

Spectra of the Energy Operator of Four-Electron Systems in the Impurity Hubbard Model. Triplet State

S. M. Tashpulatov, R. T. Parmanova

Institute of Nuclear Physics of Academy of Science of Republic of Uzbekistan, Tashkent, Uzbekistan
Email: sadullatashpulatov@yandex.ru, toshpul@mail.ru, toshpul@inp.uz

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Abstract

We consider the energy operator of four-electron systems in an impurity Hubbard model and investigated the structure of essential spectra and discrete spectrum of the system in the first triplet state in a one-dimensional lattice. For investigation the structure of essential spectra and discrete spectrum of the energy operator of four-electron systems in an impurity Hubbard model, for which the momentum representation is convenient. In addition, we used the tensor products of Hilbert spaces and tensor products of operators in Hilbert spaces and described the structure of essential spectrum and discrete spectrum of the energy operator of four-electron systems in an impurity Hubbard model. The investigations show that there are such cases: 1) the essential spectrum of the system consists of the union of no more than eight segments, and the discrete spectrum of the system consists of no more than three eigenvalues; 2) the essential spectrum of the system consists of the union of no more than sixteen segments, and the discrete spectrum of the system consists of no more than eleven eigenvalues; 3) the essential spectrum of the system consists of the union of no more than three segments, and the discrete spectrum of the system is the empty set. Consequently, the essential spectrum of the system consists of the union of no more than sixteen segments, and the discrete spectrum of the system consists of no more than eleven eigenvalues.

Keywords

Hubbard Model, Essential Spectrum, Discrete Spectrum, Four Electron Systems, Quintet State, Triplet State, Singlet State, Spectra

1. Introduction

In the early 1970s, three papers [1] [2] [3], where a simple model of 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

$$H = t \sum_{m,\gamma} a_{m,\gamma}^+ a_{m,\gamma} + U \sum_m a_{m,\uparrow}^+ a_{m,\uparrow} a_{m,\downarrow}^+ a_{m,\downarrow}, \quad (1)$$

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] [2] [3] was called the Hubbard model after John Hubbard, who made a fundamental contribution to studying the statistical mechanics of that system, although the local form of Coulomb interaction was first introduced for an impurity model in metal by Anderson [4]. We also recall that the Hubbard model is a particular case of the Shubin-Wonsowsky polaron model [5], which had appeared 30 years before [1] [2] [3]. In the Shubin-Wonsowsky model, along with the on-site Coulomb interaction, the interaction of electrons on neighboring sites is also taken into account.

The Hubbard model is currently one of the most extensively studied multielectron models of metals [6] [7] [8] [9] [10]. 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 [6]. It is known that two-electron systems can be in two states, triplet and singlet [6] [7] [8] [9] [10]. It was proved in [6] that the spectrum of the system Hamiltonian H^t in the triplet state is purely continuous and coincides with a segment $[m, M] = [2A - 4Bv, 2A + 4Bv]$, and the operator H^s of the system in the singlet state, in addition to the continuous spectrum $[m, M]$, has a unique antibound state for some values of the quasimomentum.

The spectrum and wave functions of the system of three electrons in a crystal described by the Hubbard Hamiltonian were studied in [11]. The three-electron systems exist quartet state, and two type doublet states.

The spectrum of the energy operator of a system of four electrons in a crystal described by the Hubbard Hamiltonian in the triplet state was studied in [12]. The four-electron systems exist quintet states, and three type triplet states, and two type singlet states. The triplet state corresponds to the basic functions

$${}^1t_{m,n,p,r}^1 = a_{m,\uparrow}^+ a_{n,\uparrow}^+ a_{p,\uparrow}^+ a_{r,\downarrow}^+ \varphi_0, \quad {}^2t_{m,n,p,r}^1 = a_{m,\uparrow}^+ a_{n,\uparrow}^+ a_{p,\downarrow}^+ a_{r,\uparrow}^+ \varphi_0,$$

$${}^3t_{m,n,p,r}^1 = a_{m,\uparrow}^+ a_{n,\downarrow}^+ a_{p,\uparrow}^+ a_{r,\uparrow}^+ \varphi_0.$$

The spectrum of the energy operator of four-electron systems in the Hubbard model in the quintet and singlet states was studied in [13]. The quintet state corresponds to the free motion of four electrons over the lattice with the basic

functions $q_{m,n,p,r}^2 = a_{m,\uparrow}^+ a_{n,\uparrow}^+ a_{p,\uparrow}^+ a_{r,\uparrow}^+ \varphi_0$. The work [13] proved, that the spectrum of the system in a quintet state is purely continuous and coincides with the segment $[4A - 8B\nu, 4A + 8B\nu]$, and the four-electron bound states or the four-electron antibound states are absent. The singlet state corresponds to the basic functions ${}^1s_{p,q,r,t}^0 = a_{p,\uparrow}^+ a_{q,\uparrow}^+ a_{r,\downarrow}^+ a_{t,\downarrow}^+ \varphi_0$, ${}^2s_{p,q,r,t}^0 = a_{p,\uparrow}^+ a_{q,\downarrow}^+ a_{r,\uparrow}^+ a_{t,\downarrow}^+ \varphi_0$, and these two singlet states have different origins.

The use of films in various areas of physics and technology arouses great interest in studying a localized impurity state (LIS) of a magnet. Therefore, it is important to study the spectral properties of electron systems in the impurity Hubbard model. The spectrum of the energy operator of three-electron systems in the Impurity Hubbard model in the second doublet state was studied [14]. The structure of essential spectra and discrete spectrum of three-electron systems in the impurity Hubbard model in the Quartet state were studied in [15].

2. Hamiltonian of the System

We consider the energy operator of four-electron systems in the Impurity Hubbard model and describe the structure of the essential spectra and discrete spectrum of the system for the first triplet states in the one-dimensional lattice. The Hamiltonian of the chosen model has the form

$$\begin{aligned} H = & A \sum_{m,\gamma} a_{m,\gamma}^+ a_{m,\gamma} + B \sum_{m,\tau,\gamma} a_{m,\gamma}^+ a_{m+\tau,\gamma} + U \sum_m a_{m,\uparrow}^+ a_{m,\uparrow} a_{m,\downarrow}^+ a_{m,\downarrow} \\ & + (A_0 - A) \sum_{\gamma} a_{0,\gamma}^+ a_{0,\gamma} + (B_0 - B) \sum_{\tau,\gamma} (a_{0,\gamma}^+ a_{\tau,\gamma} + a_{\tau,\gamma}^+ a_{0,\gamma}) \\ & + (U_0 - U) a_{0,\uparrow}^+ a_{0,\uparrow} a_{0,\downarrow}^+ a_{0,\downarrow}. \end{aligned} \quad (2)$$

Here $A(A_0)$ is the electron energy at 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 $\gamma = \downarrow$, \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 $m \in Z^\nu$.

