforward procedure is sufficient in the present case. Motivated by the structure of the SAC method of Sec. S2, we construct a minimization based on linear regression to achieve the decomposition of Eq. (S30). We parameterize

\[ \hat{\rho}(\varepsilon) = \sum_{i=1}^{N_c} a_i \delta(\varepsilon - \varepsilon_i) \]  

(S31)

using \( N_c \) equally spaced \( \delta \)-functions, whose weights \( \{a_i\} \) are the free parameters. By inserting Eq. (S31) into Eq. (S30), we obtain the function

\[ \rho(\omega) = \frac{1}{\pi} \sum_{i=1}^{N_c} d\varepsilon \left[ \frac{\delta}{(\omega - \varepsilon_i)^2 + \delta^2} + \frac{\delta}{(\omega + \varepsilon_i)^2 + \delta^2} \right] a_i, \]

by which we approximate the SCBA \( \rho(\omega) \). We define the goodness-of-fit parameter

\[ \chi^2 = \sum_{i=1}^{N_c} \left( \rho(\omega_i) - \rho'(\omega_i) \right)^2, \]

(S33)

whose minimization by a linear regression method determines the values \( \{a_i\} \). Because the number, \( N_c \), of data points in \( \varepsilon \) in Eq. (S31) can only be equal to or smaller than the number, \( N_\omega = 600 \), of points in the SCBA \( \rho(\omega) \), such a minimization can always be achieved.

Two examples of the intrinsic d.o.s. functions, \( \hat{\rho}(\varepsilon) \), underlying our computed SCBA functions, \( \rho(\omega) \), are shown in Fig. S5, where we have chosen \( U = 6 \) and the temperatures \( T = 0.125 \) (Fig. S5a) and \( T = 0.25 \) (Fig. S5b); in both cases we used \( N_\omega = 300 \). The \( \hat{\rho}(\varepsilon) \) functions show a clear suppression of the d.o.s. at low frequencies, with the reappearance of this weight occurring primarily around the peaks. These intrinsic functions also show the clear presence of additional states building systematically into the zero-temperature gap as \( T \) is increased.

To extract the effective Mott gap from \( \hat{\rho}(\varepsilon) \) at each temperature, we define \( \Delta_{Mott}(T) \) as the frequency at which the weights \( a_i \) in \( \hat{\rho}(\varepsilon) \) start to rise from zero. More precisely, we use the criterion that \( a_i \) should be less than 1% of the average d.o.s. at the band centre, \( \rho(\omega) \approx 0.1 \), i.e., \( a_i < 0.001 \). As shown in the insets of Figs. S5a and S5b, this criterion appears to offer a reliable means of distinguishing real reconstructed finite-\( T \) features from thermal and numerical noise.

By applying these considerations at \( U = 6 \), we obtain the data shown in Fig. 3(c), with a well-defined lower bound from \( T = 0.0625 \) to \( T = 0.2857 \). At our next higher temperature, \( T = 0.333 \), \( a_i > 0.001 \) even at \( \omega = 0 \), and thus the lower bound has become zero; we estimate the temperature at which this occurs to be \( T \approx 0.31 \), and represent this by the dashed line in Fig. 3(c). We conclude that these results can be taken to provide an accurate lower bound for \( \Delta_{Mott}(T) \), and that the closing of the Mott gap by this estimate provides the lower bound, \( T_{c,l} \approx 0.31 \), for the associated temperature.

As noted above, for a Mott insulator with no thermal fluctuations, one expects that \( \hat{\rho}(\omega) = 0 \) in the energy interval \( [-\Delta_{Mott}/2, \Delta_{Mott}/2] \), whence

\[ \rho(\omega) = \frac{2}{\pi} \int_{\Delta_{Mott}/2}^{\infty} d\varepsilon \frac{\delta}{(\omega - \varepsilon)^2 + \delta^2} \hat{\rho}(\varepsilon). \]  

(S30)

The process of using \( \rho(\omega) \), as calculated by SCBA at each value of \( T \), to extract the underlying function \( \hat{\rho}(\varepsilon) \) and the single constant \( \Delta_{Mott}(T) \) is analogous to an analytic continuation. Although a full SAC treatment of the SCBA data is complicated by a lack of statistical errors, a more straightforward procedure is sufficient in the present case. Motivated by the structure of the SAC method of Sec. S2, we construct a minimization based on linear regression to achieve the decomposition of Eq. (S30). We parameterize

\[ \hat{\rho}(\varepsilon) = \sum_{i=1}^{N_c} a_i \delta(\varepsilon - \varepsilon_i) \]  

(S31)

using \( N_c \) equally spaced \( \delta \)-functions, whose weights \( \{a_i\} \) are the free parameters. By inserting Eq. (S31) into Eq. (S30), we obtain the function

\[ \rho(\omega) = \frac{1}{\pi} \sum_{i=1}^{N_c} d\varepsilon \left[ \frac{\delta}{(\omega - \varepsilon_i)^2 + \delta^2} + \frac{\delta}{(\omega + \varepsilon_i)^2 + \delta^2} \right] a_i, \]

by which we approximate the SCBA \( \rho(\omega) \). We define the goodness-of-fit parameter

\[ \chi^2 = \sum_{i=1}^{N_c} \left( \rho(\omega_i) - \rho'(\omega_i) \right)^2, \]

(S33)

whose minimization by a linear regression method determines the values \( \{a_i\} \). Because the number, \( N_c \), of data points in \( \varepsilon \) in Eq. (S31) can only be equal to or smaller than the number, \( N_\omega = 600 \), of points in the SCBA \( \rho(\omega) \), such a minimization can always be achieved.

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(S30)
(ii) Turning now to the establishment of an upper bound on the Mott transition temperature, it is clear from Fig. 3b of the main text (SCBA) and from Fig. S4 (QMC) that \( \rho(\omega) \) changes from a low-\( T \) form with an absolute minimum at \( \omega = 0 \) to a high-\( T \) form with a peak at \( \omega = 0 \). This peak grows in size and spectral weight as a function of temperature beyond a given \( T \) value. We take this temperature for the appearance of the zero-frequency peak as an unequivocal indication that the Mott gap has closed: at this point the convolution of the overlapping lower and upper Hubbard bands gives a clear local maximum in the single-particle response. In practice, the Mott gap may have closed before the peak can emerge as a feature stronger than the d.o.s. at neighbouring finite frequencies, and hence this temperature, \( T_{\text{Mott}}^{c,u} \), can be taken as an upper bound for the closing of the Mott gap. At \( U = 6 \) we find, as shown in Fig. 3c of the main text, that \( T_{\text{Mott}}^{c,l} \approx 0.31 \) and \( T_{\text{Mott}}^{c,u} \approx 0.44 \). Comparison with the closing temperature of the holon-doublon gap, \( T_{\text{hd}} \approx 0.45 \), establishes firmly the existence of the pseudogap regime.