Communications in Physics, Vol. 29, No. 3SI (2019), pp. 305-312
DOI:10.15625/0868-3166/29/3SI/14265

MOTT TRANSITION IN THE MASS IMBALANCED IONIC HUBBARD MODEL AT HALF FILLING

NGUYEN THI HAI YEN[1], LE DUC ANH[2], HOANG ANH TUAN[1,3,†], NGUYEN TOAN THANG[1] AND TRAN THI THU TRANG[4]

[1]*Institute of Physics, Vietnam Academy of Science and Technology (VAST)*
[2]*Hanoi National University of Education*
[3]*Graduate University of Science and Technology, VAST*
[4]*Ha Long University*

[†]*E-mail:* hatuan@iop.vast.ac.vn

Received 20 August 2019
Accepted for publication 28 September 2019
Published 22 October 2019

Abstract. *The Mott - Hubbard metal - insulator transition in the half-filled mass imbalanced ionic Hubbard model is investigated using the two-site dynamical mean field theory. We find that for a fixed mass imbalanced parameter r the critical interaction U_c increases when the ionic energy Δ is increased. In the other hand, for a fixed Δ, U_c decreases with increasing the mass imbalance. We also show the existence of a band insulating phase in the system for the case $\Delta \neq 0, U = 0$ and calculate the staggered charge density $n_B - n_A$ as a function of the interaction for different values of the mass imbalance. Our results in the limiting cases ($r = 1, \Delta \neq 0$ or/and $\Delta = 0, r \neq 1$) are in good agreement with those obtained from the full dynamical mean field theory.*

Keywords: ionic Hubbard model; mass imbalance; Mott transition.

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

I. INTRODUCTION

In recent years, with the achievement of laser cooling technique, ultracold atoms in optical lattices have attracted a lot of studies that give new insight into the complex behavior of quantum many-body systems [1, 2]. By manipulating the interaction strength using the Feshbach resonance [3], it is possible to enable the observation of many-body phenomena from weak to strong coupling. Thus the conventional Hubbard model has been realized in optical lattices and investigated experimentally [4–6]. Furthermore, optical lattices can be generated in various geometries, including bipartite lattices with different potential minima on the two sublattices [7]. In addition, by varying the parameters of lasers being used, one can separately vary the hopping parameter of each spin component in the Hubbard model. As a result, this creates a mass imbalance between the spin components in the Hubbard model [8–11]. In condensed-matter physics mixtures of fermions with different effective masses are realized in rare-earth-metal compounds where a localized f level crosses a wide conduction band [12, 13]. The possibility of having bipartite lattices with different potential minima on the two sublattices with different parameter of each spin component in the Hubbard model enables one to set up the mass-imbalanced ionic Hubbard model. Therefore, it would be interesting to theoretically study how the phase diagram in the ionic Hubbard model is affected by a mass imbalance.

Dynamical mean field theory (DMFT) is a very successful method to investigate the physics of strongly correlated electrons on a lattice. However, the CPU time required by DMFT calculation is fairly large. On the other hand, the two-site DMFT proposed by Potthoff [14], who showed that a minimum realization of DMFT is achieved by mapping a correlated lattice model onto an impurity model that consists of two sites, one for the impurity and one for the bath of conduction electrons. This method provides a simple and attractive technique to obtain fairly good results for the Mott transition and the Fermi liquid phase in the single band Hubbard model. The two-site DMFT was also successfully applied for studying the Mott transition of the Hubbard model with mass imbalance [15–17].

In this paper we employ the two-site DMFT to study the Mott transition in the mass-imbalanced ionic Hubbard model at half filling, where the translational symmetry is reduced and the spin SU(2) symmetry is explicitly broken. It is found that for a fixed ionic energy, the critical interaction decreases with increasing the mass imbalance. We also calculate the staggered charge density $n_B - n_A$ as a function of the interaction for different values of the mass imbalance.

This paper is organized as follows. In Section II we present the model and solving method, the two-site DMFT. In Sec. III we show and discuss the numerical results for the Mott transitions in the model. Finally, a brief conclusion is presented in Sec. IV.

