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СПЕКТР ПЯТИ-ЭЛЕКТРОННЫХ СИСТЕМ В МОДЕЛИ ХАББАРДА

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Исследуется структура существенного спектра и дискретный спектр оператора энерги пяти-электронных систем в модели Хаббарда для первых и вторых дублетных состояний. Доказывается, что спектры этих двух дублетных состояний различные.

Ключевые слова: модель Хаббарда, пяти-электронных систем, существенный спектр, дискретный спектр, дублетное состояние, секстетное состояние, квартетное состояние, пяти-электронных связанных состояний, пяти-электронных антисвязанных состояний..

SPECTRA OF FIVE-ELECTRON SYSTEMS IN THE HUBBARD MODEL

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We investigated the structure of essential spectra and discrete spectrum of five-electron systems in the Hubbard model in the first and second doublet states. We proved the spectra of this two doublet states is different.

Keywords: Hubbard model, five-electron system, essential spectra, discrete spectrum, doublet state, sextet state, quartet state, five-electron bound state, five-electron anti-bound state.

Introduction

The Hubbard model is currently one of the most extensively studied multielectron models of metals. 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 therefore of great interest. The spectrum and wave functions of the system of two electrons in a crystal described by the Hubbard Hamiltonian were studied in [1]. The structure of essential spectrum and discrete spectra of the energy operator of three-electron and four-electron systems in the Hubbard model were investigated in the work [2, 3]. We consider the energy operator of five-electron systems in the Hubbard model and described the structure of essential spectrum and discrete spectra of the system in the doublet states. Hamiltonian of considering system has the form

$$H = A\sum_{m,\gamma} a^{+}_{m,\gamma}a_{m,\gamma} + B\sum_{m,\tau,\gamma} a^{+}_{m,\gamma}a_{m+\tau,\gamma} + U\sum_{m} a^{+}_{m,\uparrow}a_{m,\uparrow}a^{+}_{m,\downarrow}a_{m,\downarrow}.$$

Here, A is the electron energy at a lattice site, B is the transfer integral between neighboring sites (we assume that $B > 0$ for convenience), τ which means that summation is taken over the nearest neighbors, U is the parameter of the on-site Coulomb interaction of two electrons, γ is the spin index, 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 five-electron systems exists five type doublet states. The Hamiltonian H acts in the antisymmetric Fo'ck space $\mathcal{H}_{as}$. Let φ_0 be the vacuum vector in the space $\mathcal{H}_{as}$.

Main results

The first doublet state corresponds the basis functions ${}^1d^{1/2}_{m,n,p,q,r} = a^+_{m,\downarrow}a^+_{n,\downarrow}a^+_{p,\uparrow}a^+_{q,\uparrow}a^+_{r,\uparrow}\varphi_0$. The subspace ${}^1\widetilde{\mathcal{H}}^d_{1/2}$, corresponding to the first doublet state is the set of all vectors of the form ${}^1\psi^d_{1/2} = \sum_{m,n,p,q,r\in Z^\nu} \widetilde{f}(m,n,p,q,r){}^1d^{1/2}_{m,n,p,q,r}$, $\widetilde{f} \in l^{as}_2$, where l^{as}_2 is the subspace of antisymmetric functions in the space $l_2((Z^\nu)^5)$.

Theorem 1. *The subspace* ${}^1\widetilde{\mathcal{H}}^d_{1/2}$ *is invariant under the operator* H, *and the restriction* ${}^1H^d_{1/2}$ *of* H *to the subspace* ${}^1\widetilde{\mathcal{H}}^d_{1/2}$ *is a bounded self-adjoint operator. It generates a bounded self- adjoint operator* ${}^1\overline{H}^d_{1/2}$, *acting in the space* l^{as}_2.

