Thermal fluctuation driven nonequilibrium resistive and magnetic transitions in a voltage biased Mott insulator

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We use a Langevin dynamics approach to map out the thermal phases of an antiferromagnetic Mott insulator pushed out of equilibrium by a large voltage bias. The Mott insulator is realised in the half-filled Hubbard model in a three dimensional bar geometry with leads at voltage ±V/2 connected at the two ends. We decouple the strong Hubbard interaction via the combination of an auxiliary vector field, to capture magnetic fluctuations, and a homogeneous scalar field to maintain half-filling. The magnetic fluctuations are assumed to be slow on electronic timescales. At zero temperature our method reduces to Keldysh mean field theory and yields a voltage driven insulator-metal transition with hysteresis. The Langevin scheme generalises this, allowing us to study the finite temperature nonequilibrium steady state. We find an initially slow and then progressively rapid suppression of the Neel temperature $T_N$ and pseudogap temperature $T_{pg}$ with bias, and discover that the bias leads to a finite temperature insulator-metal transition. We explain the thermal results in terms of strong amplitude fluctuation of the local moments in the first order landscape.

Strongly correlated systems driven out of equilibrium define a frontier in condensed matter. Experiments have probed the response to large bias in Mott insulators [1–11], ‘pump-probe’ phenomena where a material is subjected to an intense pulse of radiation [11–15], and the effect of strong laser fields [16]. Among these, the voltage biased Mott insulator is widely studied due to the well understood equilibrium state and the occurrence of a bias driven insulator-metal transition (IMT). The breakdown of the ‘collectively localised’ Mott state is expected to be very different from that of a band insulator.

Experiments across multiple materials suggest that the current-voltage (I-V) characteristic across the bias driven transition has a common form [6–12]. These include (i) a low temperature hysteresis in the current with respect to voltage sweep - changing abruptly from low current to high current at some voltage $V^+_c$ on the upward sweep, and showing the reverse switching at $V^-_c < V^+_c$ on the downward sweep, and (ii) reduction of $V^+_c$ and also $\Delta V_c = V^+_c - V^-_c$ with increasing temperature, with hysteresis vanishing above some temperature $T^*$. These features have been observed in samples of nanometer [8] to millimeter [11] size.

Multiple theories have tried to model the voltage induced breakdown [18–36] Most microscopic approaches suggest a Landau Zener (LZ) like mechanism [18–22]. The resulting I-V characteristic fails to capture the discontinuous nature of breakdown, and the strong temperature dependence observed in a wide variety of compounds. Phenomenological network models invoking the ideas of percolation[26, 27] capture the low $V$ transport for some materials but their applicability in the strongly nonequilibrium state remains uncertain. It is only for narrow gap “dirty” Mott insulators, with in-gap states, that a successful theory [28] based on ideas of Frohlich [29–31] seems to be available. In our understanding the limitations for strong coupling systems arise from the neglect of spatial symmetry breaking (due to the bias), the difficulty in accessing the long time, steady state, current, and ignoring the magnetic order that occurs at low temperature.

This paper addresses the whole set of issues using a scheme that is non perturbative in both the interaction strength and the applied bias and only exploits the “slowness” of the magnetic fluctuations on electronic timescales. Our Keldysh based Langevin equation approach - somewhat of a novelty in correlated electron systems - retains the effects of dissipation channels (the leads), the applied bias, strong interaction, and thermal fluctuations, and yields the nonequilibrium electronic state at long times. The approach is a ‘twofold’ generalisation of the standard magnetic mean field theory of the Hubbard model: (i) at zero temperature ($T = 0$) we get a Keldysh mean field theory for magnetism in the biased open system, while (ii) at finite temperature a ‘thermal noise’ generates magnetic fluctuations in the driven system. The result is a stochastic evolution equation for the magnetic moments $\hat{M}_i(t)$ (see later) which define the background for electron physics.

We work with the half filled Hubbard model in a 3D geometry, set Hubbard repulsion $U = 6t$, where $t$ is the hopping, and probe the bias ($V$) and temperature dependence of the nonequilibrium state. At $V = 0$ the system shows a Neel transition at $T \sim 0.25t$, where $t$ is the hopping scale in the system. We discover the following. (1) The ground state shows a voltage sweep dependent transition at $V^*_c$, between an antiferromagnetic insulator (AF-I) and a paramagnetic metal (PM). The hysteretic window narrows with increasing temperature and vanishes at $T_{cex}$ $\sim 0.02t$. (2) The Neel temperature $T_N$ reduces slowly with $V$ up to $V \sim 0.5V^*_c$ and then falls sharply - vanishing at $V \sim 3.6t$. This is related to a thermally induced broad distribution of moment magnitudes, with a low mean value. (3) Apart from the expected insulating and metallic temperature dependence at small and large $V$, respectively, we observe a window of thermally induced insulator-metal transition. (4) Like $T_N$, the pseudogap temperature $T_{pg}$ - signalling the crossover from gapped to pseudogapped density of states (DOS) falls with $V$, vanishing at $V \sim 3.6t$ (5) We show that thermally induced amplitude fluctuation of the moments, and a suppression of mean magnitude, when $V$ approaches $V^*_c$ is the primary driver behind the collapse of $T_N$, $T_{pg}$, and the thermally induced IMT.
We consider the repulsive 3D Hubbard model in a finite geometry, connected to leads along the long direction. 

\[
\mathcal{H} = \mathcal{H}_{\text{sys}} + \mathcal{H}_{\text{bath}} + \mathcal{H}_{\text{coup}}
\]

\[
\mathcal{H}_{\text{sys}} = -t_s \sum_{<ij>} (d_{i\sigma}^\dagger d_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu N
\]

\[
\mathcal{H}_{\text{bath}} = -t_b \sum_{<ij>,\sigma} \left( \sum_{\beta} \left( \langle \hat{d}_{i\sigma}^{\dagger} \hat{n}_{\beta}^R \rangle + h.c. \right) - \sum_{\beta} \mu_{\beta} \hat{n}_{i\beta}^{\dagger} \right)
\]

\[
\mathcal{H}_{\text{coup}} = \sum_{<ij>,\beta} -v_{ij} \left( c_{i\sigma}^{\dagger} d_{j\sigma} + c_{i\sigma} d_{j\sigma} + h.c. \right)
\]

where \( t_s, \mu \) and \( U \) are the nearest-neighbour hopping amplitude, chemical potential and onsite Coulomb repulsion strength in the system, respectively. \( t_b \) is the hopping and \( \mu_{\beta} \) are the chemical potentials in the metallic baths, where \( \beta = (L,R) \), with \( L \) being the left lead and \( R \) the right lead. \( \mu_{L,R} = \mu \pm (V/2) \), \( V \) being the applied bias. \( v_{ij} \) denotes the system-bath hopping.

