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Effects of mass imbalance on metal-insulator transitions in the ionic Hubbard model

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Abstract. *We investigated the effects of mass imbalance on the metal-insulator phase diagram in the half-filled ionic Hubbard model using dynamical mean field theory (DMFT) and the equations of motion (EOM) method to solve the impurity problem. Our results show that the band insulator region changes less significantly compared to the Mott insulator region, while the metallic region shrinks as the mass imbalance increases. Additionally, the staggered charge density was calculated and analyzed for various values of mass imbalance, providing further insight into the critical Coulomb interaction values that govern phase transitions.*

Keywords: ionic Hubbard model; metal-insulator transition; dynamic mean field theory.

Classification numbers: 71.27.+a; 71.10.Fd; 71.30.+h.

1. Introduction

Recent experiments using laser cooling techniques with ultracold atoms in optical lattices have emerged as promising tools for investigating strongly correlated electron systems in condensed matter physics [1, 2]. Compared to traditional electron systems, ultracold gases offer several advantages in terms of control and versatility. The interactions between atoms can be finely tuned using Feshbach resonances [3, 4], enabling the observation of many-body phenomena that range from non-interacting to strongly correlated regimes by adjusting the magnetic field. Additionally, optical lattices can be constructed to have different potential minima across two sublattices [5, 6]. Consequently, the ionic Hubbard model with a difference in site energy can be generated. In addition, one can load two species of fermionic atoms (e.g., ^{6}Li, ^{40}K) within an optical lattice [7–9] that correspond to the mass imbalance of two components in the ion Hubbard model.

In 2019, Nguyen et al studied the ionic Hubbard model with mass imbalance using a two-site DMFT approach as an impurity solver [10]. However, previous studies were only able to

delineate the boundary between the metallic and Mott insulating regions, while the boundary of the transition from the band insulator state to the metallic state occurred only at $U = 0$ for all values of the mass imbalanced parameter ($r = t_\downarrow/t_\uparrow$). In the normal ionic Hubbard model ($r = 1$), the critical value of the Coulomb interaction U was found to be non-zero in both one-dimensional and high-dimensional cases [11–14]. To further clarify the effect of mass imbalance on the transition from band insulator to metal, we revisit the phase diagram of the ionic Hubbard model using an alternative method to address the impurity problem. Specifically, we apply the DMFT with the equations of motion (EOM) as the solver for the impurity problem. Although EOM is a relatively simple method, it proves effective for complicated problems, particularly when approaches like exact diagonalization (ED) or renormalization group theory (RG) demand substantial computational resources. In Section 2, we introduce the model and methods used for the bipartite lattice fermion system. The impurity Green function is obtained from the equations of motion. Section 3 details the nonmagnetic phase diagram. This phase diagram is derived from the band gap around the Fermi level of the density of states (DOS). Additionally, we illustrate the staggered charge density. The final section summarizes the conclusions of this study, indicating that the region of the Mott insulator expands, the band insulator region undergoes negligible changes, and the metallic region contracts as the mass imbalance increases.

2. Models and Methods

We begin with the Hamiltonian of the mass-imbalanced ionic Hubbard model

$$H = -\sum_{i\in A, j\in B, <ij>\sigma} t_\sigma \left(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}\right) + \varepsilon_A \sum_{i\in A,\sigma} n_{i\sigma} + \varepsilon_B \sum_{i\in B,\sigma} n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} - \sum_{i\sigma}\mu_\sigma n_{i\sigma}. \quad (1)$$

on a bipartite lattice (two sublattices A and B). The index σ refers to the light ($\uparrow$) and heavy ($\downarrow$) fermionic species, and they can be viewed as pseudo-spins of the particle. The first term is the kinetic energy, t_σ is the hopping parameter of the electron with pseudo-spin σ between two nearest neighbor sites $< i, j >$. $c_{i\sigma}$ and $c^\dagger_{i\sigma}$ are the annihilation and creation operators for the electron at site i with pseudo-spin σ. The second and third terms are the energy of an electron on each sublattice A and B. Here, we set $\varepsilon_A = \Delta > 0$, $\varepsilon_B = -\Delta$. $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$ is the occupation number operator. Next term is the Coulomb interaction U at one site. The last term μ_σ is the chemical potential. In this paper, we consider the half-filling case that means $\mu_\uparrow = \mu_\downarrow = U/2$, $n_A + n_B = 2$.

