Hubbard physics in the symmetric half-filled periodic Anderson-Hubbard model

I. Hagymási*

Institute for Solid State Physics and Optics,
Wigner Research Centre for Physics,
Hungarian Academy of Sciences, Budapest,
H-1525 P.O. Box 49, Hungary and
Institute of Physics, Eötvös University, Budapest,
Pázmány Péter sétány 1/A, H-1117, Hungary

K. Itai and J. Sólyom

Institute for Solid State Physics and Optics,
Wigner Research Centre for Physics, Hungarian Academy of Sciences,
Budapest, H-1525 P.O. Box 49, Hungary

Abstract

Two very different methods – exact diagonalization on finite chains and a variational method – are used to study the possibility of a metal-insulator transition in the symmetric half-filled periodic Anderson-Hubbard model. With this aim we calculate the density of doubly occupied d sites (ν_d) as a function of various parameters. In the absence of on-site Coulomb interaction (U_f) between f electrons, the two methods yield similar results. The double occupancy of d levels remains always finite just as in the one-dimensional Hubbard model. Exact diagonalization on finite chains gives the same result for finite U_f, while the Gutzwiller method leads to a Brinkman-Rice transition at a critical value (U_d^c), which depends on U_f and V.

PACS numbers: 71.10.Fd, 71.27.+a, 75.30.Mb

Keywords: strongly correlated system, periodic Anderson model, exact diagonalization, Gutzwiller method

*E-mail: hagymasi.imre@mta.wigner.hu

I. INTRODUCTION

The periodic Anderson-Hubbard model defined by the Hamiltonian

$$\mathcal{H} = \sum_{\boldsymbol{k},\sigma} \varepsilon_d(\boldsymbol{k}) \hat{d}^\dagger_{\boldsymbol{k},\sigma} \hat{d}_{\boldsymbol{k},\sigma} + U_d \sum_{\boldsymbol{j}} \hat{n}^d_{\boldsymbol{j}\uparrow} \hat{n}^d_{\boldsymbol{j}\downarrow} + \varepsilon_f \sum_{\boldsymbol{j},\sigma} \hat{n}^f_{\boldsymbol{j},\sigma} + U_f \sum_{\boldsymbol{j}} \hat{n}^f_{\boldsymbol{j}\uparrow} \hat{n}^f_{\boldsymbol{j}\downarrow} - V \sum_{\boldsymbol{j},\sigma} \left(\hat{f}^\dagger_{\boldsymbol{j},\sigma} \hat{d}_{\boldsymbol{j},\sigma} + \hat{d}^\dagger_{\boldsymbol{j},\sigma} \hat{f}_{\boldsymbol{j},\sigma} \right) \tag{1}$$

is meant to describe the physics of systems in which two types of electrons, one filling a relatively broad conduction band, the other a narrow band, are allowed to hybridize. In what follows we call them d and f electrons. The interactions within the bands are denoted by U_d and U_f, respectively. In the present work we restrict ourselves to the half-filled paramagnetic case, that is, when there are $N_\uparrow = N_\downarrow = N$ up- and down-spin electrons in an arbitrary dimensional lattice with N lattice sites, each of which has one d and one f orbital. Moreover, we restrict ourselves to the symmetric case, where an equal number of d and f electrons is present on the average. This is realized when $\varepsilon_f = (U_d - U_f)/2$, if the energy is measured from the center of the d band [1].

In our previous study of this model [1], in which we used two very different methods: a variational calculation using the Gutzwiller type wave function and exact diagonalization, we were mainly interested in the effect of the on-site interaction U_d between conduction electrons on the f-electron physics. In the present study we examine the effect of d-f hybridization (V) and of the interaction U_f between f electrons on the Hubbard physics, that is on the eventual metal-insulator transition at half filling.

In the Gutzwiller-type treatment of the half-filled Hubbard model, the metal-insulator transition, which is known in this case as the Brinkman-Rice transition [2], occurs at a finite U_d, where the number of doubly occupied d sites becomes zero. A similar transition was obtained by the Gutzwiller method in the half-filled periodic Anderson-Hubbard model, too [1], when the f electrons in the narrow band are strongly correlated.

In contrast to that, exact diagonalization of the half-filled periodic Anderson-Hubbard model on finite chains gave a finite number of doubly occupied d sites for any U_d, just as in the one-dimensional half-filled Hubbard model, where this number is finite for arbitrary U_d [3], even though the ground state is conducting only for $U_d = 0$ and insulating for $U_d > 0$.