The four-electron systems have a quintet state, and two type singlet state, and three type triplet states. The energy of the system depends on its total spin S . Along with the Hamiltonian, the N_e electron system is characterized by the total spin S , $S = S_{\max}, S_{\max} - 1, \dots, S_{\min}$, $S_{\max} = \frac{N_e}{2}$, $S_{\min} = 0, \frac{1}{2}$.

Hamiltonian (2) 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 Fock space \mathcal{H}_{as} .

3. Four-Electron First Triplet State in the Impurity Hubbard Model

Let φ_0 be the vacuum vector in the space \mathcal{H}_{as} . The first triplet state corresponds to the free motion of four electrons and their interactions over the lattice with the basic functions ${}^1t^1_{p,q,r,k \in Z^v} = a_{p,\uparrow}^+ a_{q,\uparrow}^+ a_{r,\uparrow}^+ a_{k,\downarrow}^+ \varphi_0$. The subspace ${}^1\mathcal{H}_1^t$, corresponding to the first triplet state is the set of all vectors of the form ${}^1\psi_1^t = \sum_{p,q,r,k \in Z^v} f(p,q,r,k) {}^1t^1_{p,q,r,k \in Z^v}$, $f \in l_2^{as}$, where l_2^{as} is the subspace of antisymmetric functions in the space $l_2\left(\left(Z^v\right)^4\right)$. We denote by ${}^1H_1^t$ the restriction of operator H to the subspace ${}^1\mathcal{H}_1^t$. We let $\varepsilon_1 = A_0 - A$, and $\varepsilon_2 = B_0 - B$, and $\varepsilon_3 = U_0 - U$.

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

$$\begin{aligned} {}^1\bar{H}_1^t {}^1\psi_1^t = & 4Af(p,q,r,k) + B \sum_{\tau} [f(p+\tau,q,r,k) + f(p,q+\tau,r,k) \\ & + f(p,q,r+\tau,k) + f(p,q,r,k+\tau)] + U [\delta_{p,k} + \delta_{q,k} + \delta_{r,k}] f(p,q,r,k) \\ & + \varepsilon_1 [\delta_{p,0} + \delta_{q,0} + \delta_{r,0} + \delta_{k,0}] f(p,q,r,k) + \varepsilon_2 \sum_{\tau} [\delta_{p,0} f(\tau,q,r,k) \\ & + \delta_{q,0} f(p,\tau,r,k) + \delta_{r,0} f(p,q,\tau,k) + \delta_{k,0} f(p,q,r,\tau) + \delta_{p,\tau} f(0,q,r,k) \\ & + \delta_{q,\tau} f(p,0,r,k) + \delta_{r,\tau} f(p,q,0,k) + \delta_{k,\tau} f(p,q,r,0)] \\ & + \varepsilon_3 [\delta_{p,0} \delta_{k,0} + \delta_{q,0} \delta_{k,0} + \delta_{r,0} \delta_{k,0}] f(p,q,r,k). \end{aligned} \tag{3}$$

The operator ${}^1H_1^t$ acts on a vector ${}^1\psi_1^t \in {}^1\mathcal{H}_1^t$ as

$${}^1H_1^t {}^1\psi_1^t = \sum_{p,q,r,k \in Z^v} ({}^1\bar{H}_1^t f)(p,q,r,k) {}^1t^1_{p,q,r,k \in Z^v}. \tag{4}$$

Proof. We act with the Hamiltonian H on vectors ${}^1\psi_1^t \in {}^1\mathcal{H}_1^t$ using the standard anticommutation relations between electron creation and annihilation operators at lattice sites, $\{a_{m,\gamma}, a_{n,\beta}^+\} = \delta_{m,n} \delta_{\gamma,\beta}$, $\{a_{m,\gamma}, a_{n,\beta}\} = \{a_{m,\gamma}^+, a_{n,\beta}^+\} = \theta$, and also take into account that $a_{m,\gamma} \varphi_0 = \theta$, where θ is the zero element of ${}^1\mathcal{H}_1^t$. This yields the statement of the theorem. \square

Lemma 1. *The spectra of the operators ${}^1H_1^t$ and ${}^1\bar{H}_1^t$ coincide.*

Proof. Because the operators ${}^1H_1^t$ and ${}^1\bar{H}_1^t$ are bounded self-adjoint operators, it follows that if $\lambda \in \sigma({}^1H_1^t)$, then the Weyl criterion (see [16], chapter VII, paragraph 3, pp. 262-263) implies that there is a sequence $\{\psi_n\}_{n=1}^\infty$ such that $\|\psi_n\| = 1$ and $\lim_{n \rightarrow \infty} \|({}^1H_1^t - \lambda)\psi_n\| = 0$. We set

$\psi_n = \sum_{p,q,r,k} f_n(p,q,r,k) a_{p,\uparrow}^+ a_{q,\uparrow}^+ a_{r,\uparrow}^+ a_{k,\downarrow}^+ \varphi_0$. Then

$$\begin{aligned} \|({}^1H_1^t - \lambda)\psi_n\|^2 &= \|({}^1H_1^t - \lambda)\psi_n, ({}^1H_1^t - \lambda)\psi_n\| \\ &= \sum_{p,q,r,k} \|({}^1\bar{H}_1^t - \lambda)f_n(p,q,r,k)\|^2 (a_{p,\uparrow}^+ a_{q,\uparrow}^+ a_{r,\uparrow}^+ a_{k,\downarrow}^+ \varphi_0, a_{p,\uparrow}^+ a_{q,\uparrow}^+ a_{r,\uparrow}^+ a_{k,\downarrow}^+ \varphi_0) \\ &= \sum_{p,q,r,k} \|({}^1\bar{H}_1^t - \lambda)F_n(p,q,r,k)\|^2 (a_{k,\downarrow}^+ a_{r,\uparrow}^+ a_{q,\uparrow}^+ a_{p,\uparrow}^+ \varphi_0, a_{k,\downarrow}^+ a_{r,\uparrow}^+ a_{q,\uparrow}^+ a_{p,\uparrow}^+ \varphi_0) \end{aligned}$$

$$\begin{aligned}
 &= \sum_{p,q,r,k} \left\| \left({}^1\bar{H}_1^t - \lambda \right) F_n(p,q,r,k) \right\|^2 (\varphi_0, \varphi_0) \\
 &= \sum_{p,q,r,k} \left\| \left({}^1\bar{H}_1^t - \lambda \right) F_n(p,q,r,k) \right\|^2 \rightarrow 0, \text{ as } n \rightarrow \infty
 \end{aligned}$$

where $F_n = \sum_{p,q,r,k} f_n(p,q,r,k)$. It follows that $\lambda \in \sigma({}^1\bar{H}_1^t)$. Consequently, $\sigma({}^1H_1^t) \subset \sigma({}^1\bar{H}_1^t)$.