Starting from the complex time Keldysh action for the above Hamiltonian we decouple the quartic term by performing a Hubbard-Stratonovich transformation and introducing real auxiliary fields at each instant, which couple to the instantaneous density and spin of the electrons - henceforth called the charge field \( \phi_i(t) \) and spin field \( \tilde{M}_i(t) \) respectively. The action becomes quadratic in the Grassmann fields which can be formally integrated out. We fix the charge field at it’s equilibrium saddle point value. Using assumptions related to the slowness of the \( \tilde{M}_i(t) \), and a simplified noise kernel, both discussed in the Supplement, we arrive at a stochastic dynamical equation for \( \tilde{M}_i(t) \).

\[
\frac{d\tilde{M}_i}{dt} + \alpha \left( \langle \hat{\sigma}_i \rangle_{\tilde{M}} \times \frac{d\tilde{M}_i}{dt} \right) = \gamma \left( \tilde{M}_i - \langle \hat{\sigma}_i \rangle_{\tilde{M}} \right) + \xi_i
\]

\[
\langle \xi_i(t) \xi_j(t') \rangle = 2\gamma T \delta_{ij} \delta_\alpha \delta_\beta \delta(t - t')
\]

\[
\langle \hat{\sigma}_i \rangle_{\tilde{M}(t)} = \int T \int [\text{Im} \left( \mathcal{G}_i^K(t,\omega) \hat{\sigma}_i \right)] d\omega
\]

where \( \alpha, \beta \) denote O(3) indices, \( \mathcal{G}_i^K \) denotes the adiabatic Keldysh Green’s function, and the trace is over the local 2 \times 2 spin subspace. \( \hat{\sigma}_i = \frac{1}{2} \sum_{\alpha,\beta} d_{i\alpha}^\dagger \tau_{\alpha,\beta} d_{i\beta} \), \( \tau \equiv (\tau^x, \tau^y, \tau^z) \) being the 2 \times 2 Pauli vector, is the local fermion spin. Its average is computed on the instantaneous \( \{\tilde{M}\} \) background. \( \langle \hat{\sigma}_i \rangle \) is a non-linear, non local, function of the \( \tilde{M} \) field and encodes the strong correlation effects in the problem. \( \gamma \) and \( \alpha \) are dimensionless phenomenological parameters which are fixed by benchmarking the scheme against equilibrium Monte-Carlo results. \( \gamma \) controls the relaxation rate of the moment magnitudes while \( \alpha \) controls the relaxation rate of the angular variables.

The equation is solved using a stochastic Heun discretisation scheme [40] to generate a time series for \( \tilde{M}_i(t) \). Upon obtaining the time series the electronic observables are computed on the instantaneous configurations (assuming that electronic timescales are much shorter than spin fluctuation scales) and averaged over the time series.

The results presented in the main text pertain to a 8 \times 4 \times 4 system, with \( L = 8 \) being the longitudinal (transport) direction. Starting with an arbitrary \( \{\tilde{M}\} \) configuration the system is evolved for \( \sim 10^6 \) steps with a time discretisation of \( 10^{-4} \tau_0 \), where \( \tau_0 \sim 1/J_{eff} \) with \( J_{eff} \sim \frac{\gamma}{2t} \) is the characteristic timescale of the auxiliary field. After allowing the system to equilibrate for 100\( \tau_0 \), the rest of the configurations have been saved to construct the time series for \( \tilde{M}_i(t) \).

The equilibrium system at half-filling has been well studied using Monte Carlo techniques [37, 38]. For any finite \( U \) the ground state is an antiferromagnetic insulator (AF-I), \( |\tilde{M}| \) grows with increasing \( U \) and saturates to unity as \( U/t \to \infty \). As the temperature is increased the system loses long range order (LRO) at a scale \( T_N(U) \). Beyond \( T_N \), the system is a paramagnetic metal (PM) for \( U < 4t \) and a paramagnetic insulator (PI) for \( U > 4t \). The crossover region from PM to PI shows a pseudogapped density of states (DOS).

Connecting leads, without a bias, modifies the moment magnitude at the edges, explored earlier in 1D [34, 35] as well as in 2D [36]. In the 3D geometry that we explore the presence of leads (at \( V = 0 \)) does not affect the structure factor significantly when \( U > 4t \). Since the magnetic structure factor shows a pseudogapped density of states (DOS) and the gap closes, and the system carries a large current. In the downward sweep, the current carrying low moment state continues till \( V_c^- \), after which the system switches back to the insulating state.

We construct a nonequilibrium \( V \sim T \) phase diagram, Fig.1(a), highlighting the magnetic, transport and spectral

![FIG. 1. (a) Phase diagram of the voltage biased repulsive Hubbard model at \( t = 0t \). The AF-I, P-M and P-I are the antiferromagnetic insulator, paramagnetic metal and paramagnetic insulator phases respectively. Insulating regimes have \( \partial I/\partial T > 0 \) and the metal has \( \partial I/\partial T < 0 \). CX marks the hysteric window. The solid blue line indicates \( T_N(V) \), the dashed white line \( T_{3x3}(V) \) and the broken grey line indicates \( T_{3x3}(V) \). (b) The magnetic ordering peak, \( S(\pi, \pi, \pi) \) as a function of temperature (\( T \)) for upward (open circles) and downward (solid squares) voltage (\( V \)) sweeps. Beyond \( T = 0.02t \) the two curves coincide for all values of \( V \). The inflection point for each curve gives the Néel temperature (\( T_N \)) for the corresponding \( V \).](image-url)
regimes that occur in the biased problem. There are three phases, AF-I, P-I and P-M, and a low
temperature coexistence (CX) window of thermally induced insulator-metal transition, and $T_{\text{coex}}$ for crossover from gapped to pseudogap DOS.