In this paper we will consider the half-filled symmetric Anderson-Hubbard model in the paramagnetic regime in the full $U_d \geq 0$, $U_f \geq 0$ sector, when it is not necessarily

in the strongly correlated Kondo region, and will study the possibility of metal-insulator transition. We should note here that in the present model a "metallic" phase is in fact a band insulator with hybridization gap. Therefore, we should be speaking about insulator-insulator transition, though its physics is the same as a metal-insulator transition due to the interactions between electrons. We calculate the number of doubly occupied d sites as a function of U_d for various values of V and U_f by both methods at the symmetric Anderson point, where the average number of f and d electrons per site (denoted by n_f and n_d, respectively) is exactly 1, and examine the effects of these couplings on the one- and higher dimensional Hubbard physics.

II. CALCULATION BY EXACT DIAGONALIZATION

First, we perform exact diagonalization of the model on finite chains, where the kinetic energy of conduction electrons moving along the chain is described by hopping between nearest-neighbor d orbitals with hopping rate t.

We consider the periodic Anderson-Hubbard model on a chain consisting of six sites with periodic boundary conditions. The results are shown in Figs. 1 and 2, where the density of doubly occupied d sites, ν_d, is shown as a function of U_d for $V = 0.1W$ and $0.3W$, respectively ($W = 4t$ is the bandwidth), and for $U_f = 0$ and $5W$. The values calculated with the Bethe Ansatz for the pure Hubbard model are also shown in the figure by a solid line.

One can see that when the conduction electrons of the d band are hybridized with non-interacting electrons in the f band ($U_f = 0$), the larger the hybridization the more the number of doubly occupied sites. The curves are reasonably close to the results obtained by the Gutzwiller method. The agreement gets better for stronger hybridization, while for weak hybridization it holds for small U_d values only.

The values of ν_d decrease for finite U_f and get close to those of the pure Hubbard model for large U_f. This suggests that the d-electron subsystem becomes decoupled from the f electrons when the f electrons are strongly correlated.

The results in this section are valid for a chain, for a one-dimensional model. In the next section we discuss a variational method, which might be relevant for higher dimensional models.

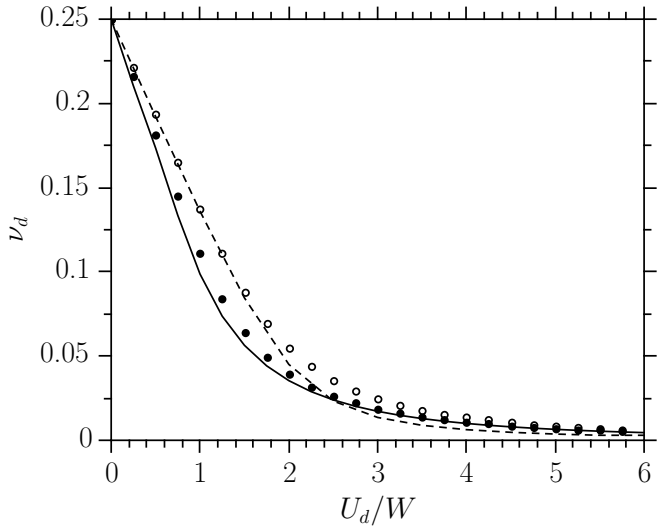

Fig. 1. ν_d as a function of U_d for $V = 0.1W$. The empty and filled circles indicate the results of exact diagonalization for $U_f/W = 0$ and 5, respectively. The dashed line is the result of the Gutzwiller method for $U_f/W = 0$. The solid line is the exact solution of the one dimensional Hubbard-model.

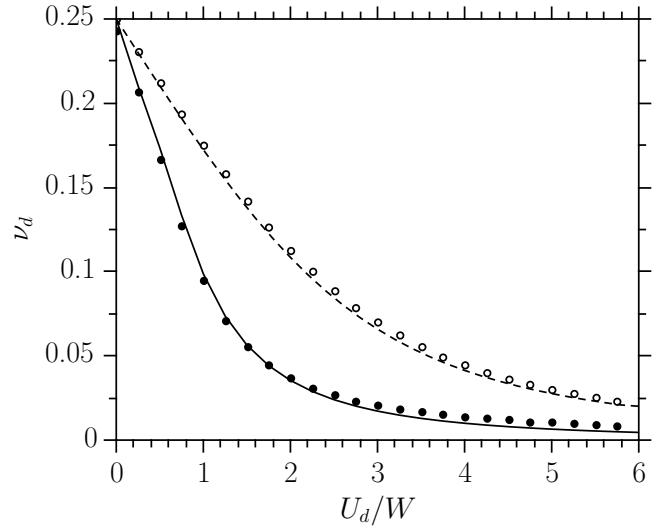

Fig. 2. The same as Fig. 1 except that $V = 0.3W$.

