Voltage bias driven resistive switching in a Mott insulator

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We develop a real space picture of the voltage bias driven transition from a Mott insulator to a correlated metal. Within our Keldysh mean field approach the problem reduces to self-consistency equations for the charge and spin auxiliary fields that decouple the Hubbard interaction. We solve these, obtain the nonlinear current-voltage (I-V) characteristic of the system, and illustrate the behaviour of the local density of states across the sample in different voltage bias regimes. We find that the effect of bias penetrates deeper into the system with increasing voltage, with a characteristic penetration depth $\xi(V)$ which rises sharply close to the breakdown voltage. We set up an approximate scheme to explain the features in the local density of states close to the insulator-metal transition.

Keywords: Mott breakdown, nonequilibrium mean field

I. INTRODUCTION

The field driven breakdown of band insulators is a well understood phenomenon owing to the early work of Landau and Zener[1]. In these insulators electron correlation effects are neglected and the breakdown is understood in terms of field assisted quantum tunnelling of electrons across the band gap. In contrast, Mott insulators are strongly correlated, with a charge gap of many body origin due to Coulomb repulsion between electrons. The breakdown of Mott insulators has garnered a lot of attention in recent times. Many studies, theoretical as well as experimental, have tried to capture the effect of the strong electron correlation on nonlinear transport in these insulators. On the theoretical front, the first studies were performed more than a decade ago for the 1D Hubbard model by numerically solving the time-dependent Schrodinger equation[2] and using time-dependent density matrix renormalisation group (DMRG) techniques[3].

A generalisation of dynamical mean field theory (DMFT) to nonequilibrium situations has also been widely used to study breakdown problems in different scenarios. Earlier approaches introduced the electric field through time dependent gauge fields, and coupling every site to dissipative baths to achieve a steady state[4]. Such an approach essentially reduces the problem to a single site interacting theory embedded in a self-consistent bath, but, in the process, misses out on the possible spatial features of the breakdown process. More recently there have been approaches employing DMFT which introduce the field by imposing a linear voltage gradient across the system[5]. This is somewhat artificial as the potential inside the system can get renormalised due to interaction effects, and hence, must be obtained self-consistently. Moreover in all these works the current-voltage characteristics do not show any threshold behaviour, in contrast to what is seen in experiments[6,7].

A mean field treatment of the bias driven transition has been attempted very recently for the Hubbard model in 1D[8]. They compute the instabilities of the system to spatially modulated patterns of the order parameter, and ascribe the metallisation of the Mott state to the emergence of these patterns. Some evidence for such modulated phases arising in the driven Mott insulator has already been found in an experiment[9]. In this work, we focus on developing an intuitive real space steady state picture of the breakdown. We work with the 2D Hubbard model connected to metallic leads, which impose a bias across the system, and develop a mean field picture for the Mott breakdown problem.

Our main results, working at zero temperature, are the following: (i) We obtain the current-voltage, $I - V$, characteristics for different values of Hubbard interaction, $U$, mapping out the $U - V$ metal-insulator phase diagram. (ii) We find that the breakdown voltage $V_b(U)$ remains essentially independent of system size, while the saturation current $I_{sat}$ decreases with increasing size. (iii) We track the changes in local density of states (LDOS) as a function of bias and distance from the edges, and identify signatures of breakdown as well as current saturation. (iv) Analysis of the spatial patterns suggest that close to the breakdown only a few modes around the dominant zero bias modes dominate the physics. (v) We provide an interpretation of the breakdown phenomenon in terms of (a) an increasing ‘penetration depth’ $\xi(V)$ (over which the bias modifies the zero bias state) which diverges as the breakdown voltage is approached, and (b) an approximate calculation of the local density of states in the biased situation.

II. MODEL AND METHOD

A. Model

We consider a 2D Mott insulator connected to non-interacting leads via tight-binding coupling. The leads serve two purposes: (i) The bias is introduced through a population imbalance in leads, and (ii) they provide dissipative channels for the system to relax. The isolated Mott insulator when subjected to a field does not thermalise for a significantly long time, but instead gets trapped in a prethermalised metastable state. On the other hand, the presence of metallic leads at the two edges allows it to relax more readily into a nonequilibrium steady state.