II. MODEL AND SOLVING METHOD

We consider the ionic Hubbard model with a mass – imbalance on a bipartite lattice

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

where $c_{i\sigma}(c^\dagger_{i\sigma})$ annihilates (creates) an electron with spin σ at site i, $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ and the sum $< i, j >$ is the sum over the nearest neighbor sites of a Bethe lattice. U is the one-site Coulomb repulsion. $\varepsilon_A = -\varepsilon_B = \Delta$ are the ionic energies, and Δ is chosen as a positive value. t_σ is the

spin-dependent nearest - neighbor hopping parameter and μ_σ the chemical potential, which is chosen so that the average occupancy is 1 (half - filling). The mass imbalance is introduced via $r = t_\downarrow/t_\uparrow$. When $r \neq 1$ the spin SU(2) symmetries are explicitly broken. In the mass balanced case, $r = 1, \Delta > 0$ the model (1) is reduced to the conventional ionic Hubbard Hamiltonian.

We apply DMFT to investigate the Hamiltonian model (1). In DMFT, the original lattice model is mapped onto an effective single impurity Anderson model embedded in an uncorrelated bath of electrons. In this case, an impurity orbital $d^\dagger_\sigma|0>$ is coupled to a bath of non-interacting orbitals via the hybridization $V_{\alpha\sigma}$ which depends on the sublattice α and spin σ. The lattice Green function is then obtained via self-consistent conditions imposed on the impurity problem. On a bipartite lattice $A-B$ the local Green function is given by

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

where $\alpha = A\,(\overline{\alpha} = B)$, $\xi_{\alpha\sigma} = \omega + \mu_{\alpha\sigma} - \Sigma_{\alpha\sigma}(\omega)$ with $\mu_{\alpha\sigma} = \mu_\sigma - \varepsilon_\alpha$, $\Sigma_{\alpha\sigma}$ the local self - energy for sublattice α and spin σ, $\rho^0_\sigma(z)$ the spin-dependent non-interacting density of states (DOS). For the Bethe lattice with infinite coordination number

$$\rho^0_\sigma(z) = \frac{1}{2\pi t^2_\sigma}\sqrt{4t^2_\sigma - z^2}, \tag{3}$$

the self - consistent condition is given by

$$\Delta_{\alpha\sigma}(\omega) = t^2_\sigma G_{\overline{\alpha}\sigma}(\omega), \tag{4}$$

where $\Delta_{\alpha\sigma}(\omega) = \omega + \mu_{\alpha\sigma} - G^{-1}_{0\alpha\sigma}(\omega)$ is the hybridization function with $G_{0\alpha\sigma}(\omega)$ being the non-interacting Green function of the effective impurity model for sublattice α. To proceed further we use the two-site DMFT. We focus on the paramagnetic case at half-filling, for which $\langle n_{\alpha\uparrow}\rangle = \langle n_{\alpha\downarrow}\rangle = \langle n_\alpha\rangle/2$ and $\mu_\uparrow = \mu_\downarrow = U/2$. In the two-site DMFT, the full DMFT self - condition $G^{imp}_{\alpha\sigma}(\omega) = G_{\alpha\sigma}(\omega)$ is replaced by the following self-consistency conditions [14]

$$n^{imp}_\alpha = n_\alpha \tag{5}$$

$$V^2_{\alpha\sigma} = Z_{\overline{\alpha}\sigma}t^2_\sigma, \tag{6}$$

where n^{imp}_α is the average occupancy of the impurity orbital in α-sublattice, $Z_{\overline{\alpha}\sigma} = \left(1 - \frac{dRe\Sigma_{\overline{\alpha}\sigma}(0)}{d\omega}\right)^{-1}$ is the quasi-particle weight.

The equations (2)- (6) must now be solved with $n_A + n_B = 2$, where at zero temperature $n_\alpha = -1/\pi\sum_\sigma\int^0_{-\infty}\Im G_{\alpha\sigma}(\omega)d\omega$. From the self - consistent solutions one can determine the occupation numbers n_A, n_B and $Z_{\alpha\sigma}$ as functions of the model parameters U, Δ, r and study the metal-insulator transitions in the system.