Fig. 2(b) shows the peak, $S_{\bar{Q}}(T)$, in the magnetic structure factor $S(\vec{q})$ defined by:

$$S(\vec{q}) = \int_0^{t_M} \frac{dt}{t_M} \sum_{ij} \vec{M}(t, \vec{r}_i) \cdot \vec{M}(t, \vec{r}_j) e^{i\vec{q}(\vec{r}_i-\vec{r}_j)}$$

For the present problem, $\bar{Q} = (\pi, \pi, \pi)$, pertaining to Néel AF order. For each $V$ the Néel temperature is estimated from the point of inflection of the $S_{\bar{Q}}(T)$ curve. There exists a coexistence region at $T = 0$ in the interval $2.2 < V/t < 4.3$, which extends up to $T_{\text{coex}} = 0.02t$. The state in this region depends on the direction of voltage sweep. In Fig. 1(b), the open circles denote the $T$ dependence of $S(\bar{Q})$ for upward sweep, while the solid squares denote the same for the downward sweep. The solid blue curve in Fig. 1(a) shows the dependence of $T_N$ on $V$ for the upward sweep. $T_N$ decreases slowly initially, with $V$, and then quicker for $V > 0.5V_c$ and vanishes at $V \approx 3.6t$.

The charge transport is characterised by the current-voltage (I-V) characteristics, with the current given by:

$$I_j(V) = \int_0^{t_M} \frac{dt}{t_M} \int_{-D}^{D} \frac{d\omega}{2\pi} Tr \left[ G^<_{j+1,j;\sigma}(t,\omega) - G^<_{j,j+1;\sigma}(t,\omega) \right]$$

$I_j(V)$ is the bond current between sites $j$ and $j'$'s neighbouring site in the longitudinal direction and $G^<$ is the adiabatic lesser Green’s function and the trace is over the $2 \times 2$ spin subspace. Within our approximation the Green’s function with label $t$ depends only on the instantaneous configuration $\{\vec{M}(t)\}$. Due to current conservation $I_j(V)$ must be independent of $j$.

The I-V characteristics is plotted in Fig. 2(a) for different temperatures. The inset shows hysteresis for $T < T_{\text{coex}} \approx 0.02t$ while the main panel shows the response for $T \approx 0.02t$. Above $T_{\text{coex}}$ and up to $T \approx 0.3t$ the I-V characteristic has a “threshold” at some $V_c(T)$ below which, the current remains exponentially suppressed. Beyond $V_c$, the current rises sharply with increasing $V$ and saturates as $V$ approaches the bandwidth $D$ of the connected system. With increasing $T$, the threshold reduces, vanishing for $T \approx 0.3t$. The current saturation at large $V$ is similar to what has been observed in the 2D problem at zero $T$ [36]. The suppression of $V_c$ with increasing $T$ has been observed in experiments on various driven Mott systems [5–11].

Figs. 2(b) show $I(T)$ at different $V$. The results reveal three regimes: (i) insulating, where the system becoming more conducting with increasing $T$: formally $\partial I/\partial T > 0$ at all $T$ (happens for $V/t \leq 2$), (ii) metallic, showing $\partial I/\partial T < 0$ at all $T$ (occurs for $V/t > 3.8$), and (iii) showing insulator to metal transition: crossing over from $\partial I/\partial T > 0$ to $\partial I/\partial T < 0$ with increasing $T$. We label the temperature at which $\partial I/\partial T = 0$ as $T_{\text{IMT}}$. The thermal IMT happens for $2 < V/t < 3.8$.

The corresponding ‘resistance’ $R = V/I$ is shown in Fig. 2(c) on a logarithmic scale. In the deep insulating regime $R$ decreases exponentially with increasing $T$ and well in the metal it rises monotonically with $T$. At intermediate $V$ it shows non monotonic $T$ dependence. This feature, arising from thermal fluctuations in a non equilibrium situation, is the most important result of our paper. We will discuss the physical basis further on. Note that within a linear response treatment of the Mott insulator $V/I$ is independent of $V$ and solely dependent on $T$. This would be true of the $V \lesssim 1$ window (the top right curve). The effective resistance at all other voltages depends crucially on the applied bias.

Another quantity of great interest is the system averaged
FIG. 3. (a) Map of DOS for varying temperature and voltage, on the upward sweep. For $V/t \leq 2.6$, the low $T$ DOS remains gapped and becomes pseudogapped for $T > T_{ps}$, in both the sweep cycles. For $2.6 < V/t < 3.4$ the DOS remains gapped at low temperature, develops subgap weight with increasing $T$, even in the insulating phase, and ultimately becomes pseudogapped at large $T$. For the downward sweep, the DOS in this regime retains subgap weight even to the lowest temperature. For $T/t \geq 3.4$ the DOS remains ungapped at low $T$, broadens with increasing $T$, and develops a pseudogap at high $T$. (b-d) The variation of density of states (DOS) with temperature for $V/t = 1.8, 2.4$ and $3.4$.

(a) The $T = 0$ transition can be modeled by extremizing a functional of the form:

$$F(M) = \frac{a(V)}{2} M^2 - \frac{b}{3} M^3 + \frac{c}{4} M^4$$

where $M$ is the magnitude of the local moment, assumed to be uniform across the system. $a(V) = a_0 \left(e^{-V'/V} - e^{-V'/V_c}\right)$; $a_0, V', b, c$ are fitting parameters which take positive values. The quality of fit for the order parameter $M(V)$, and the hysteretic window, is shown in the Supplement Fig.3. A power law dependence of $a(V)$ on voltage leads to a stronger dependence of the $M$ on bias. The coefficients $a, b, c$ should ideally be extracted from the $T = 0$ Keldysh mean field theory. While the $T = 0$ moment magnitude sets a reference it does not explain the behaviour of $T_N$ which falls in a continuous manner despite $M(V)$ at $T = 0$ being sharply discontinuous.

(b) We can promote the $F(M)$ to a ‘Boltzmann weight’ for local fluctuation of moment magnitude, and couple these moments via a nearest neighbour exchange $J_{eff}$ that reproduces the $V = 0$ Neel temperature. This did not work since the configurational weights seem to have a non-trivial $T$ dependence near $V_c$. We therefore tried to use the computationally determined moment magnitude distribution $P(M, T)$, picked moments from these, and paired them using $J_{eff}$. This, as the Supplement (Fig. 4(c)-(d)) shows, does a reasonable job except very near $V_c$. Overall, thermal amplitude fluctuation of the moments, as $V \rightarrow V_c$, is a crucial ingredient in the thermal response of this system. A softening of the moment also implies stronger charge fluctuation and greater metallicity.

The behaviour of moment magnitude and angular fluctuation directly affects the DOS. Deep in the AF-I phase the large ordered moments generate a large ‘gap’ in the DOS, albeit with exponentially suppressed low energy DOS and current. With increasing $T$ the angular fluctuations of the moments smear the gap and increase the current. As the voltage increases, amplitude fluctuations of the moments also join in, creating additional low energy DOS and larger current.

