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Mott–Hubbard transition in the N-orbital Hubbard model

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Abstract

The Mott–Hubbard insulator–metal transition (MHT) is studied for the N-orbital symmetrical Hubbard model with diagonal (t_1) and non-diagonal (t_2) hopping matrix elements. In the paramagnetic state (PM) for an $n = 1$ filling the non-diagonal hopping gives rise to two wide Hubbard sub-bands with small spectral weight of the order of $\sim 1/N$ and $2N - 2$ narrow sub-bands with a large weight $\sim (1 - 1/N)$. No orbital polarization arises in this solution. In some directions in the (t_1, t_2)-plane the insulating energy gap in the density of states is closed in the vicinity of a critical Hubbard repulsion of $U_c \sim z(t_1 + (N - 1)t_2)$ (z-coordination number), whereas the narrow bands in this region of parameters still correspond to a deeply correlated phase (with bandwidth $z(t_1 - t_2)$).

Keywords: Hubbard model; Mott–Hubbard transition; d^1 systems

The properties of the classical Hubbard model [1], describing an s-band of width W with an on-site Coulomb repulsion U, are determined by two parameters: U/W and the electron density n (number of electrons per atom). The metal–insulator Mott–Hubbard transition (MHT) may occur only for a half-filled band, $n = 1$. For this case one can expect that a MHT takes place at $U/W \simeq 1$, with slight variations depending on the lattice. This is indeed shown in the original work by Hubbard [2] $U_c = \sqrt{3}/2 \cdot W$. In nature the strongly correlated electron systems (SCES) occur for d- and f-systems, where the number of orbitals $N = 2l + 1$ is 5 and 7. The generalization to many orbitals rather than s-shell introduces two additional parameters: (a) the number of orbitals N and (b) the matrix element of *non-diagonal* hopping. Therefore, the question arises, how these additional parameters change the physics of the MHT in SCES in comparison with the Hubbard model for an s-band. We consider here the MHT physics with the perturbation theory from the atomic limit and show that the approximation, taking into account the fluctuations of the population numbers, contains a MHT. We will not address the magnetic aspect of the problem, but rather present an attempt to first get an answer for the easiest case, namely, for the paramagnetic state with $n = 1$ filling.

Let us consider the following symmetrical model:

$$\mathscr{H} = \sum U \hat{n}_{i,\lambda} \hat{n}_{i,\nu} (1 - \delta_{\lambda,\nu}) + \sum t_{ij}^{\lambda,\nu} f_{i,\lambda}^{\dagger} f_{j,\nu},$$

where i, j are site indices, $\lambda = (m_l, \sigma_\lambda)$ are orbitals, $\hat{n}_{i,\lambda} = f_{i,\lambda}^{\dagger} f_{i,\lambda}$ and $t^{\lambda,\nu} = \delta_{\lambda,\nu} t_1 + (1 - \delta_{\lambda,\nu}) \delta_{\sigma_\lambda,\sigma_\nu} t_2$. We will start from the limit $U \gg t_1, t_2$ and search for MHT by increasing the corresponding bandwidths w_1 and w_2. If we put U to zero the Hamiltonian gives rise to a degenerate narrow band, with bandwidth $z(t_1 - t_2)$, and a wide band, with bandwidth $z(t_1 + (N - 1)t_2$. Assuming that the transition takes place at $U/W \sim 1$ we have a simple estimation of the critical U_c of $z(t_1 + (N - 1)t_2$. When $U \neq 0$ the bands are split. A convenient tool for developing a perturbation theory from atomic limit is the diagram technique for the Hubbard operators [3]. The latter was introduced by Hubbard [1,4] describing many electron intra-ion transitions in the following way: $\mathscr{H}(U)|p\rangle = E_p|p\rangle, X^{p,q} = |p\rangle\langle q|$, where in the present case of interest $p = 0, \gamma, \Gamma, \Lambda$; $\gamma = (m_l, \sigma)$, $|\Gamma\rangle = |\gamma, \gamma'\rangle$, $|\Lambda\rangle = |\gamma, \gamma', \gamma''\rangle$. Therefore, the

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Matsubara's Green's functions (GF) for fermions $F_{\gamma,\gamma'}(i\omega_n) = \langle T_\tau \hat{f}_\gamma(\tau)\hat{f}^\dagger_{\gamma'}(\tau')\rangle_{i\omega_n}$ in this limit is also split into a series of X-operator GF $G_{a,-b}(\tau,\tau') = \langle T_\tau X^a(\tau)X^{-b}(\tau')\rangle$, describing the partial transitions $\boldsymbol{a} = (p, q)$, $\boldsymbol{b} = (p', q')$, $-\boldsymbol{b} = (q', p')$. The zero X-operator GF are $G^0_{[(p,q)(q',p')]}(i\omega_n) = \delta_{qq'}\delta_{pp'}[i\omega_n - \Delta^0_{q,p}]^{-1}\cdot(N^0_p + N^0_q)$, where $\Delta^0_{q,p} = E^0_q - E^0_p$, $(p, q) = (0, \gamma)$, (γ, Γ), (Γ, Λ) and $(q', p') = (\gamma, 0)$, (Γ, γ), (Λ, Γ). The population numbers are $N^0_p = \langle X^{pp}\rangle^{(0)} = Z_0^{-1}e^{-(E^0_p - n_p\mu)/T}$, $Z_0 = \sum_p e^{-(E^0_p - n_p\mu)/T}$. Due to the fact that $U \gg T$ and the absence of the exchange shifts of bands in the paramagnetic state N^0_p actually do not depend on temperature T and are numbers, which can be found from the sum rules and the filling of the bands.