Conversely, let $\bar{\lambda} \in \sigma({}^1\bar{H}_1^t)$. Then, by the Weyl criterion, there is a sequence $\{F_n\}_{n=1}^\infty$ such that $\|F_n\|=1$ and $\lim_{n \rightarrow \infty} \left\| \left({}^1\bar{H}_1^t - \bar{\lambda} \right) \psi_n \right\| = 0$. Setting

$$F_n = \sum_{p,q,r,k} f_n(p,q,r,k), \quad \|F_n\| = \left(\sum_{p,q,r,k} |f_n(p,q,r,k)|^2 \right)^{\frac{1}{2}},$$

we conclude that

$\|\psi_n\| = \|F_n\| = 1$ and $\left\| \left({}^1\bar{H}_1^t - \bar{\lambda} \right) F_n \right\| = \left\| \left({}^1\bar{H}_1^t - \bar{\lambda} \right) \psi_n \right\| \rightarrow 0$ as $n \rightarrow \infty$. This means that $\bar{\lambda} \in \sigma({}^1H_1^t)$ and hence $\sigma({}^1\bar{H}_1^t) \subset \sigma({}^1H_1^t)$. These two relations imply $\sigma({}^1H_1^t) = \sigma({}^1\bar{H}_1^t)$. □

We call the operator ${}^1H_1^t$ the four-electron first triplet state operator in the impurity Hubbard model.

Let $\mathcal{F} : L_2\left(\left(T^\nu\right)^4\right) \rightarrow L_2\left(\left(T^\nu\right)^4\right) \equiv {}^1\tilde{H}_1^t$ be the Fourier transform, where T^ν is the ν -dimensional torus endowed with the normalized Lebesgue measure $d\lambda$, i.e. $\lambda(T^\nu) = 1$.

We set ${}^1\tilde{H}_1^t = \mathcal{F} {}^1\bar{H}_1^t \mathcal{F}^{-1}$. In the quasimomentum representation, the operator ${}^1\bar{H}_1^t$ acts in the Hilbert space $L_2^{as}\left(\left(T^\nu\right)^4\right)$, where L_2^{as} is the subspace of antisymmetric functions in $L_2\left(\left(T^\nu\right)^4\right)$.

Theorem 2. (quasimomentum representation of the action of operator ${}^1H_1^t$)
 The Fourier transform of operator ${}^1\bar{H}_1^t$ is an operator ${}^1\tilde{H}_1^t = \mathcal{F} {}^1\bar{H}_1^t \mathcal{F}^{-1}$ acting in the space $L_2^{as}\left(\left(T^\nu\right)^4\right)$ be the formula

$$\begin{aligned}
 {}^1\tilde{H}_1^t {}^1\psi_1^t &= h(\lambda, \mu, \gamma, \theta) f(\lambda, \mu, \gamma, \theta) + U \left[\int_{T^\nu} f(s, \mu, \gamma, \lambda + \theta - s) ds \right. \\
 &\quad + \int_{T^\nu} f(\lambda, u, \gamma, \mu + \theta - u) du + \int_{T^\nu} f(\lambda, \mu, v, \gamma + \theta - v) dv \left. \right] \\
 &\quad + \varepsilon_1 \left[\int_{T^\nu} f(s, \mu, \gamma, \theta) ds + \int_{T^\nu} f(\lambda, u, \gamma, \theta) du + \int_{T^\nu} f(\lambda, \mu, v, \theta) dv \right. \\
 &\quad + \int_{T^\nu} f(\lambda, \mu, \gamma, \xi) d\xi \left. \right] + 2\varepsilon_2 \left[\int_{T^\nu} \sum_{i=1}^{\nu} [\cos \lambda_i + \cos s_i] f(s, \mu, \gamma, \theta) ds \right. \\
 &\quad + \int_{T^\nu} \sum_{i=1}^{\nu} [\cos \mu_i + \cos u_i] f(\lambda, u, \gamma, \theta) du \\
 &\quad + \int_{T^\nu} \sum_{i=1}^{\nu} [\cos \gamma_i + \cos v_i] f(\lambda, \mu, v, \theta) dv \\
 &\quad + \left. \int_{T^\nu} \sum_{i=1}^{\nu} [\cos \theta_i + \cos \xi_i] f(\lambda, \mu, \gamma, \xi) d\xi \right] \tag{5} \\
 &\quad + \varepsilon_3 \int_{T^\nu} \int_{T^\nu} \left[f(s, \mu, \gamma, \xi) ds d\xi + f(\lambda, u, \gamma, \xi) du d\xi \right. \\
 &\quad \left. + f(\lambda, \mu, v, \xi) dv d\xi \right],
 \end{aligned}$$

where $h(\lambda, \mu, \gamma, \theta) = 4A + 2B \sum_{i=1}^{\nu} [\cos \lambda_i + \cos \mu_i + \cos \gamma_i + \cos \theta_i]$, and L_2^{as} is the subspace of antisymmetric functions in $L_2\left(\left(T^\nu\right)^4\right)$.

Proof. The proof is by direct calculation in which we use the Fourier transformation in formula (3). □

In the impurity Hubbard model, the spectral properties of the considered operator of the energy of four-electron systems are closely related to those of its two-particle subsystems (one-electron systems with impurity). We first study the spectrum and localized impurity electron states of the one-electron impurity systems.

4. One-Electron Systems in the Impurity Hubbard Model

The Hamiltonian of one-electron systems in the impurity Hubbard model also has form (2). We let \mathcal{H}_1 denote the space of one-electron states of the operator H . It is clear that the space \mathcal{H}_1 is also invariant under operator H . We let H_1 denote the restriction of H to the space \mathcal{H}_1 .

