Dielectric Breakdown in Spin-Polarized Mott Insulator

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Nonlinear response of a Mott insulator to external electric field, corresponding to dielectric breakdown phenomenon, is studied within of a one-dimensional half-filled Hubbard model. It is shown that in the limit of nearly spin-polarized insulator the decay rate of the ground state into excited holon-doublon pair can be evaluated numerically as well to high accuracy analytically. Results show that the threshold field depends on the charge gap as $F_{\mathrm{th}} \propto \Delta^{3/2}$. Numerical results on small systems indicate on the persistence of a similar mechanism for the breakdown for decreasing magnetization down to unpolarized system.

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The nonlinear response to external fields and more general nonequilibrium properties of strongly correlated electrons and Mott insulators in particular [1] are getting more attention in recent years, also in connection with powerful novel experimental techniques, e.g., the pump-probe experiments on Mott insulators [2], as well as novel systems, the prominent example being the driven ultracold atoms within the insulating phase [3]. In this connection, one of the basic phenomena to be understood is the dielectric breakdown in Mott insulators, studied experimentally in effectively one-dimensional (1D) systems more than a decade ago [4]. The concept of Landau-Zener (LZ) single-electron tunneling [5,6] as a standard approach to dielectric breakdown of band insulators [7] is not straightforward to generalize to correlated electrons [8–10]. Theoretical efforts have been so far restricted to the prototype Hubbard model at half-filling. In 1D numerical approaches have given some support to analytical approximations for the most interesting quantity being the threshold field F_{th} and its dependence on the charge gap Δ [9], typically revealing a LZ-type dependence $F_{\mathrm{th}} \propto \Delta^2$. Different dependence is found numerically within the dynamical-mean-field-theory approach [11] as relevant for high dimensions $D \gg 1$.

In this Letter we approach the problem of a dielectric breakdown from a partially spin-polarized Mott insulator. We use the fact that the ground state (g.s.) of the 1D Hubbard model is insulating at any spin polarization with the charge gap modestly dependent on the magnetization m. In particular, a single spin excitation in fully polarized system $m \sim 1/2$, i.e. $\Delta S = 1$ state, can be studied exactly numerically as well as to high accuracy analytically. The relevant mechanism for the decay of the g.s. under constant external field F is the creation of holon-doublon (HD) pair. We show that due to the dispersionless g.s. the similarity to the LZ tunneling is only partial and leads to a different scaling $F_{\mathrm{th}} \propto \Delta^{3/2}$. Furtheron we study numerically on small systems also the model with $\Delta S > 1$, $m < 1/2$ in a finite field F. Results indicate that the decay mechanism remains qualitatively and even quantitatively similar at polarizations $m < 1/2$, in particular, for larger Δ.

We study the prototype 1D Hubbard model,

$$H = -t\sum_{i\sigma}(e^{i\phi} c^{\dagger}_{i+1,\sigma} c_{i\sigma} + \mathrm{H.c.}) + U\sum_{i} n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

with periodic boundary conditions (PBC) where $c^{\dagger}_{i\sigma}$, $c_{i\sigma}$ are creation (annihilation) operators for electrons at site i and spin $\sigma = \uparrow, \downarrow$. The action of an external electric field F is induced via the Peierls phase ϕ (vector potential) and its time dependence, i.e. $\dot{\phi}(\tau) = e_0 F(\tau) a_0/\hbar$. Furtheron we use units $\hbar = e_0 = a_0 = 1$ as well as put $t = 1$ defining the unit of energy. In such a model we investigate finite systems of length L at half-filling $N_u + N_d = L$ in general at finite total spin, $S^z = (N_u - N_d)/2$ and magnetization $m = S^z/L$.

