STRUCTURE OF ESSENTIAL SPECTRA AND DISCRETE SPECTRUM OF THE ENERGY OPERATOR OF SIX-ELECTRON SYSTEMS IN THE HUBBARD MODEL. SECOND SINGLET STATE

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Introduction. In the early 1970s, three papers [1]-[3], where a simple model of a metal was proposed that has become a fundamental model in the theory of strongly correlated electron systems, appeared almost simultaneously and independently. In that model, a single nondegenerate electron band with a local Coulomb interaction is considered. The model Hamiltonian contains only two parameters: the matrix element t of electron hopping from a lattice site to a neighboring site and the parameter U of the on-site Coulomb repulsion of two electrons. In the secondary quantization representation, the Hamiltonian can be written as $H = t\sum_{m,\gamma} a^+_{m,\gamma} a_{m,\gamma} + U\sum_m a^+_{m,\uparrow} a_{m,\uparrow} a^+_{m,\downarrow} a_{m,\downarrow}$, where $a^+_{m,\gamma}$ and $a_{m,\gamma}$ denote Fermi operators of creation and annihilation of an electron with spin γ on a site m and the summation over τ means summation over the nearest neighbors on the lattice. The model proposed in [1]-[3] 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 [4]. The spectrum and wave functions of the system of two electrons in a crystal described by the Hubbard Hamiltonian were studied in [4]. The spectrum and wave functions of the system of three electrons in a crystal described by the Hubbard Hamiltonian were studied in [5]. In the three-electron systems are exists quartet state, and two type doublet states.

HAMILTONIAN OF THE SYSTEM. We consider the energy operator of six-electron systems in the Hubbard model and describe the structure of the essential spectra and discrete spectrum of the system for second singlet state in the lattice. The Hamiltonian of the chosen model 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), $\tau = \pm e_j$, $j = 1, 2, ..., \nu$, where e_j are unit mutually orthogonal vectors, 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, $\gamma = \uparrow$ or $\gamma = \downarrow$, $\uparrow$ and $\downarrow$ denote the spin values $\frac{1}{2}$ and $-\frac{1}{2}$, 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 has a octet state, and quintet states, and triplet states, and singlet states. The energy of the system depends on its total spin S. Hamiltonian H commutes with all components of the total spin operator $S = (S^+, S^-, S^z)$, and the structure of eigenfunctions and eigenvalues of the system therefore depends on S. The Hamiltonian H acts in the antisymmetric Fo'ck space $\mathcal{H}_{as}$.

SIX-ELECTRON SECOND SINGLET STATE IN THE HUBBARD MODEL.

Let φ_0 be the vacuum vector in the space $\mathcal{H}_{as}$. The second singlet state corresponds to the free motion of six electrons over the lattice and their interactions with the basic functions ${}^2s^0_{p,q,r,t,k,n\in Z^\nu} = a^+_{p,\uparrow} a^+_{q,\downarrow} a^+_{r,\uparrow} a^+_{t,\downarrow} a^+_{k,\uparrow} a^+_{n,\downarrow}\varphi_0$. The subspace ${}^2\mathcal{H}^s_0$, corresponding to the second singlet state is the set of all vectors of the form ${}^2\psi^s_0 = \sum_{p,q,r,t,k,n\in Z^\nu} f(p,q,r,t,k,n)\,{}^2s^0_{p,q,r,t,k,n\in Z^\nu}$, $f \in l^{as}_2$,

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where l_2^{as} is the subspace of antisymmetric functions in the space $l_2((Z^\nu)^6)$. We denote by ${}^2H_0^s$ the restriction of operator H to the subspace ${}^2\mathcal{H}_0^s$.

Theorem 1. (coordinate representation of the actions of operator ${}^2H_0^s$) The subspace ${}^2\mathcal{H}_0^s$ is invariant under the operator H, and the restriction ${}^2H_0^s$ of operator H to the subspace ${}^2\mathcal{H}_0^s$ is a bounded self-adjoint operator. It generates a bounded self-adjoint operator ${}^2\overline{H}_0{}^s$ acting in the space l_2^{as} as

$${}^2\overline{H}_0^s{}^2\psi_0^s = 6Af(p,q,r,t,k,n)+B\sum_\tau[f(p+\tau,q,r,t,k,n)+f(p,q+\tau,r,t,k,n)+f(p,q,r+\tau,t,k,n)+$$

$$+f(p,q,r,t+\tau,k,n)+f(p,q,r,t,k+\tau,n)+f(p,q,r,t,k,n+\tau)]+U[\delta_{p,q}+\delta_{p,t}+\delta_{p,n}+\delta_{q,r}+\delta_{q,k}+\delta_{r,t}+$$

$+\delta_{r,n}+\delta_{t,k}+\delta_{k,n}]f(p,q,r,t,k,n)$. The operator ${}^2H_0^s$ acts on a vector ${}^2\psi_0^s \in {}^2\mathcal{H}_0^s$ as

$${}^2H_0^s{}^2\psi_0^s = \sum_{p,q,r,t,k,n\in Z^\nu} ({}^2\overline{H}_0^s f)(p,q,r,t,k,n){}^2s^0_{p,q,r,t,k,n\in Z^\nu}. \qquad (4)$$

Lemma 1. The spectra of the operators ${}^2H_0^s$ and ${}^2\overline{H}_0^s$ coincide.

