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Структура существенного спектра и дискретный спектр оператора энергии шести электронных систем в модели Хаббарда. Первое синглетное состояние[1]

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Рассматривается оператор энергии шести электронных систем в модели Хаббарда и исследуется структура существенного спектра и дискретный спектр системы в одно из синглетных состояний. Показано, что в одномерном случае, существенный спектр системы в рассматриваемом случае, состоит из объединений семьи отрезков, а дискретный спектр системы состоит из не более одного собственного значение. В трехмерном случае, либо существенный спектр системы состоит из объединений семьи отрезков, а дискретный спектр системы состоит из не более одного собственного значения, либо существенный спектр системы есть объединений четырех отрезков, а дискретный спектр системы пуст, либо существенный спектр системы есть объединений двух отрезков, а дискретный спектр системы пуст, либо существенный спектр системы состоит из единственного отрезка, а дискретный спектр системы пуст.

Ключевые слова: модель Хаббарда, шести электронная система, существенный спектр, дискретный спектр, синглетное состояние.

Structure of essential spectra and discrete spectrum of the energy operator of six-electron systems in the Hubbard model. First Singlet state[1]

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We consider of the energy operator of six electron systems in the Hubbard model and investigated the structure of essential spectra and discrete spectrum of the system in the first singlet state. Show to in the one-dimensional case, the essential spectra of the system is consists of the union of seven segments, and discrete spectrum of the system is consists of no more than one eigenvalue. In the three-dimensional case, or the essential spectra of the system is consists of the union of seven segments, and discrete spectrum of the system is consists of no more than one eigenvalue, or the essential spectra of the system is consists of the union of four segments, and discrete spectrum of the system is empty set, or the essential spectra of the system is consists of the union of two segments, and discrete spectrum of the system is empty set, or the essential spectra of the system is consists of single segment, and discrete spectrum of the system is empty set.

Keywords: Hubbard model, six-electron system, essential spectra, discrete spectrum, singlet state.

Introduction

In the early 1970s, paper [1], where a simple model of a metal was proposed that has become a fundamental model in the theory of strongly correlated electron systems. The model proposed in [1] was called the Hubbard model after John Hubbard, who made a fundamental contribution to studying the statistical mechanics of that system. The Hubbard model is currently one of the most extensively studied multielectron models of metals [2]. Therefore, obtaining exact results for the spectrum and wave functions of the crystal described by the Hubbard model is 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 [2]. The spectrum and wave functions of the system of three and four electrons in a crystal described by the Hubbard Hamiltonian were studied in [3] and [4]. The spectrum and wave functions of the system of five electrons in a crystal described by the Hubbard Hamiltonian were studied in [5].

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 six-electron systems exists singlet and triplet and quintet and octet 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 singlet state corresponds the basis functions ${}^1s^0_{m,n,p,q,r,t} = a^{+}_{m,\uparrow}a^{+}_{n,\uparrow}a^{+}_{p,\uparrow}a^{+}_{q,\downarrow}a^{+}_{r,\downarrow}a^{+}_{t,\downarrow}\varphi_0$. The subspace ${}^1\widetilde{\mathcal{H}}^s_0$, corresponding to the first singlet state is the set of all vectors of the form ${}^1\psi^s_0 = \sum_{m,n,p,q,r,t\in Z^{\nu}} \widetilde{f}(m,n,p,q,r,t)^1 s^0_{m,n,p,q,r,t}$, $\widetilde{f} \in l^{as}_2$, where l^{as}_2 is the subspace of antisymmetric functions in the space $l_2((Z^{\nu})^6)$.

Theorem 1. *The subspace ${}^1\widetilde{\mathcal{H}}^s_0$ is invariant under the operator H, and the restriction ${}^1H^s_0$ of H to the subspace ${}^1\widetilde{\mathcal{H}}^s_0$ is a bounded self-adjoint operator. It generates a bounded self- adjoint operator ${}^1\overline{H}^s_0$, acting in the space l^{as}_2.*

In the quasimomentum representation, the operator ${}^1\overline{H}^s_0$ acts in the Hilbert space $L^{as}_2((T^{\nu})^6)$ as $({}^1\widetilde{H}^s_0\widetilde{f})(\lambda,\mu,\gamma,\theta,\eta,\xi) = \{6A + 2A\sum_{i=1}^{\nu}[\cos\lambda_i +$

