FILLING ELECTRON BANDS IN THE PERIODIC ANDERSON MODEL

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The filling sequence for correlated energy bands is investigated in the periodic Anderson model (PAM) (the Anderson model on a lattice) with strong electron-electron interaction. The approach involving correlated Hubbard sub-bands is shown to be compatible with the standard band theory approach. The structure of allowed energy bands is found for the PAM in the absence of the order parameter. The dependence of the chemical potential on the electron filling is obtained.

1. Introduction

The electron structure of a variety of narrow-band materials with appreciable electron-electron interactions is specified by the co-existence of collectivized conduction electrons and the localized electrons of unfilled atomic shells. One of the popular models covering this situation is the periodic Anderson model (the Anderson model on a lattice) (PAM). It has been used to solve various problems within approaches based on diagonalization of the one-site Hamiltonian component [1, 2], by $1/N$ expansion [3], the slave-boson technique [4], and on different forms of perturbation theory (e.g., [5]). However, the filling of energy bands by correlated electrons and the positions of their chemical potentials were not analyzed in the above approaches. This analysis is necessary when applying the method of strong coupling of correlated electrons [6] to systems described by the PAM and to clarify the problem of the Luttinger or Fermi-liquid character of the correlated electrons.

A similar problem of filling bands with electrons was studied in [7] by decoupling the equations of motion for Green’s functions in the analysis of the model proposed by Müller to describe copper-oxide superconductors. In the present paper, using the Hubbard method [8] (which coincides with the loopless approximation of the diagram method for degenerate systems [9]), we investigate the filling sequence for energy bands in the PAM in the limiting case of a narrow (as compared with level splitting) priming band of collectivized electrons. The relationship between the chemical potential of the electrons and their concentration is investigated in the paramagnetic phase.

2. Diagonalization of one-site Hamiltonians and the diagram method

The PAM Hamiltonian with hybridization of the band $(c)$ and localized $(d)$ electrons of unfilled atomic shells has the form

$$ H = H_0 + H_{\text{hopp}}, $$

$$ H_0 = \varepsilon \sum_{i\sigma} n^d_i \sigma + U \sum_i n^d_i \sigma n^d_i \sigma + V \sum_{i\sigma} (c^+_i \sigma d_i \sigma + d^+_i \sigma c_i \sigma) - \mu \sum_{i\sigma} (n^d_i \sigma + n^c_i \sigma). \quad (1) $$

$$ H_{\text{hopp}} = -t \sum_{\langle ij \rangle \sigma} c^+_i \sigma c_j \sigma, \quad U = \infty. $$

where $c^+_i \sigma$ ($c_i \sigma$) are the band electron creation (annihilation) operators with the projection of the spin $\sigma$ at the $i$th lattice site. $d^+_i \sigma$ ($d_i \sigma$) are the localized electron creation (annihilation) operators with the projection...
of the spin $\sigma$ at the $i$th site, the hybridization parameter $V$ relates the local combinations of the bands $c$ and core $d$ electrons, $t$ is the integral of band electron hopping between neighboring sites, and $\epsilon < 0$ determines the positions of one-electron $d$ levels relative to the $c$-electron band.

Corresponding to the eigenfunctions of the one-site Hamiltonian $H$.

$$|\sigma l\rangle = (\cos \varphi c^+_l - \sin \varphi d^+_l)|0\rangle, \quad |\sigma u\rangle = (\sin \varphi c^+_l + \cos \varphi d^+_l)|0\rangle,$$

$$|2l\rangle = \left(\cos \alpha c^+_l c^+_l + \frac{\sin \alpha}{\sqrt{2}}\right)|0\rangle, \quad |2u\rangle = \left(\sin \alpha c^+_l c^+_l - \frac{\cos \alpha}{\sqrt{2}}\right)|0\rangle,$$

$$|20\rangle = \frac{d^+_l + d^+_u}{\sqrt{2}}, \quad |2\sigma\rangle = c^+_l d^+_l|0\rangle, \quad |3\sigma\rangle = c^+_l c^+_l d^+_\sigma|0\rangle,$$