We call the operator ${}^2H_0^s$ the six-electron second singlet state operator in the Hubbard model.

Let $\mathcal{F} : l_2((Z^\nu)^6) \to L_2((T^\nu)^6) \equiv {}^2\widetilde{\mathcal{H}}_0^s$ be the Fourier transform, where T^ν is the $\nu-$dimensional torus endowed with the normalized Lebesgue measure $d\lambda$, i.e. $\lambda(T^\nu) = 1$.

We set ${}^2\widetilde{H}_0^s = \mathcal{F}\,{}^2\overline{H}_0^s\mathcal{F}^{-1}$. In the quasimomentum representation, the operator ${}^2\overline{H}_0^s$ acts in the Hilbert space $L_2^{as}((T^\nu)^6)$, where L_2^{as} is the subspace of antisymmetric functions in $L_2((T^\nu)^6)$.

Theorem 2. (quasimomentum representation of the actions of operator ${}^2H_0^s$) The Fourier transform of operator ${}^2\overline{H}_0^s$ is an operator ${}^2\widetilde{H}_0^s = \mathcal{F}\,{}^2\overline{H}_0^s\mathcal{F}^{-1}$ acting in the space $L_2^{as}((T^\nu)^6)$ be the formula

$${}^2\widetilde{H}_0^s{}^2\psi_0^s = h(\lambda,\mu,\gamma,\theta,\eta,\chi)f(\lambda,\mu,\gamma,\theta,\eta,\chi) + U[\int_{T^\nu} f(t,\lambda+\mu-t,\gamma,\theta,\eta,\chi)dt+$$

$$+\int_{T^\nu} f(t,\mu,\gamma,\lambda+\theta-t,\eta,\chi)dt+\int_{T^\nu} f(t,\mu,\gamma,\theta,\eta,\lambda+\chi-t)dt+\int_{T^\nu} f(\lambda,t,\mu+\gamma-t,\theta,\eta,\chi)dt+$$

$$+\int_{T^\nu} f(\lambda,t,\gamma,\theta,\mu+\eta-t,\chi)dt+\int_{T^\nu} f(\lambda,\mu,t,\gamma+\theta-t,\eta,\chi)dt+\int_{T^\nu} f(\lambda,\mu,t,\theta,\eta,\gamma+\chi-t)dt+$$

$+\int_{T^\nu} f(\lambda,\mu,\gamma,t,\theta+\eta-t,\chi)dt+\int_{T^\nu} f(\lambda,\mu,\gamma,\theta,t,\eta+\chi-t)dt]$, where $h(\lambda,\mu,\gamma,\theta,\eta,\chi) = 6A+2B\sum_{i=1}^\nu[cos\lambda_i+cos\mu_i+cos\gamma_i+cos\theta_i+cos\eta_i+cos\chi_i]$, and L_2^{as} is the subspace of antisymmetric functions in $L_2((T^\nu)^6)$.

STRUCTURE OF THE ESSENTIAL SPECTRUM AND DISCRETE SPECTRUM OF OPERATOR ${}^2\widetilde{H}_0^s$.

Using tensor products of Hilbert spaces and tensor products of operators in Hilbert spaces, and taking into account that the function $f(\lambda,\mu,\gamma,\theta,\eta,\chi)$ is an antisymmetric function, we can describe the structure of essential spectra and discrete spectrum the operator ${}^2H_0^s$:

