Effect of Electric Field on One-Dimensional Insulators: A DMRG study

Sudipta Dutta, S. Lakshmi and Swapan K Pati

Theoretical Sciences Unit and DST unit on Nanoscience
Jawaharlal Nehru Centre For Advanced Scientific Research
Jakkur Campus, Bangalore 560064, India.

(Dated: February 2, 2008)

We perform density matrix renormalization group (DMRG) calculations extensively on one dimensional Mott and Peierls chains with explicit inclusion of the static bias to study the insulator-metal transition in those systems. We find that the electric field induces a number of insulator-metal transitions for finite size systems and at the thermodynamic limit, the insulating system breaks down into a completely conducting state at a critical value of bias which depends strongly on the insulating parameters. Our results indicate that the breakdown, in both the Peierls and Mott insulators, at thermodynamic limit, does not follow the Landau-Zener mechanism. Calculations on various size systems indicate that an increase in the system size decreases the threshold bias as well as the charge gap at that bias, making the insulator-metal transition sharper in both cases.

PACS number: 71.30.+h

Strongly correlated low-dimensional electronic systems have attracted much interest because of their unique low-energy characteristics. These systems are almost always insulators due to various interactions in reduced dimensions and are commonly described by Hubbard, Peierls or related Hamiltonians. While the ground state of a half-filled Hubbard system is a Mott insulator, the electron-lattice interactions lead to Peierls instability in low dimensions and are commonly described by Hubbard, Peierls or related Hamiltonians. Recent experiments on low-dimensional Mott insulators, namely, Sr$_2$CuO$_2$, SrCuO$_2$ and La$_{2-x}$Sr$_x$NiO$_4$ suggest a dielectric breakdown in presence of an external electric field. While the Peierls case is relatively easier, a tractable computational method which takes into account the static electric field and its response on the excited correlated electronic states is still lacking. One of the earliest theoretical approaches considering electric field was the Bethe-ansatz method, where, asymmetric tunneling terms towards the left and right were considered in order to describe the non-equilibrium situation and hence capture the flavor of an electric field. However, the imaginary gauge term giving rise to a non-hermitian Hamiltonian makes it very difficult to relate this to a system in presence of a real electric field. In order to account for this, another approach to this problem has been to employ the time-dependent Schrödinger equation to study the time evolution of the many-body wave functions and levels, where the electric field is applied via a time-dependent Aharonov-Bohm flux. However, in this case the calculations are restricted to only ring structures (to avoid ambiguities arising from the electrodes) and for system sizes ≤ 10 sites. Recently, however, there have been a number of studies using the real time evolution of the ground state in the presence of a source drain potential. However, a microscopic understanding of the insulator-metal transition and the quantification of the critical static electric field, required to induce it in real extended systems is still lacking.

For a clear understanding of the effect of electric field on finite size systems as well as in the thermodynamic limit, in this letter, we use the Density Matrix Renormalization Group (DMRG) method which is known to be highly accurate for low-dimensional interacting systems. For the first time, we have included static electric field in the DMRG algorithm and have obtained ground and low-energy eigen states of a one-dimensional system with various sizes. The static electric field is included as a ramp potential and we find that the electric field can induce a number of insulator-metal transitions for finite size systems, with the transition depending on the Hamiltonian parameters. We analyze our results at thermodynamic limit in the light of Landau-Zener mechanism, for both the Peierls and Mott insulating systems. To get the thermodynamic behavior we consider the total bias instead of field.

We consider a one dimensional chain representing a conjugated polymer or any other one-dimensional system, described by the Peierls-Hubbard Hamiltonian,

\[ H = \sum_i (t + (-1)^{i+1}\delta)(a_i^\dagger a_{i+1} + h.c) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

where \( t \) is the hopping term, \( U \) is the Hubbard term and \( \delta \) is the bond alternation parameter. We set \( t = 1 \) and for the Mott-insulator, we consider \( \delta = 0 \) and nonzero \( U \), while for the Peierls-insulator, \( U \) is set to zero with nonzero \( \delta \).
FIG. 1: (a) $N \rightarrow \infty$ values of $\mu_+$(square) and $\mu_-$(circle) at zero bias as a function of $U$. The dotted lines correspond to exact Bethe-ansatz results. (b) Converged ground state energy per site $\frac{E}{N}$ for half-filled system (N electrons) vs applied bias $(V)$ for $U = 0$ (X), 1 (circle), 2 (square), 3 (diamond), 4 (triangle) and 5 (star). (c) shows the energy of the systems with $N+1$ (up triangle (square)), and $N-1$ (down triangle (circle)) electrons for $U = 3(5)$ for a chain of 40 sites as a function of bias. The dashed lines represent the corresponding ground state energy $(E(N))$.