To find the phase diagram corresponding to Hamiltonian (1), we use the DMFT at the high-dimensional limit. In the scheme of the DMFT, the problem of many bodies is to reduce a single impurity that is embedded in a bath of non-interacting electrons corresponding to a self-consistent field. The bipartite lattice leads to the following impurity Green function [15]

$$G_{\alpha\sigma}(\omega) = G_{ii\alpha\sigma}(\omega) = \int_{-\infty}^{\infty} \frac{\xi_{\overline{\alpha}\sigma}(\omega)\rho^0_\sigma(z)dz}{\xi_{A\sigma}(\omega)\xi_{B\sigma}(\omega) - z^2}, \quad (2)$$

where $\alpha = A, B\,(\overline{\alpha} = B, A)$, $\xi_{\alpha\sigma} = \omega + \mu_\sigma - \varepsilon_\alpha - \Sigma_{\alpha\sigma}(\omega)$ with $\Sigma_{\alpha\sigma}$ is the local self - energy for each sublattice α with pseudo-spin σ. The calculation is performed on the Bethe lattice of the

infinity connective. The DOS of this lattice is given

$$\rho_\sigma^0(z) = \frac{1}{2\pi t_\sigma^2}\sqrt{4t_\sigma^2 - z^2}. \tag{3}$$

With the help of Eq. (3) we obtain the self-consistent condition of the form

$$\eta_{\alpha\sigma}(\omega) = t_\sigma^2 G_{\bar{\alpha}\sigma}(\omega), \tag{4}$$

$$G_{0\alpha\sigma}^{-1}(\omega) = \omega + \mu_\alpha - \varepsilon_\alpha + \frac{U}{2} - \eta_{\alpha\sigma}(\omega). \tag{5}$$

The impurity interacts with the electrons in the bath through the hybridization function $\eta_{\alpha\sigma}(\omega)$. $G_{0\alpha\sigma}$ is the non-interacting Green function of the effective impurity model for sublattice α. We use the EOM as the impurity solver for this problem. Then, the impurity Green function can be obtained as follows [16, 17]

$$\begin{aligned} G_{\alpha\sigma}(\omega) = &\frac{1- < n_{\alpha\bar{\sigma}} > /2}{G_{0\alpha\sigma}^{-1} + U\Pi_{1\alpha\sigma}(\omega)[G_{0\alpha\sigma}^{-1} - U - \Pi_{3\alpha\sigma}(\omega)]^{-1}} \\ &+ \frac{< n_{\alpha\bar{\sigma}} > /2}{G_{0\alpha\sigma}^{-1} - U - U\Pi_{2\alpha\sigma}(\omega)[G_{0\alpha\sigma}^{-1} - \Pi_{3\alpha\sigma}(\omega)]^{-1}}, \end{aligned} \tag{6}$$

where the "self-energies" Π_i are

$$\Pi_{i\alpha\sigma}(\omega) = \int_{-\infty}^{\infty} dz \Gamma_{\alpha\bar{\sigma}}(z) F_i(z) \left[\frac{1}{\omega + \mu_{\alpha\sigma} - \mu_{\alpha\bar{\sigma}} - z} + \frac{1}{\omega + \mu_{\alpha\sigma} + \mu_{\alpha\bar{\sigma}} - U + z}\right]. \tag{7}$$

Here, $\mu_{\alpha\sigma} = \mu_\sigma - \varepsilon_\alpha$ and $F_1 = f(z)$, $F_2 = 1 - f(z)$, $F_3 = 1$, $f(z) = 1/(e^{z/T} + 1)$ is the Fermi-Dirac function, $\Gamma_{\alpha\sigma}(z) = -\frac{1}{\pi}\,\mathrm{Im}\,\eta_{\alpha\sigma}(z + i0^+)$.

