The nonequilibrium thermal state of a voltage biased Mott insulator

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We establish the nonequilibrium thermal phases of a voltage driven antiferromagnetic Mott insulator in three dimensions, realised at steady state under a voltage bias. Starting from the Keldysh action for the half filled Hubbard model we derive an effective Langevin equation for the ‘slow’ magnetic variables. The coupling of electrons to degrees of freedom determine the transport properties. At low temperature we find a voltage-driven discontinuous insulator-metal transition, along with hysteresis. We map the suppression of the Néel temperature $T_N$ and pseudogap temperature $T_{pg}$ with increasing voltage, and discover that the biased Mott insulator has a finite temperature insulator-metal transition. The low temperature results resolve an experimental puzzle about hysteresis, and the thermal results make testable predictions on spectra and nonlinear transport.

I. INTRODUCTION

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, the effect of intense pulsed radiation in ‘pump-probe’ experiments 14–16, and metastable hidden phases 17–21. 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 ($I$-$V$) characteristics in Mott insulators have some generic features 6–12. These are (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 to millimeter size. Scanning near field optical microscopy (s-SNOM) measurements reveal that the voltage induced breakdown has a progressive spatial character 13.

Multiple theories have tried to model the voltage induced breakdown 22–36,41–45. Most microscopic approaches suggest a Landau-Zener (LZ) like mechanism 22–26. The resulting $I$-$V$ 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 31,32 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 33 based on ideas of Frohlich 34–36 seems to be available.

The main limitation of current methods arise from the neglect of broken translation symmetry (due to the bias) and the difficulty in accessing the long time steady state. This paper addresses the metallisation of a Mott insulator, in a three dimensional (3D) geometry, using a method that is non perturbative in both the interaction strength and the applied bias and handles thermal fluctuations exactly. Our Keldysh based Langevin dynamics approach exploits the ‘slowness’ of the magnetic fluctuations on electronic timescales, retains the effects of dissipation channels (the leads) 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 $\vec{M}(t)$ (see later) which define the background for electron physics.

We work with the half filled Hubbard model in a 3D geometry, set the onsite repulsion $U/t = 6$, where $t$ is the nearest neighbour hopping, and probe the bias ($V$) and temperature ($T$) dependence of the nonequilibrium state. At $V = 0$ our approach yields a Néel transition at $T \sim 0.28t$ which compares well with the quantum Monte Carlo value of $T_N \sim 0.3t$.

On introducing the bias we discover the following. (i) The $T = 0$ state shows a voltage sweep dependent transition at $V_c^\pm$, between an antiferromagnetic insulator (AF-I) and a paramagnetic metal (P-M). The hysteretic window narrows with increasing temperature and vanishes at $T_{coex} \sim 0.02t$. (ii) The Neel temperature $T_N$ reduces slowly with $V$ up to $V \sim 0.5V_c^+$ and then falls sharply - vanishing at $V \lesssim V_c^+$. This correlates with a thermally induced broad distribution of moment magnitudes, with a low mean value, at large $V$. The pseudogap formation temperature $T_{pg}$, signalling the crossover from gapped to pseudogapped density of states (DOS), follows a trend similar to $T_{coex}$, and then falls sharply - vanishing at $V \lesssim V_c^+$.

The paper is organised as follows. We start by defining the model for the open system that describes the biased Mott insulator, and introduce the dynamical equation at the heart of our method. The next section highlights results on the nonequi-
librium $V - T$ phase diagram, the current response $I(V,T)$, and the density of states $A(\omega,V,T)$. This if followed by a Discussion section, that places our method in the context of other approaches to the correlated electron problem, an analysis of the magnetic configurations that arise with varying $V$ and $T$, and the numerical checks that we have implemented. A Supplement\textsuperscript{37} shows how the Langevin equation arises in the 'semiclassical' limit from a Keldysh field theory.

II. MODEL AND METHOD

A. Model

The Hamiltonian for system, baths and their coupling is,

\[
\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{Hubb}} + \mathcal{H}_{\text{bath}} + \mathcal{H}_{\text{coupl}}
\]

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

\[
\mathcal{H}_{\text{bath}} = \sum_{\nu,\sigma,\beta \in \{L,R\}} \epsilon_{\nu} c_{i\nu\sigma}^\dagger c_{i\nu\beta}^\dagger
\]

\[
\mathcal{H}_{\text{coupl}} = - \sum_{<ij>,\sigma} v_{ij} \left( \epsilon_{i\uparrow}^L d_{i\sigma} + \epsilon_{i\downarrow}^R d_{j\sigma} + h.c. \right)
\]

In the equations above $n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ and $\epsilon_{\nu}$ are the bath eigenenergies. $v_{ij}$ denote the system-bath couplings. We assume the density of states of the bath to be Lorentzian. The chemical potential $\mu$ in the system is tuned to ensure half-filling. A voltage bias is applied by tuning the chemical potential $\tilde{\mu}$.

We set $\mu_{L(R)} = \mu \pm (V/2)$.

B. Method

Starting from the Keldysh\textsuperscript{38} action for the above Hamiltonian (see Supplement\textsuperscript{37}) we decouple the quartic term by Hubbard-Stratonovich transformation. This introduces real auxiliary fields at each instant, henceforth we call the charge field $\phi_i(\tau)$ and spin field $\tilde{M}_i(\tau)$, that couple respectively to the instantaneous density and spin of the electrons. $\tau$ is our time variable, $t$ being used for the hopping. The action becomes quadratic in the Grassmann fields which can be formally integrated out. We fix $\phi_i$ to its half-filling equilibrium saddle point value. Using assumptions related to the slowness of $\tilde{M}_i(\tau)$, and a simplified noise kernel, both discussed in the Supplement\textsuperscript{37}, we derive a stochastic dynamical equation for $\tilde{M}_i(\tau)$.

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

\[
\langle \xi_i^\alpha(\tau) \xi_j^\beta(\tau') \rangle = \frac{4T}{U\gamma_i(\tau)} \delta_{ij} \delta_{\alpha\beta} \delta(\tau - \tau')
\]

\[
\langle \tilde{\sigma}_i \rangle_{\{\tilde{M}\}} = \int d\omega \text{Tr} \left[ \hat{G}^K_{ii}(\tau,\omega) \tilde{\sigma}_i \right]
\]

where $a, b$ denote $O(3)$ indices. From consistency arguments, discussed in the Supplement\textsuperscript{37}, $\gamma_i(\tau) = \frac{2U}{(1 + \alpha^2 |\tilde{M}_i(\tau)|^2)}$, where $\alpha = (U/t)^2$ is the Gilbert damping\textsuperscript{39,40}.

$\hat{G}^K$ denotes the adiabatic Keldysh Green’s function, and the trace is over the local $2 \times 2$ spin subspace (assumed henceforth). $\tilde{\sigma}_i = \frac{1}{2} \sum_{\alpha\beta} \tilde{\sigma}_{i\alpha\beta} \hat{d}_{i\alpha} \hat{d}_{i\beta}$, $\tilde{\sigma}_P \equiv (\sigma^x, \sigma^y, \sigma^z)$ being the $2 \times 2$ Pauli vector, is the local fermion spin. Its average is computed on the instantaneous $\{\tilde{M}\}$ background. $\langle \tilde{\sigma}_i \rangle$ is a nonlinear, non local, function of the $\tilde{M}$ field and encodes the strong correlation effects in the problem. The computationally hard part in the evolution equation is calculation of $\hat{G}^K_{ii}(\tau,\omega)$, briefly indicated next. We also need $\hat{G}^<_{i+\hat{z},i\sigma}(\tau,\omega)$ for the transport calculation, and $\hat{G}^R_{ii}(\tau,\omega)$ for the density of states.

\[
\hat{G}^R(\tau,\omega) = \left( \omega - \hat{H}(\tau) + \hat{\Gamma}(\omega) \right)^{-1} = \left[ \hat{G}^A(\tau,\omega) \right]^\dagger
\]

\[
\hat{H}_{ij}(\tau) = \left( -\hat{M}_i(\tau) \cdot \hat{\sigma}_P + \phi_i \right) \delta_{ij} - t_{<ij>}
\]

\[
\left[ \hat{G}^{-1} \right]^K_{ij;\alpha\beta}(\tau,\omega) = -2i|\nu|^2 \rho_B(\omega) \left[ \tanh \left( \frac{\omega - \mu}{2T} \right) \right] \delta_{ij} \delta_{\alpha\beta}
\]

\[
\hat{G}^K(\tau,\omega) = \hat{G}^R(\tau,\omega) \left[ \hat{G}^{-1} \right]^K_{ij;\alpha\beta}(\tau,\omega) \hat{G}^A(\tau,\omega)
\]

\[
\hat{G}^<(\tau,\omega) = \frac{1}{2} \left[ \hat{G}^K(\tau,\omega) - \hat{G}^R(\tau,\omega) + \hat{G}^A(\tau,\omega) \right]
\]

where $\rho_B(\omega)$ is the density of states of the baths, $\mu_{L(R)}$ denote the sites at the left (right) edge.