III. VARIATIONAL CALCULATION

We summarize the main steps of the variational calculation following Ref. [4]. The trial wave function is chosen in the form

$$|\Psi\rangle = \hat{P}_{\rm G}^{d}\hat{P}_{\rm G}^{f}\prod_{\boldsymbol{k}}\prod_{\sigma}\left[u_{\boldsymbol{k}}\hat{f}_{\boldsymbol{k}\sigma}^{\dagger} + v_{\boldsymbol{k}}\hat{d}_{\boldsymbol{k}\sigma}^{\dagger}\right]|0\rangle, \tag{2}$$

where the Gutzwiller projectors, $\hat{P}_{\rm G}^{d}$ and $\hat{P}_{\rm G}^{f}$, which contain the variational parameters η_d and η_f, are written as

$$\hat{P}_{\rm G}^{d} = \prod_{\boldsymbol{j}} \left[1 - (1-\eta_d)\hat{n}_{j\uparrow}^{d}\hat{n}_{j\downarrow}^{d}\right], \tag{3}$$

$$\hat{P}_{\rm G}^{f} = \prod_{\boldsymbol{j}} \left[1 - (1-\eta_f)\hat{n}_{j\uparrow}^{f}\hat{n}_{j\downarrow}^{f}\right]. \tag{4}$$

The variational parameters, η_d and η_f, depend on U_d and U_f, respectively. Performing the optimization with respect to the mixing amplitudes, $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$, we get

$$\mathcal{E} = \frac{1}{N}\sum_{\boldsymbol{k}\in \rm FS}\left[q_d\varepsilon_d(\boldsymbol{k}) + \tilde{\varepsilon}_f - \sqrt{\left[q_d\varepsilon_d(\boldsymbol{k}) - \tilde{\varepsilon}_f\right]^2 + 4\tilde{V}^2}\right] + (\varepsilon_f - \tilde{\varepsilon}_f)n_f + U_d\nu_d + U_f\nu_f \tag{5}$$

for the ground-state energy density, where q_d denotes the kinetic energy renormalization factor of d electrons given by

$$q_d = \frac{1}{\left(1-\frac{n_d}{2}\right)\frac{n_d}{2}}\left[\sqrt{\left(\frac{n_d}{2}-\nu_d\right)\nu_d} + \sqrt{\left(\frac{n_d}{2}-\nu_d\right)\left(1-n_d+\nu_d\right)}\right]^2, \tag{6}$$

which is formally identical to the expression found in the Hubbard model [5]. The renormalized hybridization amplitude is now $\tilde{V} = V\sqrt{q_d q_f}$; the other notations are the same as in our previous paper [4], and the self-consistency condition is given by

$$n_f = \frac{1}{N}\sum_{\boldsymbol{k}\in \rm FS}\left[1 + \frac{q_d\varepsilon_d(\boldsymbol{k}) - \tilde{\varepsilon}_f}{\sqrt{\left[q_d\varepsilon_d(\boldsymbol{k}) - \tilde{\varepsilon}_f\right]^2 + 4\tilde{V}^2}}\right] = 1. \tag{7}$$

The summation over $\boldsymbol{k}$ can be carried out assuming a constant density of states, $\rho(\varepsilon) = 1/W$, in the interval $\varepsilon \in [-W/2, W/2]$. The values of ν_f, and ν_d are obtained by optimizing the energy density with respect to these parameters numerically. For $V \ll W$ and $n_d = n_f = 1$ the optimization condition with respect to ν_d and ν_f results in the following coupled equations:

$$\frac{U_d}{W} - \left[\frac{1}{4} + 2\left(\frac{V}{W}\right)^2\frac{q_f}{q_d}\right]8(1-4\nu_d) = 0, \tag{8}$$

$$\frac{U_f}{W} + 2\left(\frac{V}{W}\right)^2 \ln\left[4\frac{q_f}{q_d}\left(\frac{V}{W}\right)^2\right]8(1-4\nu_f) = 0. \tag{9}$$

When either of U_d or U_f is zero, the equations are decoupled. Note that in the absence of hybridization Eq. (8) reduces to the result for the ordinary Hubbard model.

