STRUCTURE OF ESSENTIAL SPECTRA AND DISCRETE SPECTRUM OF THE ENERGY OPERATOR OF FOUR ELECTRON SYSTEMS IN THE IMPURITY HUBBARD MODEL. THIRD TRIPLET STATE

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Рассматривается четырехэлектронная система в примесной модели Хаббарда. Описана структура существенного спектра и дискретный спектр в этой модели в случае третьего триплетного состояния. Доказывается, что, в одномерном случае, существенный спектр системы есть объединение не более чем шестнадцать отрезков, а дискретный спектр системы состоит из не более одиннадцать собственного значение.

Ключевые слова: модель Хаббарда, примесной модель Хаббарда, четырехэлектронная система, триплетное состояние, существенный спектр, дискретный спектр.

We consider of the energy operator of four electron systems in the Impurity Hubbard model and investigated the structure of essential spectra and discrete spectrum of the system in the third triplet state. We proved, that the if $\nu = 1$, then the essential spectra of the operator is consists of the union of no mote than sixteen segments, and discrete spectrum of the operator is consists of no more then eleven eigenvalues.

Keywords: Hubbard model, Impurity Hubbard model, four electron systems, triplet state, essential spectra, discrete spectrum.

The Hubbard model and impurity Hubbard model is currently one of the most extensively studied multielectron models of metals [1,2]. But little is known about exact results for the spectrum and wave functions of the crystal described by the Hubbard model, and obtaining the corresponding statements is great interest problem.

We consider the energy operator H of four-electron systems in the Impurity Hubbard model, where $H = A \sum_{m,\gamma} a_{m,\gamma}^+ a_{m,\gamma} + B \sum_{m,\tau,\gamma} a_{m,\gamma}^+ a_{m+\tau,\gamma} + U \sum_m a_{m,\uparrow}^+ a_{m,\uparrow} a_{m,\downarrow}^+ a_{m,\downarrow} + (A_0 - A) \sum_{\gamma} a_{0,\gamma}^+ a_{0,\gamma} + (B_0 - B) \sum_{\tau,\gamma} (a_{0,\gamma}^+ a_{\tau,\gamma} + a_{\tau,\gamma}^+ a_{0,\gamma}) + (U_0 - U) a_{0,\uparrow}^+ a_{0,\uparrow} a_{0,\downarrow}^+ a_{0,\downarrow}$. Here A (A_0) is the electron energy at

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a regular (impurity) lattice site, B (B_0) is the transfer integral between (between electron and impurities) neighboring sites (we assume that $B > 0$ ($B_0 > 0$) for convenience), $\tau = \pm e_j$, $j = 1, 2, \dots, \nu$, where e_j are unit mutually orthogonal vectors, which means that summation is taken over the nearest neighbors, U (U_0) is the parameter of the on-site Coulomb interaction of two electrons in the regular (impurity) sites, γ is the spin index, $\gamma = \uparrow$ or $\gamma = \downarrow$, and $a_{m,\gamma}^+$ and $a_{m,\gamma}$ are the respective electron creation and annihilation operators at a site $m \in Z^\nu$.

In the four electron systems has a quintet state, and two type singlet state, and three type triplet states. The third triplet state corresponds to the free motion of four electrons over the lattice and their interactions with the basic functions: ${}^3t_{p,q,r,t \in Z^\nu}^1 = a_{p,\uparrow}^+ a_{q,\downarrow}^+ a_{r,\uparrow}^+ a_{t,\uparrow}^+ \varphi_0$. The subspace ${}^3\tilde{\mathcal{H}}_t^1$, corresponding to the third triplet state is the set of all vectors of the form ${}^3\psi_t^1 = \sum_{p,q,r,t \in Z^\nu} f(p, q, r, t) {}^3t_{p,q,r,t}^1$, $f \in l_2^{as}$, where l_2^{as} is the subspace of antisymmetric functions in $l_2((Z^\nu)^4)$. In this case, the Hamiltonian H acts in the antisymmetric Fock space $\tilde{\mathcal{H}}_{as}$. Let φ_0 be the vacuum vector in the antisymmetrical Fock space $\tilde{\mathcal{H}}_{as}$. Let ${}^3\tilde{H}_t^1$ be the restriction H to the subspace ${}^3\tilde{\mathcal{H}}_t^1$.