Theorem 3. Let $\nu = 1$ and $U < 0$. Then the essential spectrum of the operator ${}^2H_0^s$ is consists of the union of seven segments: $\sigma_{ess}({}^2H_0^s) = [a+c+e, b+d+f]\cup[a+c+z_3, b+d+z_3]\cup[a+e+z_2, b+f+z_2]\cup[a+z_2+z_3, b+z_2+z_3]\cup[c+e+z_1, d+f+z_1]\cup[c+z_1+z_3, d+z_1+z_3]\cup[e+z_1+z_2, d+z_1+z_2]$, and discrete spectrum of the operator ${}^2H_0^s$ is consists of unique eigenvalue $\sigma_{disc}({}^2H_0^s) = \{z_1+z_2+z_3\}$, here and hereafter $a = 2A-4B\cos\frac{\Lambda_1}{2}$, $b = 2A+4B\cos\frac{\Lambda_1}{2}$, $c = 2A-4B\cos\frac{\Lambda_2}{2}$, $d = 2A+4B\cos\frac{\Lambda_2}{2}$, $e = 2A-4B\cos\frac{\Lambda_3}{2}$, $f = 2A+4B\cos\frac{\Lambda_3}{2}$, $z_1 = 2A-\sqrt{9U^2+16B^2cos^2\frac{\Lambda_1}{2}}$,

$z_2 = 2A - \sqrt{9U^2 + 16B^2 cos^2 \frac{\Lambda_2}{2}}$, $z_3 = 2A - \sqrt{9U^2 + 16B^2 cos^2 \frac{\Lambda_3}{2}}$, and $\Lambda_1 = \lambda + \mu$, $\Lambda_2 = \gamma + \theta$, $\Lambda_3 = \eta + \chi$.

Theorem 4. Let $\nu = 1$ and $U > 0$. Then the essential spectrum of the operator ${}^2H_0^s$ is consists of the union of seven segments: $\sigma_{ess}({}^2H_0^s) = [a+c+e, b+d+f] \cup [a+c+\widetilde{z}_3, b+d+\widetilde{z}_3] \cup [a+e+\widetilde{z}_2, b+f+\widetilde{z}_2] \cup [a+\widetilde{z}_2+\widetilde{z}_3, b+\widetilde{z}_2+\widetilde{z}_3] \cup [c+e+\widetilde{z}_1, d+f+\widetilde{z}_1] \cup [c+\widetilde{z}_1+\widetilde{z}_3, d+\widetilde{z}_1+\widetilde{z}_3] \cup [e+\widetilde{z}_1+\widetilde{z}_2, d+\widetilde{z}_1+\widetilde{z}_2]$, and discrete spectrum of the operator ${}^2H_0^s$ is consists of unique eigenvalue $\sigma_{disc}({}^2H_0^s) = \{\widetilde{z}_1+\widetilde{z}_2+\widetilde{z}_3\}$, where $\widetilde{z}_1 = 2A + \sqrt{9U^2 + 16B^2 cos^2 \frac{\Lambda_1}{2}}$, $\widetilde{z}_2 = 2A + \sqrt{9U^2 + 16B^2 cos^2 \frac{\Lambda_2}{2}}$, $\widetilde{z}_3 = 2A + \sqrt{9U^2 + 16B^2 cos^2 \frac{\Lambda_3}{2}}$.

Theorem 5. Let $\nu = 3$ and $U > 0$, and $\Lambda_1 = \lambda + \mu$, $\Lambda_2 = \gamma + \theta$, $\Lambda_3 = \eta + \chi$, and $\Lambda_1 = (\Lambda_1^0, \Lambda_1^0, \Lambda_1^0)$, $\Lambda_2 = (\Lambda_2^0, \Lambda_2^0, \Lambda_2^0)$, and $\Lambda_3 = (\Lambda_3^0, \Lambda_3^0, \Lambda_3^0)$.

a). If $U > \frac{4B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_3^0}{2}$, and $\cos\frac{\Lambda_2^0}{2} < \cos\frac{\Lambda_3^0}{2}$, or $U > \frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < \cos\frac{\Lambda_2^0}{2}$, and $\cos\frac{\Lambda_3^0}{2} < \cos\frac{\Lambda_2^0}{2}$, or $U > \frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_2^0}{2} < \cos\frac{\Lambda_1^0}{2}$, and $\cos\frac{\Lambda_3^0}{2} < \cos\frac{\Lambda_1^0}{2}$, then the essential spectrum of the operator ${}^2H_0^s$ is consists of the union of seven segments: $\sigma_{ess}({}^2H_0^s) = [a+c+e, b+d+f] \cup [a+c+\widetilde{z}_3, b+d+\widetilde{z}_3] \cup [a+e+\widetilde{z}_2, b+f+\widetilde{z}_2] \cup [a+\widetilde{z}_2+\widetilde{z}_3, b+\widetilde{z}_2+\widetilde{z}_3] \cup [c+e+\widetilde{z}_1, d+f+\widetilde{z}_1] \cup [c+\widetilde{z}_1+\widetilde{z}_3, d+\widetilde{z}_1+\widetilde{z}_3] \cup [e+\widetilde{z}_1+\widetilde{z}_2, d+\widetilde{z}_1+\widetilde{z}_2]$, and discrete spectrum of the operator ${}^2H_0^s$ is consists of unique eigenvalue $\sigma_{disc}({}^2H_0^s) = \{\widetilde{z}_1+\widetilde{z}_2+\widetilde{z}_3\}$, where $a = 2A - 12B\cos\frac{\Lambda_1^0}{2}$, $b = 2A + 12B\cos\frac{\Lambda_1^0}{2}$, $c = 2A - 12B\cos\frac{\Lambda_2^0}{2}$, $d = 2A + 12B\cos\frac{\Lambda_2^0}{2}$, $e = 2A - 12B\cos\frac{\Lambda_3^0}{2}$, $f = 2A + 12B\cos\frac{\Lambda_3^0}{2}$, $\widetilde{z}_1$, $\widetilde{z}_2$, $\widetilde{z}_3$ are the same concrete numbers and W is the Watson integral.