III. RESULTS AND DISCUSSION

Before numerically solving the above equations, let us briefly consider limiting cases. In the non - interaction $(U = 0)$ limit, the integral (2) is evaluated analytically with result

$$G_{\alpha\sigma}(\omega) = \frac{1}{2t^2_{\bar{\sigma}}}\left\{\omega - \varepsilon_{\bar{\alpha}} - \left[(\omega - \varepsilon_{\bar{\alpha}})^2 - \frac{\omega - \varepsilon_{\bar{\alpha}}}{\omega - \varepsilon_\alpha}4t^2_\sigma\right]^{1/2}\right\}, \tag{7}$$

which is clear that the total DOS at the Fermi level is zero ($\rho(0) = \sum_{\alpha\sigma} \rho_{\alpha\sigma}(0) = 0$), i. e. the system is a band insulator (BI) for all values of r and finite Δ.

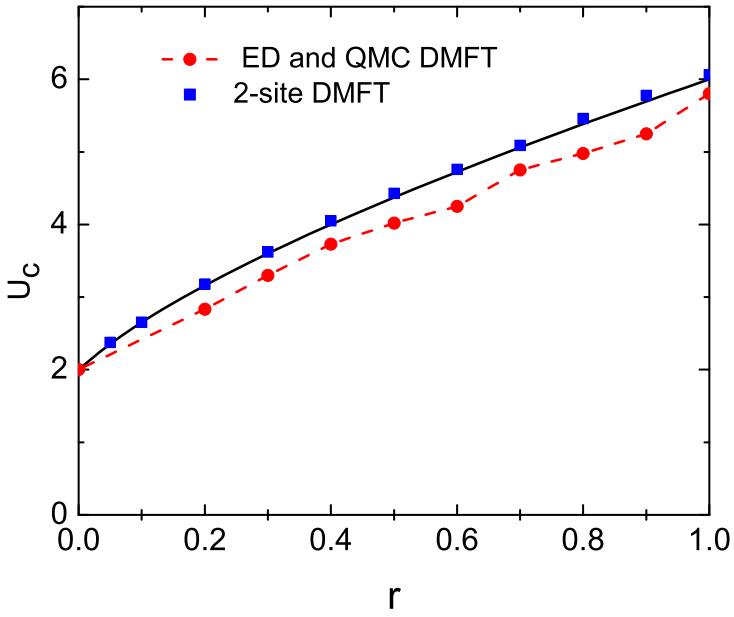

Fig. 1. Critical interaction in the half-filled mass imbalanced Hubbard model ($\Delta = 0$) as a function of the mass imbalanced parameter r: a comparison between the two-site and the full DMFT results in Ref. [15]. The squares correspond to our numerical results, and the solid line corresponds to the results obtained by using the two-site analytic expression from Ref. [17].

We return now to present our numerical results. The systems of equations are solved numerically by simple iterations to determine the self - energy $\Sigma_{\alpha\sigma}(\omega)$ and the Green function $G_{\alpha\sigma}(\omega)$. The algorithm is summarized as follows: Start with a guess for the one-particle energy of the bath site and the hybridization strength $V_{\alpha\sigma}$, the two - site impurity model can be solved to find its self-energy, Green function and the average occupancy of the impurity level n_α^{imp}. Then, the quasi - particle weight $Z_{\overline{\alpha}\sigma}$ is calculated and from the condition (6) a new value for the hybridization strength $V_{\alpha\sigma}$ is found. Inserting $\Sigma_{\alpha\sigma}(\omega)$ into Eq. (2), one finds the local lattice Green function $G_{\alpha\sigma}$ and the filling n_α which must be compared with n_α^{imp}. Finally, a new value for the one-particle energy of the bath site of each sublattice is chosen such that the different $n_\alpha - n_\alpha^{imp}$ is reduced in the next cycle. The cycles have to be iterated until convergence is reached. In actual numerical calculations, we replace the real frequency by the complex one $\omega \to \omega + i\eta$, where η is a positive infinitesimal number. If η is too small the convergence is never reached. Thus, η must take a finite small value (should be in range from 10^{-3} to 10^{-2}) to make the iterations converge. Then we use the spline extrapolation to reach the limit when $\eta \to 0$ to get sharp pictures for the quasi -