In the quasimomentum representation, the operator ${}^1\overline{H}^d_{1/2}$ acts in the Hilbert space $L^{as}_2((T^\nu)^5)$ as $({}^1\widetilde{H}^d_{1/2}\widetilde{f})(\lambda,\mu,\gamma,\theta,\eta) = \{5A + 2A\sum_{i=1}^\nu[\cos\lambda_i + \cos\mu_i + \cos\gamma_i + \cos\theta_i + \cos\eta_i]\}\widetilde{f}(\lambda,\mu,\gamma,\theta,\eta) + U\int_{T^\nu}[\widetilde{f}(s,\mu,\lambda+\gamma-s,\theta,\eta) + \widetilde{f}(s,\mu,\gamma,\lambda+\theta-s,\eta) + +\widetilde{f}(s,\mu,\gamma,\theta,\lambda+\eta-s) + \widetilde{f}(\lambda,s,\mu+\gamma-s,\theta,\eta) + \widetilde{f}(\lambda,s,\gamma,\mu+\theta-s,\eta) + \widetilde{f}(\lambda,s,\gamma,\theta,\mu+\eta-s)]ds$, where L^{as}_2 is the subspace of antisymmetric functions in $L_2((T^\nu)^5)$.

Theorem 2. *Let* $\nu = 1$ *and* $U < 0$. *Then the essential spectrum of operator* ${}^1\widetilde{H}^d_{1/2}$ *is the union of four segments and the discrete spectrum is empty.*

Let $\nu = 3$, $\Lambda_1 = \lambda+\gamma$, $\Lambda_2 = \mu+\theta$, $\Lambda_i = (\Lambda^0_i, \Lambda^0_i, \Lambda^0_i), i = 1,2;$

Theorem 3. *a). If* $U < -\frac{6B\cos\frac{\Lambda^0_1}{2}}{W}, \cos\frac{\Lambda^0_1}{2} > \cos\frac{\Lambda^0_2}{2}$, *or* $U < -\frac{6B\cos\frac{\Lambda^0_2}{2}}{W}$, $\cos\frac{\Lambda^0_1}{2} < \cos\frac{\Lambda^0_2}{2}$, *then the essential spectrum of operator* ${}^1\widetilde{H}^d_{1/2}$ *is the union of four segments and the discrete spectrum of operator* ${}^1\widetilde{H}^d_{1/2}$ *is empty.*

b). If $-\frac{6B\cos\frac{\Lambda^0_1}{2}}{W} \le U < -\frac{6B\cos\frac{\Lambda^0_2}{2}}{W}, \cos\frac{\Lambda^0_1}{2} > \cos\frac{\Lambda^0_2}{2}$, *or* $-\frac{6B\cos\frac{\Lambda^0_2}{2}}{W} \le U <$

$-\frac{6B\cos\frac{\Lambda_1^0}{2}}{W}, \cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, *then the essential spectrum of operator* ${}^1\widetilde{H}^d_{1/2}$ *is the union of two segments and the discrete spectrum of operator* ${}^1\widetilde{H}^d_{1/2}$ *is empty.*

c). If $-\frac{6B\cos\frac{\Lambda_1^0}{2}}{W} \leq U < 0, \cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$ *or* $-\frac{6B\cos\frac{\Lambda_2^0}{2}}{W} \leq U < 0, \cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$, *then the essential spectrum of* ${}^1\widetilde{H}^d_{1/2}$ *is the single segment and the discrete spectrum of operator* ${}^1\widetilde{H}^d_{1/2}$ *is empty.*

The basis functions ${}^2d^{1/2}_{m,n,p,q,r} = a^+_{m,\downarrow}a^+_{n,\uparrow}a^+_{p,\downarrow}a^+_{q,\uparrow}a^+_{r,\uparrow}\varphi_0$ corresponds to the second doublet state. The subspace ${}^2\widetilde{\mathcal{H}}^d_{1/2}$, corresponding to the second doublet state is the set of all vectors of the form ${}^2\psi^d_{1/2} = \sum_{m,n,p,q,r\in Z^\nu}\widetilde{f}(m,n,p,q,r){}^2d^{1/2}_{m,n,p,q,r}$. Denote ${}^2H^d_{1/2}$ the restriction of operator H to the subspace ${}^2\mathcal{H}^d_{1/2}$. Let $\Lambda_1 = \lambda + \mu$, $\Lambda_2 = \gamma + \theta$.

