Structure of essential spectra and discrete spectrum of the energy operator of five-electron systems in the Hubbard model. Fifth doublet state

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Abstract: We consider the energy operator of five-electron systems in the Hubbard model and describe the structure of essential spectrum and discrete spectrum of the system in the fifth doublet state. 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 $\gamma = \downarrow$, and $a^+_{m,\gamma}$ and $a_{m,\gamma}$ are the respective electron creation and annihilation operators at a site $m \in Z^\nu$. Let ${}^5\widetilde{H}^d_{1/2}$ denote the operator of fifth doublet state of five-electron systems and W and m are the positive numbers.

Theorem. Let $\nu = 3$. **a).** *If $U < -\frac{4B}{m}$, $m < \frac{4}{3}W$, or $U < -\frac{3B}{W}$, $m > \frac{4}{3}W$, then the essential spectrum of operator ${}^5\widetilde{H}^d_{1/2}$ is exactly the union of seven segments and the discrete spectrum of ${}^5\widetilde{H}^d_{1/2}$ consists of no more one point.*

b). *If $-\frac{3B}{W} \le U < -\frac{4B}{m}$, then the essential spectrum of ${}^5\widetilde{H}^d_{1/2}$ is the union of four segments and the discrete spectrum of ${}^5\widetilde{H}^d_{1/2}$ is empty.*

c). *If $-\frac{4B}{m} \le U < 0$, $m > \frac{4}{3}W$, or $-\frac{3B}{W} \le U < -\frac{3B}{m}$, and $m < \frac{4}{3}W$, then the essential spectrum of ${}^5\widetilde{H}^d_{1/2}$ is the union of two segments and the discrete spectrum of ${}^5\widetilde{H}^d_{1/2}$ is empty.*

d). *If $-\frac{4B}{m} \le U < 0$, $m > \frac{4}{3}W$, or $-\frac{3B}{W} \le U < 0$, $m < \frac{4}{3}W$, then the essential spectrum of operator ${}^5\widetilde{H}^d_{1/2}$ is the single segment and the discrete spectrum of operator ${}^5\widetilde{H}^d_{1/2}$ is empty.*

Keywords: Hubbard Model, Essential and Discrete spectrum, five-electron systems, sextet state, quartet state, doublet states,bound and antibound states.

2010 Mathematics Subject Classification: 47Axx, 46XX, 46L60,11F72, 35Pxx,62M15,58C40