We model the Mott insulator (system) by the repulsive Hubbard model defined on a square lattice, while the leads are modeled as tight-binding electron reservoirs. Each site at the left and the right edges of the Mott insulator is coupled to the...
Stratonovich (HS) transformation. The first transformation introduces a charge field $\phi_i$: 

$$i\hbar \int dt \left( \sum_{\sigma} n_{i\sigma}^e \right)^2 \propto \int d\phi_i^e \frac{i}{\hbar} \int dt \left( \frac{\phi_i^e}{\hbar} \sum_{\sigma} n_{i\sigma}^e \right)$$  \hspace{1cm} (3a)$$

While the HS transformation on the second term introduces a spin field $M$: 

$$i\hbar \int dt \left( \sum_{\sigma} \sigma n_{i\sigma}^e \right)^2 \propto \int dM_i^e \frac{i}{\hbar} \int dt \left( -\frac{M_i^e}{\hbar} \sum_{\sigma} \sigma n_{i\sigma}^e \right)$$  \hspace{1cm} (3b)$$

with $\sigma_z = +1$ for $\uparrow$ and $-1$ for $\downarrow$. In the previous three equations we have suppressed the time arguments for brevity.

As a result of these transformations the problem gets mapped to a quadratic Lagrangian with additional fluctuating noise fields.

$$Z \propto \int \mathcal{D}\{\bar{c}, c, \bar{d}, d; \phi, M\} e^{i\hat{S}[c, \bar{c}, \bar{d}, d; \phi, M]}$$  \hspace{1cm} (4)

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

We can write the continuous time form of the action by imposing the boundary condition that, far in the past the system and the leads were not connected.

$$S = \int_{-\infty}^{\infty} dt \left[ \mathcal{L}_S(t) + \mathcal{L}_B(t) + \mathcal{L}_C(t) \right]$$  \hspace{1cm} (2a)$$

$$\mathcal{L}_S(t) = \sum_{i,j,s} s d_{i\sigma}^\dagger(t) (i\partial_t + t_s) d_{j\sigma}(t) - U \sum_{i,s} n_{i\uparrow}^e(t) n_{i\downarrow}^e(t)$$  \hspace{1cm} (2b)$$

$$\mathcal{L}_B(t) = \sum_{i,j,s,\sigma} s c_{i\sigma\alpha}^\dagger(t) (i\partial_t + t_\sigma) c_{j\sigma\alpha}(t)$$  \hspace{1cm} (2c)$$

$$\mathcal{L}_C(t) = \sum_{i,j,s,\sigma} t_c \left( c_{i\sigma}^L(t) d_{j\sigma}(t) + c_{i\sigma}^R(t) d_{j\sigma}(t) + g.c. \right)$$  \hspace{1cm} (2d)$$

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:

$$Un_{i\uparrow}^e n_{i\downarrow}^e = \frac{U}{4} \left[ (n_{i\uparrow}^e + n_{i\downarrow}^e)^2 - (n_{i\uparrow}^e - n_{i\downarrow}^e)^2 \right]$$  \hspace{1cm} (2e)$$

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

$$i\hbar \int dt \left( \sum_{\sigma} n_{i\sigma}^e \right)^2 \propto \int d\phi_i^e \frac{i}{\hbar} \int dt \left( \frac{\phi_i^e}{\hbar} \sum_{\sigma} n_{i\sigma}^e \right)$$  \hspace{1cm} (3a)$$

The first transformation in-
\( \Gamma_{R,A,K}(\omega) \) are dissipation terms which enter the action as a result of integrating out the leads.