Theorem 4. *If* $\nu = 1$ *and* $U < 0$, *then the essential spectra of the operator* ${}^2H^d_{1/2}$ *is the union of seven segments and the discrete spectrum of operator* ${}^2H^d_{1/2}$ *is consists of no more one point.*

Let $\nu = 3$, $\Lambda_3 = \lambda + \mu$, $\Lambda_4 = \gamma + \theta$, $\Lambda_j = (\Lambda_j^0, \Lambda_j^0, \Lambda_j^0), j = 3, 4$.

Theorem 5.

a). If $\nu = 3$ *and* $U < -\frac{3B}{W}$, $\cos\frac{\Lambda_3^0}{2} < \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} > \cos\frac{\Lambda_4^0}{2}$, *or* $U < -\frac{3B}{W}$, $\cos\frac{\Lambda_4^0}{2} < \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} < \cos\frac{\Lambda_4^0}{2}$, *or* $U < -\frac{6B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_3^0}{2} > \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} > \cos\frac{\Lambda_4^0}{2}$, *then the essential spectra of operator* ${}^2H^d_{1/2}$ *is the union of seven segments and the discrete spectrum of operator* ${}^2H^d_{1/2}$ *is consists of no more one point.*

b). If $\nu = 3$ *and* $-\frac{3B}{W} \leq U < -\frac{6B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_3^0}{2} < \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} \geq \cos\frac{\Lambda_4^0}{2}$, *or* $-\frac{6B\cos\frac{\Lambda_3^0}{2}}{W} \leq U < -\frac{3B}{W}$, $\cos\frac{\Lambda_3^0}{2} > \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} > \cos\frac{\Lambda_4^0}{2}$, *or* $-\frac{6B\cos\frac{\Lambda_4^0}{2}}{W} \leq U < -\frac{3B}{W}$, $\cos\frac{\Lambda_4^0}{2} > \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} < \cos\frac{\Lambda_4^0}{2}$, *or* $-\frac{6B\cos\frac{\Lambda_3^0}{2}}{W} \leq U < -\frac{6B\cos\frac{\Lambda_4^0}{2}}{W}$, $\cos\frac{\Lambda_3^0}{2} > \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} > \cos\frac{\Lambda_4^0}{2}$, *then the essential spectra of operator* ${}^2H^d_{1/2}$ *is the union of four segments and the discrete spectrum of* ${}^2H^d_{1/2}$ *is empty.*

c). If $-\frac{6B\cos\frac{\Lambda_3^0}{2}}{W} \leq U < -\frac{6B\cos\frac{\Lambda_4^0}{2}}{W}$, $\cos\frac{\Lambda_3^0}{2} < \frac{1}{2}$, *or* $-\frac{3B}{W} \leq U < -\frac{6B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_3^0}{2} < \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} < \cos\frac{\Lambda_4^0}{2}$, *or* $-\frac{6B\cos\frac{\Lambda_4^0}{2}}{W} \leq U < -\frac{3B}{W}$, $\cos\frac{\Lambda_4^0}{2} < \frac{1}{2}$, *then the essential spectra of operator* ${}^2H^d_{1/2}$ *is the union of two segments and the discrete spectrum of operator* ${}^2H^d_{1/2}$ *is empty.*

d). If $-\frac{6B\cos\frac{\Lambda_4^0}{2}}{W} \leq U < 0$, $\cos\frac{\Lambda_4^0}{2} < \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} > \cos\frac{\Lambda_4^0}{2}$, *or* $-\frac{6B\cos\frac{\Lambda_3^0}{2}}{W} \leq$

$U < 0$, $\cos\frac{\Lambda_3^0}{2} < \frac{1}{2}$, $\cos\frac{\Lambda_3^0}{2} < \cos\frac{\Lambda_4^0}{2}$, or $-\frac{3B}{W} \leq U < 0$, $\cos\frac{\Lambda_3^0}{2} > \cos\frac{\Lambda_4^0}{2}$, $\cos\frac{\Lambda_4^0}{2} > \frac{1}{2}$, then the essential spectra of operator ${}^2H_{1/2}^d$ is single segment and the discrete spectrum of ${}^2H_{1/2}^d$ is empty.

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