Ground-state properties of fermionic mixtures with mass imbalance in optical lattices

P. Farkašovský

Institute of Experimental Physics, Slovak Academy of Sciences - Watsonová 47, 040 01 Košice, Slovakia, EU

received 19 June 2008; accepted in final form 1 October 2008
published online 29 October 2008

PACS 71.10.-w – Theories and models of many-electron systems
PACS 71.30.+h – Metal-insulator transitions and other electronic transitions
PACS 05.30.Fk – Fermion systems and electron gas

Abstract – Ground-state properties of fermionic mixtures confined in a one-dimensional optical lattice are studied numerically within the spinless Falicov-Kimball model with a harmonic trap. A number of remarkable results are found. i) At low particle filling the system exhibits phase separation with heavy atoms in the center of the trap and light atoms in the surrounding regions. ii) Insulating phases always coexist with metallic phases. iii) Atomic-density waves are observed in the insulating regions for all particle fillings near the half-filled lattice case. iv) The variance of the local density exhibits universal behavior (independent of the particle filling, the Coulomb interaction and the strength of a confining potential) over the whole region of the local density values.

Copyright © EPLA, 2008

Introduction. – Experiments on ultracold atomic gases in optical lattices [1] open new routes for exploring the physics of long-standing problems of condensed-matter theory, like the phase separation, metal-insulator transitions, charge ordering, superconductivity, and so forth. A noteworthy advantage of atomic gases over condensed-matter systems such as solids or liquids, is that they allow for versatile tuning of the model parameters so that the particle hopping between the nearest-neighbor sites, the dimensionality of the system (from one to three), and the on-site interaction between particles (from attractive to repulsive) can all be varied and controlled with high precision [2]. On the other hand, the quadratic confining potential, present in addition to the regular “lattice” potential, leads to a number of fundamentally new phenomena. For example, it was shown [3,4] that in the presence of a confining potential the Mott-insulating phase is restricted to the domain that coexists with a metallic phase, in contrast to the global character typical of solid-state systems. Moreover, mixtures of two-component atoms with different masses (e.g., ⁴Li and ⁸⁷Rb) introduce an additional parameter, namely, the difference between the hopping amplitudes associated with each species of atoms in the optical lattice. This may affect the stability of the possible quantum phases or even induce new ones [5–7]. For these reasons the mixtures of ultracold atoms in optical lattices belong to the most intensively studied subjects of contemporary experimental and theoretical physics.

In this paper we investigate the ground-state properties of mixtures of two species of fermionic atoms with strongly different masses in a harmonic potential. Since the tunneling rate decreases exponentially with the square root of the mass of the atom, and particles of different species on the optical lattice interact only through the on-site interaction, this leads naturally to the Hamiltonian of the Falicov-Kimball model (FKM) [8] with a confining potential [3]

$$H = \sum_{ij} t_{ij} d_i^\dagger d_j + U \sum_i d_i^\dagger d_i f_i^\dagger f_i + \left(\frac{2}{L}\right)^2 \times V \sum_i \left(i - \frac{L}{2}\right)^2 (d_i^\dagger d_i + f_i^\dagger f_i),$$

(1)

where $f_i^\dagger$ ($f_i$) and $d_i^\dagger$ ($d_i$) are the creation (annihilation) operators of heavy (f) and light (d) particles at lattice site $i$. The number of lattice sites is $L$ and is selected so that all the fermions are confined in the trap. We denote the total number of fermions in the trap as $N$ and consider equal number of heavy ($N_f = \sum_i f_i^\dagger f_i$) and light ($N_d = \sum_i d_i^\dagger d_i$) atoms.

The first term of eq. (1) is the kinetic energy corresponding to the quantum-mechanical hopping of the
light-$d$-atoms between the nearest-neighbor sites $i$ and $j$. These intersite hopping transitions are described by the matrix elements $t_{ij}$, which are $-t_d$ if $i$ and $j$ are the nearest neighbors and zero otherwise (in the following all energies are measured in units of $t_d$). The second term represents the on-site Coulomb interaction ($U > 0$) between the light and heavy atoms. The last term is the energy of light and heavy atoms in the harmonic trapping potential. In accordance with similar studies for the asymmetric Hubbard model (HM) [9], we consider here the confining potential the electronic importance to analyze the interplay between the on-site Coulomb interaction and the confining potential.