Let us first consider the problem of a single overturned spin, i.e., $\Delta S^z = L/2 - S^z = 1$. Here, wavefunctions $|\varphi_{jm}\rangle$ correspond to an empty site (holon) at site j and a doubly occupied site (doublon) at site m. Taking into account the translational symmetry of the model (1) with PBC [even with time-dependent $\phi(\tau)$] at given (total) momentum $q = 2\pi m_q/L$ the relevant basis is $|\Psi^l_q\rangle = (1/\sqrt{L})\sum_j e^{iqj}|\varphi_{j,j+l}\rangle$, $l \in [0, L-1]$. At fixed ϕ adiabatic eigenfunctions can be then searched in the form $|\psi\rangle = \sum_j d_j |\Psi^j_q\rangle$ leading to the eigenvalue equation,

$$-\frac{1}{U} = \frac{1}{L}\sum_{q'} \frac{1}{E - U + 2[\cos(q'-\phi) + \cos(q'-\phi-q)]}. \quad (2)$$

In the limit $L \to \infty$ the g.s. energy E_0 representing the holon-doublon (HD) bound state can be expressed explicitly as $E_0 = U - [U^2 + 16\cos^2(q/2)]^{1/2}$. We note that (in spite of the q-dependence) g.s. states for all q are non-conducting since from Eq. (2) it follows that the charge stiffness $\mathcal{D}_0 \propto \partial^2 E_0/\partial\phi^2 \to 0$ for $L \to \infty$. On the other hand, excited states form a continuum with lower edge at $E_1 = U - 4\cos(q/2)$.

Since $\phi(\tau)$ conserves total q we further on consider only solutions within the $q = 0$ subspace representing the absolute g.s. wave function $|0\rangle$ with $d_j^0 = Ae^{-\kappa|j|}e^{i\phi j}$ and $A = \sqrt{\tanh\kappa}$. Here, the charge gap $\Delta = E_1 - E_0$ and the related g.s. localization parameter κ are given by

$$\Delta = -4 + \sqrt{U^2 + 16} = 4(\cosh\kappa - 1). \tag{3}$$

When we consider the time-dependent $\phi(\tau)$ we have to deal at finite L with adiabatic states $E_n(\phi)$ as, e.g., shown in Fig. 1 for finite L. At finite $L \gg 1/\kappa$ E_0 is essentially ϕ-independent but the same holds as well for lowest excited states E_n, $n \gtrsim 1$ which makes an usual application of two-level LZ approach not straightforward to apply. If we suppose that due to field $F > 0$ the transition probability between neighboring excited states is high (neglecting finite size gaps between them) excited states are well represented by 'free' HD pair states with $d_j^k = e^{ikj}/\sqrt{L}$, $\epsilon_k = U - 4\cos(\phi - k)$, $k = 2\pi m_k/L$. As shown further relevant transitions due to time-dependent $\phi(\tau)$ happen to effective states $|k\rangle$ with $|m_k| \gg 1$ since the g.s. $|0\rangle$ is well localized.

Let us consider the decay of the g.s. $|0\rangle$ after switching constant field $F(\tau > 0) = F$, $\phi = F\tau$. We present an analysis for the initial decay where most weight is still within the g.s., i.e. $|a_0(\tau)| \gg |a_{n\neq 0}(\tau)|$. In such case the excited state amplitude time-dependence $a_n(\tau)$ is given by

$$a_n(\tau) = -F\int_0^\tau d\tau'\Phi_n(\tau')\exp\left[i\int_0^{\tau'}\omega_n(\tau'')d\tau''\right], \tag{4}$$

where $\Phi_n = \langle n|\partial/\partial\phi|0\rangle$ and $\omega_n(\tau) = E_n(\phi) - E_0$.