### B. Static Path Approximation (SPA)

Till this point the formulation has been exact. We have traded off the quartic interaction term for a quadratic theory with two fluctuating noise fields. In order to make further progress we introduce the static path approximation in which we retain just the zero frequency auxiliary fields and ignore their finite frequency modes. We introduce the notation:

\[
\phi_i \equiv \phi_i^0, \quad \phi_i^q \equiv \phi_i^q
\]

\[
M_i^q \equiv M_i^q, \quad M_i^q \equiv M_i^q
\]

Hence, we arrive at an effective steady state description given by the SPA action:

\[
S_{SPA}[\phi, M] = -iTr \ln \left[ iG^{-1}(\omega) \right] + \frac{1}{2\pi U} \sum_i \left( \phi_i^c \phi_i^0 - M_i^q M_i^q \right)
\]

with

\[
\left( G^{-1} \right)^R_{ij,\alpha\alpha'} = \left[ (\omega + i\eta - \phi_i^c)\delta_{\alpha\alpha'} + M_i^q \sigma_{\alpha\alpha'}^c \right] \delta_{ij} + \left[ t_{<ij} + i\Gamma_{ij}(\omega) \right] \delta_{\alpha\alpha'}
\]

\[
\left( G^{-1} \right)^{12}_{ij,\alpha\alpha'} = -\frac{1}{2} \left( \phi_i^q \delta_{\alpha\alpha'} - M_i^q \sigma_{\alpha\alpha'}^c \right) \delta_{ij} + \Gamma_{ij}(\omega) \delta_{\alpha\alpha'}
\]

\[
\left( G^{-1} \right)^{21}_{ij,\alpha\alpha'} = -\frac{1}{2} \left( \phi_i^c \delta_{\alpha\alpha'} - M_i^c \sigma_{\alpha\alpha'}^c \right) \delta_{ij} + \Gamma_{ij}(\omega) \delta_{\alpha\alpha'}
\]

\[
\left( G^{-1} \right)^{A}_{ij,\alpha\alpha'} = \left[ (\omega - i\eta - \phi_i^c)\delta_{\alpha\alpha'} + M_i^q \sigma_{\alpha\alpha'}^c \right] \delta_{ij} + \left[ t_{<ij} + i\Gamma_{ij}(\omega) \right] \delta_{\alpha\alpha'}
\]

We arrive at the mean-field consistency conditions by extremising with respect to the auxiliary fields. At each site we get a set of four saddle point equations:

\[
\frac{\delta S_{SPA}}{\delta \phi_i^c} \bigg|_{\phi^e, M^e=0} = 0; \quad \frac{\delta S_{SPA}}{\delta M_i^q} \bigg|_{\phi^e, M^e=0} = 0 \quad (7a)
\]

\[
\frac{\delta S_{SPA}}{\delta \phi_i^q} \bigg|_{\phi^e, M^e=0} = 0; \quad \frac{\delta S_{SPA}}{\delta M_i^c} \bigg|_{\phi^e, M^e=0} = 0 \quad (7b)
\]

The saddle point conditions w.r.t. the classical components in eq. \([7a]\) reduce to an identity and hence give us no new information. Those w.r.t. the quantum components in eq. \([7b]\) give us the local consistency conditions:

\[
Tr \left[ G^{K}_{ij,\alpha\alpha'}(\omega) \right] = \frac{\phi_i^e}{2\pi U}
\]

\[
Tr \left[ G^{K}_{ij}(\omega) \cdot \sigma^z \right] = \frac{M_i^q}{2\pi U}
\]

### C. Implementation of mean field consistency

The mean field consistency equations and are solved iteratively for each site until the system converges. Starting with an initial guess for \(\{\phi\}\) and \(\{M\}\), we calculate the local traces by performing the frequency integrals of the locally projected Green’s functions. We have benchmarked the scheme against the analytically tractable zero temperature mean-field limit of the equilibrium Hubbard model in 2D with periodic boundary conditions.

### III. RESULTS

We discuss the results for our implementation of the scheme in a 2D system, which is finite in the longitudinal direction, while being periodic in the transverse direction. In this paper we focus strictly at zero temperature. The results are shown for a system with 32 sites in the longitudinal(x) direction and 8 sites in the transverse(y) direction. The system size dependence of our results has also been discussed. Unless otherwise mentioned, all energies are measured in units of hopping in the system \(t_s\), and all currents are measured in units of \(2et_s^2/h\).