Since in this spinless version of the FKM with a confining potential the $f$-heavy atom occupation number $f_i^d f_i$ of each site $i$ commutes with the Hamiltonian (1), the $f$-heavy atom occupation number is a good quantum number, taking only two values: $w_i = 1$ or 0, according to whether or not the site $i$ is occupied by the heavy atom. Therefore, the Hamiltonian (1) can be written as

$$H = \sum_{ij} h_{ij} d_i^\dagger d_j + \left( \frac{2}{L} \right)^2 V \sum (i - \frac{L}{2})^2 w_i,$$

where $h_{ij}(w) = t_{ij} + \left( U w_i + \left( \frac{2}{L} \right)^2 V (i - \frac{L}{2})^2 \right) \delta_{ij}$. Thus for a given configuration of heavy atoms $w = \{w_1, w_2, \ldots, w_L\}$ defined on the one-dimensional lattice, the Hamiltonian (2) is the second-quantized version of the single-particle Hamiltonian $h(w)$, so the investigation of the model (2) is reduced to the investigation of the spectrum of $h$ for different configurations of heavy atoms.

It is well known that in the absence of harmonic confinement ($V = 0$) the one-dimensional FKM exhibits a rich spectrum of solutions including phase-separated ($U$ small) as well as most homogeneous distributions of heavy atoms [10]. However, due to the confining potential the lattice sites become inequivalent, and thus, it is of fundamental importance to analyze the interplay between the on-site Coulomb interaction and the confining potential.

To describe the system at nonzero $V$ we have calculated various local quantities, like the local density of heavy atoms ($n_i^f = \langle f_i^f f_i \rangle$), the total density of light atoms ($n_i^d = \langle d_i^d d_i \rangle$), the total site occupation ($n_i = \langle f_i^f f_i + d_i^d d_i \rangle$), the variance of the local density $\langle \Delta_i = \langle f_i^f f_i + d_i^d d_i \rangle^2 - (f_i^f f_i + d_i^d d_i)^2 \rangle$ and the local double occupation ($\langle D_i = \langle d_i^d d_i f_i^f f_i \rangle \rangle$), as functions of the total number of the confined atoms, the Coulomb interaction $U$ and the
Ground-state properties of fermionic mixtures with mass imbalance in optical lattices

The ground states are calculated by a well-controlled numerical method that we have elaborated [11] for a description of the conventional FKM (V = 0). Later, the method was successfully used for various generalizations of the FKM and different physical problems [12]. The generalization of the algorithm on systems with a harmonic potential is straightforward and consists of the following steps. i) Choose a trial configuration \( w = \{ w_1, w_2, \ldots, w_L \} \). ii) Having \( w, U \) and \( V \) fixed, find all eigenvalues \( \lambda_k \) of \( h(w) \). iii) For a given \( N_f = \sum_i w_i \) determine the ground-state energy \( E(w) = \sum_{k=1}^{N_L} \lambda_k + \left( \frac{3}{2} \right)^2 V \sum_i (i - \frac{1}{2})^2 w_i \) of a particular \( f \)-atom configuration \( w \) by filling in the lowest \( N_d \) energy levels. iv) Generate a new configuration \( w' \) by moving a randomly chosen \( f \)-atom to a new position which is chosen also as random. v) Calculate the ground-state energy \( E(w') \). If \( E(w') < E(w) \) the new configuration is accepted, otherwise \( w' \) is rejected. Then the steps ii)–v) are repeated until the convergence (for given \( U \) and \( V \)) is reached.

**Results and discussion.** In fig. 1 we present results of our numerical calculations for \( n_f^i, n_d^i, n_i, D_i \) and \( \Delta_i \) obtained on the one-dimensional cluster of \( L = 120 \) sites at \( U = 4, V = 4 \) and different fillings. We have added also the profiles of the local compressibility that has been proposed by Rigol et al. [3] as a local order parameter to characterize the insulating regions. This quantity is defined as [3]

\[
\kappa_i^f = \sum_{|j| < \xi(U)} \chi_{i,i+j},
\]

where

\[
\chi_{i,j} = \langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle
\]

is the density-density correlation function and \( l(U) \sim b \xi(U) \), with \( \xi(U) \) the correlation length of \( \chi_{i,j} \) in the unconfined system at half-filling for a given \( U \). The factor \( b \) is chosen within a range where \( \kappa^f \) becomes qualitatively insensitive to its precise value [4]. The insulating regions are then characterized by \( \kappa^f_i = 0 \). For the values of \( U \) used here we usually have \( b \sim 4–8 \) with \( \xi(U) \sim 1 \).