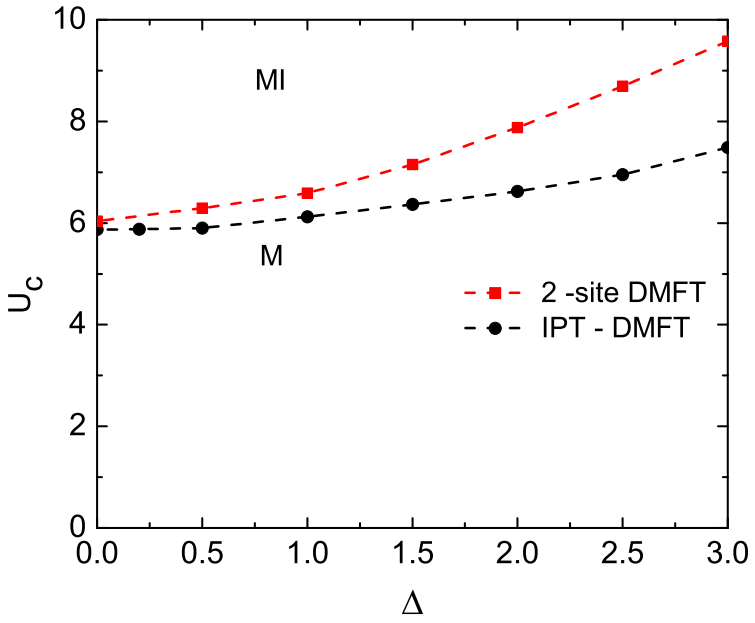

Fig. 2. Critical interaction in the half-filled mass balanced ionic Hubbard model $(r = 1)$ as a function of the ionic energy Δ: a comparison between the two-site and the full DMFT results in Ref. [18]. MI and M denote Mott insulator and metal, respectively.

particle weight, from which one can determine the critical interaction for the Mott metal - insulator transition. Hereafter, we take $t_\uparrow$ as the energy unit, zero temperature and $\eta = 0.01$ in the numerical calculations. Firstly, we estimate the reliability of the two-site DMFT by comparing the results of the Mott critical interaction U_c with the ones obtained from full DMFT in the limiting cases. Within our method the Mott metal - insulator transition is signaled by $Z_{\alpha\sigma}(U \to U_c) \to 0$. In Fig. 1 our two-site DMFT results for U_c as a function of the mass imbalanced parameter r in the mass imbalanced Hubbard model $(\Delta = 0)$ are compared with those obtained from the full DMFT [15]. The numerical results from two-site DMFT are almost identical with the analytic ones [17] and in very good agreement with the full DMFT results over the whole r range. In Fig. 2 our two-site DMFT results for U_c as a function of Δ in the conventional ionic Hubbard model $(r = 1)$ are compared with those of the full DMFT from Ref. [18]. In this case, although the two-site DMFT overestimates U_c in the whole Δ range, we find that they are semi-quantitatively the same and in both methods the critical interaction increases as ionic energy increases. It should also be noted that even DMFT with the same impurity solver but different ansatz for the self-energy can lead to very different quantitative results, such as the metal - insulator phase diagrams of the IHM found in Refs. [18, 19]. Therefore, the difference between the two-site and the full DMFT results is understandable and we believe that the two-site DMFT gives satisfactory results for Mott transition in the mass imbalanced IHM.