#### A. Current Profile and Phase Diagram

The bond currents between the nearest neighbour sites are given by the expression:

\[
I_{j,j+1}(V) = \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \left[ G^{<}_{j,j+1;\sigma}(\omega) - G^{<}_{j,j+1;\sigma}(\omega) \right]
\]

with

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

For a system with periodic boundary conditions along the transverse direction the current can depend only on the longitudinal direction. At steady state one further expects the current to be the same on all bonds along the longitudinal axis. This has been checked to be true in the limit \(\eta \to 0\).

One can construct a phase diagram (FIG.1) from the \(I - V\) characteristics (FIG.2) by tracking the breakdown \(V_c(U)\). Within our scheme we find \(V_c(U)\) to be independent of system size.

For any finite \(U\), the \(I - V\) character has three different regions: I. exponentially suppressed current, II. breakdown and III. saturation, as is evident in FIG.2 where we plot the current (I) as a function of bias (V) for various interaction strengths (U). In regime I the current goes as \(\propto e^{-\alpha(U)/V}\), essentially independent of system size, up to a certain \(V_c(U)\) after which the system enters regime II. In regime II the current rises rapidly, with a linear profile close to \(V_c\) and then approaches saturation as it enters regime III. In regime III the current remains constant with \(V\), while the saturation value \(I_{sat}\) depends on \(U\) and the system size \(L\) (FIG.3).
FIG. 1. Phase diagram illustrating the metallic and insulating states in the $U - V$ plane. The solid blue curve demarcates the phase boundary, which grows linearly for large $U$. The dashed curve in black shows the dependence of equilibrium Mott gap on $U$. The two curves nearly coincide with each other, which signifies that the Mott insulator breaks down when the bias becomes equal to the zero bias gap.

The phase diagram (FIG.1) demarcates the insulating (regime I) and the metallic (regimes II and III) regions in the $U - V$ plane. It is imperative to note that within our scheme the Mott insulator supports exponentially weak current at $V < V_c(U)$ (ref. inset FIG.3).

FIG. 2. The $I - V$ character for different values of interaction strength $U$. For any finite $U$, the $I - V$ curve marks the transition from an insulating Mott state to a metallic state in which the current rises sharply after a critical bias $V_c$ and finally saturates to a constant value $I_{sat}$.

FIG. 3. Size dependence of $I - V$ curves at $U = 6$. The inset shows the zoomed in picture around $V_c$. Although $I_{sat}$ shows weak dependence on system size, $V_c$ remains robust.

B. Density of states

The density of states (DOS), $A(\omega)$, is obtained by averaging the local DoS (LDOS), $A_{ii}(\omega)$ given by:

$$A_{ii}(\omega) = -\frac{1}{\pi} \Im \left[ G_{ii}^R(\omega) \right]$$

with $1/L \sum_{i=1}^{L} A_{ii}(\omega)$)

In the zero bias problem LDOS remains gapped throughout the system except for the edge sites and the sites just next to the edge. These get renormalised due to coupling with the baths. The sites away from the edges remain essentially unaffected in absence of any bias, as is evident in the first column of FIG.4. With increasing bias the effect of the leads propagates further and further into the system. Even at $V_c$ the central site DOS remains weakly renormalised, with the gap intact, while the sites close to the edge become gapless - as illustrated in FIG.4 second column.

For $V < V_c$, the effect of bias decays exponentially inside the system, with the penetration depth controlled by the bias voltage ($V$). This shall be discussed in detail in a latter section. After the onset of breakdown, $V > V_c$, all the sites feel the effect of bias and the gap for the central site starts getting depleted (FIG.4 third column). At large $V$ the spectrum freezes and increasing bias further doesn’t affect the system. This marks the onset of the saturation regime.

The total density of states shows a gap at zero bias. As the system is biased one can observe the occurrence of subgap features in the full DOS even before $V$ hits $V_c$ (FIG.5). This contribution must come from the sites near the edges, as local DOS at these sites pick up weight at the Fermi level while sites close to the center remain gapped still. Until the effect of bias propagates to the center of the system the current remains exponentially suppressed.