Analytically progress can be made by using effective HD states $|k\rangle$ as approximate excited states with $\omega_k(\xi) = \epsilon_k - E_0 = 4(\cosh\kappa - \cos\xi)$, $\xi = F\tau - k$. By using the relation

$$\langle k|0\rangle\omega_k = \langle k|H_0 + U - H|0\rangle = U\langle k|n_{0\downarrow}|0\rangle = UA/\sqrt{L}, \tag{5}$$

where H_0 denotes only kinetic term in Eq. (1), one can express Φ_k in Eq. (4) as

$$\Phi_k = \langle k|\frac{\partial}{\partial\phi}|0\rangle = \frac{\partial}{\partial\phi}\langle k|0\rangle = \frac{UA}{\sqrt{L}}\frac{\partial\omega_k^{-1}}{\partial\phi}. \tag{6}$$

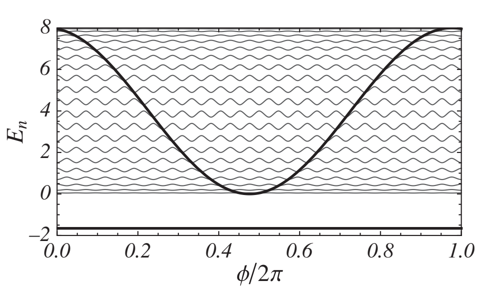

FIG. 1. Energy levels E_n (in units of t) vs phase ϕ in the system with $L = 21$ sites and $U = 4$. Thick line represents the g.s. and the effective holon-doublon pair state dispersion.

Here, we can already realize some essential differences to the usual concept of LZ tunneling, i.e., Φ_k and Eq. (4) do not favor transitions to lowest lying excited state but rather to $|k - \phi| \sim \kappa/\sqrt{3}$, hence the reduction to a two-level problem is not appropriate.

The rate of $a_k(\tau)$ following from Eqs. (4) and (6) is not steady. Since we are interested in low F we average it over the Bloch period $\tau_B = 2\pi/F$ to get $\bar{a} = a_k(\tau_B)$ which is approximately the same for majority of k (fixing here $k = \pi$),

$$\bar{a} = -\frac{AU}{\sqrt{L}}\int_{-\pi}^{\pi}d\xi\left[\frac{1}{\omega_\pi(\xi)}\right]'\exp\left[\frac{i}{F}\int_{-\pi}^{\xi}d\xi'\omega_\pi(\xi')\right] \tag{7}$$

$$\sim\frac{iAU}{F\sqrt{L}}\int_{-\pi}^{\pi}d\xi\exp\left[\frac{i}{F}\int_{-\pi}^{\xi}d\xi'\omega_\pi(\xi')\right], \tag{8}$$

after per partes integration of Eq. (7) and neglecting the first fast oscillating part, smaller also due to an additional prefactor F. Final simplification for small F can be made by replacing $\cosh\kappa - \cos\xi \sim \xi^2/2 + \Delta/4$ and consequently extending integrations in Eq. (8) to $\xi = \pm\infty$. This leads to an analytical expression for the decay rate Γ, defined by $|a_0|^2 \sim \exp(-\Gamma\tau)$ where $\Gamma = L|\bar{a}|^2/\tau_B$,

$$\Gamma = \frac{\Delta^{3/2}B(\Delta)}{3\pi F}K_{1/3}^2\left(\frac{\sqrt{2}\Delta^{3/2}}{3F}\right) \sim \frac{B(\Delta)}{\sqrt{8}}\exp\left[-\frac{(2\Delta)^{3/2}}{3F}\right], \tag{9}$$

where $K_{1/3}(x)$ is the modified Bessel function and $B(\Delta) = \Delta(\Delta + 8)^{3/2}/(\Delta + 4)$, and the last exponential approximation is valid for small enough Γ. The main conclusion of the analysis is that Γ in Eq. (9) depends on $\Delta^{3/2}/F$ unlike usual LZ theory applications [8,9] yielding Δ^2/F. As the threshold field is usually defined with the expression $\Gamma \propto \exp(-\pi F_{\mathrm{th}}/F)$, Eq. (9) directly leads $F_{\mathrm{th}} = (2\Delta)^{3/2}/(3\pi)$.