their eigenvalues are

$$\lambda_{\sigma l} = \frac{\epsilon - \sqrt{\epsilon^2 + 4V^2}}{2} - \mu, \quad \lambda_{\sigma u} = \frac{\epsilon + \sqrt{\epsilon^2 + 4V^2}}{2} - \mu,$$

$$\lambda_{2l} = \frac{\epsilon - \sqrt{\epsilon^2 + 8V^2}}{2} - 2\mu, \quad \lambda_{2u} = \frac{\epsilon + \sqrt{\epsilon^2 + 8V^2}}{2} - 2\mu,$$

$$\lambda_{20} = \epsilon - 2\mu, \quad \lambda_{2\sigma} = \epsilon - 2\mu, \quad \lambda_{3\sigma} = \epsilon - 3\mu,$$

$$\cos \varphi = \frac{\epsilon + \sqrt{\epsilon^2 + 4V^2}}{\sqrt{2}\epsilon^2 + 4V^2}, \quad \cos \alpha = \frac{\epsilon + \sqrt{\epsilon^2 + 4V^2}}{\sqrt{(\epsilon + \sqrt{\epsilon^2 + 4V^2})^2 + 8V^2}}.$$

Note that this means of taking the hybridization interaction into account was previously offered in an analysis of exciton states in the “black” and “gold” phases of SmS [10]. The self-energies (3) account for all characteristic electron energies. The indices $l$ and $u$ denote the lower and upper energy levels, respectively.

The generalized Hubbard (atomic) operators $X^l_q = |p\rangle\langle q|$ shift the site from the energy state $|q\rangle$ to the state $|p\rangle$ from the set (2). The diagram technique for the Hubbard operators of nondegenerate $s$ electrons is naturally generalized to the atomic operator for systems of orbitally degenerate electrons [6, 9]. It is based on the generalized Wick theorem [11] as applied to the $X$ operators of the classical Hubbard model [12–14] and then [15], by analogy, to the spin operators in the Heisenberg model [16]. We expand the one-electron operators in atomic operators as follows:

$$c^+_\sigma = \cos \varphi X^\sigma_{0l} + \sin \varphi X^\sigma_{0u} + \sigma \left(\cos \varphi \cos \alpha + \frac{\sin \varphi \sin \alpha}{\sqrt{2}}\right)X^\sigma_{2l} + \left(\cos \varphi \sin \alpha + \frac{\sin \varphi \cos \alpha}{\sqrt{2}}\right)X^\sigma_{2u} + \sigma \left(\sin \alpha \sin \varphi - \frac{\cos \alpha \cos \varphi}{\sqrt{2}}\right)X^\sigma_{3l} + \left(\sin \alpha \cos \varphi - \frac{\cos \alpha \sin \varphi}{\sqrt{2}}\right)X^\sigma_{3u} + \sigma \left(\cos \alpha \sin \varphi - \frac{\cos \alpha \cos \varphi}{\sqrt{2}}\right)X^\sigma_{4l} + \left(\sin \alpha \cos \varphi - \frac{\cos \alpha \sin \varphi}{\sqrt{2}}\right)X^\sigma_{4u},$$

$$d^+_\sigma = -\sin \varphi X^\sigma_{0l} + \cos \varphi X^\sigma_{0u} - \sigma \left(-\sin \alpha \cos \varphi \right)X^\sigma_{2l} - \sigma \left(-\cos \alpha \cos \varphi \right)X^\sigma_{2u} + \sigma \left(-\sin \alpha \sin \varphi \right)X^\sigma_{3l} + \left(-\cos \alpha \cos \varphi \right)X^\sigma_{3u} + \sigma \left(-\cos \alpha \sin \varphi \right)X^\sigma_{4l} + \left(-\sin \alpha \cos \varphi \right)X^\sigma_{4u},$$

Unlike the expansion in Hubbard $X$ operators, the expansion coefficients in (4) depend on the energy parameters of the problem. Substituting (4) into (1), we get the Hamiltonian in terms of generalized $X$