Theorem 3. (coordination representation of the action of operator H_1) *The space \mathcal{H}_1 is an invariant under operator H , and restriction H_1 of operator H to the subspace \mathcal{H}_1 is a bounded self-adjoint operator. It generates a bounded self-adjoint operator \bar{H}_1 , acting in the space l_2^{as} as*

$$(\bar{H}_1 f)(p) = Af(p) + B \sum_{\tau} [f(p + \tau)] + \varepsilon_1 \delta_{p,0} f(p) + \varepsilon_2 \sum_{\tau} [\delta_{p,0} f(\tau) + \delta_{p,\tau} f(0)], \tag{6}$$

where $\delta_{k,j}$ is the Kronecker symbol. The operator H_1 acts on a vector $\psi \in \mathcal{H}_1$ as

$$H_1 = \sum_{p,\tau} (\bar{H}_1 f)(p) a_{p,\uparrow}^+ \varphi_0. \tag{7}$$

Lemma 2. *The spectra of the operators H_1 and \bar{H}_1 coincide.*

We let \mathcal{F} denote the Fourier transform: $\mathcal{F}: l_2(Z^v) \rightarrow L_2(T^v)$. We set $\tilde{H}_1 = \mathcal{F} \bar{H}_1 \mathcal{F}^{-1}$. In the quasimomentum representation, the operator \bar{H}_1 acts in the Hilbert space $L_2(T^v)$.

Theorem 4. (quasimomentum representation of the action of operator \tilde{H}_1) *The Fourier transform of the operator \bar{H}_1 is a bounded self-adjoint operator \tilde{H}_1 acting in the space $\tilde{\mathcal{H}}_1$ be the formula*

$$(\tilde{H}_1 f)(\lambda) = \left[A + 2B \sum_{i=1}^v \cos \lambda_i \right] f(\lambda) + \varepsilon_1 \int_{T^v} f(s) ds + 2\varepsilon_2 \int_{T^v} \sum_{i=1}^v [\cos \lambda_i + \cos s_i] ds. \tag{8}$$

Comparing the formulas (5) and (8), and using tensor products of Hilbert spaces and tensor products of operators in Hilbert spaces [17], and taking into account that the function $f(\lambda, \mu, \gamma, \theta)$ is an antisymmetric function, we can verify that the operator ${}^1\tilde{H}_1'$ can be represented in the form

$${}^1\tilde{H}_1' = \{ \tilde{H}_1 \otimes I + \otimes I \otimes \tilde{H}_1 + K \} \otimes I \otimes I + I \otimes I \otimes \{ \tilde{H}_1 \otimes I + I \otimes \tilde{H}_1 \}, \tag{9}$$

where I is the unit operator in space $\tilde{\mathcal{H}}_1$, and $K = K_{1\Lambda_1} + K_2$, and $(K_{1\Lambda_1} f)(\lambda) = U \int_{T^v} f_{\Lambda_1}(s) ds$, and $(K_2 f)(s, t) = \int_{T^v} \int_{T^v} f(s, t) ds dt$, and $f_{\Lambda_1}(s) = f(s, \Lambda_1 - s)$, $\Lambda_1 = \lambda + \theta$.

It is known that the continuous spectrum of operator \tilde{H}_1 fills the entire segment $[m_\nu, M_\nu] = [A - 2B\nu, A + 2B\nu]$. We set

$D_\nu(z) = (b_2 - b_3)^{\nu-1} \{a_1 [b_2 + (\nu - 1)b_3] - \nu a_2 b_1\}$, where

$$a_1 = 1 + \int_{T^\nu} \frac{[\varepsilon_1 + 2\varepsilon_2 \sum_{i=1}^\nu \cos s_i] ds_1 \cdots ds_\nu}{A + 2B \sum_{i=1}^\nu \cos s_i - z},$$

$$a_2 = \int_{T^\nu} \frac{\cos s_i [\varepsilon_1 + 2\varepsilon_2 \sum_{i=1}^\nu \cos s_i] ds_1 \cdots ds_\nu}{A + 2B \sum_{i=1}^\nu \cos s_i - z},$$

$$b_1 = 2\varepsilon_2 \int_{T^\nu} \frac{ds_1 \cdots ds_\nu}{A + 2B \sum_{i=1}^\nu \cos s_i - z}, b_2 = 1 + 2\varepsilon_2 \int_{T^\nu} \frac{\cos s_i ds_1 \cdots ds_\nu}{A + 2B \sum_{i=1}^\nu \cos s_i - z},$$

$$b_3 = 2\varepsilon_2 \int_{T^\nu} \frac{\cos s_i ds_1 \cdots ds_\nu}{A + 2B \sum_{i=1}^\nu \cos s_i - z},$$

and ν is lattice dimensionality.

Lemma 3. *A number $z_0 \notin [m_\nu, M_\nu]$ is an eigenvalue of operator \tilde{H}_1 if and only if it is a zero of the function $D_\nu(z)$.*

Definition 1. *The eigenfunction $\varphi \in L_2(T^\nu)$ of the operator \tilde{H}_1 corresponding to an eigenvalue $z \notin [m_\nu, M_\nu]$ is called a local impurity state (LIS) of \tilde{H}_1 , and z is called the energy of this state.*

The following Theorem describes the exchange of the spectrum of operator \tilde{H}_1 in the case $\nu = 1$.

Theorem 5. *(description of the spectra of the operator \tilde{H}_1)*

A) *If $\varepsilon_2 = -B$ and $\varepsilon_1 < -2B$ (respectively, $\varepsilon_2 = -B$ and $\varepsilon_1 > 2B$), then the operator \tilde{H}_1 has a unique eigenvalue $z = A + \varepsilon_1$, lying below (respectively, above) the continuous spectrum of the operator \tilde{H}_1 .*

B) *If $\varepsilon_2 = -2B$ and $\varepsilon_1 < 0$ or $\varepsilon_2 = 0$ and $\varepsilon_1 < 0$ (respectively, $\varepsilon_2 = -2B$ and $\varepsilon_1 > 0$ or $\varepsilon_2 = 0$ and $\varepsilon_1 > 0$), then the operator \tilde{H}_1 has a unique eigenvalue $z = A - \sqrt{4B^2 + \varepsilon_1^2}$ (respectively, $z = A + \sqrt{4B^2 + \varepsilon_1^2}$), lying the below (respectively, above) of continuous spectrum of the operator \tilde{H}_1 .*

C) *If $\varepsilon_1 = 0$ and $\varepsilon_2 > 0$ (respectively, $\varepsilon_1 = 0$ and $\varepsilon_2 < -2B$), then the operator \tilde{H}_1 has a unique eigenvalue $z = A - \frac{2BE}{\sqrt{E^2 - 1}}$, (respectively,*

$z = A + \frac{2BE}{\sqrt{E^2 - 1}}$), where $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, lying the below (respectively, above)

of continuous spectrum of the operator \tilde{H}_1 .