The Langevin equation is solved using a stochastic Heun discretisation scheme\textsuperscript{31} to generate a time series for $\tilde{M}_i(\tau)$. 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.

We benchmark the scheme against equilibrium Monte-Carlo results on the adiabatic problem (see Appendix B). The nonequilibrium results pertain to a $8 \times 4 \times 4$ system, with $L = 8$ being the longitudinal (transport) direction. We discuss size dependence in the Discussion section. Starting with an arbitrary $\{\tilde{M}\}$ configuration the system is evolved for $\sim 10^6$ steps with a time discretisation of $10^{-3}\tau_0$, where $\tau_0 \sim 1/J_{ij}\sim 1/J_{ij}$ (with $J_{eff} \sim J^2/U$) is the characteristic timescale of the auxiliary field. After allowing the system to equilibrate for $100\tau_0$ (this is taken to be $\tau = 0$ in the definition of time averaging of observables), the rest of the configurations have been saved to construct the time series for $\tilde{M}_i(\tau)$. The maximum time of the simulation is $\tau_M \sim 1000\tau_0$.
FIG. 1. (a) Temperature ($T$) vs voltage ($V$) phase diagram of the voltage biased repulsive Hubbard model at $U/t = 6$. The AF-I, P-M and P-I are the antiferromagnetic insulator, paramagnetic metal and paramagnetic insulator phases respectively. Insulating (metallic) regimes have $\partial I/\partial T > (<) 0$, where $I$ is the steady state current. CX marks the hysteric window. The solid blue line indicates $T_{N}(V)$, the dashed white line $T_{IMT}(V)$ and the broken grey line indicates $T_{pp}(V)$. (b) The magnetic ordering peak, $S_q(T)$ for upward (open circles) and downward (solid squares) $V$ sweeps. For $T/t ≥ 0.02$ the two curves coincide for all values of $V$. The inflection point for each curve gives the $T_N$ for the corresponding $V$.

III. RESULTS

A. Phase diagram

The $V = 0$ ground state at half-filling is an antiferromagnetic insulator (AF-I) for any finite $U^{46,47}$. $|\vec{M}|$ grows with increasing $U$ and saturates to unity as $U/t → ∞$. As the temperature is increased the system loses long range order (LRO) at a scale $T_N(U)$. For $T > T_N$, the system is a paramagnetic metal (P-M) for $U/t ≤ 4$ and a paramagnetic insulator (P-I) for $U/t ≥ 4$. The crossover region from P-M to P-I shows a pseudogapped density of states (DOS). The equilibrium physics and how our method accurately captures it is discussed in detail in the Discussion section.

We construct a nonequilibrium $V - T$ phase diagram at $U = 6t$, Fig.1(a), highlighting the magnetic, transport and spectral regimes that occur in the biased problem. There are three phases, AF-I, P-I and P-M, and a low $T$ coexistence (CX) window bounded by $V_c^\pm$. The bias dependent temperature scales are $T_{N}$, for the magnetic transition, $T_{IMT}$ for the narrow window of thermally induced insulator-metal transition, and $T_{pp}$ for crossover from gapped to pseudogap DOS. The indicators in terms of which we infer magnetic order, transport behaviour, and spectral features, are discussed below.

Fig.1(b) shows the peak, $S_{q}(T)$ in the magnetic structure factor $S_{q}$, where $S_{q}$ is defined by,

$$ S_{q} = \frac{1}{N^2} \sum_{ij} \int^{\tau_{M}}_{0} \frac{d\tau}{\tau_{M}} \vec{M}(\tau, \vec{r}_{i}) \cdot \vec{M}(\tau, \vec{r}_{j}) e^{i\vec{q} \cdot (\vec{r}_{i} - \vec{r}_{j})} \tag{4} $$

The $\tau = 0$ point corresponds to the start of the measurement period in the nonequilibrium steady state and is 100$\tau_{0}$.

$\vec{q} = \vec{Q} = (\pi, \pi, \pi)$ pertains to Néel AF order. For the cubic lattice with nearest neighbour hopping the peak in the structure factor remains at $(\pi, \pi, \pi)$ at all $V$. For each $V$ the Néel temperature is estimated from the point of inflection of the $S_{q}(T)$ curve. There exists a coexistence region at $T = 0$ for $2.2 ≤ V/t < 4.3$, which extends upto $T_{coex}/t = 0.02$. The state in this region depends on the direction of voltage sweep. In Fig1.(b), the open circles denote the $T$ dependence of $S_{q}$ for upward sweep, while the solid squares denote the same for the downward sweep. The solid blue curve in Fig1.(a) shows the dependence of $T_N$ on $V$. $T_N$ decreases slowly initially, with $V$, and then quicker for $V ≥ 0.5V_c^+$ and vanishes for the upward sweep at $V/t ≈ 3.6$.

FIG. 2. (a) The current-voltage ($I$-$V$) characteristics with changing temperature ($T$). The hysteretic behaviour at low $T$ is shown in inset. The solid (dashed) lines and open circles (filled squares) correspond to upward (downward) voltage sweeps. The arrows indicate the sweep direction. For $T < 0.02t$, $I$ changes discontinuously at $V_c^\pm(T)$ for the upward and downward sweeps, respectively. Beyond the coexistence region the $I$-$V$ has a unique threshold at $V_c^{\mp}(T)$ which reduces with increasing $T$ and vanishes for $T > 0.1t$. (b) $I$ vs $T$ for different $V$. $\partial I/\partial T > (<) 0$ indicates an insulating (metallic) phase. A peak in the $I(V,T)$ curve for a fixed $V$ indicates a temperature driven IMT. (c) Log of resistance ($R = V/I$) vs $T$ for different $V$. Analogously, a minimum in the $R(T,V)$ curve for a fixed $V$ indicates IMT.
FIG. 3. (a) Map of DOS for varying temperature and voltage, on the upward sweep. (b-d) Temperature variation for $V/t = 0, 2.2$ and $3.2$. For $V \leq 2.2t$, the low T DOS remains gapped and becomes pseudogapped for $T > T_{pg}$, in both the sweep cycles. For $2.2 < V/t < 3.4$ the DOS remains gapped at low temperature, develops subgap weight with increasing $T$, even in the insulating phase, and becomes pseudogapped at large $T$. For the downward sweep, the DOS in this regime retains subgap weight even to the lowest temperature, as shown in (d) with a dashed line. For $V \geq 3.4t$ the DOS remains ungapped at low $T$ and broadens with increasing $T$.

B. Transport

The charge current across a transverse cross-section at site $j$ is given by

$$I_x(V) = \sum_{y,z} \int_0^{\tau_M} \frac{d\tau}{\tau M} \int_{-D}^D \frac{d\omega}{2\pi} \text{Tr}[\delta G_{j+\hat{x},j+\sigma}^<(\tau,\omega)]$$

where $G^<$ is the adiabatic lesser Green’s function and the sum is over all sites in the transverse cross-section containing the site $j$. Due to charge conservation $I_x(V)$ must be independent of $x$. However, there is a weak violation ($\lesssim 10\%$) of current conservation at very low temperatures due to a finite convergence factor $\eta \approx 0.01t$, which is needed for numerical stability of the scheme. The current conservation is better satisfied with increasing $T$ and $V$. The $I-V$ characteristics are plotted in Fig.2(a) for different temperatures. The inset shows hysteresis for $T < T_{cex} \approx 0.02t$ while the main panel shows the response for $T/t \gtrsim 0.02$. Above $T_{cex}$ and up to $T/t \approx 0.3$ it has a ‘threshold’ at some $V_c(T)$ (below which the current remains exponentially suppressed) that reduces with increasing $T$. Beyond $V_c$, the current rises sharply with increasing $V$ and saturates as $V$ approaches the bandwidth $D$ of the connected system. The current saturation at large $V$ is similar to what has been observed in the 2D problem at zero $T$.