We now turn to the discussion of the d-electron subsystem. We calculate the density of doubly occupied d sites, ν_d, as a function of U_d. The results are displayed in Fig. 3 for several values of U_f for a relatively weak hybridization, $V = 0.1W$, and in Fig. 4 for a stronger hybridization.

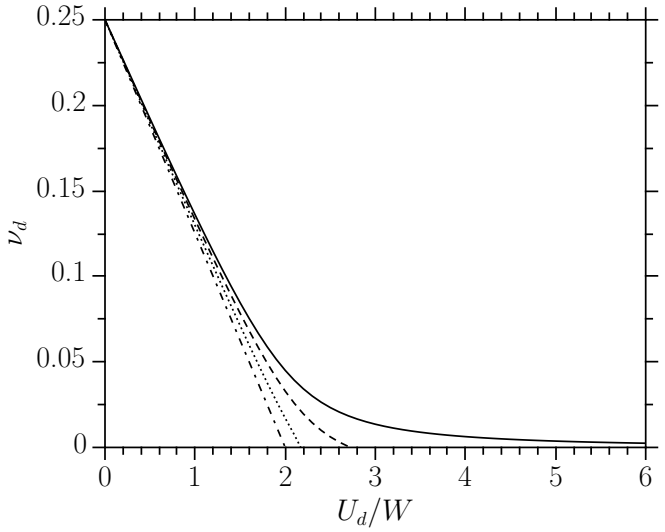

Fig. 3. ν_d as a function of U_d. The solid, dashed, dotted and dot-dashed lines correspond to $U_f/W = 0, 0.3, 0.5, 5$ respectively. $V = 0.1W$ in all cases.

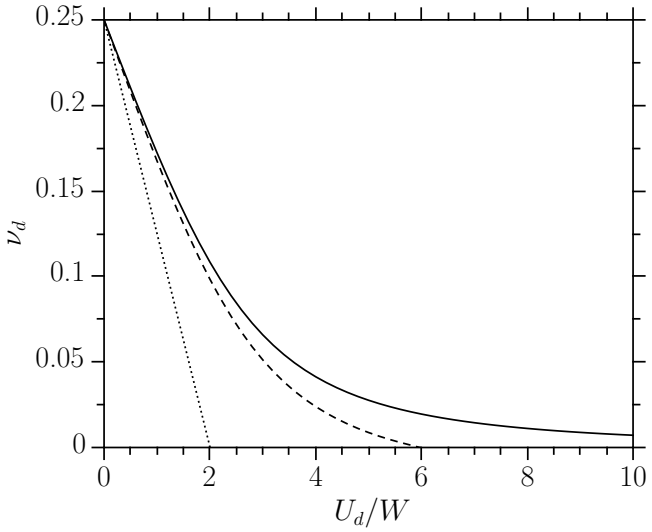

Fig. 4. ν_d as a function of U_d. The solid, dashed and dotted lines correspond to $U_f/W = 0, 1, 10$ respectively. $V = 0.3W$ in all cases.

First, we find that for $U_f = 0$, ν_d never becomes zero, just as it was obtained by the exact diagonalization for a finite chain, that is, the Brinkman-Rice transition does not occur. We

can calculate the asymptotic behavior of ν_d for large value of U_d from the following analysis. When $U_f = 0$, $q_f = 1$ irrespective of U_d, and Eq. (8) can be solved for ν_d. For $U_d \gg W$ in leading order we arrive at:

$$\nu_d \propto \frac{2V^2}{U_d}. \tag{10}$$

Second, we find that the Gutzwiller method leads to a Brinkman-Rice transition for any $U_f > 0$, that is, there exists a finite value, U_d^c, where ν_d becomes zero. For $U_d > 0$ and $U_f > 0$ the optimization conditions, Eqs. (8) and (9) for ν_f and ν_d are coupled, and thus both ν_d and ν_f decrease when either of the interactions increases. Therefore, even for very small U_f, when U_d is large enough, ν_f also becomes small, and finally both ν_d and ν_f simultaneously become zero at U_d^c. As a matter of fact, U_d and U_f play a rather similar role. If we fix U_d at a certain value larger than $2W$, a Brinkman-Rice transition occurs at a certain U_f^c. The difference in the condition ($U_d > 2W$ and $U_f > 0$) necessary for occurrence of a transition is due to the different widths of the d and f bands (W and 0, respectively) in the present model.