Equations (2), (4)-(7) establish self-consistent equations for $G_{\alpha\sigma}(\omega)$ ($\alpha = A, B$, $\sigma = \uparrow, \downarrow$). These equations must be solved with the condition $n_A + n_B = 2$, where $n_\alpha = -\frac{1}{\pi}\int_{-\infty}^{0} d\omega \sum_\sigma \mathrm{Im}\, G_{\alpha\sigma}(\omega)$. Therefrom one can derive critical insights into the electronic properties of the system based on the pseudo-spin-dependent DOS $\rho_{\alpha\sigma}(\omega)$. $n_B - n_A$ is the staggered charge density that can be calculated from the model parameters. A total DOS at the Fermi level is finite that indicates a metallic behavior, while a vanishing DOS signal insulating properties.

3. Results and Discussions

In this framework, we study the paramagnetic case, i.e., $< n_{\alpha\uparrow} > = < n_{\alpha\downarrow} > = < n_\alpha > /2$ and we set the half bandwidth with pseudo-spin-up $D = 2t_\uparrow$ as the unit of energy. The mass imbalance parameter denotes $r = t_\downarrow/t_\uparrow$. We chose $t_\uparrow$ and $t_\downarrow$ as corresponding to the hoping parameter of the heavy and light particles, respectively, that means $0 < r < 1$. To investigate the influence of mass imbalance on the phase diagram of the ionic Hubbard model, we fix the mass imbalance at $r = 0.5$ and plot the density of states depend on pseudo-spin σ for the sublattices α ($\alpha = A, B$) for $\Delta = 1.0$ at $U = 0.5, 2.5$, and 3.5 in Fig. 1. There are three phases in the phase diagram: (1) a band insulator phase at weak interaction, (2) a Mott insulator phase at strong interaction, and (3) a metallic intermediate phase between the two insulating phases. In the small U region ($U = 0.5$), the system behaves as a band insulator with a gap around the band center ($\omega = 0$) for both sublattices. In contrast, in the larger U region ($U = 3.5$), the system corresponds to a Mott insulator with a smaller gap around $\omega = 0$, and there are two gaps in the pseudo-spin-dependent

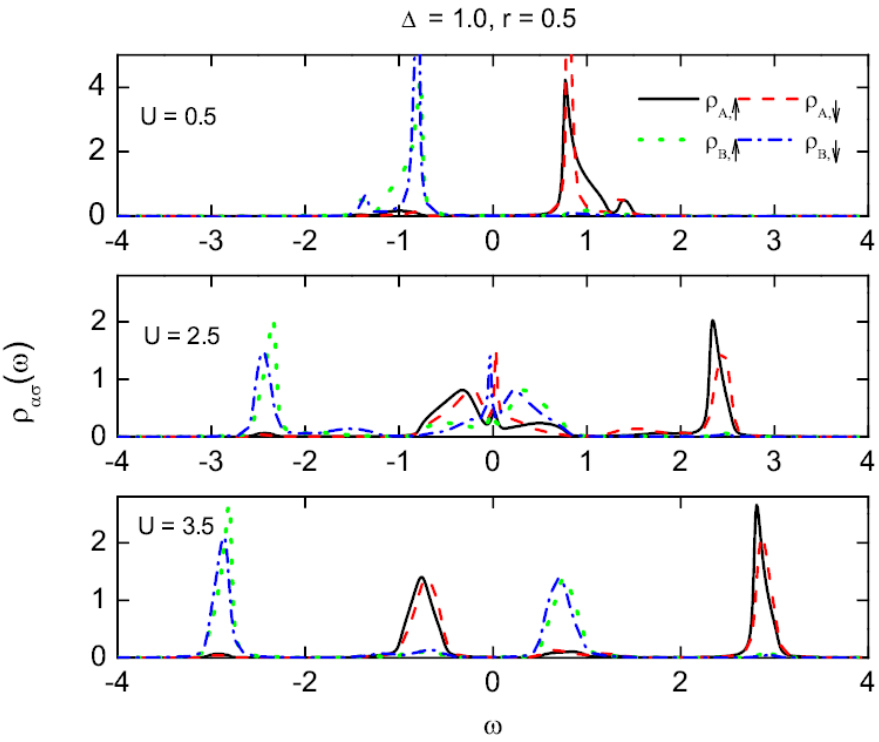

Fig. 1. (Color online) Density of states depend on pseudo-spin σ for the sublattices ($\alpha = A, B$) for $\Delta = 1.0$ at the mass imbalance $r = 0.5$. Top panel: a band insulator state for $U = 0.5$; Center panel: a metallic state at $U = 2.5$; Bottom panel: a Mott insulator state for $U = 3.5$.