It is straightforward to verify the validity of approximations for $N_d = 1$ via a direct numerical solution of the time-dependent Schrödinger equation (TDSE) with $\phi = F\tau$ within the full basis at $q = 0$ and finite but large $L > 100$. Time dependence of the g.s. weight $|a_0(\tau)|^2$ is presented in Fig. 2 for typical case $U = 4$ and different fields $F = 0.2$–0.5. Results for the case of an instantaneous switching $F(\tau > 0) = F$ (shown for $F = 0.5$) reveal some oscillations (with the frequency proportional to the gap Δ) but otherwise clear exponential decay with well defined Γ. In order to minimize the fast-switching effect we use in Fig. 2 and further on mostly smooth transient [11], i.e., field increases as $F(\tau < 0) = F\exp(3\tau/\tau_B)$ to its final value $F(\tau > 0) = F$.

In Fig. 3 we compare results for Γ as obtained via three different methods: (a) direct numerical solution of TDSE, (b) analytical approximation with an average decay rate into free HD states, numerically integrating Eq. (7), and (c) the explicit expression (9) where additional simplification of the parabolic dispersion of excited states is used.

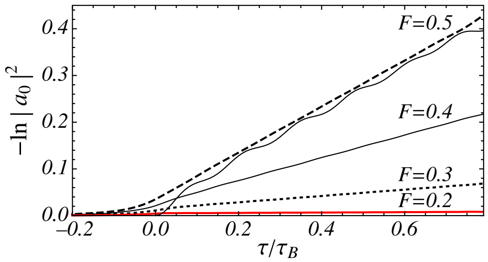

FIG. 2 (color online). Ground state weight $\ln|a_0|^2$ vs time τ/τ_B for $U = 4$ and different fields $F = 0.2$–0.5. For $F = 0.5$ comparison of results for smoothly and instantaneously switched $F(\tau)$ is presented while for $F < 0.5$ only smooth switching is used.

The agreement between different methods is satisfactory essentially within the whole regime of small Γ and deviations between analytical and numerical results become visible only for large $\Gamma \sim 0.1$. Moreover, results confirm the expected variation $\ln\Gamma \propto 1/F$ essentially in the whole investigated range of F.

One can assume that a similar mechanism of the dielectric breakdown via the decay into free HD pairs remains valid at finite deviations $N_d > 1$ and $m < 1/2$. In order to test this scenario we perform the numerical solution of TDSE for the model, Eq. (1), with the finite field $F(\tau)$. Calculation for all S^z sectors covering the whole regime $0 \le m < 1/2$ are performed on finite Hubbard chains with up to $L = 16$ sites using the Lanczos procedure both for the determination of the initial g.s. wave function $|0\rangle$ as well as for the time integration of the TDSE [12] within the full basis for given quantum numbers N_d, N_u, q reaching up to $N_{\rm st} \sim 10^7$ basis states. We use everywhere smooth transient for the field $F(\tau)$. Since the decay rate of the g.s. weight $|a_0|^2$ is expected to scale with the number of overturned spins N_d the relevant quantity to follow and compare is $(1/N_d)\ln|a_0|^2(\tau)$.

In Fig. 4 we present numerical results for time dependence of normalized g.s. weight $\ln|a_0|^2/N_d$ as obtained via a direct solution of the TDSE for $L = 16$ with the whole range of magnetization $1/2 > m \ge 0$ (relevant $1 \le N_d \le L/2$) for two cases of $U = 4$, 10, respectively, and the span of appropriate fields F. Examples are chosen such to represent charge gap (for a single HD pair) being small $\Delta \sim 1.3 < W$ and large $\Delta \sim 6.5 > W$, respectively, relative to the noninteracting bandwidth $W = 4$.

The main conclusion following from Fig. 4 is that the g.s. weight $|a_0|^2$ indeed decays proportional to N_d confirming the basic mechanism of the field-induced creation of (nearly independent) HD pairs. The decay rate Γ defined as $|a_0|^2 \propto \exp(-\Gamma N_d \tau)$ is only moderately dependent on N_d and m. Results confirm that Γ is essentially independent of N_d in well polarized systems with $m \ge 1/4$, which is compatible with independent decay into low concentration of HD pairs. For larger $U = 10$ in Fig. 4(b) the invariance of Γ extends even to unpolarized situation $m = 0$ ($N_d/L = 1/2$) for intermediate fields $F \ge 2.2$.