Third, when U_f is large enough and ν_f is exponentially small even for small U_d, that is, when the system is the Kondo regime, the $\nu_d - U_d$ curves become straight lines and coincide to the known behavior of the Hubbard-model. In the limit $U_f \gg W$ we obtain:

$$\nu_d = \frac{1}{4} - \frac{U_d}{8(W + 4E_{\rm K})}, \tag{11}$$

where

$$E_{\rm K} = \frac{W}{2} \exp\left\{-\frac{U_f}{16V^2/W}\right\}. \tag{12}$$

The scenario is the same for weak or strong hybridizations.

The results described above indicate that a phase boundary can be defined in the three-dimensional parameter space of U_d, U_f and V, which separates the region where $\nu_d = \nu_f = 0$ from that where both ν_d and ν_f are finite. The former is a Mott insulator region and the latter is a hybridized band insulator region (for small U_f) or a Kondo insulator region (for large U_f). The phase boundaries in the U_d–U_f plain are shown in Fig. 5. (About the boundary between a hybridized band insulator and a Kondo one, see Ref. [1].)

IV. CONCLUSIONS

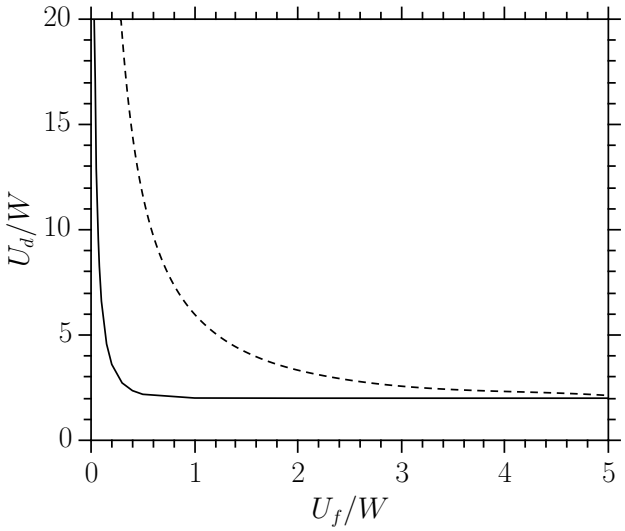

Fig. 5. The phase boundaries in the U_d–U_f plain separating the metallic and insulating regimes. The solid and dashed lines correspond to $V = 0.1W$ and $0.3W$, respectively.

In this paper we discussed the periodic Anderson-Hubbard model focusing our attention on the physics of the conduction electron subsystem, using two different methods: exact diagonalization on finite chains and a variational method of the Gutzwiller-type. We studied the effects of the d-f hybridization (V) and of the on-site interaction between f electrons (U_f) on the number of doubly occupied d sites, ν_d. When $U_f = 0$, both methods gave similar results. For larger U_f, however, the results of exact diagonalization in the one-dimensional model showed that ν_d approaches that obtained from the Bethe-Ansatz solution of the pure Hubbard model, while the Gutzwiller method indicates a Brinkman-Rice-type scenario for a metal-insulator transition.

It is interesting from theoretical point of view that $\nu_d \propto 1/U_d^2$ according to the Bethe-Ansatz solution for $U_d \gg W$, while the Gutzwiller method gives a slower asymptotic behavior, $\nu_d \propto 1/U_d$ for $U_f = 0$.

ACKNOWLEDGMENTS

This work was supported in part by the Hungarian Research Fund (OTKA) through Grant No. T 68340. One of the authors (I. H.) acknowledges the support of TÁMOP Grant No. 4.2.2/B-10/1-2010-0030.

REFERENCES

[1] I. Hagymási, K. Itai and J. Sólyom, to be published in *Phys. Rev. B*, cond-mat/1106.4999

[2] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).

[3] F. Woynarovich, J. Phys. C: Solid State Phys. **16**, 6593 (1983).

[4] K. Itai and P. Fazekas, *Phys. Rev. B* **54**, R752 (1996).

[5] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963), Phys. Rev. **134**, A923 (1964), Phys. Rev. **137**, A1726 (1965); see also D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).