The most interesting result obtained at low particle fillings (we note that \( N_f = N_d = N/2 \)) is the observation of the complete phase separation with heavy atoms in the center of the trap \( (n_f^i = 1, n_d^i \sim 0) \) and light atoms in the surrounding regions \( (n_f^i = 0, n_d^i < 1) \). Such a behaviour is found for all particle fillings from \( N_f = 1 \) to some critical value \( N_f^c \) that rapidly decreases with increasing \( V \) and is weakly dependent upon \( U \) (see the first inset in fig. 3). In the regions where \( n_f^i = 0 \) \( (0 < n_d^i < 1) \) the variance of the

Fig. 2: The site occupation \( n_i \) as a function of the site position \( i \) calculated for different \( V \) (the first column) and different \( U \) (the second column).
local density $\Delta_i$ and the local compressibility $\kappa_i^l$ are finite (the metallic phase), while in the middle of the trap where $n_f^d = 1$ ($n_f^d$ exponentially decreases in this region) both $\Delta_i$ and $\kappa_i^l$ are equal to zero (the insulating phase). Thus in accordance with results obtained for the HM [3] (the hopping probabilities are same for both types of atoms) we have found that also in the FKM insulating domains coexist with metallic regions, such that global quantities are not appropriate to describe the system.

At higher particle fillings the situation is more complex. Above the critical filling $N_f^c$ ($N_f^c = 24$, for $V = 4, U = 4$) the connected cluster by heavy atoms occupied sites (in the center of the trap) splits on smaller clusters, usually of the same size, separated by the empty site. As $N_f$ increases the size of clusters decreases from $N_f$ to 1. Of course, the redistribution of heavy atoms has dramatic consequences on the distribution of light atoms. Now, the light atoms occupy preferably the empty sites in the middle of the trap ($n_i = 1$) what leads to the atomic-density waves (ADWs) in $n_f^d$ and $n_f$ profiles. In the region where $n_i = 1$ the variance of the local density is finite but smaller than in surrounding metallic regions indicating [3,4] the presence of an insulating phase in the center of the trap. This conjecture supports the behaviour of the local compressibility $\kappa_i^l$ that is equal to zero in the corresponding region.

Increasing the number of particles up to $N_f = 52$, the connected cluster of heavy atoms ($n_f^d = 1$) starts to form in the middle of the trap. In this region both the variance of the local density and the local compressibility are finite what indicates the presence of a metallic phase in the center of the trap. Upon adding more fermions, this new metallic phase widens spatially, while the insulating regions of the ADWs are pushed to the borders and completely disappear at $N_f = 90$. At this filling practically the whole region of the trap, except the edges (where $n_f^d = 0, n_f^l \sim 1$), is metallic. With still a higher filling this metallic phase is further stabilized, but at some critical filling ($N_f = 95$) a new insulating phase (“a band insulator”) starts to develop in the center of the trap ($n_f^d = 1, n_f^l = 1$). This trend holds also for the highest particle fillings, the width of the band-insulating phase increases and the surrounding metallic regions are gradually suppressed.

To reveal the role of the Coulomb interaction $U$ and the confining potential $V$ on a formation of metallic and insulating domains, similar calculations have been also
Fig. 4: (a), (b) The site occupation $n_i$ of the asymmetric HM with a harmonic trap as a function of the site position $i$ calculated within the well-controlled numerical method [15] for different values of $t_f$ and $N_f$ on a finite cluster of $L = 24$ sites. (c) The critical values of $t_f$ (below which the physics of the FKM dominates) as functions of $1/L$. (d) The variance of the local density $\Delta$ as a function of the local density $n$ calculated for different values of $U, V$ and $N_f$. 

performed for various combinations of $U$ and $V$. The results of numerical calculations for the site occupation $n_i$ as a function of $i$ are displayed in fig. 2. One can see that the Coulomb interaction $U$ and the confining potential $V$ exhibit precisely opposite effects on the stability of metallic and insulating domains. Indeed, with increasing $V$ (at fixed $U$) the insulating domain ($n_i \sim 1$) is suppressed and the metallic domains are stabilized, while with increasing $U$ (at fixed $V$) the metallic domains are suppressed and the insulating domain is stabilized.