D) *If $\varepsilon_1 = \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_1 = -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the oper-*

ator \tilde{H}_1 has a unique eigenvalue $z = A + \frac{2B(E^2 + 1)}{E^2 - 1}$ (respectively,

$z = A - \frac{2B(E^2 + 1)}{E^2 - 1}$), where $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, lying the above (respectively, below)

of continuous spectrum of the operator \tilde{H}_1 .

E) If $\varepsilon_2 > 0$ and $\varepsilon_1 > \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_2 < -2B$ and $\varepsilon_1 > \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the operator \tilde{H}_1 has a unique eigenvalue $z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}$, where $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and the real number $\alpha > 1$, lying the above of continuous spectrum of the operator \tilde{H}_1 .

F) If $\varepsilon_2 > 0$ and $\varepsilon_1 < -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_2 < -2B$ and $\varepsilon_1 < -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the operator \tilde{H}_1 has a unique eigenvalue $z_1 = A - \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}$, where $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and the real number $\alpha > 1$, lying the below of continuous spectrum of the operator \tilde{H}_1 .

K) If $\varepsilon_2 > 0$ and $-\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} < \varepsilon_1 < \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_2 < -2B$ and $-\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} < \varepsilon_1 < \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the operator \tilde{H}_1 has a exactly two eigenvalues $z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} < m_1$, and $z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} > M_1$, where $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and real number $|\alpha| < 1$, lying the above and below of continuous spectrum of the operator \tilde{H}_1 .

M) If $-2B < \varepsilon_2 < 0$, then the operator \tilde{H}_1 has no eigenvalue lying the outside of continuous spectrum of the operator \tilde{H}_1 .

Proof. In the case $\nu = 1$, the continuous spectrum of the operator \tilde{H}_1 coincide with the segment $[m_1, M_1] = [A - 2B, A + 2B]$. Expressing all integrals in the equation $D_1(z) = 0$ through the integral $J(z) = \int_T \frac{ds}{A + 2B \cos s - z}$, we find that the equation $D_1(z) = 0$ is equivalent to the equation

$$[\varepsilon_1 B^2 + (\varepsilon_2^2 + 2B\varepsilon_2)(z - A)]J(z) + (B + \varepsilon_2)^2 = 0. \tag{10}$$

Moreover, the function $J(z)$ is a differentiable function on the set $\mathbb{R} \setminus [m_1, M_1]$, in addition, $J'(z) = \int_T \frac{ds}{[A + 2B \cos s - z]^2} > 0$, $z \notin [m_1, M_1]$. Thus the function

$J(z)$ is a monotone increasing function on $(-\infty, m_1)$ and on $(M_1, +\infty)$. Furthermore, $J(z) \rightarrow +0$ as $z \rightarrow -\infty$, $J(z) \rightarrow +\infty$ as $z \rightarrow m_1 - 0$, $J(z) \rightarrow -\infty$ as $z \rightarrow M_1 + 0$, and $J(z) \rightarrow -0$ as $z \rightarrow +\infty$.

If $\varepsilon_1 B^2 + (\varepsilon_2^2 + 2B\varepsilon_2)(z - A) \neq 0$ then from (10) follows that

$$J(z) = -\frac{(B + \varepsilon_2)^2}{\varepsilon_1 B^2 + (\varepsilon_2^2 + 2B\varepsilon_2)(z - A)}$$

The function $\psi(z) = -\frac{(B + \varepsilon_2)^2}{\varepsilon_1 B^2 + (\varepsilon_2^2 + 2B\varepsilon_2)(z - A)}$ has a point of asymptotic

discontinuity $z_0 = A - \frac{B^2 \varepsilon_1}{\varepsilon_2^2 + 2B\varepsilon_2}$. Since $\psi'(z) = \frac{(B + \varepsilon_2)^2 (\varepsilon_2^2 + 2B\varepsilon_2)}{[\varepsilon_1 B^2 + (\varepsilon_2^2 + 2B\varepsilon_2)(z - A)]^2}$

for all $z \neq z_0$ it follows that the function $\psi(z)$ is a monotone increasing (decreasing) function on $(-\infty, z_0)$ and on $(z_0, +\infty)$ in the case $\varepsilon_2^2 + 2B\varepsilon_2 > 0$ (respectively, $\varepsilon_2^2 + 2B\varepsilon_2 < 0$), in addition, and if $\varepsilon_2 > 0$, or $\varepsilon_2 < -2B$, then $\psi(z) \rightarrow +0$ as $z \rightarrow -\infty$, $\psi(z) \rightarrow +\infty$ as $z \rightarrow z_0 - 0$, $\psi(z) \rightarrow -\infty$ as $z \rightarrow z_0 + 0$, $\psi(z) \rightarrow -0$ as $z \rightarrow +\infty$ (respectively, if $-2B < \varepsilon_2 < 0$, then $\psi(z) \rightarrow -0$ as $z \rightarrow -\infty$, $\psi(z) \rightarrow -\infty$ as $z \rightarrow z_0 - 0$, $\psi(z) \rightarrow +\infty$ as $z \rightarrow z_0 + 0$, $\psi(z) \rightarrow +0$ as $z \rightarrow +\infty$).

A) If $\varepsilon_2 = -B$ and $\varepsilon_1 < -2B$ (respectively, $\varepsilon_2 = -B$ and $\varepsilon_1 > 2B$), then the equation for eigenvalues and eigenfunctions (10) has the form

$$\{\varepsilon_1 B^2 - B^2(z - A)\} J(z) = 0. \tag{11}$$

It is clear, that $J(z) \neq 0$ for the values $z \notin \sigma_{cont}(\tilde{H}_1)$. Therefore, $\varepsilon_1 - z + A = 0$, i.e., $z = A + \varepsilon_1$. If $\varepsilon_1 < -2B$, then this eigenvalue lying the below of continuous spectrum of the operator \tilde{H}_1 , if $\varepsilon_1 > 2B$, then this eigenvalue lying the above of continuous spectrum of the operator \tilde{H}_1 .