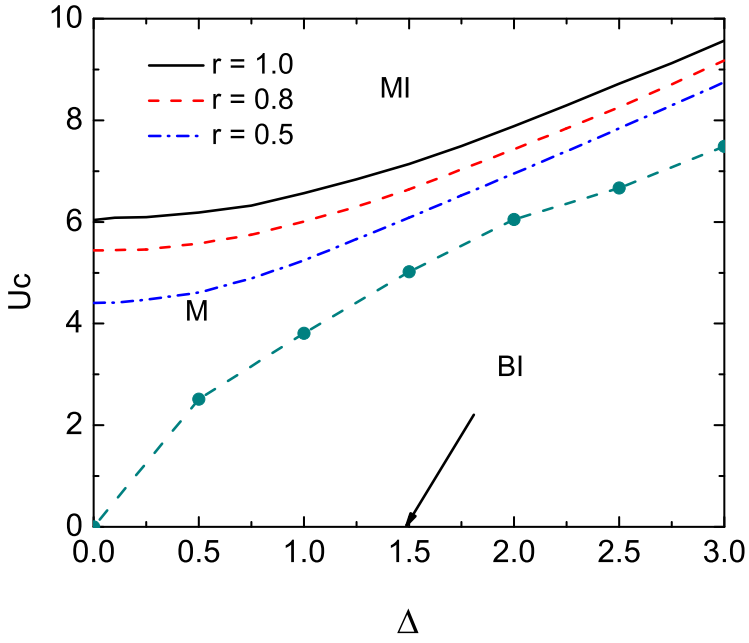

Fig. 3. Critical interaction in the half-filled mass imbalanced Hubbard model as a function of the ionic energy Δ for different values of r. MI, M and BI denote Mott insulator, metal and band insulator, respectively. The dashed line with dots corresponds to the boundary between metal and band insulator in the mass balanced IHM obtained from Ref. [18].

We plot in Fig. 3 the Mott critical interaction U_c as functions of Δ for $r = 1.0$, 0.8 and 0.5. Like the balanced case $(r = 1)$, in the mass imbalanced IHM U_c increases when Δ is increased. In the other hand, for a fixed Δ, the critical interaction decreases with decreasing r, i.e. with increasing the mass imbalance. The latter can be understood because at fixed $t_\uparrow$ the larger the difference in the bare mass means the smaller $t_\downarrow$, hence the easier it is to localize the system. As we showed in the beginning of this Section when $U = 0$ the system is a band insulator for all values of r and finite Δ, i. e. the metallic, the Mott and band insulating phases are found in the $(U - \Delta)$ phase diagram of the mass imbalanced IHM at half filling. In Fig. 3 we also present the boundary between the metal and the band insulator for the mass balanced IHM obtained from Ref. [18]. We expect a similar result for the mass imbalanced IHM, however within the two-site DMFT we cannot find a proper order parameter of the band insulating phase as well as the BI-metal transition points. Next, in Fig. 4 we show the two-site result for the staggered charge density $n_B - n_A$ as a function of U for different values of r at $\Delta = 0.5$. For fixed r the charge density decreases with increasing U and approaches zero for $U = U_c$. Our results for $r = 1.0$ (the mass balanced case) and $(U < U_c)$ are in good agreement with those obtained within the full DMFT in [18], keeping in mind that in [18] n_α denotes the occupation number for only one spin direction. However, we

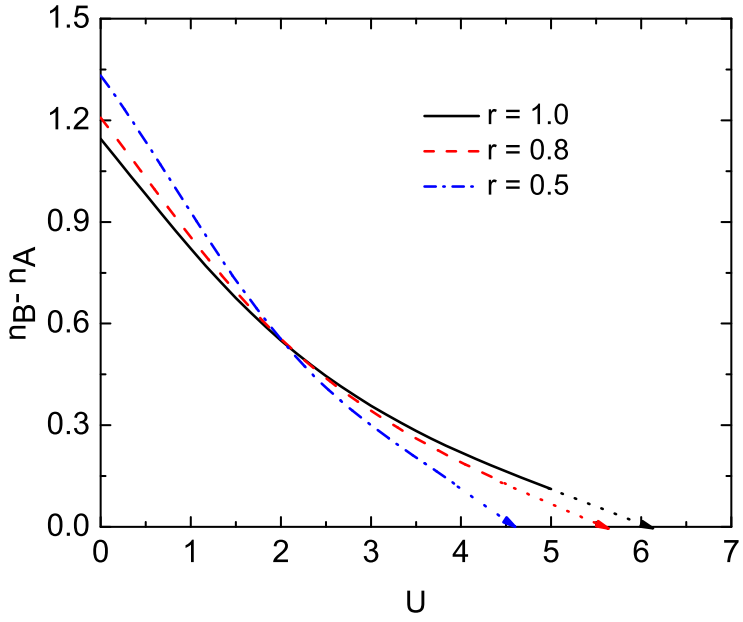

Fig. 4. Staggered charge density $n_B - n_A$ as a function of U for different values of the mass imbalanced parameter r at $\Delta = 0.5$. Our results for $r = 1.0$ (the mass -balanced case) and $(U < U_c)$ are in good agreement with those obtained within the full DMFT in [18]. The dotted lines are obtained by using the spline extrapolation to reach the limit when $\eta \to 0$.

cannot properly determine the staggered charge density near the transition point between the MI and the metallic phase, therefore we cannot identify its nature of phase transition.