DOS of both sublattices at $\omega \approx \pm 2.0$. The distinction between the two insulating phases is further illustrated by the staggered charge density $n_B - n_A$. Additionally, $n_B - n_A$ is approximately zero ($n_B \approx n_A \approx 1$) for a Mott insulator state, while n_B is greater than n_A for a band insulator state. In contrast, the pseudo-spin-dependent DOS at the Fermi level of both sublattices A and B is nonzero for $U = 2.5$, corresponding to a metallic phase.

Next, we build the phase diagram to show the influence of the mass imbalance into the ionic Hubbard model at half-filling, which includes various values of $r = 1.0, 0.5$, and 0.1 as shown in Fig. 2. This diagram comprises three phases: a correlated metal, a Mott insulator phase, and a band insulator. We denote this phases are M, MI and BI, respectively. This phase diagram resolves the limitations of the two-site DMFT for this model reported in our Ref. [10], which only identified the Mott transition. There are two transitions in the phase diagram. As the Coulomb interaction increases, the system transitions from a band insulator to a metallic phase first, and then it undergoes a metal to a Mott insulator transition. The critical values U_{c1} for the first transition in the weak Coulomb interaction region for $r = 1.0, 0.5$, and 0.1 can be determine as a function of Δ. The results show that U_{c1} changes insignificantly and approximates 2Δ as decreasing the mass imbalanced parameter r. In this region $U \ll 2\Delta$, the charge density at site B (lower energy) is

larger than at site A (higher energy), meaning both of two component pseudo-spins (up and down) of electrons are primarily localized at site B, making the influence of the hopping integral for both pseudo-spins very small compared to the staggered energy 2Δ. In contrast, for fixed staggered energy Δ in a larger U region, the critical value of Coulomb interaction U_{c2} for the second transition from metal to Mott insulator decreases significantly as the mass imbalance increases. Physically this situation can be imagine that for fixed $t_\uparrow$, the increasing mass difference between the two pseudo-spin components means that $t_\downarrow$ is smaller, which makes it easier to localize the system. These results show qualitative agreement with the findings obtained from the two-site DMFT method in [10] (keep in mind that results in [10] using $t_\uparrow$ is a unit energy). However, the metallic region in our current phase diagram is smaller than that found in the previous study [10] due to the different approximations employed. This is not unusual; for example, the critical interaction in the conventional Hubbard model ($\Delta = 0$) $Uc = D$ as obtained by CPA, while this value equals $1.8D$ by our EOM-DMFT, $2.4D$ by ED-DMFT, and $3.0D$ by two-site DMFT [18]. The metallic phase represents an intermediate region between the two insulator phases. In the case of $\Delta = 0$, the model becomes the asymmetric Hubbard model. The critical values $U_{c2} \approx 1.80, 1.38$ and 1.12 for $r = 1.0, 0.5$ and 0.1, respectively, are similar to the results shown in Fig. 7 of D. A. Le's paper [19], and these results are consistent with Eq. (17) in A. T. Hoang's paper [20], which corresponding to the Hubbard III approximation.