Figs.2(b) show $I(T)$ at different $V$. The results reveal three regimes: (i) insulating, where the system becomes more conducting with increasing $T$, i.e., $\partial I/\partial T > 0$ at all $T$ (happens for $V/t \approx 2$), (ii) metallic, showing $\partial I/\partial T < 0$ at all $T$ (occurs for for $V/t > 3.8$), and (iii) showing insulator to metal transition: $\partial I/\partial T$ changing sign at $T_{IMT}$. This 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 in the strongly metallic regime 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 $V/t \lesssim 1$ window (the top right curve). The effective re-
sistance at all other voltages depends crucially on the applied bias.

C. Density of states

The system averaged single particle density of states (DOS) is given by

$$\mathcal{A}(\omega) = -\frac{1}{2\pi N} \sum_i \int_0^{\tau_M} d\tau \text{Im}[\text{Tr}[G^R_i(\tau, \omega)]]$$

(6)

where $G^R$ is the adiabatic retarded Green’s function. $N$ is the total no. of sites. Its behaviour with increasing $T$ in different voltage regimes is shown in Fig.3(a). For $0 \leq V/t \leq 2.2$ (Fig.3(b),(c)), at low $T$, the DOS has a gap independent of the sweep direction, which gets smeared with increasing $T$ and ultimately becomes a pseudogap beyond $T_{pg}$. For $2.2 < V/t < 3.4$ (Fig.3(d)), in the upward sweep the DOS remains gapped at low temperatures, but develops subgap weight upon increasing $T$. Upon heating beyond $T_{IMT}(V)$ the DOS becomes pseudogapped and broadens with increasing $T$ further. For the downward voltage sweep in this regime, the DOS remains ungapped even to the lowest temperature, as shown in Fig.3(d) with a dashed line.

IV. DISCUSSION

In our Model and Method section we introduced the Langevin approach without any discussion of its place within the larger scheme of many body theory for nonequilibrium systems. Similarly, most of the results presented till now has been experimental data, which makes it difficult for the reader to observe a certain kind of behavior. We adopted this approach to get across the basic results quickly without digression. This section, the Appendices, and the Supplement, aim to fill up the gaps, by placing our method in context, and motivating the results we have shown.

The first subsection focuses on the method that we have used. It addresses where our method lies in the spectrum between full fledged quantum Monte Carlo (QMC) and simple mean field theory (MFT), and the benchmarks it satisfies at equilibrium.

The subsections thereafter focus on features of the magnetic configurations $\bar{M}(\tau)$ that arise from the Langevin evolution. Since the electron response time is assumed to be much shorter than the magnetic fluctuation time the electronic properties are computed on magnetic configurations on individual ‘time slices’, $\tau$, and then averaged.

In what follows we (i) locate our method within the larger family of many body approximations and distinguish it from mean field theory, (ii) highlight some aspects of the distribution $P(M,V,T)$, (iii) suggest a Landau like functional at $T = 0$ for the bias driven first order transition, (iv) propose a plausible mechanism for the suppression of $T_N$ with $V$, and (v) quantify the scattering mechanism that seems to decide the current in the bias stabilized metallic phase. We also comment (vi) on the spatial variation of the electron density and local moment magnitude and (vii) on the size and dimension dependence of our results. Finally, (viii) we briefly discuss the connection of our results to experiments on bias driven Mott materials.

A. Locating our method

In our methods section we directly moved to the Langevin equation in the nonequilibrium problem. This would be a case of double unfamiliarity for many readers since (i) the Langevin approach is not standard even in the equilibrium problem, and (ii) the driven problem additionally complicates the formulation by bringing in leads and a bias. In what follows we quickly discuss the equilibrium formulation that generalises to our nonequilibrium scheme, differentiate it from simple mean field theory, and schematically show how the nonequilibrium method arises. The detailed derivation of the nonequilibrium scheme is given in the Supplement.

1. At equilibrium

The equilibrium problem corresponds to disconnecting the Hubbard block from the leads (and setting the bias $V = 0$). There are three levels at which the Hubbard model can be approached. The flow chart in Fig.4 illustrates these.

$$H_{Hubb} \rightarrow \mathcal{L}^H_{Hubb} \rightarrow H^{SPA}_{Hubb} \rightarrow H^{MF}_{Hubb}$$

In the above $H_{Hubb}$ is the Hubbard model, $\mathcal{L}^H_{Hubb}$ is the corresponding Lagrangian after rewriting the interaction in terms of charge and spin auxiliary fields, $\phi_i(\tau)$ and $\bar{M}_i(\tau)$, respectively. Till this is exact. The approximation we use is to treat the auxiliary fields as only spatially fluctuating, neglecting the $\tau$ dependence. This is called the ‘static path approximation’ and leads to $H_{SPA}$. It retains all spatial thermal fluctuations but no temporal fluctuations. A possible further simplification is to drop the spatial fluctuations as well, retaining only the ‘order parameter mode’. This is the mean field model, $H_{MF}$, retaining only the $\bar{q} = (\pi, \pi, \pi)$ mode of the $\bar{M}$ field.

A fourth approach, not listed above, corresponds to dynamical mean field theory (DMFT) which would retain the temporal fluctuations of the auxiliary fields and drop the spatial dependence. We write the exact, the SPA, and the mean field models below. For SPA in the half-filling case we ignore fluctuations of the charge field $\phi_i$.

The models are, successively,

$$H_{Hubb} = -t \sum_{<ij>,\sigma} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H^{SPA}_{Hubb} = -t \sum_{<ij>,\sigma} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_i \bar{M}_i \sigma_i + U \sum_i M^2$$

$$H^{MF}_{Hubb} = -t \sum_{<ij>,\sigma} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_i M e^{iQ \cdot \bar{r}_i} \sigma_{iz} + U N M^2$$
1. Isolated system: \[ H_{\text{Hubb}} \rightarrow L_{\text{Hubb}}^{HS} \rightarrow H_{\text{Hubb}}^{\text{SPA}} \rightarrow H_{\text{Hubb}}^{\text{MF}} \]
\[ + (H_{\text{comp}} + H_{\text{bath}}) \]
\[ \downarrow \]
\[ H_{\text{tot}} \]
\[ \downarrow \]
2. Open system: \[ S_{\text{tot}} \rightarrow S_{\text{tot}}^{HS} \rightarrow S_{\text{tot}}^{\text{SC}} \rightarrow S_{\text{tot}}^{\text{MF}} \]

| Exact | Our method | MFT |
|-------|------------|-----|

FIG. 4. Sequence of approximations in the isolated equilibrium system (top) and the open nonequilibrium system (bottom). The single arrows indicate exact transformations while the double arrows indicate approximations. Our method, described in the text, approximates the magnetic variables as "slow" but retains fluctuation effects far beyond mean field theory (MFT). The notation is described in the text below.

The full model can be studied via exact diagonalisation, severely size limited, or determinantal QMC in terms of the auxiliary fields \( \phi_i(\tau) \) and \( \tilde{M}_i(\tau) \). The SPA model can be studied by Monte Carlo sampling of the field \( \tilde{M}_i \) (the \( \phi_i \) being dropped at half-filling), or by the Langevin approach - assuming the \( M_i \) dynamics to be much slower than electron dynamics. The MF model, as well known, can be immediately diagonalised due to the assumed periodic nature of the \( \tilde{M}_i \) background. Mean field theory restricts \( \tilde{M}_i \) to \( Me^{i\tilde{Q}.\tilde{r}} \), with \( \tilde{Q} = (\pi, \pi, \pi) \), for the Neel state.

Within MFT there is only a site independent magnitude to be determined - the size \( M \) of the magnetic moment. There are no angular variables anymore. As a result, MFT has only two possible phases: (a) an AF-I when \( M \neq 0 \), and (b) a trivial P-M when \( M = 0 \). Magnetic order and insulating gap are intimately connected. \( M \) would vanish when the temperature is comparable to the \( T = 0 \) gap, for \( U \gg t \) this is \( T_N^c \sim U \). At our parameter point it is \( T_N^c \sim t \). The mean field spectrum is either gapped or tight binding, there is no pseudogap phase.