Once the bias voltage reaches the scale of zero bias gap $\Delta (U)$ the entire system feels its effect, and as a result there is a sharp rise in current through the system. In the break-
FIG. 4. The evolution of local density of states along the longitudinal direction with changing bias at $U = 6$. The three rows stand for different kinds of sites. Row (a) tracks the site at the left edge, row (b) tracks the site which is at quarter distance from the left edge and row (c) tracks the central site. The columns illustrate bias dependence for the corresponding sites. The edge site (row (a)) remains ungapped even at $V = 0$, and with increasing bias the peak shifts to the right. In row (b) the zero bias gap in the LDOS gets depleted by the time $V$ reaches $V_c$, and by the time $V$ goes into the saturation regime it picks up significant weight at the Fermi level. For the central site (row (c)), we find that the zero bias gap remains intact till the breakdown point. In the breakdown regime the central site gap starts getting depleted with increasing $V$ till the point where it vanishes, and the system enters saturation regime, after which, the spectrum ceases to change with increasing $V$. The picture for right half of the system is an exact mirror image of the picture described above. The plot has been shown for a system with 32 sites in the longitudinal direction but the size dependence of the behaviour of LDOS has been checked for longitudinal sizes upto 48 sites.

down regime the DOS unfurls from a bunched profile to an evenly spread profile, and by the time system goes into saturation regime the eigenstates become evenly distributed over the entire bandwidth. In order to get a more intuitive picture for behaviour of the DOS, we investigate the effect of bias on the auxiliary fields.

C. Auxiliary fields

Within our framework the effect of the bias gets encapsulated within the auxiliary fields through the self-consistency. The electrons respond to the local auxiliary field patterns and, as a result, sense the bias through them. For the unbiased open system the charge field $\phi$ vanishes throughout the system, whereas the spin field $M$ attains a uniform value ($\leq 1$) on all sites, except for the edge sites where is remains small ($< 10\%$ of bulk value). Also, due to the antiferromagnetic nature of the ground state the $M$’s alternate from site to site for all values of $U$ and $V$.

If the bias is applied symmetrically, i.e. $\mu_L = -\mu_R$ condition is satisfied, then the auxiliary fields must remain antisymmetric with respect to the center of the system for all values of $V$. The bias dependence of the $\phi$ field and the $|M|$ field has been plotted for a typical value of $U$ in FIG. 6. We can notice that till $V_c$ the effect of the bias remains confined to the edges. Beyond $V_c$ the auxiliary fields throughout the system get significantly renormalised due to the bias.

Additionally, the fields support a modulation which rides on top of a finite mean value for the $\phi$ field, whereas the $M$ field has modulations over zero mean value. The modulation in the $\phi$ field is more pronounced, and in order to analyse the mode content of it we subtract out the mean value and then fourier analyse the modulating field $\tilde{\phi}(x)$. The mean $\phi$ field $\bar{\phi}$ falls linearly through the system and since it is antisymmetric across the system, hence it can be characterised just by its value at the left edge $\bar{\phi}_L$. They are related by the expression $\bar{\phi}_L = \bar{\phi}_L(U,V) \left(1 - \frac{x}{L_x}\right)$, where $L_x$ is the longitudinal size of the system.

Before breakdown the fourier profile is dominated by the
FIG. 5. The behaviour of density of states with changing bias for $U = 6$ has been plotted. From left to right the columns illustrate the DoS for the open system at zero bias, to the left of critical bias, at critical bias and at large bias (deep into the saturation current regime). We observe the occurrence of in-gap states at $V = 4.4$ which is below the critical bias ($V_c = 5$). As the system is driven into breakdown regime the spectrum unfurls from a bunched to an evenly spread profile. Once $V$ hits the saturation regime the spectrum ceases to change further.