There are some visible deviations at $m \le 1/4$ for weakest fields both in Fig. 4(b) for $F = 1.6$ and even more for smaller $U = 4$ and $F = 0.3$ in Fig. 4(a), indicating on larger Γ and correspondingly faster decay of unpolarized g.s. with $m = 0$ relative to nearly saturated $m \sim 1/2$. Part of this enhancement of Γ can be attributed to the dependence of the charge gap on the magnetization $\Delta(m)$. The thermodynamic ($L \to \infty$) value $\Delta_0 = \Delta(m = 0)$ is known via the Bethe Ansatz solution $\Delta_0 = (16/U) \times \int_1^\infty dx\sqrt{x^2 - 1}/\sinh(2\pi x/U)$ [13,14]. Values for $\Delta(m \sim 1/2)$ as given by Eq. (3) are somewhat larger than Δ_0 with the relative difference becoming more pronounced for $U < 4$. Still taking into account actual $\Delta(m)$ some enhancement seems to remain at $m \sim 0$ at least for weaker fields F and smaller U. This could indicate that the decay into HD pairs are not independent processes but correlations due to finite concentration of N_d/L enhance decay.

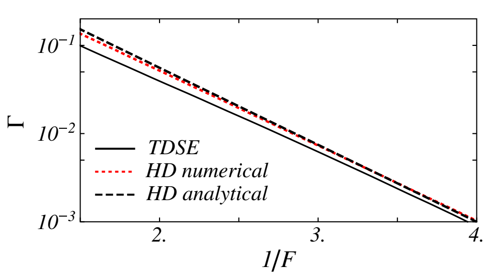

FIG. 3 (color online). Ground state decay rate Γ (log scale) vs $1/F$ for $U = 4$ as evaluated by direct numerical solution of TDSE (full line), decay into free HD states, numerically integrating Eq. (7) (dotted), and analytical expression, Eq. (9) (dashed).

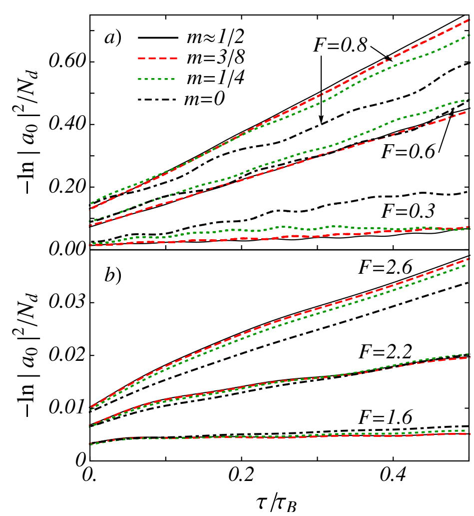

FIG. 4 (color online). Normalized g.s. weight $(1/N_d)\ln|a_0|^2$ vs time τ/τ_B for (a) $U = 4$ and fields $F = 0.3$, 0.6, 0.8, (b) $U = 10$ and $F = 1.6$, 2.2, 2.6, for various spin states $1 \le N_d \le L/2$.

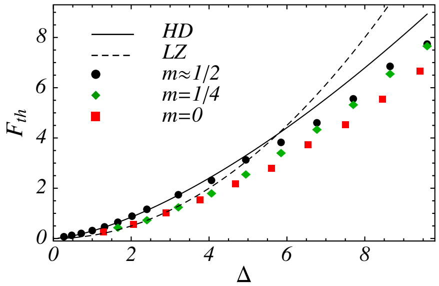

FIG. 5 (color online). Threshold field F_{th} vs charge gap Δ for different magnetizations $m \sim 1/2$ (given by $N_d = 1$) and $m = 1/4$, 0 as obtained numerically for $L = 16$. Full curve (HD) represent the analytical approximation, Eq. (9), while the dashed curve is the LZ approach result from Ref. [9].