Our approach is SPA, when using Monte Carlo, or the equivalent Langevin scheme when using dynamics (see Appendices). Within these the magnitude as well as the direction associated with the \( \tilde{M}_i \) can fluctuate and the electronic properties are computed in these backgrounds. Retaining these thermal fluctuations leads to two major differences in our results compared to mean field theory: (i) The loss of AF order arises from angular fluctuations of the moments rather than \( |\tilde{M}_i| \rightarrow 0 \). The \( T_N^{SPA} \) scale we obtain compares very well with full QMC, our result at \( U = 6t \) is \( T_N \sim 0.28t \) compared to the QMC value \( \sim 0.3t \). (ii) The gap at large \( U \) is related to the magnitude of \( \tilde{M}_i \) not its long range order. The difference between the \( T < T_N \) and \( T > T_N \) phases is mainly in the angular correlation between the moments, not their magnitude.

As a result, even in the \( T > T_N \) phase a gap can survive - this is the paramagnetic insulator (P-I). When \( U/t \) is in the intermediate coupling window, as in our case, the \( T \gtrsim T_N \) window shows a pseudogap rather than a clean gap.

All these features are visible in the \( V = 0 \) results in various figures. Fig.1(a) shows the \( T_N \) (see Fig.4 of a QMC reference\(^{50} \)) and also the temperature where the low temperature gapped phase transits to a higher \( T \) pseudogap phase. Fig.2(b) shows that at low \( V \) insulating behaviour persists well beyond \( T_N \) - the signature of a P-I phase. Fig.3(b) shows the DOS at \( V = 0 \). The plot corresponding to \( T = 0.4t \) shows the PG in the spectrum. These \( V = 0 \) results gave us the confidence to treat the bias problem using the Langevin scheme.

2. Out of equilibrium

For the nonequilibrium problem \( H_{\text{Hubb}} \) is augmented by \( H_{\text{comp}} + H_{\text{bath}} \) as in Eqn.1. There is no longer a ‘Hamiltonian’ that describes the system degrees of freedom and we need to use an action. Following the notation of Eqn.1 we have the sequence of approximations:

\[ H_{\text{tot}} \rightarrow S_{\text{tot}} \rightarrow S_{\text{tot}}^{HS} \rightarrow S_{\text{tot}}^{SC} \rightarrow S_{\text{tot}}^{MF} \]

The sequence from \( H_{\text{tot}} \rightarrow \ldots S_{\text{tot}}^{SC} \) is described in the Supplement\(^{27} \). Upto \( S_{\text{tot}}^{HS} \) the formulation is exact. Beyond this we do a semiclassical (SC) expansion, assuming that the \( \tilde{M}_i \) fields are much slower than the electrons, to obtain \( S_{\text{tot}}^{SC} \). This is the equivalent of the SPA approximation in the equilibrium problem. One can further simplify the SC scheme by neglecting dynamics and thermal fluctuation altogether to obtain the mean field action \( S_{\text{tot}}^{MF} \). This is what we used at \( T = 0 \) in an earlier paper\(^{45} \).
B. Moment magnitude distribution

At steady state the magnetic configurations are characterised by their local distribution \( P_{i}(M) \) and the system averaged distribution \( P(M) \), where

\[
P_{i}(M) = \frac{1}{\tau_M} \int_{0}^{\tau_M} d\tau \delta(M - |\vec{M}_{i}(\tau)|)
\]

\[
P(M) = \frac{1}{N} \sum_{i} P_{i}(M)
\]  \( (7) \)

The magnitude \( |\vec{M}_{i}| \) plays an important role since \( \langle M \rangle = \langle |\vec{M}| \rangle \) and \( M \rightarrow 1 \) indicates that the double occupancy \( d_{i} = \langle n_{i\uparrow} n_{i\downarrow} \rangle \rightarrow 0 \), i.e., no charge fluctuation, while \( M \rightarrow 0 \) implies a tight binding metal. The \( V \) and \( T \) dependence of \( P(M) \) is the primary determinant of insulating and metallic behaviour.

The effect of bias and temperature on \( P(M) \) has been plotted in Fig.5. There are broadly three regimes. (a) For \( V/t \leq 2 \), and \( T \ll T_N \), the moments remain almost pinned to their equilibrium ground state value. Hence, the \( \langle M \rangle \) is sharply peaked around 0.8. As temperature increases the distribution broadens around the 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 \( T \). (b) Between \( 2.2 < V/t \leq 4.3 \) the low \( T \) moment distribution changes from being unimodal to bimodal, and acquires a sweep dependence. This is because the “effective potential” governing the moment distribution develops a metastable low moment minimum, as we shall discuss in the next section. (c) Beyond \( V = 4.3t \), where the system is in a metallic phase, the low temperature \( P(M) \) peak gets pushed towards \( M = 0 \) as the moments collapse throughout the system. With increasing \( T \), the distribution broadens while the mean shifts towards larger \( M \) values.

C. The zero temperature transition

The \( T = 0 \) transition can be modeled by extremising an effective functional \( F \) of the form:

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

\[
a(V) = a_0 \left( e^{-V^*/V} - e^{-V^*/V_c} \right)
\]  \( (8) \)

where \( M \) is the magnitude of the local moment, assumed to be uniform across the system. \( a_0 \), \( V^* \), \( b \), \( c \) are fitting parameters which take positive values. \( a_0 \), \( V^* \) and \( b \) can be determined in terms of the moment magnitude at \( V = 0 \) and \( V = V_c^+ \), and \( V_c^+ \). The peculiar form of \( a(V) \) ensures that the finite \( M \) minimum of \( \bar{F} \) remains almost pinned at \( M = M(V = 0) \) till \( V \lesssim V_c^+ \) and changes sharply across \( V_c^+ \). 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 assumed the moment amplitude in the large \( V \) state to vanish. We find that \( V^* \approx 4.8t \). The \( V \) dependence of \( F \) has been shown in Fig.6(a) and the resulting moment profile has been shown in Fig.6(b).

D. Finite temperature magnetism

As we have seen, the Néel temperature decreases with increasing \( V \). Making the crude assumption that the bare Heisenberg exchange scale, \( J = t^2/U \) at strong coupling, remains unchanged with \( V \), we attempt to correlate the reduction in \( T_N \) with the behaviour of the average moment magnitude \( \langle M(V,T) \rangle \). Fig.7(a) shows the variation of \( \langle M(V,T) \rangle \) with increasing \( T \), for different \( V \) values. We find that \( \langle M(V,T) \rangle \) behaves nonmonotonically with temperature for \( 1 < V/t < 4 \), and develops a minimum at a temperature \( T_*(V) \sim T_N(V) \). Fig.7(b) we have compared \( T_N(V)/T_N(0) \) with \( \frac{\langle M^2(V,T) \rangle}{\langle M^2(0,0) \rangle} \) and find that they follow a similar trend with increasing \( V \).

This correspondence suggests that an effective Heisenberg
model for the local moments may be able to describe the underlying physics. To make progress we assume that the amplitude distributions of the local moments are same across the system, given by \( P(M,V,T) \) and shown in Fig.5. In the insulating phase, increasing \( T \) leads to reduction in the local moment amplitudes, which is negligible at low \( V \) but becomes significant near \( V \lesssim V_c \) (above the coexistence region). In the metal, however, the thermal broadening of \( P(M) \) leads to an increase in mean moment size with \( T \). A combination of these two effects leads to the nonmonotonic \( T \) dependence at intermediate \( V \).

Motivated by this, we attempt 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 shown earlier. The effective Heisenberg model is then given by

\[
H_{eff} = i^2 U \sum_{ij} \vec{M}_i \cdot \vec{M}_j
\]

where the magnitude of \( \vec{M}_i \) at a site, at a given \( V \) and \( T \), is obtained by sampling \( P(M,V,T) \). This approach, building in “amplitude fluctuation” of the moments, gives a reasonable match with the full Langevin calculation, for the structure factor Fig.7(c) as well as the Néel temperature Fig.7(d), except very near \( V_c \).

Rather than use the computed \( P(M,V,T) \) we had tried to use \( P \propto e^{-F(M,V)/T} \) as amplitude weight. That approach did not work, suggesting that the finite temperature \( F \) has a non trivial \( T \) dependence.

The discussion above about moment magnitude and its magnetic order pertains to the insulating state. At large \( V \) the low \( T \) state is a metal, with essentially zero magnetic moment. However there are thermally induced moments in the metal, and their fluctuation serves as a source of scattering. The next section provides an analytic basis for this effect.

### E. The bias stabilised metal

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 \( G^<_{\alpha} (\tau, \omega) \), 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.

\[
G^< = \frac{1}{2} \left( G^K - (G^R - G^A) \right)
\]

with,

\[
\Sigma_{\alpha,\beta}^{R,A,K}(\tau, \omega) = U^2 M^\tau_i (M^\beta_j) g^{R,A,K}_{ij}(\omega)
\]

The discussion of the dependence of \( T_N(V) \) has been marked with a black cross on the trace. \( M(T) \) shows a minimum at a temperature \( T_c(V) \).

