EXACT GROUND-STATES FOR THE PERIODIC ANDERSON MODEL IN RESTRICTED REGIONS OF THE PARAMETER SPACE*

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Exact localised ground-states are presented for the one- and two-dimensional periodic Anderson model at finite $U > 0$ in restricted regions of the parameter space, which extends from the low U to the high U regions as well. The physical properties of this phase are analysed in detail.

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1. Introduction

The periodic Anderson model (PAM) is a basic model describing strongly correlated systems, largely applied in characterising heavy-fermion materials [1], intermediate-valence compounds [2], and even high T_c superconductors [3]. In contrast with other models used in the understanding of strong correlation effects, the exact solution of the model even in 1D is not known, so the physics provided by PAM is almost exclusively interpreted based on approximations. Concerning ground-state (GS) properties, notable exceptions from this rule are GS deduced in restricted regions of the parameter space for decorated hypercubic lattices [4] and one-dimensional case with restrictions on parameter values [5], both obtained at $U = \infty$, and extended later on to higher dimensions [6]. The advancement leading to exact GS at finite and non-zero U becomes to be possible almost after one decade [7–9]. This has been achieved by a proper decomposition of the Hubbard interaction combined with the use of positive semidefinite operators collecting contributions from a direct space region with the extension of an unit cell (I) [7]. The procedure has been applied for 1D [7,8], and 2D [9] cases as well. The obtained GS solutions describe highly non-trivial itinerant and localised wave-functions. From these, the itinerant case, presenting non-Fermi

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liquid characteristics in normal phase has been described previously [7, 9]. Herewith, we are characterising the properties of the localised solutions obtained in conditions in which all hopping matrix elements from the unit cell are taken into consideration.

2. The model, used procedure, and obtained results

The PAM Hamiltonian we use is defined as

$$\hat{H}_{\rm PAM} = \hat{T}_{\rm c} + \hat{T}_f + \hat{E}_f + \hat{V}_0 + \hat{V}_1 + \hat{U}\,, \tag{1}$$

where $\hat{T}_b = \sum_{\boldsymbol{j},\boldsymbol{r},\sigma}(t_{b,\boldsymbol{r}}\hat{b}^{\dagger}_{\boldsymbol{j},\sigma}\hat{b}_{\boldsymbol{j}+\boldsymbol{r},\sigma} + \text{H.c.})$ are kinetic energies for $b = c, f$ electrons, $\hat{E}_f = E_f\sum_{\boldsymbol{j},\sigma}\hat{n}^f_{\boldsymbol{j},\sigma}$, is the on-site f-electron energy, $\hat{V}_0 = \sum_{\boldsymbol{j},\sigma}(V_0\hat{c}^{\dagger}_{\boldsymbol{j},\sigma}\hat{f}_{\boldsymbol{j},\sigma} + \text{H.c.})$, and $\hat{V}_1 = \sum_{\boldsymbol{j},\boldsymbol{r},\sigma}(V_1(\boldsymbol{r})\hat{c}^{\dagger}_{\boldsymbol{j},\sigma}\hat{f}_{\boldsymbol{j}+\boldsymbol{r},\sigma} + \text{H.c.})$ are the local and non-local hybridizations, and $\hat{U} = U\sum_{\boldsymbol{j}}\hat{n}^f_{\boldsymbol{j},\uparrow}\hat{n}^f_{\boldsymbol{j},\downarrow}$, $U > 0$, represents the interaction term. The $\boldsymbol{r}$ vector has an unique value in 1D (lattice spacing $\boldsymbol{a}$), and in 2D it has 4 possible values: $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}+\boldsymbol{y}, \boldsymbol{y}-\boldsymbol{x}$, where $\boldsymbol{x}$ and $\boldsymbol{y}$ are the primitive vectors of I. The presence of $\hat{T}_f$ is motivated by experiments [10].