IV. DISCUSSION

A. Visualising the transition in terms of auxiliary fields

In this section, we wish to develop an understanding of the behaviour of the auxiliary fields across the transition. For that purpose, we inspect the real space auxiliary field patterns further by looking at their deviation from the zero bias values $\Delta \phi(x, V)$, $|\Delta M(x, V)|$. The left panel in FIG. 8 shows the fits of the deviation fields with the hypothesis functions:

$$\Delta \phi_{hyp}(x) = A \left( e^{-x/\xi} - e^{-(L_x-x)/\xi} \right)$$

(11a)

$$\Delta M_{hyp}(x) = A \left( e^{-x/\xi} + e^{-(L_x-x)/\xi} \right)$$

(11b)

where $L_x$ is the length in the longitudinal direction. The bias dependence of the deviation fields enters through the parameters $A$, an overall scale factor, and $\xi$, the penetration depth.

The right panel in fig. 8 shows the bias dependence of fitting parameters.

For $V << V_c$ the effect of bias remains localised to the edges, since $\Delta \phi$ and $|\Delta M|$ decay exponentially beyond a cou-
The effect of bias enters the action through the deviation fields. To the first order in deviation fields the self-energy is given by:

$$\Sigma_{i,j;\sigma}^R(\omega,V) = -\frac{U}{2} \sum_l \left( \Delta \phi_l - \sigma^2 \Delta M_l \right) g_{i,l;\sigma}^R(\omega) g_{j,l;\sigma}^R(\omega)$$

(12b)

Using this form of the self-energy we can invert the Dyson’s equation to obtain the resummed $G^R(\omega,V)$.

Since even the zero-bias problem is off diagonal we had to invert $\left[ g^{-1}_l(\omega) \right]^R_{\omega}$ numerically for each $\omega$ in order to construct the self-energy. From the resummed $G^R(\omega)$ we could calculate the local density of states using eq. [10]. The perturbative calculation indeed captures the qualitative features of the LDOS in the regime where the deviation fields are small, as demonstrated in FIG. 9.

For sites sufficiently away from the edges, the perturbation theory works till we hit $V_c$. Inside the breakdown regime the

![FIG. 8. The left panel shows fits for the deviations of auxiliary fields from their corresponding zero bias profiles - $\Delta \phi(x)$, $|\Delta M(x)|$, at bias values close to the transition (shown in colour), for three different system sizes with $U$ fixed at 6. With respect to the center of the system the $\Delta \phi(x)$, $|\Delta M(x)|$ fields are antisymmetric and symmetric respectively. Hence, the fits are shown till the center of the system. The data points are denoted by open circles, while the fitted curves are denoted by solid lines. The right panel shows the evolution of fitting parameters - penetration depth $\xi$ and scale factor $A$ as a function of bias $V$, across the transition. The behaviour for the three sizes is demarcated with different colours. The error bars indicate goodness of fit.

![FIG. 9. Comparison of local density of states across the system obtained via first order perturbation in the deviation fields with the exact result at $U = 6$, $V = 4.8$. The $V = 0$ DoS is plotted in grey to emphasize the change due to bias. $x$ labels the site from the left edge of the system having 32 sites in the longitudinal direction. The behaviour on the right half would be mirror symmetric.](image-url)
deviation fields grow rapidly (FIG. 8) and attain large values throughout the system. As a result the area around the center to which perturbation theory remains applicable shrinks, and ultimately vanishes.

V. CONCLUSION

We studied the metallisation of the Mott insulator in response to a voltage bias, using Keldysh based mean field theory at zero temperature. We obtained the current-voltage characteristics for a finite sized system and studied it’s size dependence. The $I − V$ curves which we obtain show a threshold behaviour, unlike those obtained from DMFT\cite{6,7} or DMRG\cite{4} studies. Such a behaviour is consistent with the experimental findings\cite{10,11,12}. We studied the effect of bias on the local density of states along the longitudinal direction: the LDOS goes from ‘gapped’ to ‘ungapped’ as one moves from the center to the edge at large bias, $V ≲ V_c$. This behaviour can be probed by STM measurements. We extract a lengthscale $ξ(V)$ from the spatial behaviour that shows a divergence as $V → V_c$. All response functions can be calculated, approximately, based on a knowledge of this lengthscale. Our method can be readily generalised to disordered systems, as well as frustrated geometries, and finite temperatures.

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