Finally, let us consider the threshold field for the decay F_{th} as defined by $\Gamma \propto \exp(-\pi F_{\mathrm{th}}/F)$. We present results in Fig. 5 for F_{th} as function of the gap Δ. To extract F_{th} vs Δ we use numerical data for $\Gamma(F)$ obtained from numerical $|a_0|^2(\tau)$ as, e.g., shown in Figs. 2 and 4. For the reference charge gap $\Delta(m)$ we use for $m \sim 1/2$ and $m = 1/4$ Eq. (3), while for $m = 0$ we use exact Δ_0. Some deviation between $m \sim 1/2$ and $m = 1/4$ results can be still attributed to actually slightly smaller gap for the latter magnetization. For comparison we plot also the analytical result emerging from Eq. (9), $F_{\mathrm{th}} \propto \Delta^{3/2}$, as well as the dependence following from the LZ approach [9] with $F_{\mathrm{th}} = \Delta^2/8$. From Fig. 5 we conclude that the general trend $F_{\mathrm{th}}(\Delta)$ is quite well represented by the single HD pair result which deviates significantly from the LZ dependence at least for larger $\Delta > 6$. At the same time, we should note that our numerical results in the range $1 < \Delta < 2.1$ agree well with data analyzing numerically the g.s. decay using the time-dependent density-matrix renormalization group method (at $m = 0$) for the same model but bigger $L \sim 50$ [9].

In conclusion, we have presented an analysis of the dielectric breakdown within the Mott-Hubbard insulator starting from a spin-polarized ground state. Such an approach has clearly an advantage since the problem can be solved up to desired accuracy numerically but as well captured analytically. As such the situation can serve at least as well controlled test for more demanding situations of an arbitrary magnetization.

The case of a nearly polarized state $N_d = 1$ describes the mechanism of the field-induced decay of the g.s. into single HD pair. Differences to usual LZ-type approaches are: a) the g.s. is localized and dispersionless, b) the transition is not between two isolated levels but rather to a continuum, moreover it follows from Eqs. (4) and (6) that matrix elements do not favor transitions to lowest excited states, c) exact excites states can be approximated by effective free HD states with dispersion that is unlike in LZ applications not hyperbolic, e.g., $\omega_k \propto (k^2 + \kappa^2)^{1/2}$ but rather parabolic $\omega_k \propto k^2 + \kappa^2$ which is presumably the main origin for qualitatively different behavior of the threshold field $F_{\mathrm{th}} \propto \Delta^{3/2}$ which is a final manifestation of the distinction to usual LZ applications. However there are some similarities. In particular the analytical expression for the average transition rate, Eq. (8), where matrix element is integrated out, appears analogous to two-level problem and ready for phase-integral transformation into imaginary plane as used originally by Landau [5] then generalized [15,16] and applied also to breakdown problem [10,17]. Still it is straightforward to verify that for the levels under consideration ω_k do not satisfy criteria for its application, but the analogy rather emerges through the application of the steepest descent approximation to Eq. (8).

The picture of the decay of the driven Mott insulator into HD pairs remains attractive for magnetization approaching the unpolarized g.s. There seem to be two characteristic length scales controlling the mechanism, the HD pair localization length $\zeta = 1/\kappa$ and the Stark (Bloch) localization scale $L_S = 8/F$. Our results for magnetization approaching the unpolarized case indicate that for larger Δ (small ζ) and well localized HD pairs the mechanism of decay into nearly independent HD pairs remains at least qualitatively valid. Nevertheless, we find indications that for smaller Δ and weaker F (larger L_S), the decay is enhanced, i.e., pointing into the direction of more collective driven excitations favored also in the interpretation of experiments [4]. It should be pointed out that the phenomenon of HD pair generation is not particularly specific to 1D systems discussed here but can be generalized to higher dimensional nearly polarized Mott insulators as well.

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