This suggests that a Heisenberg model with varying moment magnitude but \( V, T \) independent coupling may describe the finite \( V \) magnetism.

(\( c \)) Temperature dependence of the magnetic structure factor at \( \vec{Q} = (\pi, \pi, \pi) \) in the effective Heisenberg model for different \( V \), computed via Monte Carlo. (\( d \)) Comparison of the full Langevin based \( T_N \) and that extracted from the effective Heisenberg model. The correspondence works well up to intermediate \( V \) and breaks down in the metallic phase.
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., $(M_i^I(\tau)M_j^J(\tau')) \approx T\delta_{ij}\delta(\tau-\tau')$. So the averaged self-energy

$$
\langle \Sigma^{R,A,K}_{j,j+i,j,j-i}(\omega) \rangle = U^2T\delta_{ij}\delta(\omega)g^{R,A,K}_{ij}(\omega)
$$

(10)

can be used to approximate the mean current. Fig.8 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. This suggests that the current in the metallic phase is essentially given by the tight-binding result for $V/t \geq 6$ as $T \to 0$. For a finite system this has a finite value, and scales linearly with the number of conduction channels which is proportional to the cross sectional area $A$. Hence the resistance in the metallic phase is finite even as $T \to 0$ within a finite sized calculation, as is evident in Fig.8, and would vanish only if $A \to \infty$. As the temperature increases, thermal fluctuations of the background moments leads to enhanced scattering which depletes the current further.

F. Spatial variation of charge and magnetic moment

In Fig.9, we show the charge deviation (from $n_i = 1$) and moment magnitude, defined as,

$$
\langle \delta n_i \rangle = 1 - \sum_{\tau_y,\tau_z} \int_0^{L_y} \int_0^{L_z} \frac{d\tau}{\tau_M} \frac{d\omega}{2\pi} \text{Tr} \left[ g^{K}_{ii}(\tau,\omega) \right]
$$

(11a)

$$
\langle |\delta_1| \rangle = \sum_{\tau_y,\tau_z} \int_0^{L_y} \int_0^{L_z} \frac{d\tau}{\tau_M} \frac{d\omega}{2\pi} \text{Tr} \left[ g^{K}_{ii}(\tau,\omega)\sigma_3 \right]
$$

(11b)

where the trace is over the $2 \times 2$ local spin subspace. At $V/t = 0$, the charge deviation from $n_i = 1$ is vanishingly, as required, at all temperature, while the moment magnitude falls as the system is heated beyond $T_N$. For $0 < V/t \leq 2.2$, the charge deviation is small and concentrated at the edge 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 $2.2 < V/t < 3.6$, the charge 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 flat and with magnitude increasing with $T$.

G. Size dependence

The Langevin scheme presented here leads to a numerically intensive computation primarily because of the presence of leads in the nonequilibrium problem, and is worsened by the presence of multiplicative noise. As a result, for each site in every time step we need to diagonalise the electronic Hamiltonian twice. Moreover, one needs to have a sufficiently long run length in order to achieve a steady state. All these considerations constrain us to a modest size, $8 \times 4 \times 4$.

However, to our benefit, we discovered that the voltage driven insulator-metal transition is strongly first order for the 3D system. This means the transition should be realised even in larger systems although the coexistence region may pick up a size dependence. Furthermore, the magnetic transition at equilibrium is easily captured within our working size and several other studies have used even smaller systems to study it. For the voltage driven problem, a larger size may provide more resolution around the low temperature insulator-metal transition region of the phase diagram, but it should not change the essential features highlighted in this study. We have also checked the size independence of results for a few parameter points on a $10 \times 4 \times 4$ system.

H. Dimension dependence

It is important to highlight the nature of the transition as we go from a 3D bar geometry to a 2D rectangular geometry by removing one layer at a time, as shown in Fig.10. We find that the low temperature transition becomes progressively less abrupt as we reduce the number of layers, and for a single layer 2D system it becomes a crossover, which was studied in detail in Ref.55. The hysteresis region systematically shrinks with reducing number of layers, and for the single layer system no hysteresis is found. The “softening” of the jump in $I$-$V$ with reducing thickness of the sample has also been reported in an experiment11.
FIG. 9. (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.

I. Connection with experiments

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), 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. An experiment$^{11}$ has also reported that the jump in the $I-V$ becomes less abrupt upon reducing sample thickness, which is also captured within our scheme (Fig. 10). An experiment on a multiorbital ruthenate has reported suppression of Néel temperature with increasing current$^1$. 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.

V. CONCLUSIONS

We have been able 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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Appendix A: Accessing equilibrium dynamics

The Langevin scheme yields a time series for the auxiliary field $\vec{M}(\tau)$ starting from an initial configuration which may be arbitrary. Thus the scheme allows for thermalisation of the system to the equilibrium state. However, it remains to be ascertained that the system reaches the correct equilibrium state, which is nontrivial, given the multiplicative nature of the noise. Moreover, the dissipation coefficient $\gamma_i(\tau)$ and the diffusion $D_i(\tau)$ not only vary over sites, but also depend on the instantaneous configuration of the auxiliary fields. Nevertheless, we shall show that even with such nontrivial parameters, the Langevin scheme converges to the correct long time equilibrium state. To do this we write the Fokker-Planck equation for the distribution function of the moments $P(\{\vec{m}_i(\tau)\}, \tau) = \langle \prod_i \delta(m_i^a - M_i^a) \rangle$.

$$\begin{aligned}
\frac{\partial P}{\partial \tau} &= -\frac{\partial}{\partial m_i^a} \left[ \left( \epsilon_{abc} m_i^b F_i^c + \alpha m_i^a m_i^b \right) \left( F_i^b - T \tilde{D}_i \frac{\partial}{\partial m_j^b} \right) \right. \\
&\quad \left. + \frac{1}{\alpha} \left( F_i^a - T \tilde{D}_i \frac{\partial}{\partial m_i^a} - (\delta_{ab} + m_i^a m_i^b) T \frac{\partial}{\partial m_i^b} \right) \right] P \\
&A1
\end{aligned}$$

where the repeated indices are to be summed over, and $\tilde{D}_i = \frac{D_i \gamma_i}{2\alpha^2}$ is the effective diffusion coefficient, and $\tilde{F}_i = \langle \tilde{F}_i \rangle = \langle \vec{m}_i \rangle - \vec{m}_i$ is a generalised force. At steady state $\frac{\partial P}{\partial \tau} = 0$ leading to conservation of probability current. For the dynamics at equilibrium, the following conditions are additionally met:

- The force is conservative, and hence, can be derived from the spin-fermion Hamiltonian as $\tilde{F}_i = -\frac{\partial H}{\partial m_i^a}$, where,

$$H = -t \sum_{\langle ij \rangle, \sigma} d_i^\dagger_{\sigma} d_j_{\sigma} - U \sum_i (\vec{m}_i \cdot \vec{\sigma}_i^P + |\vec{m}_i|^2) \quad A2$$

is the same Hamiltonian which was introduced in Eq. 3g in the Supplement, with the scaling $\tilde{H} \rightarrow U \tilde{H}$ and including the classical stiffness of the auxiliary moments. The charge field is fixed to the half-filling saddle point value.

- The distribution is given by a Boltzmann form,

$$P(\{\vec{m}_i(\tau)\}) \propto \text{Tr}_{el} \left( e^{-\beta H} \right) \quad A3$$

Using this form in Eq. A1, we find that the distribution becomes stationary if we assume $D_i = 1$ which leads to,

$$D_i = \frac{2U}{\gamma_i} \times \frac{\alpha}{1 + \alpha^2 |\vec{m}_i(\tau)|^2} \quad A4$$

This determines the diffusion coefficient in terms of the known parameters and the instantaneous background configuration.

Hence, we find that with a suitable choice of the dissipation and diffusion coefficients, the Langevin scheme indeed leads to the correct equilibrium state.

Appendix B: Benchmarks

We benchmark our formulation against the classical Monte Carlo (MC) formulation at equilibrium. We compare the temperature dependence of the structure factor (Eq.3 in the main text) peak across the two formulations, in Fig.11(a). The two curves coincide for almost the entire range of temperature. The magnetic transition temperature within Quantum Monte Carlo (QMC) at $U/t = 6$ in 3D is about $0.34$.