In the deep metallic phase the moment magnitude is small at low $T$. This closes the Mott gap and allows a large current to flow. As $T$ increases, the moment distribution broadens, the mean moment increases, and its angular fluctuation scatters the electrons. This suppresses the current. At intermediate $V$ a combination of activation induced current increase competes with scattering induced current decrease leading to the thermal IMT.

The Langevin equation we use involves two key assumptions: (i) adiabaticity, and (ii) thermal noise. The adiabatic assumption would be valid if the typical frequency associated with magnetic fluctuations were self consistently smaller than the electron frequency. We have not shown the magnetic spectra here but at $U = 6t$ the magnetic bandwidth is $2J_{eff} \sim \frac{8t^2}{U}$, while the electron bandwidth is $\sim U$. At $U = 6t$, the ratio is $\sim 1/5$. This argument does not hold in the deep metallic state where $U$ is rendered ineffective. The ‘thermal noise’ is used in
the spirit of a first approximation, consistent with mean field theory at $T = 0$. In a scheme with quantum fluctuations built in, the noise would need self consistent modification.

Finally, the relevance of our results to real Mott materials. Experimentally, the I-V characteristics have a generic form across the transition metal oxides, TMO’s, (e.g. vanadium oxides [6,7], ruthenates [10,11], magnetites [8,9]) and some organics [12]. All these show a first order transition at low $T$ which gets weaker with increasing temperature. This aspect is well captured by our theory, unlike other microscopic approaches. Some TMOs also undergo a temperature driven structural transition at equilibrium. However, the transport measurements have been made below this equilibrium transition temperature. Our theory suggests that the transport characteristics can be explained via a purely electronic mechanism. An experiment on a multiorbital ruthenate has also reported suppression of Néel temperature with increasing current [1].

Conclusions: Our main achievement has been to construct a real time finite temperature scheme to approach nonequilibrium effects in a strongly correlated system. This Langevin equation approach simplifies the underlying Keldysh field theory by assuming adiabaticity, i.e., electrons are much faster than magnetic degrees of freedom, and a thermal noise. With these assumptions we could implement a numerical study of a Mott insulator in a finite 3D geometry. We established a voltage sweep driven hysteretic insulator-metal transition at low temperature, the collapse of the Néel and pseudogap temperature with increasing bias, and a thermally induced insulator-metal transition at finite bias. In our analysis the primary driver of the finite temperature effects is strong amplitude fluctuation of the local moments in the bias induced first order landscape. This Langevin approach would open up other nonequilibrium problems that have remained inaccessible.

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REAL TIME PATH INTEGRAL

Assuming the leads were connected far in the past, one can write the steady-state action for the system by discretizing the complex time Keldysh contour. The generating functional is given by:

$$ Z = \int \mathcal{D}\{\bar{c}, c; \bar{d}, d\} e^{iS[\bar{c}, c; \bar{d}, d]} $$

(1)

where $(\bar{c}, c)$ and $(\bar{d}, d)$ are the Grassmann fields for the lead and system fermions respectively. $S[\bar{c}, c; \bar{d}, d]$ is the complex time Keldysh action defined on the contour.

$$ S = \int_{-\infty}^{\infty} dt \left[ \mathcal{L}_{\text{sys}}(t) + \mathcal{L}_{\text{bath}}(t) + \mathcal{L}_{\text{coup}}(t) \right] $$

(1a)

$$ \mathcal{L}_{\text{sys}}(t) = \sum_{<ij>; \sigma, \alpha, s} s d_{i\sigma}^*(t) (i\partial_t + t_s) d_{j\sigma}^* (t) - U \sum_{i, s} s n_{i\uparrow}^s n_{i\downarrow}^s (t) $$

(1b)

$$ \mathcal{L}_{\text{bath}}(t) = \sum_{<ij>; \sigma, \alpha, s} s \overline{c}_{i\sigma \alpha}^s (t) (i\partial_t + t_s) c_{j\sigma \alpha}^s (t) $$

(1c)

$$ \mathcal{L}_{\text{coup}}(t) = \sum_{<ij>; \sigma} v_{ij} \left( \overline{c}_{i\sigma}^s (t) d_{j\sigma}^* (t) + c_{i\sigma}^s (t) d_{j\sigma} (t) + g.c. \right) $$

(1d)

where $i, j$ are the lattice indices, $\sigma$ is the spin index, $\alpha$ labels the leads and $s$ labels the contour. $s = \pm 1$ for the upper and the lower contour fields respectively. At each time slice, for every site we can rewrite the interaction term as:

$$ U n_{i\uparrow}^s n_{i\downarrow}^s = \frac{U}{4} (n_{i\uparrow}^s)^2 - U \left( S_{i\alpha}^s \cdot \hat{\Omega}_{i\alpha}^s \right)^2 $$

(2)

where we have suppressed the time label for brevity. Here, $n_{i\uparrow}^s = \overline{c}_{i\uparrow}^s c_{i\uparrow}^s + \overline{c}_{i\downarrow}^s c_{i\downarrow}^s$ is the local density, $S_{i\alpha}^s = \frac{1}{2} \sum_{\alpha, \beta} \sigma_{\alpha, \beta} c_{i\alpha}^s \overline{c}_{i\beta}^s$ is the local spin operator and $\hat{\Omega}_{i\alpha}^s$ is an arbitrary SO(3) vector.

Each of the two terms can be decomposed by a Hubbard-Stratonovich (HS) transformation. The first transformation introduces a “charge field” $\phi_i(t)$:

$$ e^{-i\frac{\phi_i^c(t)}{U} (n_{i\uparrow}^s)^2} \propto \int d\phi_i^c (t) e^{i\left( \frac{\phi_i^c(t)}{U} (n_{i\uparrow}^s)^2 - \frac{\phi_i^c(t)}{U} \phi_i^c(t) n_{i\downarrow}^s (t) \right)} $$

(2a)

While the HS transformation on the second term can be written in terms of an O(3) “spin field” $M_i(t)$:

$$ e^{i\frac{\phi_i^s(t)}{U} (n_{i\uparrow}^s)^2} \propto \int \mathcal{D} M_i \left[ \int d^3 M_i(t) e^{i\left( \frac{\phi_i^s(t)}{U} (n_{i\uparrow}^s)^2 + s U M_i^2(t) \cdot \delta_i^c \right)} \right] $$

(2b)