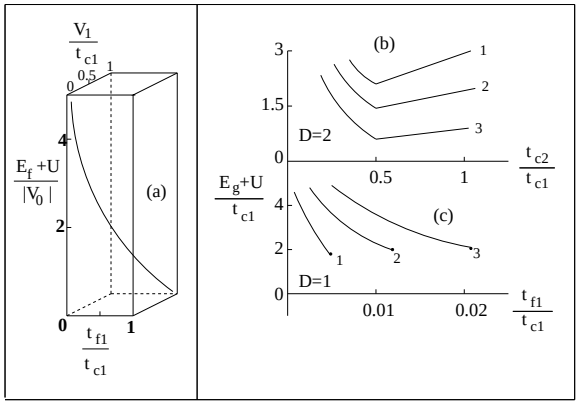

Fig. 1. The parameter space region where the described solution is present in $D = 1$ dimension (a), and the ground-state energy per site E_g in $D = 2$ (b), and $D = 1$ (c). The $\hat{H}$ parameter values are $t_{f1}/t_{c1} = 0.1,\ 0.25,\ 0.35$ for curves 1, 2, 3 in (b); and $V_0/t_{c1} = 0.1,\ 0.2,\ 0.3$ for curves 1, 2, 3 in (c).

Let us consider the operator $\hat{A}_{\boldsymbol{i},\sigma} = \sum_{\boldsymbol{i}_\alpha,b} a_{\alpha,b}\hat{b}_{\boldsymbol{i}+\boldsymbol{i}_\alpha,\sigma}$, where $\boldsymbol{i}_\alpha$, starting from $\boldsymbol{i}_1 = 0$, is summed up over all sites of I, placed at site $\boldsymbol{i}$, and $a_{\alpha,b}$ are numerical coefficients depending only on the position in I and $b = c, f$. Furthermore, $\hat{U} = U\hat{P}' + U\sum_{\boldsymbol{j},\sigma}(\hat{n}^f_{\boldsymbol{j},\sigma} - 1/2)$, where $\hat{P}' = \sum_{\boldsymbol{j}}\hat{P}'_{\boldsymbol{j}}$, and $\hat{P}'_{\boldsymbol{j}} = \prod_\sigma(1 - \hat{n}^f_{\boldsymbol{j},\sigma})$. $\hat{P}'$ is a positive semidefinite operator, whose minimum

(zero) eigenvalue is obtained when there is at least one f-electron on every lattice site. Using periodic boundary conditions, it can be observed that

$$\hat{H} = \sum_{\boldsymbol{i},\sigma} \hat{A}_{\boldsymbol{i},\sigma} \hat{A}^{\dagger}_{\boldsymbol{i},\sigma} + U\hat{P}' + C_1\hat{N} + C_2 = \hat{H}_{\mathrm{PAM}} \,, \tag{2}$$

if $a_{\alpha,b}$ and the constants C_i parametrise properly the parameters of $\hat{H}_{\mathrm{PAM}}$. This parametrisation fixes the phase diagram region $\mathcal{P}_H$ where the transformation $\hat{H}_{\mathrm{PAM}} = \hat{H}$ is valid, and taking into account that $\hat{A}^{\dagger}_{\boldsymbol{i},\sigma}\hat{A}^{\dagger}_{\boldsymbol{i},\sigma} = 0$, the GS inside $\mathcal{P}_H$ at 3/4 filling becomes $|\Psi_g\rangle = \prod_{\boldsymbol{i}}(\hat{A}^{\dagger}_{\boldsymbol{i},\sigma}\hat{A}^{\dagger}_{\boldsymbol{i},\sigma}\hat{F}^{\dagger}_{\boldsymbol{i}})|0\rangle$, where $\hat{F}_{\boldsymbol{i}} = \sum_{\sigma}\mu_{\boldsymbol{i},\sigma}\hat{f}_{\boldsymbol{i},\sigma}$, and $\mu_{\boldsymbol{i},\sigma}$ are arbitrary coefficients. The localised GS is obtained from $|\Psi_g\rangle$ by a proper choice of the $a_{\alpha,b}$ coefficients in forbidding neighbouring $\hat{A}^{\dagger}_{\boldsymbol{i},\sigma}\hat{A}^{\dagger}_{\boldsymbol{j},\sigma}$ operators to introduce particles in the same site of the lattice. This is obtained when $a_{\alpha,c}/a_{\alpha,f} = p$ for all α, and p is real. In this case $|\Psi_g\rangle$ transforms in $|\Psi_{\mathrm{loc}}\rangle$, whose properties are analysed in details below.