b). If $\frac{4B\cos\frac{\Lambda_2^0}{2}}{W} < U \leq \frac{4B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < cos\frac{\Lambda_2^0}{2}$, and $cos\frac{\Lambda_2^0}{2} < cos\frac{\Lambda_3^0}{2}$, or $\frac{4B\cos\frac{\Lambda_1^0}{2}}{W} < U \leq \frac{4B\cos\frac{\Lambda_3^0}{2}}{W}$, $\cos\frac{\Lambda_2^0}{2} < cos\frac{\Lambda_1^0}{2}$, and $cos\frac{\Lambda_1^0}{2} < cos\frac{\Lambda_3^0}{2}$, or $\frac{4B\cos\frac{\Lambda_3^0}{2}}{W} < U \leq \frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < cos\frac{\Lambda_3^0}{2}$, and $cos\frac{\Lambda_3^0}{2} < cos\frac{\Lambda_2^0}{2}$, or $\frac{4B\cos\frac{\Lambda_1^0}{2}}{W} < U \leq \frac{4B\cos\frac{\Lambda_2^0}{2}}{W}$, $\cos\frac{\Lambda_1^0}{2} < cos\frac{\Lambda_2^0}{2}$, and $cos\frac{\Lambda_3^0}{2} < cos\frac{\Lambda_1^0}{2}$, or $\frac{4B\cos\frac{\Lambda_2^0}{2}}{W} < U \leq \frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_3^0}{2} < cos\frac{\Lambda_2^0}{2}$, and $cos\frac{\Lambda_2^0}{2} < cos\frac{\Lambda_1^0}{2}$, or $\frac{4B\cos\frac{\Lambda_3^0}{2}}{W} < U \leq \frac{4B\cos\frac{\Lambda_1^0}{2}}{W}$, $\cos\frac{\Lambda_2^0}{2} < cos\frac{\Lambda_3^0}{2}$, and $cos\frac{\Lambda_3^0}{2} < cos\frac{\Lambda_1^0}{2}$, then the essential spectrum of the operator ${}^2H_0^s$ is consists of the union of four segments: $\sigma_{ess}({}^2H_0^s) = [a+c+e, b+d+f] \cup [a+e+\widetilde{z}_2, b+f+\widetilde{z}_2] \cup [c+e+\widetilde{z}_1, d+f+\widetilde{z}_1] \cup [e+\widetilde{z}_1+\widetilde{z}_2, d+\widetilde{z}_1+\widetilde{z}_2]$, or $\sigma_{ess}({}^2H_0^s) = [a+c+e, b+d+f] \cup [a+c+\widetilde{z}_3, b+d+\widetilde{z}_3] \cup [c+e+\widetilde{z}_1, d+f+\widetilde{z}_1] \cup [c+\widetilde{z}_1+\widetilde{z}_3, d+\widetilde{z}_1+\widetilde{z}_3]$, or $\sigma_{ess}({}^2H_0^s) = [a+c+e, b+d+f] \cup [a+c+\widetilde{z}_3, b+d+\widetilde{z}_3] \cup [a+e+\widetilde{z}_2, b+f+\widetilde{z}_2] \cup [a+\widetilde{z}_2+\widetilde{z}_3, b+\widetilde{z}_2+\widetilde{z}_3]$, and discrete spectrum of the operator ${}^2H_0^s$ is empty set: $\sigma_{disc}({}^2H_0^s) = \emptyset$.

There is also the case when the essential spectrum of the operator ${}^2H_0^s$ is consists of the unions of two segments, and the discrete spectrum of the operator ${}^2H_0^s$ is empty set: $\sigma_{disc}({}^2H_0^s) = \emptyset$, and the case when the essential spectrum of the operator ${}^2H_0^s$ is consists of a single segment, and the discrete spectrum of the operator ${}^2H_0^s$ is empty set: $\sigma_{disc}({}^2H_0^s) = \emptyset$.

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