Upon introducing the auxiliary fields the action becomes quadratic in the fermions, which can be integrated out to get the following effective action:

$$ S[\phi, M] = -\frac{1}{2} Tr \ln \left[ \hat{G}^{-1}(t, t') \right] + \frac{U}{2} \int dt \sum_i \left[ \phi_i^c(t) \phi_i^c(t) - M_i^2(t) \cdot \delta_i^c \right] $$

(3)

where the components of $G^{-1}$ in the $2 \times 2$ Keldysh space are given by:

$$ \hat{G}^{-1}_R (t, t') = \left( \hat{G}^{-1}_R \right) $$

(3a)

$$ \hat{G}^{-1}_A (t, t') = \left( \hat{G}^{-1}_A \right) $$

(3b)

$$ \hat{G}^{-1}_K (t, t') = \left( \hat{G}^{-1}_K \right) $$

(3c)

$$ \hat{G}^{-1}_{12} (t, t') = \left( \hat{G}^{-1}_{12} \right) $$

(3d)

$$ \hat{G}^{-1}_{21} (t, t') = \left( \hat{G}^{-1}_{21} \right) $$

(3e)

$$ \hat{H}_i^c (t) = \left( \hat{H}_i^c \right) $$

(3f)

where $\mathbb{I}_2$ is the $2 \times 2$ identity matrix. $\hat{H}_i^c(t)$ is can be interpreted as a time-dependent Hamiltonian which depends on the “classical” component of the auxiliary fields. $\Gamma_{R, A, K}(t, t')$
are dissipation terms which enter the action as a result of integrating out the leads. $F(t,t')$ is the distribution function of the disconnected system, and $\circ$ denotes convolution. The "classical" and "quantum" components of the auxiliary fields are linear combinations of the auxiliary fields introduced in the H-S transformations in Eqs.2a and 2b.

$$\tilde{M}^c = \frac{1}{2} (\tilde{M}^+ + \tilde{M}^-)$$

(4)

$$\tilde{M}^q = (\tilde{M}^+ - \tilde{M}^-)$$

(5)

where we have suppressed the time and other labels for notational brevity. A similar transformation holds for the $\phi$ fields.

**APPROXIMATIONS**

In order to make progress we make a series of approximations to make the problem tractable. (i) We fix the charge field ($\phi$) to it’s classical saddle point at equilibrium, i.e., $\phi^c, \phi^q = 0$. The fixes the overall density to half-filling, but allows local density fluctuations due to the dynamics of the spin-field ($\tilde{M}$). (ii) We perform a cumulant expansion of the action to second order in $\{M^q\}$ fields, introduce a "noise" by decoupling the quadratic terms, and evaluate the ‘classical’ saddle point to obtain a stochastic equation of motion (EOM). (iii) We simplify the EOM by performing a semiclassical expansion of the two-point functions to obtain a 'Langevin’ equation in terms of the ‘slow’ time coordinate. The noise kernel is assumed to be Gaussian.

**Cumulant expansion**

The $\tilde{G}^{-1}$ introduced in Eq.3a can be decomposed into a Green’s function $\hat{G}^{-1}$, which depends only on the ‘classical’ field and a self-energy $\tilde{\Sigma}_q$, which depends only on the ‘quantum’ field.

$$\tilde{G}^{-1} = (\tilde{1} + \tilde{\Sigma}_q \circ \hat{G}^{-1}) \circ \hat{G}^{-1}$$

$$\tilde{\Sigma}_q(t,t') = \frac{U}{4} \tilde{M}^q(t) \cdot \sigma_{\alpha\alpha'} \delta_{ij} (t-t') \otimes \sigma^\tau$$

(6)

where the $\sigma^\tau$ denotes the structure in the $2 \times 2$ Keldysh space. We expand the action in Eq.3 to second order in $\Sigma_q$.

$$\hat{S} = \hat{S}^0 + \hat{S}^1 + \hat{S}^2 + ...$$

(7)

with

$$\hat{S}^0 = -i Tr \ln [t \hat{G}^{-1}(t,t')] = 0$$

(7a)

$\hat{S}^0$ vanishes from the causality relation between the retarded and advanced Green’s functions.

$$\hat{S}^1 = \frac{U}{4} \sum_i \int dt \left [ \Im \left [ Tr \left ( \hat{G}^{-1} (t,t) \hat{\sigma} \right ) \right ] - \tilde{M}^c_i (t) \cdot \tilde{M}^c_i (t) \right ]$$

(7b)

$$\hat{S}^2 = \frac{l}{2} \left ( \frac{U}{4} \right )^2 \int dt \int dt' \sum_{ij;ab} M^q_{ii}(t) \left [ \hat{\Pi}^{K}(t,t') \right ]^{ab}_{ij} M^q_{jj}(t')$$

(7c)

where

$$\left [ \hat{\Pi}^{K}(t,t') \right ]^{ab}_{ij} = Tr \left [ \left ( \hat{G}^{K} \right )_{ij}(t,t') \sigma^a \hat{G}^{K}_{ji}(t',t) \sigma^b \right ] + \left ( \hat{G}^{K}_{ij}(t,t') \sigma^a \hat{G}^{K}_{ji}(t',t) \sigma^b \right ) + \left ( \hat{G}^{K}_{ij}(t,t') \sigma^a \hat{G}^{K}_{ji}(t',t) \sigma^b \right )$$

(7d)

Now, we decompose the term quadratic in $M^q$.

$$e^{i \hat{S}^2} = e^{-M^q \circ \hat{\Pi}^{K} \circ M^q}$$

$$\propto \int \mathcal{D}[\xi] \exp \left ( -\frac{1}{2} \xi \circ \left [ \hat{\Pi}^{K} \right ]^{-1} \circ \xi - i \xi \circ M^q \right )$$

(7e)

Hence, this adds a term to the coefficient of $M^q$ in $\hat{S}^1$ and additionally, the generating functional is reweighted by the quadratic piece in $\xi$.

We obtain the equation of motion by requiring that the first order variation w.r.t the ‘q’ fields must vanish at $\phi^q = 0, \tilde{M}^q = 0$. This gives us the following equation for the ‘c’ fields:

$$\Im \left [ Tr \left ( \hat{G}^{-1} (t,t) \hat{\sigma} \right ) \right ] = \tilde{M}^c_i (t) + \xi^c_i (t)$$

$$\langle \xi^c_i (t) \xi^c_j (t') \rangle = \left [ \hat{\Pi}^{K} (t,t') \right ]^{ab}_{ij}$$

(8)

**Semiclassical expansion**

Transforming to Wigner coordinates allows us to write.

$$\hat{G}^{K}(t,t) = \hat{G}^{K}(t,t_r = 0) = \int d\omega \hat{G}^{K}(t,\omega)$$

(9)

In what follows, we would write a series expansion for $\hat{G}^{K}(t,\omega)$ in powers of $\hbar$.