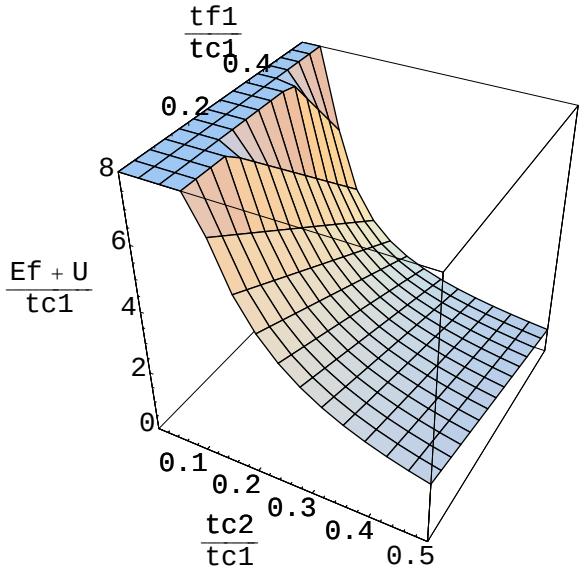

Fig. 2. The parameter space region where the described solution is present in $D = 2$ dimensions for $t_{c2}/t_{c1}, t_{f1}/t_{c1} < 1/2$. For the possible V_0/t_{c1} values see text.

The $\mathcal{P}_H$ region (in which the solutions are present) is depicted in Fig. 1(a) for 1D and Fig. 2 for 2D square-lattice case. Concerning the notations of hopping matrix elements, we use (b, n) in the lower index, $n = 1, 2$ denoting the coordination sphere. We mention that for 1D a given point of

the presented curve in Fig. 1(a) represents the plain $x + y = q|z|$ in the $(x = U/t_{c1}, y = E_f/t_{c1}, z = V_0/t_{c1})$ space, where $q = (1 - v)/\sqrt{v}$ and $v = t_{f1}/t_{c1}$. For 2D, the surface presented in Fig. 2 containing the solution extends to ∞ for $u = t_{c2}/t_{c1} \to 0$, and on the surface $|V_0/t_{c1}| = 4u\sqrt{v}$. The GS energies per site (E_g) are presented in Fig. 1(b) for 2D and Fig. 1(c) for 1D. As can be seen, the obtained behaviour is clearly D dependent: in 2D a cusp like behaviour is present in E_g at $u = 1/2$, which is absent in 1D, where the curves smoothly start from a given point of the parameter space. Leaving $\mathcal{P}_H$, the localised phase is no more defined as a GS. Inside $\mathcal{P}_H$, the GS has a large spin degeneracy and globally is paramagnetic. The GS wave function coherently controls all lattice sites and maintains constant (3) the occupation number on every lattice site, producing long-range density-density correlations and prohibits in the same time the hopping and non-local hybridization within the system. The f-electron occupancy per site exceeds one and slightly increases with v, the local f moments being present, but randomly orientated. Further development of the procedure allowing the study of the case in which not all hopping matrix elements inside the unit cell are nonzero can be found in [11]. We mention that in principle the presented solutions are representing importance even if $\mathcal{P}_{\mathcal{H}}$ is repulsive from RG point of view [12].

In conclusion, we analysed in detail the exact localized ground-states deduced for PAM at finite $U > 0$ in $D = 1, 2$ dimensions.

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