Since the FKM can be considered as a simplification of the HM (only one kind of particles, say with spin up can hop) it is interesting to compare results obtained in these two different limits. Such a comparison (see ref. [3] and ref. [4]) reveals obvious differences in the behavior of these models in the confining potential. For example, the ground state of the HM (for $V \neq 0$) is always metallic at low particle fillings, while the metallic regions coexist with the insulating region in the ground state of the FKM. Moreover, the local density profiles exhibit obvious oscillations for the FKM, while no sign of such oscillations has been observed for the repulsive HM (with the exception of Hartree-Fock [4] and variational studies [13], that were not confirmed by a projector Monte Carlo simulations, however [4]).

To exclude the possibility that oscillations are a consequence of a finite size of clusters used in our numerical calculations, we have performed an exhaustive finite-size scaling analysis on finite clusters up to $L = 600$ sites for all particle fillings from fig. 1. This analysis showed that the ground states found for $L = 120$ hold also on clusters of $L = 240$, $L = 480$ and $L = 600$ sites. In fig. 3 we present numerical results for the largest cluster accessible by our algorithm ($L = 600$) and the same values of $n_f = N_f/L, V$ and $U$ as used in fig. 1. These results clearly demonstrate that increasing $L$ suppresses the ADWs in the metallic phase, but stabilizes the ADWs in the insulating phase. The ADWs in the insulating phase are thus obviously a consequence of immobilization of one sort of particles ($t_f = 0$). As shown later these oscillations are gradually suppressed with increasing $t_f$ (see the case of $N_f = 12$ in fig. 4) and the system undergoes the transition from the FKM regime to the HM regime (without oscillations).

Since in the real experiments with ultracold atoms the hopping matrix elements (of heavy atoms) between the nearest-neighbor sites ($t_f$) are not strictly equal to zero,
it is necessary to examine the stability of our solutions obtained for \( t_f = 0 \) against the finite values of \( t_f \). For this reason we have performed exhaustive numerical studies of the asymmetric HM [14] \( (t_f \neq 0) \) in a confining potential for a wide range of model parameters \((N_f, t_f, U)\) and \((V)\) on finite clusters up to \( L = 40 \). The calculations have been done with a new numerical method that we have elaborated recently for a description of ground states of the asymmetric HM [15]. Its main advantage is the high accuracy in the strongly asymmetric limit \( t_f < 0.2 \). The representative examples of local density profiles are displayed in fig. 4 for several different values of \( N_f \) and \( t_f \). They clearly show that results obtained for \( t_f = 0 \) remain stable also at finite (small) \( t_f \). To specify more precisely the regime where the physics of the FKM dominates we have also calculated the quantity \( \delta_i = \left| n_i(t_f) - n_i(0) \right| \) on finite clusters up to \( L = 40 \). In fig. 4(c) we present the critical values of \( t_f \) below which \( \delta_i < 0.05 \) for each site \( i \). Extrapolating these results to the thermodynamic limit \( L \to \infty \) one can see that the regime of the FKM extends up to \( t_f \sim 0.2 \) and thus it includes also the case of alkali mixtures Li\(^3\) and K\(^{40}\) with \( t_f/t_f \sim 0.15 \).

Finally, we have also calculated the variance of the local density as a function of the local density \( n_i \). It is known from the study of the one-dimensional HM in a harmonic potential [3] that this quantity shows universality with respect to the confining potential for \( n_i \to 1 \). It should be noted that the universal behavior was observed only for strong Coulomb interactions \( U \), where systems have a Mott-insulating phase at \( n = 1 \). In fig. 4(d) we present numerical results for the variance of the local density obtained within the FKM with a harmonic potential as a function of the local density calculated for various particle fillings and various values of \( U \) and \( V \). One can see that all numerical data for the variance of the local density collapse on the same curve (given by \( \Delta = -\alpha(n-1) \) for \( n \leq 1 \) and \( \Delta = -(n-1)(n-2) \) for \( n > 1 \)). Thus in contrast to the similar studies on the HM [3] we have found that the variance of the local density of systems described by FKM with a harmonic potential exhibits universality not only with respect to the confining potential but also with respect to the Coulomb interaction \( U \). The universality in the FKM is obviously a consequence of the fact that for \( t_f = 0 \) the site occupation \( n_f^i \) is only zero or one, and therefore the variance in the occupation is simply related to the occupation itself. A similar universal behaviour has been observed also for other local quantities. For example, the local double occupation \( D_f = 0 \) for \( n_f \leq 1 \) and \( D_f = n_f - 1 \) for \( n_f > 1 \), independent of values of \( U, V, N_f \) and \( L \). Also the universal behavior is found for the local compressibility \( k_v^i \) when \( n_f \to 1 \). However, the value of the critical exponent for the FKM is equal to 1, unlike the nontrivial value 0.68–0.78 found for the HM [3].