**The retarded Green’s function $\hat{G}^{R}$**

The retarded Green’s function obeys the Dyson’s equation

$$\langle \hat{G}^{-1, R} \hat{G}^{R} \rangle (t,t') = \delta(t-t')$$

(10)
Transforming to Wigner coordinates allows us to expand the LHS in a Kramers-Moyal series,
\[ \left( \omega - \hat{H}^c(T) + \hat{T}^R(\omega) \right) \hat{G}^R(T, \omega) \]
\[ - i\hbar \left( \partial_T \hat{H}^c(T) \partial_\omega \hat{G}^R - \langle \hat{I} + \partial_\omega \hat{T}^R \rangle \partial_T \hat{G}^R \right) + O(\hbar^2) = \hat{I} \]  \hspace{1cm} (10a)
where \( T \) is the center-of-mass time, and \( \omega \) is the Fourier conjugate to the relative time. Furthermore, we have assumed that \( \hat{T} \) depends only on the relative time. This is true at steady state. Inverting this gives us
\[ \hat{G}^R(T, \omega) = \hat{G}^R(T, \omega) \]
\[ + i\hbar \left( \hat{G}^R \partial_T \hat{H}^c(T) \partial_\omega \hat{G}^R + \hat{G}^R (\langle \hat{I} + \partial_\omega \hat{T}^R \rangle \partial_T \hat{G}^R) \right) + O(\hbar^2) \]  \hspace{1cm} (10b)
where, \( \hat{G}^R(T, \omega) \) is the "adiabatic" retarded Green’s function given by
\[ \hat{G}^R(T, \omega) = \left( \omega \hat{I} - \hat{H}^c(T) + \hat{T}^R(\omega) \right)^{-1} \]  \hspace{1cm} (10c)

Now, for any matrix \( \hat{A} = -\hat{A} \left( \partial_\alpha \hat{A}^{-1} \right) \hat{A} \). Using this we can rewrite 10b to \( O(\hbar) \) as
\[ \hat{G}^R(T, \omega) = \left( \hat{I} - i\hbar \left[ \hat{G}^R \partial_T \hat{H}^c, \hat{G}^R (\langle \hat{I} + \partial_\omega \hat{T}^R \rangle) \right] \right) \hat{G}^R(T, \omega) \]  \hspace{1cm} (10d)
where \([, , ]\) denotes the commutator bracket.

**The Keldysh Green’s function** \( \hat{G}^K \)

Knowing \( \hat{G}^R \) and \( \hat{G}^A \) to any order in \( \hbar \) allows one to construct the \( \hat{G}^K \) to that order. From the structure of \( \hat{G}^{-1} \), it follows that
\[ \hat{G}^K(t, t') = -\hat{G}^R(t, t_1) \circ \hat{G}^{-1}(t_1, t_2) \circ \hat{G}^A(t_2, t') \]  \hspace{1cm} (11)
where \( \hat{G}^{-1}(t_1, t_2) \) has been defined in eq.3d. Transforming to Wigner coordinates and implementing the Kramers-Moyal expansion, as above, allows us to write
\[ \hat{G}^K(T, \omega) = \hat{G}^K(T, \omega) \]
\[ - i\hbar \left[ \hat{G}^R \partial_T \hat{H}^c, \hat{G}^R (\langle \hat{I} + \partial_\omega \hat{T}^R \rangle) \right] F \hat{G}^R + H.c. \]  \hspace{1cm} (11a)
\[ \hat{G}^K(T, \omega) = F(\omega) \left( \hat{G}^R(T, \omega) - \hat{G}^A(t, \omega) \right) \]
\[ - \hat{G}^R(t, \omega) \hat{G}^A(\omega) \hat{G}^A(t, \omega) \]  \hspace{1cm} (11b)

Now, we can write the matrix elements of adiabatic Green’s function in the \( 2 \times 2 \) spin subspace as:
\[ \hat{G}^R_{ij}(T, \omega) = \hat{g}^R_{ij}(T, \omega) \langle \hat{S}_i \rangle \langle \hat{S}_j \rangle + \hat{k}^R_{ij}(T, \omega) \cdot \hat{\sigma} \]  \hspace{1cm} (12a)
and similarly, defining,
\[ \hat{\Pi}^R_{ij} = -i\hbar \left[ \hat{G} \partial_T \hat{H}^c, \hat{G}^R (\hat{I} + \partial_\omega \hat{T}^R) \right] \]  \hspace{1cm} (12b)
we can write,
\[ \hat{\Pi}^R_{ij}(T, \omega) = \chi^R_{ij}(T, \omega) \hat{I}_{2x2} + \hat{Q}^R_{ij}(T, \omega) \cdot \hat{\sigma} \]  \hspace{1cm} (12c)
Plugging these in eq.11a we obtain
\[ T \hat{R} \left[ \hat{G}^K_{ii}(T, \omega) \sigma^a \right] = T \hat{R} \left[ \hat{G}^K_{ii}(T, \omega) \sigma^a \right] \]
\[ + \frac{U}{2} \sum_j \left( \gamma_{ij}(T, \omega) \partial_T M^a_j + \left( \tilde{\alpha}_{ij}(T, \omega) \times \partial_T \hat{M}_j \right) \right) \]
\[ + \tilde{\beta}^a_{ij}(T, \omega) \cdot \partial_T \hat{M}_j \]  \hspace{1cm} (12d)
where
\[ \gamma_{ij} = \left( \chi_{ij} R^R_{ij} - \hat{G}^R_{ij} \cdot \hat{R}^R_{ij} + R \rightarrow A \right) \]
\[ \tilde{\alpha}_{ij} = \left( \chi_{ij} R^R_{ij} - \hat{G}^R_{ij} g^R_{ij} + R \rightarrow A \right) \]
\[ \tilde{\beta}^a_{ij} = \left( \hat{G}^R_{ij} \tilde{R}^R_{ij} - \hat{G}^R_{ij} \cdot \hat{R}^R_{ij} + R \rightarrow A \right) \]
Finally, from eq.9 we know that the equal time Keldysh Green’s function which enters the EOM eq’8 is obtained by performing an integral over \( \omega \) of eq.12d.
\[ \int d\omega \left[ \left( \hat{G}^K_{ii}(T, \omega) \hat{\sigma} \right) \right] \]  \hspace{1cm} (13a)
where \( \hat{S}_i(t) \) is the instantaneous expectation value of the electron spin obtained under the adiabatic approximation. We further assume,
\[ \int d\omega \gamma_{ij}(t, \omega) \approx \gamma \frac{2}{U^2} \delta_{ij} \]  \hspace{1cm} (13b)
\[ \int d\omega \tilde{\alpha}_{ij}(t, \omega) \approx \alpha \frac{2\gamma}{U^2} \hat{S}_i(t) \delta_{ij} \]  \hspace{1cm} (13c)
\[ \left[ \Pi^K(t, t') \right]_{ij} \approx 2\gamma \frac{T}{U^2} \delta_{ij} \delta(t-t') \]  \hspace{1cm} (13d)
where \( \gamma, \alpha \) are dimensionless phenomenological parameters and \( \tilde{\beta}^a_{ij} \) has been neglected, \( T \) is the temperature. Hence, one obtains the final form of the evolution equation for \( \{ \hat{M} \} \), as given in Eq.2 of the main text. One can also cast this into a Landau-Lifshitz-Gilbert(LLG) form by solving for \( \frac{d\hat{M}}{dt} \), which gives,
\[ \frac{d\hat{M}}{dt} = \frac{U}{\gamma} \left( \hat{M} - \langle \hat{S}_i \rangle \langle \hat{M} \rangle + \hat{\xi}_i \rangle + \gamma \langle \hat{S}_i \rangle \langle \hat{M} \rangle \times \left( \hat{M} + \hat{\xi}_i \rangle \right) \]
\[ + \gamma \alpha \langle \hat{S}_i \rangle \times \left( \left( \hat{M} + \hat{\xi}_i \rangle \right) \times \langle \hat{S}_i \rangle \langle \hat{M} \rangle \right) \]  \hspace{1cm} (14)
where \( \hat{\gamma} = U \alpha \gamma \)\( (1+\alpha^2|\hat{S}|^2) \).
FIG. 1. (a)Comparison of temperature dependence of the structure factor peak with equilibrium ‘classical’ Monte Carlo. The two curves fall on top for low \((T/t \leq 1.2)\) and high \((T/t > 0.3)\) temperatures. The Langevin formulation overestimates the Néel temperature by \(\approx 17\%\). (b) Comparison of moment distribution for different temperatures. The distributions match for low temperatures \((T/t \leq 1.2)\). At higher temperatures the distributions deviate at low values of the moment, but match at higher values.