B) If $\varepsilon_2 = -2B$ and $\varepsilon_1 < 0$ (respectively, $\varepsilon_2 = -2B$ and $\varepsilon_1 > 0$), then the equation for the eigenvalues and eigenfunctions has the form $\varepsilon_1 B^2 J(z) + B^2 = 0$, that is, $J(z) = -\frac{1}{\varepsilon_1}$. It is clear, what the integral $J(z)$ calculated in a quadrature,

of the below (above) of continuous spectrum of the operator \tilde{H}_1 , the integral $J(z) > 0$, ($J(z) < 0$), consequently, $\varepsilon_1 < 0$ ($\varepsilon_1 > 0$.) The calculated the integral

$J(z) = \int_{r^v} \frac{ds}{A + 2B \cos s - z}$, the below of continuous spectrum of the operator

\tilde{H}_1 , we have the equation of the form $\frac{1}{\sqrt{(A - z)^2 - 4B^2}} = -\frac{1}{\varepsilon_1}$. This equation

has a solution $z = A - \sqrt{\varepsilon_1^2 + 4B^2}$, lying the below continuous spectrum of the operator \tilde{H}_1 . In the above continuous spectrum of the operator \tilde{H}_1 , the

equation takes the form $-\frac{1}{\sqrt{(z - A)^2 - 4B^2}} = -\frac{1}{\varepsilon_1}$. This equation has a solution

of the form $z = A + \sqrt{\varepsilon_1^2 + 4B^2}$, lying the above continuous spectrum of the operator \tilde{H}_1 .

C) If $\varepsilon_1 = 0$ and $\varepsilon_2 > 0$ (respectively, $\varepsilon_1 = 0$ and $\varepsilon_2 < -2B$), then the equation for the eigenvalues and eigenfunctions take in the form

$$(\varepsilon_2^2 + 2B\varepsilon_2)(z - A)J(z) = -(B + \varepsilon_2)^2, \text{ or } J(z) = -\frac{(B + \varepsilon_2)^2}{(\varepsilon_2^2 + 2B\varepsilon_2)(z - A)}$$

Denote $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$. Then $J(z) = -\frac{E}{z-A}$, or $J(z) = \frac{E}{A-z}$. In the below

of continuous spectrum of the operator \tilde{H}_1 , we have the equation of the form

$$\frac{1}{\sqrt{(A-z)^2 - 4B^2}} = \frac{E}{A-z}. \text{ This equation has a solution } z = A - \frac{2BE}{\sqrt{E^2 - 1}}. \text{ It is}$$

obviously, that $E^2 > 1$. This eigenvalue lies the below continuous spectrum of the operator \tilde{H}_1 . In the above continuous spectrum of the operator \tilde{H}_1 , the equation for the eigenvalues and eigenfunctions has the form

$$-\frac{1}{\sqrt{(z-A)^2 - 4B^2}} = -\frac{E}{z-A}. \text{ From here, we find } z = A + \frac{2BE}{\sqrt{E^2 - 1}}. \text{ This eigen-}$$

value lies the above continuous spectrum of the operator \tilde{H}_1 .

D) If $\varepsilon_1 = \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, then the equation for eigenvalues and eigenfunctions has the form $(\varepsilon_2^2 + 2B\varepsilon_2)(z - A + 2B)J(z) = -(B + \varepsilon_2)^2$, from this

$$J(z) = -\frac{(B + \varepsilon_2)^2}{(\varepsilon_2^2 + 2B\varepsilon_2)(z - A + 2B)}. \quad (12)$$

We denote $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$. In the first, we consider Equation (12) in the below

continuous spectrum of the operator \tilde{H}_1 . In Equation (12) we find the equation

$$\text{of the form } \frac{1}{\sqrt{(A-z)^2 - 4B^2}} = \frac{E}{A-z-2B}. \text{ From this, we find}$$

$$z_1 = A + \frac{2B(E^2 + 1)}{E^2 - 1}, \text{ and } z_2 = A - 2B. \text{ Now we verify the conditions}$$

$z_i < A - 2B, i = 1, 2$. The inequality $z_1 < A - 2B$, is incorrect, and inequality $z_2 < A - 2B$, is incorrect. We now consider Equation (12) in the above continuous spectrum of the operator \tilde{H}_1 . We have

$$-\frac{1}{\sqrt{(z-A)^2 - 4B^2}} = -\frac{E}{z-A+2B}. \text{ From this equation, we find the same solutions}$$

z_1 and z_2 , the outside of the domain of continuous spectrum of the operator \tilde{H}_1 . Now we verify the conditions $z_i > A + 2B, i = 1, 2$. The inequality $z_1 > A + 2B$, is correct, and inequality $z_2 > A + 2B$, is incorrect. Consequently, in this

case, the operator \tilde{H}_1 has a unique eigenvalue $z_1 = A + \frac{2B(E^2 + 1)}{E^2 - 1}$, lying the above continuous spectrum of the operator \tilde{H}_1 .

Let $\varepsilon_1 = -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, then the equation of eigenvalues and eigenfunctions

$$\text{take in the form } J(z) = -\frac{E}{z-A-2B}, \text{ where } E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}.$$

In the below of continuous spectrum of the operator \tilde{H}_1 , we have equation of

the form $\frac{1}{\sqrt{(A-z)^2 - 4B^2}} = \frac{E}{A-z+2B}$. From here we find $z_1 = A - \frac{2B(E^2 + 1)}{E^2 - 1}$,

and $z_2 = A + 2B$. Inequalities $z_1 < A - 2B$, is correct, and

$z_2 < A - 2B$, is incorrect. In the above continuous spectrum of the operator \tilde{H}_1 ,

we have equation of the form $-\frac{1}{\sqrt{(z-A)^2 - 4B^2}} = -\frac{E}{z-A-2B}$. It follows that

what $z_1 = A - \frac{2B(E^2 + 1)}{E^2 - 1}$, and $z_2 = A + 2B$. The inequality $z_1 > A + 2B$, and

$z_2 > A + 2B$, are incorrect. Therefore, in this case, the operator \tilde{H}_1 has a

unique eigenvalue $z_1 = A - \frac{2B(E^2 + 1)}{E^2 - 1}$, lying the below continuous spectrum of

the operator \tilde{H}_1 .

E) If $\varepsilon_2 > 0$ and $\varepsilon_1 > \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, (respectively, $\varepsilon_2 < -2B$ and

$\varepsilon_1 > \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then consider necessary, that $\varepsilon_1 = \alpha \times \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, where

$\alpha > 1$ -real number. Then the equation for eigenvalues and eigenfunctions has the form

$$\left\{ \alpha \times \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} \times B^2 + (\varepsilon_2^2 + 2B\varepsilon_2)(z-A) \right\} J(z) + (B + \varepsilon_2)^2 = 0,$$

or $(\varepsilon_2^2 + 2B\varepsilon_2)(z - A + 2\alpha B)J(z) + (B + \varepsilon_2)^2 = 0$. From this

$$J(z) = -\frac{(B + \varepsilon_2)^2}{(\varepsilon_2^2 + 2B\varepsilon_2)(z - A + 2\alpha B)}.$$

We denote $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, then $J(z) = -\frac{E}{z - A + 2\alpha B}$. In the first, we consid-

er this equation in the below continuous spectrum of the operator \tilde{H}_1 . Then

$\frac{1}{\sqrt{(A-z)^2 - 4B^2}} = \frac{E}{A-z-2\alpha B}$. This equation has the solutions

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}, \text{ and } z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}.$$

Now, we verify the condition $z_i < A - 2B, i = 1, 2$. The solution z_1 no satisfies

the condition $z_1 < A - 2B$, but z_2 satisfies the condition $z_2 < A - 2B$. We

now verify the conditions $z_2 < A - 2\alpha B$. The appear, this inequality is incorrect.