$\cos\mu_i+\cos\gamma_i+\cos\theta_i+\cos\eta_i+\cos\xi_i]\}\widetilde{f}(\lambda,\mu,\gamma,\theta,\eta,\xi)+U\int_{T^\nu}[\widetilde{f}(s,\mu,\gamma,\lambda+\theta-s,\eta,\xi)+\widetilde{f}(s,\mu,\gamma,\theta,\lambda+\eta-s,\xi)+\widetilde{f}(s,\mu,\gamma,\theta,\eta,\lambda+\xi-s)+\widetilde{f}(\lambda,s,\gamma,\mu+\theta-s,\theta,\xi)+\widetilde{f}(\lambda,s,\gamma,\theta,\mu+\eta-s,\xi)+\widetilde{f}(\lambda,s,\gamma,\theta,\eta,\mu+\xi-s)+\widetilde{f}(\lambda,\mu,s,\gamma+\theta-s,\eta,\xi)+\widetilde{f}(\lambda,\mu,s,\theta,\gamma+\eta-s,\xi)+\widetilde{f}(\lambda,\mu,s,\theta,\eta,\gamma+\xi-s)]ds$, where L_2^{as} is the subspace of antisymmetric functions in $L_2((T^\nu)^6)$.

Theorem 2. *Let* $\nu=1$ *and* $U<0$. *Then the essential spectrum of operator* ${}^1\widetilde{H}_0^s$ *is the union of seven segments:* $\sigma_{ess}({}^1\widetilde{H}_0^s)=[a+c+e,b+d+f]\cup[a+c+z_3,b+d+z_3]\cup[a+e+z_2,b+f+z_2]\cup[a+z_2+z_3,b+z_2+z_3]\cup[c+e+z_1,d+f+z_1]\cup[c+z_1+z_3,d+z_1+z_3]\cup[e+z_1+z_2,f+z_1+z_2]$, *and the discrete spectrum of operator* ${}^1\widetilde{H}_0^s$ *is consists of no more one eigenvalue:* $\sigma_{disc}({}^1\widetilde{H}_0^s)=\{z_1+z_2+z_3\}$, *or* $\sigma_{disc}({}^1\widetilde{H}_0^s)=\emptyset$, *here and hereafter* $a=2A-4B\cos\frac{\Lambda_1}{2}$, $b=2A+4B\cos\frac{\Lambda_1}{2}$, $c=2A-4B\cos\frac{\Lambda_2}{2}$, $d=2A+4B\cos\frac{\Lambda_2}{2}$, $e=2A-4B\cos\frac{\Lambda_3}{2}$, $f=2A+4B\cos\frac{\Lambda_3}{2}$, *and* $z_1=2A-\sqrt{9U^2+16B^2\cos^2\frac{\Lambda_1}{2}}$, $z_2=2A+\sqrt{9U^2+16B^2\cos^2\frac{\Lambda_2}{2}}$, $z_3=2A-\sqrt{U^2+16B^2\cos^2\frac{\Lambda_3}{2}}$.

Let $\nu=3$, $\Lambda_1=\lambda+\mu$, $\Lambda_2=\gamma+\theta$, $\Lambda_3=\eta+\xi$, and $\Lambda_i=(\Lambda_i^0,\Lambda_i^0,\Lambda_i^0), i=1,2,3$;

Theorem 3. *a). If* $U<0$, *and* $U<-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W},\cos\frac{\Lambda_1^0}{2}>\cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2}>3\cos\frac{\Lambda_3^0}{2}$, *or* $U<-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2}<\cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_2^0}{2}>3\cos\frac{\Lambda_3^0}{2}$, *or* $U<-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}$, *and* $\cos\frac{\Lambda_1^0}{2}<3\cos\frac{\Lambda_3^0}{2}$, *then the essential spectrum of operator* ${}^1\widetilde{H}_0^s$ *is consists of the union of seven segments:* $\sigma_{ess}({}^1H_0^s)=[a_1+c_1+e_1,b_1+d_1+f_1]\cup[a_1+c_1+z_3^{'},b_1+d_1+z_3^{'}]\cup[a_1+e_1+z_2^{'},b_1+f_1+z_2^{'}]\cup[a_1+z_2^{'}+z_3^{'},b_1+z_2^{'}+z_3^{'}]\cup[c_1+e_1+z_1^{'},d_1+f_1+z_1^{'}]\cup[c_1+z_1^{'}+z_3^{'},d_1+z_1^{'}+z_3^{'}]\cup[e_1+z_1^{'}+z_2^{'},f_1+z_1^{'}+z_2^{'}]$, *and discrete spectrum of operator* ${}^1\widetilde{H}_0^s$ *of no more one eigenvalue:* $\sigma_{disc}({}^1H_0^s)=\{z_1^{'}+z_2^{'}+z_3^{'}\}$, *or* $\sigma_{disc}({}^1H_0^s)=\emptyset$. *Here, and hereafter* $a_1=2A-12B\cos\frac{\Lambda_1^0}{2}$, $b_1=2A+12B\cos\frac{\Lambda_1^0}{2}$, $c_1=2A-12B\cos\frac{\Lambda_2^0}{2}$, $d_1=2A+12B\cos\frac{\Lambda_2^0}{2}$, $e_1=2A-12B\cos\frac{\Lambda_3^0}{2}$, $f_1=2A+12B\cos\frac{\Lambda_3^0}{2}$, *and* $z_1^{'}$, $z_2^{'}$, *and* $z_3^{'}$ *are the eigenvalue, correspondingly, of the operators* $\widetilde{H}_{2\Lambda_1}^1$, $\widetilde{H}_{2\Lambda_2}^2$, *and* $\widetilde{H}_{2\Lambda_3}^3$.