In summary, we have studied the ground-state properties of fermionic mixtures with mass imbalance in a one-dimensional optical lattice within the spinless FKM with a harmonic potential. We have found that the system exhibits phase separation at low particle fillings. In this case the heavy atoms occupy the center of the trap while the light atoms are localized in the surrounding (metallic) regions. At higher fillings we have observed a formation of insulating domains with ADWs. In all cases insulating phases coexist with metallic phases. One of the most interesting results is, however, the observation of the universal behavior of the variance of the local density (independent of the particle filling, the Coulomb interaction and the strength of the confining potential) over the whole region of the local density values.

***

This work was supported by the Slovak Grant Agency VEGA under Grant No. 2/7057/27 and Slovak Research and Development Agency (APVV) under Grant LPP-0047-06.

REFERENCES

[1] Greiner M. et al., Nature (London), 415 (2002) 39; Bloch I., Phys. World, 17 (2004) 25; Jacksch D. and Zoller P., Ann. Phys. (N.Y.), 315 (2005) 52; Hufstetler W., Philos. Mag., 86 (2006) 1891; Stöferle T. et al., Phys. Rev. Lett., 96 (2006) 030401.
[2] Bloch I. et al., arXiv:0704.3011 (2007).
[3] Rigol M., Muramatsu A., Batrouni G. G. and Scalettar R. T., Phys. Rev. Lett., 91 (2003) 130403.
[4] Rigol M. and Muramatsu A., Phys. Rev. A, 69 (2004) 053612.
[5] Ates C. and Ziegler K., Phys. Rev. A, 71 (2004) 063610; Ziegler K., Nucl. Phys. A, 790 (2007) 718C.
[6] Gu S. J., Fan R. and Lin H. Q., Phys. Rev. B, 76 (2008) 125107.
[7] Cazalilla M. A., Ho A. F. and Giamarchi T., Phys. Rev. Lett., 95 (2005) 226402; Lin G. D., Yi W. and Duan L. M., Phys. Rev. A, 74 (2006) 031604(R); Tao T. L., Georges A. and Capone M., Phys. Rev. B, 76 (2007) 104517; Conduit G. J., Conlon P. H. and Simons B. D., Phys. Rev. A, 77 (2008) 3617.
[8] Falicov L. M. and Kimball J. C., Phys. Rev. Lett., 22 (1969) 997.
[9] Gottwald T. and van Dongen P. G. J., Eur. Phys. J. B, 61 (2008) 277.
[10] Lemberger P., J. Phys. A, 25 (1992) 715; Gruber C., Ueltschi D. and Jedrzejewski J., J. Stat. Phys., 76 (1994) 125; Freericks J. K., Lieb E. H. and Ueltschi D., Phys. Rev. Lett., 88 (2002) 106401.
[11] Farkašovský P., Eur. Phys. J. B, 20 (2001) 209; Int. J. Mod. Phys. B, 17 (2003) 4897.
[12] Farkašovský P., Cenčareľová H. and Tomášovičová N., Eur. Phys. J. B, 45 (2005) 479; Farkašovský P. and Cenčareľová H., Eur. Phys. J. B, 47 (2005) 517.
[13] Fujihara Y., Koga A. and Kawakami N., J. Phys. Soc. Jpn. B, 76 (2007) 034716.
[14] Lyzwa R. and Domanski Z., Phys. Rev. B, 50 (1994) 11381.
[15] Farkašovský P., Phys. Rev. B, 77 (2008) 085110.