The appear inequalities $z_1 > A + 2B$ is correct, and $z_2 > A + 2B$, is incorrect.

We now verify the conditions $z_1 > A - 2\alpha B$. So far as, $A - 2\alpha B < A + 2B$, the

appear, this inequality is correct. Consequently, in this case, the operator \tilde{H}_1

has a unique eigenvalue $z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}$, above of continuous

spectrum of the operator \tilde{H}_1 .

F) If $\varepsilon_2 > 0$, and $\varepsilon_1 < -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, (respectively, $\varepsilon_2 < -2B$, and $\varepsilon_1 < -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then we assume that $\varepsilon_1 = -\alpha \times \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, where $\alpha > 1$ -real number. The equation for eigenvalues and eigenfunctions take in the form

$$(\varepsilon_2^2 + 2B\varepsilon_2)(z - A - 2\alpha B)J(z) = -(B + \varepsilon_2)^2.$$

From here $J(z) = -\frac{(B + \varepsilon_2)^2}{(\varepsilon_2^2 + 2B\varepsilon_2)(z - A - 2\alpha B)}$. The introduce notation

$$E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}. \text{ Then}$$

$$J(z) = -\frac{E}{z - A - 2\alpha B}. \tag{13}$$

In the below continuous spectrum of the operator \tilde{H}_1 , we have the equation

$$J(z) = \frac{E}{A - z + 2\alpha B}, \text{ from here } \frac{1}{\sqrt{(A - z)^2 - 4B^2}} = \frac{E}{A - z + 2\alpha B};$$

This equation takes the form

$$(E^2 - 1)(A - z)^2 - 4\alpha B(A - z) - 4B^2(E^2 + \alpha^2) = 0.$$

We find

$$z_1 = A - \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} \text{ and } z_2 = A - \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}.$$

We now verify the conditions $z_i < m_1 = A - 2B, i = 1, 2$. The appear, that $z_1 < A - 2B$, is correctly and $z_2 < A - 2B$, is incorrect. Now we consider Equation (13) in the above continuous spectrum of the operator \tilde{H}_1 . Then

$$J(z) = -\frac{E}{z - A - 2\alpha B}. \text{ From this } -\frac{1}{\sqrt{(z - A)^2 - 4B^2}} = -\frac{E}{z - A - 2\alpha B}. \text{ We find}$$

$$z_1 = A - \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}, \text{ and } z_2 = A + \frac{2B(-\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}.$$

We verify the conditions $z_i > A + 2B, i = 1, 2$. The appear $z_1 > A + 2B$, it is not true, and the $z_2 > A + 2B$, is true. We now verify the conditions $z_2 > A + 2\alpha B$. The appear, this inequality is incorrect. Consequently, in this case, the operator

\tilde{H}_1 have unique eigenvalue $z_1 = A - \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} < m_1$, i.e., lying the below continuous spectrum of the operator \tilde{H}_1 .

K) If $\varepsilon_2 > 0$ and $-\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} < \varepsilon_1 < \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively,

$\varepsilon_2 < -2B$ and $-\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} < \varepsilon_1 < \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, we take

$\varepsilon_1 = \alpha \times \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$, where $-1 < \alpha < 1$ -real number. Then the equation for eigenvalues and eigenfunctions has the form

$$(\varepsilon_2^2 + 2B\varepsilon_2)(z - A + 2\alpha B)J(z) = -(B + \varepsilon_2)^2, |\alpha| < 1. \tag{14}$$

We denote $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$. Then Equation (14) receives the form

$$J(z) = -\frac{E}{z - A + 2\alpha B}.$$

In the below of continuous spectrum of the operator \tilde{H}_1 we have the equation of the form

$$\frac{1}{\sqrt{(A - z)^2 - 4B^2}} = \frac{E}{A - z - 2\alpha B}, |\alpha| < 1.$$

This equation has a solutions

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}, \text{ and } z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}.$$

The inequalities $z_1 < A - 2B$, and $z_1 < A - 2\alpha B$, is incorrect. The inequalities $z_2 < A - 2B$, is correct. We now verify the conditions $z_2 < A - 2\alpha B$, since $A - 2B < A - 2\alpha B$, this inequality is true. We now consider Equation (14) in the above continuous spectrum of the operator \tilde{H}_1 . We have the equation of the form

$$-\frac{1}{\sqrt{(z - A)^2 - 4B^2}} = -\frac{E}{z - A + 2\alpha B}.$$

This equation has a solutions

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}, \text{ and } z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}.$$

The inequalities $z_1 > A + 2B$, and $z_1 > A - 2\alpha B$ is true, as $A + 2B > A - 2\alpha B$, that the inequality $z_1 > A - 2\alpha B$ is correct. The inequalities $z_2 > A + 2B$, and $z_2 > A + 2\alpha B$ is incorrect. Consequently, in this case, the operator \tilde{H}_1 has exactly two eigenvalues

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1}, \text{ and } z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1},$$

lying the above and below of continuous spectrum of the operator \tilde{H}_1 .

M) If $-2B < \varepsilon_2 < 0$, then $\varepsilon_2^2 + 2B\varepsilon_2 < 0$, and the function

$$\psi(z) = -\frac{(B + \varepsilon_2)^2}{\varepsilon_1 B + (\varepsilon_2^2 + 2B\varepsilon_2)(z - A)}$$

is a decreasing function in the intervals

$(-\infty, z_0)$ and $(z_0, +\infty)$; By, $z \rightarrow -\infty$ the function $\psi(z) \rightarrow -0$, and by $z \rightarrow z_0 - 0$, the function $\psi(z) \rightarrow -\infty$, and by $z \rightarrow +\infty$, $\psi(z) \rightarrow +0$, and by $z \rightarrow z_0 + 0$, $\psi(z) \rightarrow +\infty$. The function $J(z) \rightarrow 0$, by $z \rightarrow -\infty$, and by $z \rightarrow m_1 - 0$, the function $J(z) \rightarrow +\infty$, and by $z \rightarrow M_1 + 0$, the function $J(z) \rightarrow -\infty$, by $z \rightarrow +\infty$, the function $J(z) \rightarrow -0$. Therefore, the equation $\psi(z) = J(z)$, that's impossible the solutions in the outside the continuous spectrum of operator \tilde{H}_1 . Therefore, in this case, the operator \tilde{H}_1 has no eigenvalues lying the outside of continuous spectrum of the operator \tilde{H}_1 . \square

Consequently, the spectrum of operator \tilde{H}_1 is consisted of a continuous spectrum and at most two eigenvalues.