BENCHMARKS

We benchmark our formulation against the classical Monte Carlo (MC) formulation at equilibrium\([1]\). We compare the temperature dependence of the structure factor (Eq.3 in the main text) peak across the two formulations, in Fig.1(a). The MC predicts a transition at \(T_{MC} = 0.24t\), while the present formulation predicts it to be at \(T_{Lang} = 0.28t\). So, the Langevin formulation overestimates the Néel temperature by \(\approx 17\%\). The ordering peak height, at \(\vec{Q} = (\pi, \pi, \pi)\), matches across the two formulations for \(T \leq 0.5T_{MC}\), and also for temperatures beyond \(T_{Lang}\).

We also compare the moment distribution defined as

\[
P(m) = \frac{1}{N} \sum_i \int_0^{t_M} \frac{dt}{t_M} \delta(m - |\vec{M}_i(t)|)
\]

(15)

Fig.1(b) shows the comparison at different temperatures. At low temperatures \(T \leq 0.5T_{MC}\) the distributions match fairly well. For higher temperatures, the distributions start to differ at low moment values, but match at higher values of the moment. The \(P(m)\) → 0 as \(m → 0\), within our formulation but the same is not true for the MC at high temperatures. This might be because we have oversimplified the noise.

NATURE OF MAGNETIC STATE

Moment magnitude distribution

A quantity of interest is the probability distribution of the magnitude of the local moments as defined in Eq. The evolution of \(P(m)\) with temperature in different voltage regimes has been plotted in Fig.4. For \(V\) in the LR regime, and \(T < < T_N\), the moments remain almost pinned to their equilibrium ground state value, except for renormalisation at the edges due to the baths. Hence, the \(P(m)\) is sharply peaked around 0.8. As the system is heated up the distribution broadens around the same mean value up to \(T \approx T_N\). Beyond \(T_N\) the distribution becomes skewed and the mean starts shifting to lower values with increasing \(T\). Between \(V = 2t\) and 3.6\(t\) the low \(T\) moment distribution changes from being unimodal to bimodal. This can be understood in terms of penetration of edge effect into the bulk with increasing \(V\). As \(V\) approaches the \(V_{th}(T = 0)\) more and more sites from the edge sense the presence of the leads and, as a result, the moment on these sites weaken. This effect has been studies in detail for the 2D system in Ref.\([2]\). Beyond \(V = 3.6t\) the system goes into a metallic phase. At low \(T\), the \(P(m)\) peak gets quenched as the moments collapse throughout the system. With increasing \(T\), the distribution broadens while the mean shifts towards larger \(m\) values.

Effective theory at low \(T\)

The \(T = 0\) transition can be qualitatively explained using an effective functional \((F)\) of the form:

\[
F(M) = \frac{a(V)}{2} M^2 - \frac{b}{3} M^3 + \frac{c}{4} M^4
\]

(16)

where \(M\) is the magnitude of the local moment, assumed to be uniform across the system. \(a(V) = a_0 \left( e^{-V^\ast/V} - e^{-V^\ast/V^\ast} \right)\); \(a_0, V^\ast, b, c\) are fitting parameters which take positive values. \(a_0, V^\ast\) and \(b\) can be determined in
FIG. 3. (a) Effective functional for different values of $V/t$. For $V < V^- c$ it has a unique minimum at large $M$. For $V^- c < V \leq V^+ c$ it develops two minima (inset). For $V > V^+ c$ there is a unique minimum at $M = 0$. (b) The resulting moment profile which gets a sweep dependence in the coexistence region due to the presence of two minima. The open symbols are actual data points for $T = 0.001 t$. The red square indicates the point at which the moment profile jumps in the upward sweep according to the effective functional. In the effective description the large $V$ moment has been approximated to be zero.

terms of the moment magnitude at $V = 0$ and $V = V^+ c$, and $\Delta V c$. The moment profile does not depend on the parameter $c$, which just sets the overall scale of $F$. It can be fixed by fitting the low $T$, $P(m)$ at $V = 0$. Here, we have approximated the moment amplitude in the large $V$ state to vanish. The $V$ dependence of $F$ has been shown in Fig. 3(a) and the resulting moment profile has been shown in Fig. 3(b). For $V < V^- c$, $F$ has a unique minimum at finite $M$. For $V^- c < V \leq V^+ c$, $F$ develops another minimum at $M = 0$. Beyond $V^+ c$ only the $M = 0$ minimum survives. For the upward voltage sweep the system remains stuck in the finite $M$ minimum till $V^+ c$ and then switches to the $M = 0$ minimum discontinuously. A similar discontinuous transition happens in the downward sweep, in which the stating state corresponds to the $M = 0$ minimum, which changes abruptly at $V^- c$. This explains the low $T$ coexistence and hysteresis. However this is too simplistic to capture the finite $T$ transition, for which one must take angular fluctuations of $\{\vec{M}\}$ into account.