b). *If* $-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W}\le U<-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2}>\cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_2^0}{2}>3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W}\le U<-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2}<\cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_2^0}{2}>3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}\le U<-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2}<3\cos\frac{\Lambda_3^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2}>\cos\frac{\Lambda_2^0}{2}$, *or* $-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}\le U<-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_2^0}{2}<3\cos\frac{\Lambda_3^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2}<\cos\frac{\Lambda_2^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W}\le U<-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2}>3\cos\frac{\Lambda_3^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2}>\cos\frac{\Lambda_2^0}{2}$, *or*

$-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W} \le U < -\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, *then the essential spectrum of the operator* ${}^1\widetilde{H}_0^s$ *is consists of the union of four segments:* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1] \cup [a_1+c_1+z_3^{'}, b_1+d_1+z_3^{'}] \cup [c_1+e_1+z_1^{'}, d_1+f_1+z_1^{'}] \cup [c_1+z_1^{'}+z_3^{'}, d_1+z_1^{'}+z_3^{'}]$, *or* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1] \cup [a_1+c_1+z_3^{'}, b_1+d_1+z_3^{'}] \cup [a_1+e_1+z_2^{'}, b_1+f_1+z_2^{'}] \cup [a_1+z_2^{'}+z_3^{'}, b_1+z_2^{'}+z_3^{'}]$, *or* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1] \cup [a_1+e_1+z_2^{'}, b_1+f_1+z_2^{'}] \cup [c_1+e_1+z_1^{'}, d_1+f_1+z_1^{'}] \cup [e_1+z_1^{'}+z_2^{'}, f_1+z_1^{'}+z_2^{'}]$, *and the discrete spectrum of the operator* ${}^1\widetilde{H}_0^s$ *is empty set.*

c).*If* $-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W} \le U < -\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}, \cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_2^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W} \le U < -\frac{12B\cos\frac{\Lambda_3^0}{2}}{W}, \cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W} \le U < -\frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2} < 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W} \le U < -\frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_2^0}{2} < 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W} \le U < --\frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *and* $\cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$, $\cos\frac{\Lambda_2^0}{2} < 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W} \le U < -\frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, $\cos\frac{\Lambda_2^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, $\cos\frac{\Lambda_1^0}{2} < 3\cos\frac{\Lambda_3^0}{2}$, *then the essential spectrum of operator the operator* ${}^1\widetilde{H}_0^s$ *is the union of two segments:* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1] \cup [a_1+c_1+z_3^{'}, b_1+d_1+z_3^{'}]$, *or* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1] \cup [a_1+e_1+z_2^{'}, b_1+f_1+z_2^{'}]$, *or* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1] \cup [c_1+e_1+z_1^{'}, d_1+f_1+z_1^{'}]$, *and discrete spectrum of the operator* ${}^1\widetilde{H}_0^s$ *is empty set.*

d). *If* $-\frac{12B\cos\frac{\Lambda_3^0}{2}}{W} \le U < 0, \cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$ *and* $\cos\frac{\Lambda_2^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *or* $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$ *and* $\cos\frac{\Lambda_1^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_2^0}{2}}{W} \le U < 0, \cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$ *and* $\cos\frac{\Lambda_1^0}{2} < 3\cos\frac{\Lambda_3^0}{2}$, *or* $\cos\frac{\Lambda_1^0}{2} > \cos\frac{\Lambda_2^0}{2}$, $\cos\frac{\Lambda_1^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *or* $-\frac{4B\cos\frac{\Lambda_1^0}{2}}{W} \le U < 0, \cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$ *and* $\cos\frac{\Lambda_2^0}{2} < 3\cos\frac{\Lambda_3^0}{2}$, *or* $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, *and* $\cos\frac{\Lambda_2^0}{2} > 3\cos\frac{\Lambda_3^0}{2}$, *then the essential spectrum of the operator* ${}^1\widetilde{H}_0^s$ *is consists of a single segment:* $\sigma_{ess}({}^1H_0^s) = [a_1+c_1+e_1, b_1+d_1+f_1]$, *and discrete spectrum of the operator* ${}^1\widetilde{H}_0^s$ *is empty set:* $\sigma_{disc}({}^1\widetilde{H}_0^s) = \emptyset$.

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