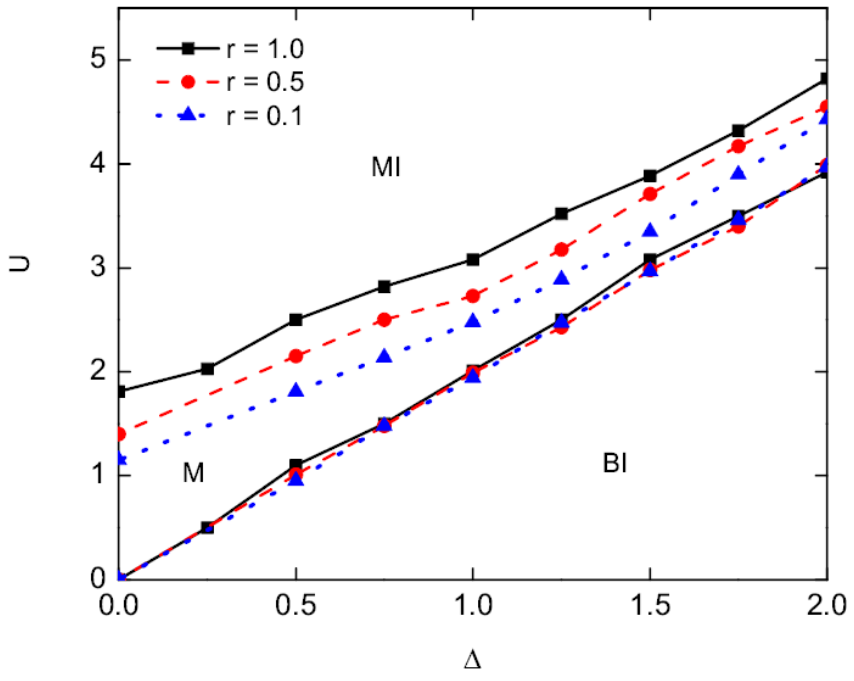

Fig. 2. Phase diagram of IHM at mass imbalance case $r = 0.5, 0.1$ compare to the mass balance case $r = 1.0$. BI, M and MI denote a band insulator phase, a correlated metal and a Mott insulator, respectively.

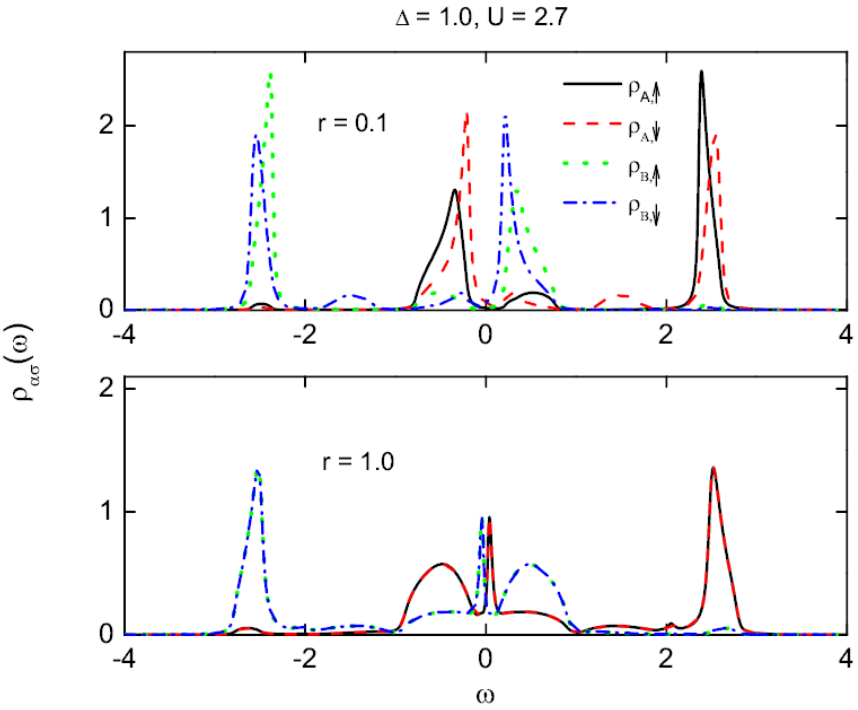

Fig. 3. pseudo-spin-dependent density of states for the sublattices ($\alpha = A, B$) for $\Delta = 0.5, U = 1.4$ at the mass-imbalanced parameter $r = 0.1$ compared to the balanced case $r = 1.0$. Upper panel for $r = 0.1$, system is a Mott insulator; Lower panel for the $r = 1.0$, system is a metal.

To clarify the influence of mass imbalance in the strong Coulomb interaction region of the phase diagram, we calculated the pseudo-spin-dependent density of states (DOS) for both sublattices A and B at $U = 2.7$ for $r = 0.1$ (upper panel) and $r = 1.0$ (lower panel) with a fixed $\Delta = 1.0$ in Fig. 3. The system transitions from a metal state to a Mott insulator as the mass imbalance parameter increases.