IV. CONCLUSIONS

In summary, we have used the two-site DMFT to investigate the Mott transition in the mass imbalanced ionic Hubbard model at half filling. We find that like the balanced case $(r = 1)$, in the mass imbalanced IHM the critical interaction increases when Δ is increased. In the other hand, for a fixed Δ, this quantity (U_c) decreases with increasing the mass imbalance. Our results in the limiting cases $(r = 1, \Delta \neq 0$ or/and $\Delta = 0, r \neq 1)$ are in good agreement with those obtained from full DMFT [15, 16, 18]. We also show the existence of BI phase in the system for the case $\Delta \neq 0, U = 0$ and calculate the staggered charge density $n_B - n_A$ as a function of the interaction for different values of the mass imbalance. However, within the two-site DMFT we cannot determine the boundary between metallic and band insulating phases and as well as the nature of phase transitions. These may be the subject of our future study.

ACKNOWLEDGMENTS

This research is funded by Vietnam National Foundation of Science and Technology Development (NAFOSTED) under Grant No. 103.01-2017.56 and High-level Researcher Support Program NVCC05.13/19-19.

REFERENCES

[1] M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen, and U. Sen, *Adv. Phys.* **56** (2007) 243.
[2] I. Bloch *et al.,*, *Rev. Mod. Phys.* **80** (2008) 885.
[3] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, *Rev. Mod. Phys.* **82** (2010) 1225.
[4] W. Hofstetter, J. I. Cirac, P. Zoller, E. Demler, and M. D. Lukin, *Phys. Rev. Lett.* **89** (2002) 220407.
[5] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, *Nature* **455** (2008) 204.
[6] T. Esslinger, *Annu. Rev. Condens. Matter Phys.* **1** (2010) 129.
[7] A. Hemmerich, D. Schropp, and T. W. Hänsch, *Phys. Rev.* A **44** (1991) 1910.
[8] S. Taie, Y. Takasu, S. Sugawa, R. Yamazaki, T. Tsujimoto, R. Murakami, and Y. Takahashi, *Phys. Rev. Lett.* **105** (2010) 190401.
[9] A. Trenkwalder, C. Kohstall, M. Zaccanti, D. Naik, A. I.Sidorov, F. Schreck, and R. Grimm, *Phys. Rev. Lett.* **106** (2011) 115304.
[10] C. Kohstall, M. Zaccanti, M. Jag, A. Trenkwalder, P. Massignan, G. M. Bruun, F. Schreck, and R. Grimm, *Nature (London)*, **485** (2013) 615.
[11] M. Jag, M. Zaccanti, M. Cetina, R. S. Lous, F. Schreck, R.Grimm, D. S. Petrov, and J. Levinsen, *Phys. Rev. Lett.* **112** (2014) 075302.
[12] P. Fazekas, *Electron Correlation and Magnetism* (World Scientific, Singapore, 1999).
[13] P. S. Riseborough and J. M. Lawrence, *Rep. Prog. Phys.* **79** (2016) 084501.
[14] M. Potthoff, *Phys. Rev.* B **64** (2001) 165114.
[15] E.A. Winograd, R. Chitra, M.J. Rozenberg *Phys. Rev.* B **84** (2011) 233102.
[16] T.L. Dao *et al.*, *Phys. Rev.* A **85** (2012) 013606.
[17] Anh-Tuan Hoang, Duc-Anh Le, *Physica* B **485** (2016) 121.
[18] L. Craco *et al., Phys. Rev.* B **78** (2008) 075121.
[19] A. Garg *et al., Phys. Rev. Lett.* **97** (2006) 046403.