We also compare the moment distribution defined in eq. 7. Fig.11(b) shows the comparison at different temperatures. The distributions match at low and high temperature, but slightly deviate for low moment values near $T_N$.

FIG. 11. (a) Comparison of temperature dependence of the structure factor peak with equilibrium ‘classical’ Monte Carlo. The Néel temperature $T_N = 0.28t$ at $U = 6t$. The two curves coincide, except very close to $T_N$. (b) Comparison of moment distribution for different temperatures. The distributions match at low and high temperature and deviate slightly for low moment values near $T_N$.

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See Supplemental Material [URL to be inserted by publisher] for derivation of the Langevin equation for the auxiliary spin field starting from the Hubbard model connected to leads.

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Supplementary Material on “The nonequilibrium thermal state of a voltage biased Mott insulator”

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I. 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 Keldysh contour shown in Fig.1. The generating functional is given by:

\[ Z = \int D\{\hat{c}, \hat{c}^\dagger, \hat{d}, \hat{d}^\dagger\} e^{iS[\hat{c}, \hat{c}^\dagger, \hat{d}, \hat{d}^\dagger]} \]  \hspace{1cm} (1)

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

\[
\begin{align*}
S &= \int_{-\infty}^{\infty} d\tau \left[ \mathcal{L}_{\text{sys}}(\tau) + \mathcal{L}_{\text{bath}}(\tau) + \mathcal{L}_{\text{coup}}(\tau) \right] \\
\mathcal{L}_{\text{sys}}(\tau) &= \sum_{\langle ij \rangle} \sum_{\sigma, s} s \hat{d}_{\sigma i}^\dagger(\tau) (i\partial_\tau + t) \hat{d}_{\sigma j}^\dagger(\tau) - U \sum_{i,s} s \hat{n}_{\sigma i}^\dagger(\tau) \hat{n}_{\sigma i}(\tau) \\
\mathcal{L}_{\text{bath}}(\tau) &= \sum_{\nu, \beta, s} s \hat{c}_{\nu i}^\dagger(\tau) (i\partial_\tau - \epsilon_\nu) \hat{c}_{\beta j}(\tau) \\
\mathcal{L}_{\text{coup}}(t) &= \sum_{\langle ij \rangle} \sum_{\sigma, s} \nu_{ij} \left( \hat{c}_{\sigma i}^\dagger(\tau) \hat{d}_{\sigma j}^\dagger(\tau) + \hat{c}_{\sigma j}(\tau) \hat{d}_{\sigma i}^\dagger(\tau) + g.c. \right)
\end{align*}
\]  \hspace{1cm} (1a, 1b, 1c, 1d)

where \(i, j\) are the lattice indices, \(\sigma\) is the spin index, \(\beta\) 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:

\[ U \hat{n}_{\sigma i}^\dagger(\tau) \hat{n}_{\sigma i}(\tau) = \frac{U}{4} \left( \hat{n}_{\sigma i}^\dagger(\tau) \right)^2 - U \left( \hat{\sigma}^\dagger_{\sigma i} \cdot \hat{\Omega}^\dagger_{\sigma i} \right)^2 \]  \hspace{1cm} (2)

where we have suppressed the time label for brevity.

\[
\hat{\sigma}^\dagger_{\sigma i} = \frac{1}{2} \sum_{\alpha, \beta} \hat{d}_{\alpha i}^\dagger \hat{d}_{\beta i}^\dagger \hat{d}_{\beta i} \hat{d}_{\alpha i}^\dagger \] is the local density, \(\hat{\Omega}^\dagger_{\sigma i} = \frac{1}{2} \sum_{\alpha, \beta} \hat{d}_{\alpha i}^\dagger \hat{d}_{\beta i}^\dagger \hat{d}_{\beta i} \hat{d}_{\alpha i}^\dagger \) is the local spin operator and \(\hat{\Omega}_{\sigma i}^\dagger\) is an arbitrary SO(3) vector. \(\hat{\sigma}^\dagger_{\sigma i}\) is the \(2 \times 2\) Pauli vector.

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

\[ e^{-i \frac{\hat{\sigma}^\dagger(\tau) \hat{\phi}(\tau)^2}{4}} \propto \int d\phi_i(\tau) e^{i(\hat{\phi}(\tau)^2 - \epsilon_\phi(\tau) \hat{n}_i(\tau))} \]  \hspace{1cm} (2a)

While the HS transformation on the second term can be written in terms of an O(3) “spin field” \(\hat{M}_i(\tau)\):

\[ e^{iU \hat{\sigma}^\dagger(\tau) \hat{\Omega}^\dagger_{\sigma i}(\tau)} \propto \int d\hat{M}^\dagger_{\sigma i}(\tau) e^{i(-\epsilon(\hat{\Delta}^\dagger_{\sigma i}(\tau)) - \hat{M}^\dagger_{\sigma i}(\tau) \cdot \hat{\sigma}^\dagger_{\sigma i}(\tau))} \]  \hspace{1cm} (2b)

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

\[
\hat{S}[\phi, M] = -iTr \ln \left[ i\hat{G}^{-1}(\tau, \tau') \right] + \frac{1}{U} \int dt \sum_i \left[ \phi_i^\dagger(\tau) \phi_i^\dagger(\tau) - \hat{M}^\dagger_i(\tau) \cdot \hat{M}_i(\tau) \right]
\]  \hspace{1cm} (3)

with

\[
\hat{G}^{-1}(t, t') = \begin{pmatrix}
\hat{G}_R(t, t') & \hat{G}_R(t, t')^{-1} \\
\hat{G}_R(t, t')^{-1} & \hat{G}_R(t, t')
\end{pmatrix}
\]  \hspace{1cm} (3a)

FIG. 1. The complex time Keldysh contour for nonequilibrium steady states. The ends of the contour corresponding to the initial time \(\tau_0\) and the maximum accessible time \(\tau_{\text{max}}\) is taken to \(\pm \infty\). In order to calculate observables, e.g., the two-point function, one makes insertions at intermediate times \(\tau_1\) and \(\tau_2\).
where the components of $G^{-1}$ in the $2 \times 2$ Keldysh space are given by:

$$
\hat{G}_R^{-1}(\tau, \tau') = \left( \frac{\partial}{\partial \tau} - \hat{H}^c(\tau) \right) \delta(\tau - \tau') + \hat{\Gamma}(\tau, \tau')
$$

(3b)

$$
\hat{G}_A^{-1}(\tau, \tau') = \left( \frac{\partial}{\partial \tau} - \hat{H}^c(\tau) \right) \delta(\tau - \tau') + \hat{\Gamma}(\tau, \tau')
$$

(3c)

$$
\hat{G}_K^{-1}(\tau, \tau') = \Gamma_{ij}(\tau, \tau') \delta_{\alpha \alpha'} + \left( \hat{G}_R^{-1} \circ F - F \circ \hat{G}_A^{-1} \right)(\tau, \tau')
$$

(3d)

$$
\left[ \hat{G}_{12}^{-1}(\tau, \tau') \right]_{ij; \alpha \alpha'} = \frac{1}{2} \left( \hat{M}^q(\tau) \cdot \hat{\sigma}_{\alpha \alpha'}^P - \phi_i(\tau) \delta_{\alpha \alpha'} \right)
$$

(3e)

$$
\delta_{ij} \delta(\tau - \tau')
$$

(3f)

$$
\hat{H}_{ij}(\tau) = \left( \phi_i(\tau) \mathbb{1}_2 - \hat{M}_i^c(\tau) \cdot \hat{\sigma}^P \right) \delta_{ij} - t_{<ij>} \mathbb{1}_2
$$

(3g)

where $\mathbb{1}_2$ is the $2 \times 2$ identity matrix. $\hat{H}^c(\tau)$ is a time-dependent Hamiltonian which depends on the 'classical' component of the auxiliary fields. $\hat{\Gamma}_{R,A,K}(\tau, \tau')$ are dissipation terms which enter the action as a result of integrating out the leads. $F(\tau, \tau')$ 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 fields introduced in the H-S transformations in Eqs. 2a and 2b.

$$
\hat{M}^c = \frac{1}{2} \left( \hat{M}^+ + \hat{M}^- \right), \quad \hat{M}^q = \left( \hat{M}^+ - \hat{M}^- \right)
$$

(4)

where we have suppressed the time and other labels for notational brevity. A similar transformation holds for the $\phi$ fields. We have mapped the original fermionic action for the dissipative Hubbard model into an action containing time dependent auxiliary fields. The mapping is formally exact up to this point.