$\delta$. The external electric field applied on the system has the form of a ramp potential, distributed over all the sites in such a way that the potential $V_i$ at site $i$ becomes $-\frac{V}{N} + a\frac{V}{N+1}$, where $V$ is the applied voltage and $N$ is the total number of sites in the 1D chain. This form of the potential ensures that the bias varies between $-V/2$ to $V/2$ across the molecule. The potential adds an extra term $\sum_i V_i a_i^\dagger a_i$ to the above Hamiltonian.

Our DMRG results compare fairly well with the $V = 0$ Bethe-ansatz ground state energy and charge gap, for all values of $U$, with a density-matrix cut-off $m = 140$. For nonzero bias, the DMRG results compare up to numerical accuracies with the exact diagonalization results of finite sizes up to $N = 16$. For $U = 0$, the problem can be exactly solved and we obtain the ground state and excitation spectrum in presence of bias using tight-binding one-electron formalism. In the Mott (Peierls) case, $U(\delta)$ has been varied from 0 to 5 (0 to 1) with bias from 0 to 6 volts in steps of 0.1 volt.

For many-body models, the charge excitation gap is defined as the difference between the energy required to add ($\mu_+$) and remove ($\mu_-$) electrons from the ground state,$^{19}$

$$\Delta_{\text{charge}} = \mu_+ - \mu_-$$

where $\mu_+ = E(N+1) - E(N)$ and $\mu_- = E(N) - E(N-1)$. $E(N)$, $E(N+1)$ and $E(N-1)$ are the energies of the half-filled system and the systems with one extra and one less electron respectively.

To understand the energy cost due to the addition or removal of electrons in the presence of bias, we have calculated $\mu_+$ and $\mu_-$ numerically using DMRG for a range of bias. In Fig.1(a), we have plotted $\mu_+$ and $\mu_-$ as a function of $U$ at zero bias. The finite size DMRG results ($\mu_+$ and $\mu_-$) are extrapolated to the thermodynamic limit ($N \rightarrow \infty$) for every $U$ value. For a clear demonstration of the accuracy of our results, we have also shown the Bethe-ansatz $\mu_+$ and $\mu_-$ values derived for every $U$ in the same plot. As can be seen, our numerical extrapolated values compare fairly well with the exact thermodynamic Bethe-ansatz results. Both $\mu_+$ and $\mu_-$ increase with increase of $U$. However, the former increases with larger slope than the latter, resulting in increase of the charge gap with increasing Hubbard repulsion. This is because, a higher value of Hubbard repulsion localizes the electrons more and leads to higher charge gap.

The ground state of the Hamiltonian with nonzero $U$ is a spin-density wave insulator with one electron at every site.$^{20}$ In Fig.1(b) we have plotted the converged (extrapolated value at $N \rightarrow \infty$ limit) ground state energy of the half-filled system as a function of applied bias for different $U$ values. As can be seen, for a fixed $U$ value, the ground state energy remains almost constant upto a certain bias, and beyond it, the system starts stabilizing rapidly with applied bias.$^{21}$ It can thus be interpreted from Fig.1(b) that the applied electric field stabilizes the system after a threshold value, required to overcome the effect of the electron repulsion, $U$. Thereafter, the system gains kinetic energy as the electrons start hopping in the direction of bias. For $U = 0$, the stabilization starts as soon as the bias is turned on.

To understand the response of the excited states of the system with electric field, for a given $U$, we have computed $E(N+1)$ and $E(N-1)$. Both the energies for a particular system size ($N = 40$) are plotted in the Fig.1(c) as a function of bias for two representative $U$ values, together with $E(N)$. As like the ground state, excitation energies
FIG. 2: Charge gap vs bias for $N = 20$ (solid line), 26 (dashed line) and 40 (dotted line) for $U = 4$. Inset shows the charge densities on first (solid lines) and last site (dashed lines) for the N-1(a), N(b) and N+1(c) electron systems as a function of bias for $U = 4$ (circle) and 5 (star) with $N = 30$.

FIG. 3: Bias at first (circle), second (square) and third (triangle) minimum as a function of $1/N$ for $U = 4$. Dashed lines show the extrapolation. Inset shows the $\mu_+$ (star) and $\mu_-$ (diamond) at first minimum as a function of $1/N$ for $U = 3$ (solid lines) and 4 (dashed lines). Dotted lines are extrapolation. Error bars are of the same size as the symbols.

(both $E(N+1)$ and $E(N−1)$) decrease with increase in bias, however, their difference always remains equal to $U$ for all values of bias, as expected. For a given value of $U$, although the slope of $E(N+1)$ and $E(N−1)$ are same, the slope of $E(N)$ is different leading to the interesting phenomenon of insulator-metal transition, as described later. Fig.1(c) also shows that the stabilization of the system with one extra/less electron needs higher bias for higher value of $U$.