**Reduction of $T_N$ with increasing $V$**

We find that the Néel temperature decreases with increasing $V$. Assuming that Heisenberg exchange scale ($J_{eff} \sim \frac{1}{T}$, at strong coupling) remains unchanged with $V$, the reduction in $T_N$ with increasing $V$ may be attributed to a reduction in the average moment magnitude $\langle |M| \rangle$, for a fixed temperature, with increasing $V$. Fig. 4(a) shows the variation of $\langle |M| \rangle$ with increasing $T$, for different $V$ values. We find that $\langle |M| \rangle$ behaves nonmonotonically with temperature between $1 < V/t < 4$, and develops a minimum at a temperature $T_c(V) > T_N(V)$. In fig. 4(b) we have compared $\frac{T_c(V)}{T_c(0)}$ with $\frac{\langle |M| \rangle(V)}{\langle |M| \rangle(0)}$, and find that they follow similar trends with increasing $V$.

Motivated by this, we attempted to explain the drastic reduction in $T_N$ beyond $V \sim 0.5V^+_c$ by invoking an effective Heisenberg model, in which the moment magnitudes are determined by the $P(m)$ distribution described in the previous section. This gives a reasonable match for both the structure factor Fig. 4(c) as well as the Néel temperature Fig. 4(d), with the full calculation, except very near $V_c$.

FIG. 4. (a) Variation of average moment magnitude with temperature ($T$) for different values of bias voltaage ($V$). For each $V$ the corresponding Néel temperature ($T_N(V)$) has been marked with a black cross on the trace. (b) Comparison of the ratios of Néel temperatures and squared average moment magnitudes.

FIG. 5. Comparison of the approximate current (solid lines) with the exact result (open circles) in the paramagnetic metal phase for $V/t = 4, 6$. 
FIG. 6. (a1-d1) Variation of the average charge profile, along the longitudinal direction, with increasing temperature for $V/t = 0, 2, 3.4$ and 6. With sufficient averaging the profile becomes antisymmetric about the center of the system, hence only the left half has been shown. (a2-d2) Variation of the average local moment magnitude along the longitudinal direction. The averaging leads to a symmetric profile across the center of the system.

CURRENT AT LARGE $V$

One can set up an approximate calculation for the current at large $V$, where the mean moment size gets quenched. One can approximate the lesser Green’s function $G^<$($t$, $\omega$), which enters the expression for the current in Eq. 4 in the main text, by setting up a perturbation theory about the tight-binding limit.

$$G^< = \frac{1}{2} (G^K - (G^R - G^A))$$ (17a)

$$(G^R \quad G^K)
\begin{pmatrix}
G^K & G^A \\
0 & G^A
\end{pmatrix}
= \begin{pmatrix}
[g^{-1}]^R - \Sigma^R & [g^{-1}]^K - \Sigma^K \\
0 & [g^{-1}]^A - \Sigma^A
\end{pmatrix}^{-1}$$ (17b)

with,

$$\Sigma^{R,A,K}_{i,j,\alpha,\beta}(t, \omega) = M^\alpha_i(t)M^\beta_j(t)g^{R,A,K}_{ij}(\omega)$$ (17c)

where $g^{R,A,K}$ are the Green’s functions of the connected tight-binding system. The mean current is computed by averaging over the time-series of $M$. This can be simplified further if one averages over the self-energy instead of the Green’s functions, assuming the distribution for $M$s to be normal, i.e.,

$$\langle M^\alpha_i(t)M^\beta_j(t) \rangle = T\delta_{ij}\delta_{\alpha\beta}.$$ So the average self-energy

$$\langle \Sigma^{R,A,K}_{i,j,\alpha,\beta}(\omega) \rangle = T\delta_{ij}\delta_{\alpha\beta}g^{R,A,K}_{ij}(\omega)$$ (18)

can be used to approximate the mean current. Fig. 3 shows compares the temperature dependence of the approximate current with the actual result in the P-M phase. They seem to compare well for sufficiently large $V$, given the ‘drastic’ nature of the approximations.

AVERAGE DENSITY AND SPIN

In Fig. 5, we show the average charge and moment magnitude which are defined as:

$$\langle \delta n_{ix} \rangle = 1 - \sum_{i_x,i_y} \frac{dt}{t_M} \int_{-D}^{D} \frac{d\omega}{2\pi} Tr(G_{ix}(t, \omega))$$ (19a)

$$\langle |\vec{S}_{ix}| \rangle = \sum_{i_x,i_y} \frac{dt}{t_M} \int_{-D}^{D} \frac{d\omega}{2\pi} Tr(G_{ix}(t, \omega)\vec{\sigma})$$ (19b)

where the trace is over the $2 \times 2$ local spin subspace. At $V/t = 0$, the average charge profile remains vanishingly small throughout the longitudinal direction at all temperatures, while the moment magnitude falls as the system is heated beyond the Néel temperature ($T_N$). For $0 < V/t < 2$, the charge profile shows deviations at the edges, even at very low $T$, and becomes linear at high $T$. The moment magnitude also shows deviations at the edges, and gets diminished throughout the system with increasing $T$. For $2 < V/t < 3.6$, the charge profile shows edge deviations in low $T$ insulating phase, but becomes linear as one heats up the system to reach the P-M phase. The moment magnitude shows nonmonotonic behaviour with temperature. For $V/t > 3.6$, the system remains in the P-M phase at all $T$. The charge profile remains linear, whose slope increases with increasing $T$, while the moment profile remains fairly constant and increases with increasing $T$.

[1] A. Mukherjee, N. D. Patel, S. Dong, S. Johnston, A. Moreo and E. Dagotto, Phys. Rev. B 90, 205133 (2014).

[2] Arijit Dutta and Pinaki Majumdar, Phys. Rev. B (2020).