**II. APPROXIMATIONS**

Next, we derive an effective thermal fluctuation theory by making a series of approximations: (i) We fix the charge field ($\phi$) to it's classical saddle point at equilibrium, i.e., $\phi_i^c, \phi_i^q = 0$. This fixes the overall density to half-filling, but allows local density fluctuations due to dynamics of the spin-field ($\hat{M}$). (ii) We perform a cumulant expansion of the action to second order in $\{M^q\}$ fields, introduce a 'noise' by decoupling the quadratic term, and evaluate the 'classical' saddle point to obtain a stochastic equation of motion (EOM) for the $\{M^c\}$. (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, which can be justified in the high temperature limit.

**A. Cumulant expansion**

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

$$
\hat{G}^{-1} = (\mathbb{1} + \Sigma_q \circ \hat{G}_c) \circ \hat{G}^{-1}_c
$$

$$
\Sigma_q(\tau, \tau') = \frac{1}{2} \hat{M}^q(\tau) \cdot \hat{\sigma}^P \delta_{ij} \delta(\tau - \tau') \otimes \sigma_K
$$

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

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

(6)

with

$$
\hat{S}^0 = -\imath \text{Tr} \ln \left[ \imath \hat{G}^{-1}_c(\tau, \tau') \right] = 0
$$

(6a)

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

$$
\hat{S}^1 = \sum_i \int d\tau \left( \text{Im} \left[ \text{Tr} \left( \hat{G}^K_{ii}(\tau, \tau) \hat{\sigma} \right) - \frac{\hat{M}^c_i(\tau)}{U} \right] \cdot \hat{M}^q_i(\tau) \right)
$$

(6b)

$$
\hat{S}^2 = \frac{1}{2} \int d\tau \int d\tau' \sum_{i,j:ab} M_{ia}^q(\tau) \left[ \hat{\Pi}^K(\tau, \tau') \right]_{ij}^{ab} M_{jb}^q(\tau')
$$

(6c)

where

$$
\left[ \hat{\Pi}^K(\tau, \tau') \right]_{ij}^{ab} = \text{Tr} \left[ \left( \hat{G}_{ij}(\tau, \tau') \sigma^a \hat{G}^K_{ji}(\tau', \tau) \sigma^b \right) + \left( \hat{G}_{ij}^A(\tau', \tau) \sigma^a \hat{G}^R_{ji}(\tau', \tau) \sigma^b \right) \right]
$$

(6d)

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

$$
e^{\imath \hat{S}^2} = e^{-\frac{1}{2} \hat{M}^q \circ \hat{\Pi}^K \circ \hat{M}^q}
$$

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

(6e)

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 φq = 0, ̄M = 0. This gives us the following equation for the ‘c’ fields:

\[
\text{Tr} \left[ \hat{G}^R_{ii}(\tau, \tau) \delta \phi \right] = \hat{M}_c(\tau) - \hat{\xi}_c(\tau)
\]

\[
\langle \xi_c^a(\tau) \xi_c^b(\tau') \rangle = \left[ \hat{\Pi}^R(\tau, \tau') \right]_{ab}^{\text{nb}} \tag{7}
\]

### B. Semiclassical expansion

Transforming to Wigner coordinates allows us to write,

\[
\hat{G}^K(\tau, \tau) = \hat{G}^K(\tau, \tau_r = 0) = \int d\omega \hat{G}^K(\tau, \omega) \tag{8}
\]

In what follows, we would write a series expansion for \( \hat{G}^K(\tau, \omega) \) in powers of \( \hbar \). For this purpose we first construct a series expansion for \( \hat{G}^R(\tau, \omega) \).

#### 1. The retarded Green’s function \( \hat{G}^R \)

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

\[
(\hat{G}^{-1}^R \circ \hat{G}^R)(\tau_1, \tau_2) = \delta(\tau_1 - \tau_2)\hat{1}
\]

Transforming to Wigner coordinates allows us to expand the LHS in a Kramers-Moyal series \(^3\),

\[
(\omega - \hat{H}^c(\tau) + \hat{\Gamma}^R(\omega)) \hat{G}^R(\tau, \omega)
\]

\[
+ \frac{i\hbar}{2} \left( \partial_\tau \hat{H}^c(\tau) \partial_\omega \hat{G}^R - (\hat{1} + \partial_\omega \hat{\Gamma}^R) \partial_\tau \hat{G}^R \right) + O(h^2) = \hat{1} \tag{9a}
\]

where \( \tau \equiv \frac{\tau - \tau_2}{2} \) is the center-of-mass time, and \( \Omega \) is the fourier conjugate to the relative time \( \tau_r \equiv \tau_1 - \tau_2 \). Furthermore, we have assumed that \( \hat{\Gamma}^R \) depends only on the relative time. This is true at steady state.

This expansion relies on the condition that \( \hbar \ll (\text{timescale for } \hat{M} \text{ fluctuations}) \times (\text{energy-scale for electronic excitations}) \). The timescale for magnetic fluctuations is set by \( J^{-1} \), where \( J \sim \frac{eU}{\hbar} \) is the magnetic exchange scale, while the energy-scale for electronic excitations is set by the electronic bandwidth given by \( U \), for \( U \ll t \). Setting \( \hbar = 1 \), we then have the condition \( J \ll U \) for the expansion to be valid.

Inverting the above Eq. gives us

\[
\hat{G}^R(\tau, \omega) = \hat{G}^R(\tau, \omega)
\]

\[
- \frac{i\hbar}{2} \left( \hat{G}^R \partial_\tau \hat{H}^c + \hat{G}^R(\hat{1} + \partial_\omega \hat{\Gamma}^R) \partial_\tau \hat{G}^R \right) + O(h^2) \tag{9b}
\]

where,

\[
\hat{G}^R(\tau, \omega) = \left( \omega \hat{1} - \hat{H}^c(\tau) + \hat{\Gamma}^R(\omega) \right)^{-1} \tag{9c}
\]

is the “adiabatic” retarded Green’s function which depends only on the instantaneous configuration of the background field, and not on its history.

Now, for any matrix \( \hat{A}(\omega) \), we have \( \partial_\omega \hat{A} = -\hat{A} \left( \partial_\omega \hat{A}^{-1} \right) \). Using this we can rewrite Eq.9b to \( O(h) \) as

\[
\hat{G}^R(\tau, \omega) = \left( \hat{1} + \frac{i\hbar}{2} \left[ \hat{G}^R \partial_\tau \hat{H}^c, \hat{G}^R \left( \hat{1} + \partial_\omega \hat{\Gamma}^R \right) \right] \right) \hat{G}^R(\tau, \omega) \tag{9d}
\]

where \([ , ]\) denotes the commutator bracket.

#### 2. 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 provided the distribution function is known apriori. In our case, the distribution function in the disconnected system \( F(\Omega) = \tanh(\omega/2T) \) gets corrections due to hybridisation with the leads, as is apparent from the form of \( \hat{G}^K(\tau, \tau') \) defined in Eq.3d. From the structure of \( \hat{G}^{-1} \), it follows that

\[
\hat{G}^K(\tau_1, \tau_2) = -\hat{G}^R(\tau_1, \tau_2) \circ \hat{G}^{-1}_K(\tau', \tau') \circ \hat{G}^A(\tau', \tau_2) \tag{10}
\]

Transforming to Wigner coordinates and implementing the Kramers-Moyal expansion, as above, allows us to write

\[
\hat{G}^K(\tau, \omega) = \hat{G}^K(\tau, \omega)
\]

\[
+ \frac{i\hbar}{2} \left[ \hat{G}^R \partial_\tau \hat{H}^c, \hat{G}^R \left( \hat{1} + \partial_\omega \hat{\Gamma}^R \right) \right] \hat{F} \hat{G}^R - H.c. + (\ldots) \tag{10a}
\]

where,

\[
\hat{G}^K(\tau, \omega) = F(\omega) \left( \hat{G}^R(\tau, \omega) - \hat{G}^A(\tau, \omega) \right)
\]

\[
- \hat{G}^R(\tau, \omega) \hat{\Gamma}^K(\omega) \hat{G}^A(\tau, \omega) \tag{10b}
\]