Finally, in Fig. 4, we present the difference of charge density of two sublattices (the staggered charge density) $n_B - n_A$ as a function of U for different values of r at $\Delta = 1.0$. The staggered charge density decreases with increasing U and approaches zero as U approaches U_{c2} at fixed r. The critical values of Coulomb interaction U_{c2} for the metal-to-Mott insulator transition at $\Delta = 1.0$ are obtained by extrapolation (see the dashed black arrow in Fig. 4), yielding approximate values 2.56, 2.66, 2.88, and 3.05 for $r = 0.1, 0.4, 0.8$, and 1.0, respectively. For the balance case $r = 1.0$ and $\Delta = 1.0$, this results are in good agreement with those obtained from the full DMFT in [13,14], and the two-site DMFT results in [10], bearing in mind that in [13,14], and [10], t is treated as the unit of energy.

Notably, the value of $n_B - n_A$ remains the same for all values of r at the $U \approx 2\Delta$ point, regardless of the mass imbalance parameter r. This point also corresponds to U_{c1} for the band insulator - metal transition. In Fig. 4, for $\Delta = 1.0$, $U_{c1} \approx 1.9$ is approximately equal to 2Δ for all

$r = 1.0, 0.8, 0.4$ and 0.1. This consistency reinforces the influence of the mass imbalance parameter on the critical Coulomb values U_{c1} illustrated in Fig. 2.

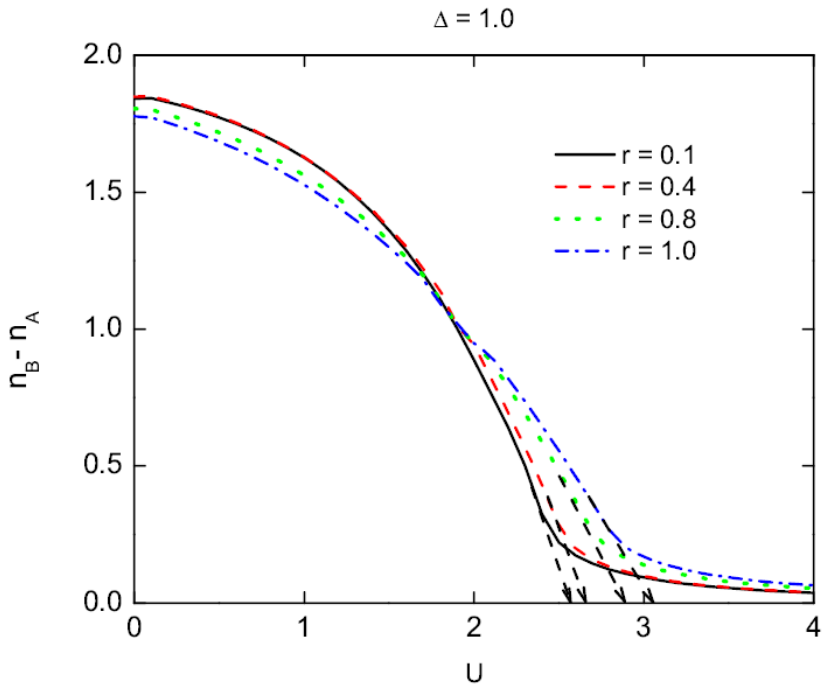

Fig. 4. Staggered charge density $n_B - n_A$ as a function of U for $r = 0.1, 0.4, 0.8$ and 1.0 at fixed $\Delta = 1.0$. The lines at difference values of r intersect at the same point, which is corresponding to the first transition from a band insulator to a metallic state

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4. Conclusions

In this paper, we used EOM within DMFT to explore the effects of mass imbalance on metal-insulator transitions in the half-filled ionic Hubbard model. Similar to the balanced case ($r = 1$) [13,14], we found that the critical Coulomb interaction (U_{c2}) for the metal to Mott insulator transition decreases with increasing mass imbalance, while the critical interaction for the band insulator to metal transition (U_{c1}) remains almost unchanged. The phase diagram reveals two phase transitions: at fixed staggered energy Δ, the system transitions from a band insulator to a metal as soon as Coulomb interaction is introduced, and then from a metallic state to a Mott insulator as the interaction strength increases. We observed that the Mott insulator region expands significantly with increasing mass imbalance, whereas the band insulator region remains relatively unchanged, and the metallic region shrinks. The staggered charge density ($n_B - n_A$) provides a reliable indicator for identifying critical interaction values U_{c1} and U_{c2} for the phase transitions. Our findings extend previous studies and address limitations of simpler DMFT approaches [10], providing a more detailed understanding of mass imbalance effects on the phase diagram of the ionic Hubbard model.