To characterise the bias at which this insulator-metal transition occurs accurately, we plot in Fig.2 the charge gap as a function of bias for different finite size systems for a representative value of $U$. It can be clearly seen that the charge gap shows an oscillation with bias, going through a number of minima and maxima. To understand the underlying physics, we have calculated the onsite charge densities as a function of bias for various system sizes with several $U$ values. We present this in the inset of Fig.2 for the half-filled state and the states with one extra and one less electron than half-filling for two representative values of $U$ for a finite chain with $N = 30$. For clarity, we plot charge densities at only the first and the last sites. At zero bias, the ground state charge density at every site of the system is the same and it remains almost the same with increase in bias upto the bias corresponding to the first minimum of the charge gap ($\Delta E$). However, after that, they show a large shift in the direction of bias, giving rise to charge inhomogeneties. A higher value of $U$ requires a higher bias to shift the charge density as can be seen from the inset of Fig.2 and thus the bias corresponding to the first $\Delta E$ minimum increases with increasing $U$. Interestingly, the repetetive period of charge gap going through minima with increase in bias is due to the role of charge stiffness. The external bias tends to shift the charge densities towards one electrode with the nullification of $U$ at the first $\Delta E$ minimum. However, beyond this, an increase in bias results in further hopping of charges leading to double occupancy of more sites, with electron repulsion overwhelming the kinetic stabilization, thereby increasing the energy gap. Further increase of bias nullifies this effective repulsion, resulting in the next charge gap minimum. Hence, such a variation in charge gap resulting in
For Peierls insulators, the limit of the Landau-Zener formula, we analyze the initial charge gap and the \( \delta \) limit (inset in Fig. 4) has a near linear dependence on the form \( V/N \). This indicates that the Landau-Zener formula which has been described previously by us \[23, 24\]. Inset of Fig. 4 displays the variation of converged bond-alternation parameter, \( \delta \). To now compare and contrast the critical bias obtained for the Peierls and Mott insulators in light of the Landau-Zener formula, we analyze the initial charge gap and the \( V_c \) dependence on the model parameters, \( \delta \) and \( U \). For Peierls insulators, the \( V = 0 \) charge gap is linear in \( \delta \), and the critical bias \( V_c \), calculated at the thermodynamic limit (inset in Fig. 4) has a near linear dependence on \( \delta \). This indicates that the Landau-Zener formula which has the form \( V_c(\delta) \propto [\Delta_{\text{charge}}(\delta)]^2 \), is not obeyed although previous studies on finite size systems indicated that tunneling occurs between the Landau quasi-degenerate valence and conduction levels \[23, 24, 25\], resulting in an exchange of their symmetries. This is because, at the large \( N \) limit, the gap at the critical bias goes to zero and the system goes to a completely conducting state. In case of the Mott insulator, the initial charge gap has a nonlinear dependence on \( U \), and as seen in Fig. 4, the critical bias also shows a nonlinear dependence on \( U \). A fitting gives \( V_c(U) \propto [\Delta_{\text{charge}}(U)]^n \), with \( n \sim 1 \), which, unlike the results from previous studies \[22\] clearly indicates that, the tunneling between many body levels does not follow Landau-Zener mechanism in thermodynamic limit. Note that, in our case \( V_c \) corresponds to the total bias applied to the chain with \( N \to \infty \), while the time dependent studies \[22, 25\] calculate the critical field \( (V_c/N) \) by converging it upto a certain finite chain length. We do not consider the effect of polarization on the applied electric field in our calculations. Because the inclusion of polarization does not change the nature of the insulator-metal transition as we have observed earlier \[24\]. It can only change the quantitative estimation of the bias at charge gap minima to some extent. Moreover, in presence of Hubbard repulsion term \( U \) the ramp nature of the electric field is retained even with inclusion of polarization effects in our calculations \[26\].
Qualitatively, the slope change of the ground state can be visualized even for a 2-sites Mott-insulating system. For $V = 0$, the ground state of the half-filled system comprising of four basis states, has large contribution from the singly occupied sites, with second order ($t^2/U$) contribution from the double occupancy sites. However, the external bias nullifies the Hubbard repulsion, leading to a mixing of the double and single occupancy sites. The ground state charge density shifts in the direction of the applied electric field, at $V \sim 3U$. On the other hand, the state with one extra electron comprising of two basis states, stabilizes with a slope which does not depend on $U$. This is because the external bias results in the hopping of electron from one site to another, leading to a preference of one of the basis states as compared to the other. But since both the basis states are energetically degenerate, this hopping occurs without any Hubbard energy cost, rather the energy reduces due to kinetic stabilization. This results in a slope that is independent of the Hubbard repulsion. Additionally, the Hubbard repulsion also does not play any role on the 2-sites one electron case. The 2-sites problem thus captures the ground state behavior, and not the transition phenomena, since the interesting features described earlier ($\Delta E$ oscillation) leading to breakdown behavior occur primarily due to the response of the excited states to an applied static electric field.