The terms denoted by \((\ldots)\) in Eq.10a can be dropped as their contribution is negligible for a gapped system. Now, we can write the matrix elements of adiabatic Green’s function in the \( 2 \times 2 \) spin subspace as:

\[
\hat{G}^R_{ij}(\tau, \omega) = g^{R}_{ij}(\tau, \omega) \hat{1}_{2	imes2} + \hat{h}^R_{ij}(\tau, \omega) \cdot \hat{\sigma} \tag{11a}
\]

and similarly, for,

\[
\hat{\chi}^R_{ij}(\tau, \omega) = -i\hbar \left[ \hat{G} \partial_\tau \hat{H}^c, \hat{G}^R \left( \hat{1} + \partial_\omega \hat{\Gamma}^R \right) \right] \tag{11b}
\]

we can write,

\[
\hat{\chi}^R_{ij}(\tau, \omega) = \rho^{R}_{ij}(\tau, \omega) \hat{1}_{2	imes2} + \hat{h}^R_{ij}(\tau, \omega) \cdot \hat{\sigma} \tag{11c}
\]

Plugging these in Eq.10a we obtain

\[
\text{Tr} \left[ \hat{G}^K_{ii}(\tau, \omega) \sigma^a \right] = \text{Tr} \left[ \hat{G}^K_{ii}(\tau, \omega) \sigma^a \right] + \sum_j \left( -\Gamma_{ij}(\tau, \omega) \partial_\tau M^a_j \right)
\]

\[
+ \left( \tilde{\chi}_{ij}(\tau, \omega) \times \partial_\tau M_j \right) \right) + \tilde{b}^R_{ij}(\tau, \omega) \cdot \partial_\tau M_j \tag{11d}
\]
where

\begin{align}
\Gamma_{ij} &= \left( \rho_{ij} R_{ji} - \vec{h}_{ij} \cdot R_{ji} + R \rightarrow A \right) \\
\vec{\Lambda}_{ij} &= \left( \rho_{ij} \vec{h}_{ji} - \vec{\lambda}_{ij} g_{ji} + R \rightarrow A \right) \\
\beta^a_{ij} &= \left( \vec{R}_{ij} R_{ji} - \vec{\lambda}_{ij} \cdot \vec{h}_{ji} + R \rightarrow A \right)
\end{align}

Finally, from eq.8 we know that the equal time Keldysh Green’s function which enters the EOM eq’7 is obtained by performing an integral over \( \omega \) of eq.11d.

\[ \int \text{Im} \left[ \text{Tr} \left( \hat{G}^R_{tt}(\tau, \omega) \hat{\sigma}^P \right) \right] d\omega \equiv \langle \vec{\sigma}(\tau) \rangle_{\{\vec{M}\}} \]

where \( \langle \vec{\sigma}(\tau) \rangle \) is the instantaneous expectation value of the electron spin obtained under the adiabatic approximation.

Evaluating the coefficients \( \Gamma_{ij}, \vec{\Lambda}_{ij} \) and \( \beta^a_{ij} \) for an arbitrary \( \{\vec{M}\} \) configuration is very hard. We simplify them by performing a strong coupling expansion and retaining just the leading order terms. \( \beta^a \) drops out in this process. Further, we postulate the following form for the remaining coefficients,

\begin{align}
\int d\omega \Gamma_{ij}(\tau, \omega) &\approx \frac{1}{\gamma_i(\tau)} \delta_{ij} \\
\int d\omega \vec{\Lambda}_{ij}(\tau, \omega) &\approx \frac{\alpha}{\gamma_i(\tau)} \vec{M}_i(\tau) \delta_{ij} \\
[\Pi^K(\tau, \tau')]^{ab}_{ij} &\approx 2D_i(\tau) T \delta_{ij} \delta_{ab}(\tau - \tau')
\end{align}

where \( \gamma_i(\tau), D_i(\tau) \) and \( \alpha \) are unknown parameters, which we shall determine subsequently, and \( T \) is the temperature. \( \alpha \) is the dimensionless Gilbert damping\(^{2,3} \) parameter which provides a relaxational torque to the angular degrees of freedom, \( \gamma_i \) contributes to longitudinal damping and \( D_i \) are position dependent diffusion coefficients. The uncorrelated form of the noise kernel can be motivated by expanding \( \Pi^K(\tau, \Omega) \) about the homogeneous antiferromagnetic state in powers of \( \Omega / \Delta \) and \( t / \Delta \), where \( \Omega \) is the characteristic scale of two particle excitation \( (J \sim t^2 / U) \) and \( \Delta \) is the gap in the single particle spectrum, and taking the limit \( \Omega \ll T \). The noise vanishes as \( T \to 0 \) as a result of this approximation, but the actual noise survives even at zero temperature in a quantum system. In Appendix A, we show \( D_i(\tau) = 2U / \gamma_i(\tau) \) for detailed balance to be satisfied at equilibrium. Hence, one obtains the form of the evolution equation for \( \{\vec{M}\} \), as given in the main text.

Next shall fix \( \gamma \). For this we cast the Langevin equation into a Landau-Lifshitz-Gilbert(LLG) form by solving for \( \frac{d\vec{M}}{dT} \).

\[ \frac{d\vec{M}_i}{dT} = -A_i(\tau) \vec{M}_i \times \left( \langle \vec{\sigma}_i \rangle + \vec{\xi}_i \right) + B_i(\tau) \vec{M}_i \times \left( \vec{M}_i \times \left( \langle \vec{\sigma}_i \rangle + \vec{\xi}_i \right) \right) + \gamma_i(\tau) \left( \vec{M}_i - \langle \vec{\sigma}_i \rangle + \vec{\xi}_i \right) \]

with, \( A_i(\tau) \equiv \frac{\gamma_i(\tau) \alpha}{1 + \alpha^2 |\vec{M}_i(\tau)|^2} \) and \( B_i(\tau) \equiv \frac{\gamma_i(\tau) \alpha^2}{1 + \alpha^2 |\vec{M}_i(\tau)|^2} \). The first term is the ‘Bloch’ term which leads to precessional motion of the spins. In order to capture the correct spin wave dispersion \( A_i = 2U \) must be satisfied, which follows from the subleading term in the strong coupling expansion of \( \langle \vec{\sigma}_i \rangle \). This means that the time dependence in \( A_i(t) \) must drop out, which leads us to the condition,

\[ \gamma_i(\tau) = \frac{2U}{\alpha} \left( 1 + \alpha^2 |\vec{M}_i(\tau)|^2 \right) \]

and hence, \( B_i = 2U / \alpha \) also becomes independent of time. \( \alpha \) remains the only free parameter in the Langevin scheme. It is dimensionless, and the static properties do not depend sensitively on \( \alpha \). It can be estimated by evaluating Eq.11f for a two site system. A tedious, but straightforward, calculation suggests \( \alpha = (U/t)^2 \). Hence, all the parameters which were introduced ‘by-hand’ get fixed upon further considerations and the final formulation does not have any free parameters. Having said that, we must note that unlike the other two parameters the value of \( \alpha \) doesn’t get fixed by any consistency condition, but rather through a calculation. We shall test the sanctity of this result by benchmarking our scheme against equilibrium Monte-Carlo results.

An alternative, and perhaps more intuitive approach, would be to show that the Langevin equation for the auxiliary fields maps to the well studied Landau-Lifshitz-Gilbert(LLG) equation at strong coupling. This is easy to see once we expand the electronic spin in powers of \( t / U \) in terms of the instantaneous background configuration,

\[ \langle \vec{\sigma}_i(t) \rangle = \vec{M}_i(t) - \frac{J}{2U} \sum_{j \in NN} \vec{M}_j(t) \]

where \( J = 4t^2 / U \). Substituting this in Eq. 13 and projecting the dynamics on the spheres defined by \( |\vec{M}_i| = 1/2 \) we get\(^4 \),

\[ \frac{d\vec{M}_i}{dT} = \vec{M}_i \times \left( \vec{B}_i + \vec{\xi}_i \right) - \alpha \vec{M}_i \times \left( \vec{M}_i \times (\vec{B}_i + \vec{\xi}_i) \right) \]

where \( \vec{B}_i = J \sum_{i+z \in NN} \vec{M}_{i+z} \) and \( \alpha = \frac{3\alpha}{4} - \frac{1}{\alpha} \). The configuration dependence of the parameters drops out. This is the celebrated LLG equation.

Thus, we find that the Langevin formulation reproduces the known limits consistently. However, in the context of Hubbard model the observable quantities are electronic correlations which can be calculated within the adiabatic approximation by solving the electronic problem in the instantaneous auxiliary field background. Thus, this gives us a time series for electronic operators as well, from which we can compute various static and dynamic correlators.
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