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Conflict of interest

The authors declare that they have no competing financial interests.

References

[1] B. DeMarco and D. S. Jin, *Onset of fermi degeneracy in a trapped atomic gas*, Science **285** (1999) 1703.
[2] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch and I. Bloch, *Quantum phase transition from a superfluid to a mott insulator in a gas of ultracold atoms*, Nature **415** (2002) 39.
[3] C. Chin, R. Grimm, P. Julienne and E. Tiesinga, *Feshbach resonances in ultracold gases*, Rev. Mod. Phys. **82** (2010) 1225.
[4] S. Inouye, M. Andrews, J. Stenger, H.-J. Miesner, D. M. Stamper-Kurn and W. Ketterle, *Observation of feshbach resonances in a bose–einstein condensate*, Nature **392** (1998) 151.
[5] S. Taie, Y. Takasu, S. Sugawa, R. Yamazaki, T. Tsujimoto, R. Murakami *et al.*, *Realization of a* $\mathrm{SU}(2) \times \mathrm{SU}(6)$ *system of fermions in a cold atomic gas*, Phys. Rev. Lett. **105** (2010) 190401.
[6] F. Abudinén, I. Adachi, K. Adamczyk, L. Aggarwal, H. Ahmed, H. Aihara *et al.*, *Hydrodynamic expansion of a strongly interacting fermi-fermi mixture*, Phys. Rev. Lett. **106** (2011) 115304.
[7] P. Fazekas, *Lecture Notes on Electron Correlation and Magnetism*, vol. 5. World Scientific, 1999, 10.1103/PhysRevLett.95.226402.
[8] P. S. Riseborough and J. M. Lawrence, *Mixed valent metals*, Rep. Prog. Phys. **79** (2016) 084501.
[9] M. Cazalilla, A. Ho and T. Giamarchi, *Two-component fermi gas on internal-state-dependent optical lattices*, Phys. Rev. Lett. **95** (2005) 226402.
[10] N. T. H. Yen, D. A. Le, H. A. Tuan, N. T. Thang, T. T. T. Trang and N. T. Huong, *Mott transition in the mass imbalanced ionic hubbard model at half filling*, Comm. Phys. **29** (2019) 305.
[11] M. Fabrizio, A. O. Gogolin and A. A. Nersesyan, *From band insulator to mott insulator in one dimension*, Phys. Rev. Lett. **83** (1999) 2014.
[12] T. Wilkens and R. M. Martin, *Quantum monte carlo study of the one-dimensional ionic hubbard model*, Phys. Rev. B, **63** (2001) 235108.
[13] H. R. K. A. Garg and M. Randeria, *Can correlations drive a band insulator metallic?*, Phys. Rev. Lett. **97** (2006) 04640.
[14] L. Craco, P. Lombardo, R. Hayn, G. I. Japaridze and E. Müller-Hartmann, *Electronic phase transitions in the half-filled ionic hubbard model*, Phys. Rev. B **78** (2008) 075121.
[15] A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg, *Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions*, Rev. Mod. Phys. **68** (1996) 13.
[16] A.-T. Hoang, T.-H.-Y. Nguyen and D.-A. Le, *Conductivity in the half-filled disordered hubbard model: A typical medium dynamical mean-field study*, Mod. Phys. Lett. B **38** (2024) 2450226.
[17] Y. Meir, N. S. Wingreen and P. A. Lee, *Transport through a strongly interacting electron system: Theory of periodic conductance oscillations*, Phys. Rev. Lett. **66** (1991) 3048.
[18] Y. Ōno, R. Bulla and A. Hewson, *Phase diagram of the mott transition in a two-band hubbard model in infinite dimensions*, Eur. Phys. J. B **19** (2001) 375.
[19] D. A. Le, T. T. T. Tran, A. T. Hoang, T. T. Nguyen, M. T. Tran *et al.*, *Mass-imbalanced hubbard model in optical lattice with site-dependent interactions*, Phys. B: Condens. Matter **532** (2018) 204.
[20] A. T. Hoang, T.-H.-Y. Nguyen, T. T. T. Tran and D. A. Le, *Two-component fermions in optical lattice with spatially alternating interactions*, J. Phys. Soc. Jpn. **85** (2016) 104702.