In conclusion, we have shown that, in thermodynamic limit, the insulator-metal transition in presence of an external static electric field does not follow Landau-Zener mechanism in both Peierls and Mott insulators. Our DMRG calculation is the first of its kind, which allows us to study various system sizes with better understanding of the general insulator-metal transition, with quantitative predictability.

SD acknowledges the CSIR for the research fellowship and SKP acknowledges the research support from DST and CSIR, Govt. of India.

[1] Geller Michael R. 2001 cond-mat/0106256
[2] Torrance J. B., Vazquez J. E., Mayerle J. J. and Lee V. Y. 1981 Phys. Rev. Lett., 46 253; Del Freo L, Painelli A. and Soos Z. G. 2002 Phys. Rev. Lett., 89 027402; Anusova Y., Soos Z. G. and Painelli A. 2001 Phys. Rev. B, 63 205118.
[3] Dagotto E. 2005 Science, 309 257; Yanase Y. et al. 2003 Physics Report, 387 1.
[4] Wiegmann P. B. 1988 Phys. Rev. Lett., 60 821.
[5] Ogota M., Anderson P. W. 1993 Phys. Rev. Lett., 70 3087
[6] Gutzwiller M. C. 1963 Phys. Rev. Lett., 10 159; Hubbard J. 1963 Proc. Roy. Soc. (London), Ser. A 276, 238 and 1964 Proc. Roy. Soc. (London), Ser. A 277, 237.
[7] Su W. P., Schreiffer J. R. and Heeger A. J. 1979 Phys. Rev. Lett. 42 171; 1980 Phys. Rev. B, 22 2099.
[8] Chen J., Reed M. A., Rawlett A. M. and Tour J. M. 2001 Science, 286 1550; 2000 Appl. Phys. Lett., 77 1224.
[9] Lakshmi S. and Pati S. K. 2005 Phys. Rev. B, 72 193410.
[10] Taguchi Y., Matsumoto T. and Tokura Y. 2000 Phys. Rev. B, 62 7015.
[11] Yamanouchi S., Taguchi Y. and Tokura Y. 1999 Phys. Rev. Lett., 83 5555.
[12] Fukui T. and Kawakami N. 1998 Phys. Rev. B, 58 16051.
[13] Deguchi T. et al. 1998 J. Phys. A, 31 7315.
[14] Oka T., Arita R. and Aoki H. 2003 Phys. Rev. Lett., 91 066406.
[15] Al-Hassanieh K. A. et al. 2006 Phys. Rev. B., 73 195304; Schneider G. and Schmitteckert P. 2006 cond-mat/0601389.
[16] White S. R. 1992 Phys. Rev. Lett., 69 2863; 1993 Phys. Rev. B, 48 10345.
[17] Schollwöck U. 2005 Rev. Mod. Phys., 77 259; Pati S. K., Ramasesha S. and Sen D. in Magnetism: molecules to materials IV, Miller J. S. and Drillon M. Eds. Wiley-VCH, Weinheim, 2003, 199; Lakshmi S., Datta A. and Pati S. K. 2005 Phys. Rev. B., 72 045131.
[18] Landau L. D. 1932 Phys. Z. Sowjetunion., 2 46; Zener C. 1932 Proc. R. Soc. London A, 137 696. Stückelberg E. C. G. 1932 Helv. Phys. Acta, 5 369.
[19] Lieb E.H. and Wu F.Y. 1968 Phys. Rev. Lett., 20 1445.
[20] Campbell D. K., Baeriswyl D., Majumdar S., in Conjugated Conducting Polymers, edited by H. Kiess, Springer Series in Solid-State Science, 102, (Springer, New York, 1992).
[21] Souza I., Iniguez J. and Vanderbilt D. 2002 Phys. Rev. Lett., 89 117602.
[22] Oka T. and Aoki H. 2005 Phys. Rev. Lett., 95 137601.
[23] Lakshmi S. and Pati S. K. 2004 J. Chem. Phys., 121 11998.
[24] Sengupta S., Lakshmi S. and Pati S. K. 2006 J. Phys. Cond. Mat., 18 9189.
[25] Oka T., Arita R. and Aoki H. 2005 Physica B: Condens. Matter, 359 759.
[26] Lakshmi S.and Pati S. K. 2003 Proc. Ind. Acad. Sc. 115 533.