It is known from the original Hubbard work [1,2], that the Hubbard I approximation is unable to describe the Mott insulator–metal transition. For this reason we consider the one-loop approximation. In the paramagnetic state for the filling $n_e = 1$ all the Green's Functions (GF), describing $(0, \gamma)$-transitions, coincide. The same is valid for the upper sub-band. Therefore, the zero-order fermion GF is

$$F^0 = \frac{\alpha/2}{i\omega + U/2} + \frac{1-\alpha/2}{i\omega - U/2}.$$

Here $\alpha \equiv 1/N$ and the reference point on the energy axis is shifted to the middle of the gap. We introduce the locator $L^{a,-b}$, describing single-site transitions $(\boldsymbol{a}, -\boldsymbol{b})$, as an irreducible graphical element, which cannot be separated into two unlinked parts by cutting the interaction line , i.e. in our case, the hopping. The loop correction to the locator gives $\hat{G}(\boldsymbol{p}, i\omega) = [\hat{1} - \hat{L}(i\omega)\cdot\hat{t}(\boldsymbol{p})]^{-1}\cdot\hat{L}(i\omega)$. It is convenient to define the locator for the fermion GF as follows: $F^{(0)}_{\nu\mu}(i\omega_n) = \sum_{a,-b}(f_\nu)_a(f^\dagger_\mu)_{-b}L_{a,-b}(i\omega_n)$. Then one can write for the fermion GF $F_{\nu\mu}(\boldsymbol{k}, i\omega_n) = F^{(0)}_{\nu\mu}(i\omega_n) + F^{(0)}_{\nu\mu}(i\omega_n)t_{\mu'\mu''}(\boldsymbol{k})F_{\mu''\mu}(\boldsymbol{k}, i\omega_n)$. Only a diagonal, $L^{(F)}_1(i\omega_n)$, and a non-diagonal, $L^{(F)}_2(i\omega_n)$, fermion locator arises. Therefore, we find

$$F_1(\boldsymbol{k}, i\omega) = \alpha\frac{L^{(F)}_1}{1 - T_{1k}L^{(F)}_1} + (1-\alpha)\frac{L^{(F)}_2}{1 - T_{2k}L^{(F)}_2} \qquad (1)$$

and

$$F_2(\boldsymbol{k}, i\omega) = \alpha\left(\frac{L^{(F)}_1}{1 - T_{1k}L^{(F)}_1} - \frac{L^{(F)}_2}{1 - T_{2k}L^{(F)}_2}\right). \qquad (2)$$

Here $T_{1k} = t_{1k} + (N-1)t_{2k}$, $T_{2k} = t_{1k} - t_{2k}$. Using $L_i = F^0$ gives the GF in the Hubbard I approximation [1,4]. Below we perform the calculations for the model when $t_{ik} = t_i\gamma_k$, $i = 1, 2$. Using renormalized hopping $(T_{rp} \to \tilde{T}_{rp} = T_{rp}/[1 - L(i\omega_n)T_{rp}])$ in Eqs. (1) and (2), we have a system of self-consistent equations which can be solved iteratively to give the density of states. The loop correction is responsible for the non-zero imaginary part of the self-energy, which gives states inside of the gap. The density of electronic states, obtained from the self-consistent solution of this system of equations for an elliptic bare density of states, is presented in Fig. 1. Due to the small spectral weight $\sim 1/N$ the wide band in the upper panel is seen as a solid line at the x-axis, in the lower panel it is shown in a magnified form.

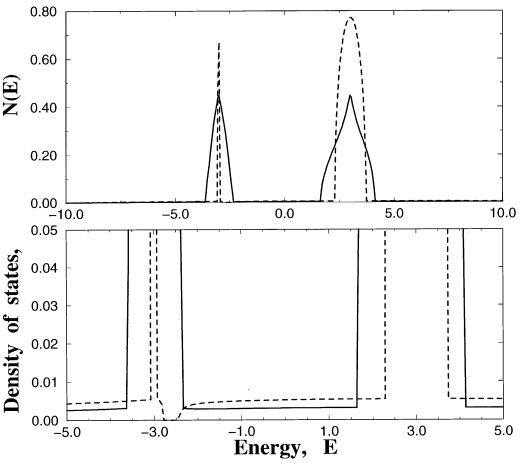

Fig. 1. DOS for $N = 5$, $U = 6.0$, $w_1 = 1.0$ and $w_2 = 2.5$ in Hubbard-I approximation (dashed line), and in one-loop approximation (solid line). In the lower panel a magnified part of the upper panel is shown. In the one-loop approximation the correlation gap is closed.

Thus, the non-diagonal hopping in the many-orbital system can give an essential increase to the bandwidth of the fully symmetrical band. This favors the metallic state (or making U_c larger). This observation leads to the conclusion, that in the metallic phase a *part of the strongly correlated electrons can be considered as weakly correlated*, since in this sub-band the electrons do not experience the correlation gap. At the same time the electrons in all the other sub-bands remain in the strong coupling regime. However, in order to reproduce the central peak [5] in the DOS in the region $U/W_1 < 1$ the approximation used should be improved.

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