Theorem 1. *The subspace ${}^3\mathcal{H}_1^t$ is invariant under the operator H , and the operator ${}^3H_1^t$ is a bounded self-adjoint operator. It generates a bounded self-adjoint operator ${}^3\bar{H}_1^t$ acting in the space l_2^{as} .*

We set ${}^3\tilde{H}_1^t = \mathcal{F} {}^3\bar{H}_1^t \mathcal{F}^{-1}$. In the quasimomentum representation, the operator ${}^3\tilde{H}_1^t$ acts in the Hilbert space $L_2^{as}((T^\nu)^4)$.

Theorem 2. *Let $\nu = 1$, and $\varepsilon_2 = -B$, and $\varepsilon_1 < -2B$ (respectively, $\varepsilon_2 = -B$, and $\varepsilon_1 > 2B$). Then the essential spectrum of the operator ${}^3\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$: $\sigma_{ess}({}^3\tilde{H}_1^t) = [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \cup [A - 2B + z + z_3, A + 2B + z + z_3] \cup [A - 2B + z + z_4, A + 2B + z + z_4]$, and the discrete spectrum of operator ${}^3\tilde{H}_1^t$ is consists of no more three eigenvalues: $\sigma_{disc}({}^3\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\}$, where $z = A + \varepsilon_1$, and z_3 and z_4 are the additional eigenvalues of operator ${}^3\tilde{H}_1^t$.*

Theorem 3. *If $\nu = 1$, and $-2B < \varepsilon_2 < 0$, then the essential spectrum of the operator ${}^3\tilde{H}_1^t$ is consists of the union of N_1 segments, where $1 \leq N_1 \leq 3$: $\sigma_{ess}({}^3\tilde{H}_1^t) = [4A - 8B, 4A + 8B] \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4]$, and the discrete spectrum of operator ${}^3\tilde{H}_1^t$ is empty set.*

Theorem 4. *Let $\nu = 1$, and $\varepsilon_2 > 0$, and $-\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} < \varepsilon_1 < \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, then the essential spectrum of the operator ${}^3\tilde{H}_1^t$ is consists of the union of the N_1 segment, where $10 \leq N_1 \leq 16$: $\sigma_{ess}({}^3\tilde{H}_1^t) = [4A - 8B, 4A + 8B] \cup$*

$[3A - 6B + z_1, 3A - 6B + z_1] \cup [3A - 6B + z_2, 3A - 6B + z_2] \cup [2A - 4B + 2z_1, 2A + 4B + 2z_1] \cup [2A - 4B + 2z_2, 2A + 4B + 2z_2] \cup [2A - 4B + z_1 + z_2, 2A + 4B + z_1 + z_2] \cup [A - 2B + 3z_1, A + 2B + 3z_1] \cup [A - 2B + 3z_2, A + 2B + 3z_2] \cup [A - 2B + 2z_1 + z_2, A + 2B + 2z_1 + z_2] \cup [A - 2B + z_1 + 2z_2, A + 2B + z_1 + 2z_2] \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [A - 2B + z_1 + z_3, A + 2B + z_1 + z_3] \cup [A - 2B + z_2 + z_3, A + 2B + z_2 + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \cup [A - 2B + z_1 + z_4, A + 2B + z_1 + z_4] \cup [A - 2B + z_2 + z_4, A + 2B + z_2 + z_4]$ and discrete spectrum of the operator ${}^3\tilde{H}_1^t$ is consists of N_2 eigenvalues, where $5 \leq N_2 \leq 11 : \sigma_{disc}({}^3\tilde{H}_1^t) = \{4z_1, 4z_2, 3z_1 + z_2, z_1 + 3z_2, 2z_1 + 2z_2, 2z_1 + z_3, z_1 + z_2 + z_3, 2z_2 + z_3, 2z_1 + z_4, z_1 + z_2 + z_4, 2z_2 + z_4\}$.

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