Now, using the obtained results and representation (9), we describe the structure of essential spectrum and discrete spectrum of the energy operator of four-electron systems in the impurity Hubbard model in the first triplet state.

Theorem 6. (essential spectra of the operator ${}^1\tilde{H}_1^t$) Let $\nu = 1$. Then

A) If $\varepsilon_2 = -B$ and $\varepsilon_1 < -2B$ (respectively, $\varepsilon_2 = -B$ and $\varepsilon_1 > 2B$), then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$:

$$\begin{aligned} \sigma_{ess}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ & \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \\ & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ & \cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and the discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than three eigenvalues:

$$\sigma_{disc}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

where $z = A + \varepsilon_1$, and z_3 and z_4 are the additional eigenvalues of operator ${}^1\tilde{H}_1^t$.

B) If $\varepsilon_2 = -2B$ and $\varepsilon_1 < 0$ or $\varepsilon_2 = 0$ and $\varepsilon_1 < 0$ (respectively, $\varepsilon_2 = -B$ and $\varepsilon_1 > 0$ or $\varepsilon_2 = 0$ and $\varepsilon_1 > 0$), then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$:

$$\begin{aligned} \sigma_{ess}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ & \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \\ & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ & \cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more three eigenvalues:

$$\sigma_{disc}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

where $z = A + \sqrt{4B^2 + \varepsilon_1^2}$, and z_3 and z_4 are the additional eigenvalues of

operator ${}^1\tilde{H}_1^t$.

C) If $\varepsilon_1 = 0$ and $\varepsilon_2 > 0$ (respectively, $\varepsilon_1 = 0$ and $\varepsilon_2 < -2B$), then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$:

$$\begin{aligned} \sigma_{\text{ess}}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ & \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \\ & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ & \cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than three eigenvalues:

$$\sigma_{\text{disc}}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

where $z = A - \frac{2BE}{\sqrt{E^2 - 1}}$, (respectively, $z = A + \frac{2BE}{\sqrt{E^2 - 1}}$), and $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$,

and z_3 and z_4 are the additional eigenvalues of operator ${}^1\tilde{H}_1^t$.

D) If $\varepsilon_1 = \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_1 = -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$:

$$\begin{aligned} \sigma_{\text{ess}}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ & \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \\ & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ & \cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than three eigenvalues:

$$\sigma_{\text{disc}}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

where $z = A + \frac{2B(E^2 + 1)}{E^2 - 1}$ (respectively, $z = A - \frac{2B(E^2 + 1)}{E^2 - 1}$), and

$E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and z_3 and z_4 are the additional eigenvalues of operator ${}^1\tilde{H}_1^t$.

E) If $\varepsilon_2 > 0$ and $\varepsilon_1 > \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_2 < -2B$ and $\varepsilon_1 > \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$:

$$\begin{aligned} \sigma_{\text{ess}}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ & \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \end{aligned}$$

$$\begin{aligned} & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ & \cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than three eigenvalues:

$$\sigma_{disc}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

where

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1},$$

and $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and the real number $\alpha > 1$, and z_3 and z_4 are the ad-

ditional eigenvalues of operator ${}^1\tilde{H}_1^t$.

F) If $\varepsilon_2 > 0$ and $\varepsilon_1 < -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_2 < -2B$ and $\varepsilon_1 < -\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$), then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $4 \leq N_1 \leq 8$:

$$\begin{aligned} \sigma_{ess}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ & \cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \\ & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ & \cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than three eigenvalues:

$$\sigma_{disc}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

where

$$z_1 = A - \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1},$$

and $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and the real number $\alpha > 1$, and z_3 and z_4 are the ad-

ditional eigenvalues of operator ${}^1\tilde{H}_1^t$.

K) If $\varepsilon_2 > 0$ and $-\frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B} < \varepsilon_1 < \frac{2(\varepsilon_2^2 + 2B\varepsilon_2)}{B}$ (respectively, $\varepsilon_2 < -2B$ 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 ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $10 \leq N_1 \leq 16$:

$$\begin{aligned} \sigma_{\text{ess}}\left({}^1\tilde{H}_1^t\right) &= [4A - 8B, 4A + 8B] \cup [3A - 6B + z_1, 3A + 6B + z_1] \\ &\cup [3A - 6B + z_2, 3A + 6B + z_2] \cup [2A - 4B + 2z_1, 2A + 4B + 2z_1] \\ &\cup [2A - 4B + z_1 + z_2, 2A + 4B + z_1 + z_2] \cup [2A - 4B + 2z_2, 2A + 4B + 2z_2] \\ &\cup [A - 2B + 3z_1, A + 2B + 3z_1] \cup [A - 2B + 2z_1 + z_2, A + 2B + 2z_1 + z_2] \\ &\cup [A - 2B + z_1 + 2z_2, A + 2B + z_1 + 2z_2] \cup [A - 2B + 3z_2, A + 2B + 3z_2] \\ &\cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ &\cup [A - 2B + z_1 + z_3, A + 2B + z_1 + z_3] \cup [A - 2B + z_1 + z_4, A + 2B + z_1 + z_4] \\ &\cup [A - 2B + z_2 + z_3, A + 2B + z_2 + z_3] \cup [A - 2B + z_2 + z_4, A + 2B + z_2 + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than eleven eigenvalues:

$$\begin{aligned} \sigma_{\text{disc}}\left({}^1\tilde{H}_1^t\right) &= \{4z_1, 3z_1 + z_2, 2z_1 + 2z_2, z_1 + 3z_2, 4z_2, 2z_1 + z_3, 2z_1 + z_4, \\ & z_1 + z_2 + z_3, z_1 + z_2 + z_4, 2z_2 + z_3, 2z_2 + z_4\}, \end{aligned}$$

where

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} < m_1,$$

and

$$z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} > M_1,$$

and $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and real number $|\alpha| < 1$, and z_3 and z_4 are the additional eigenvalues of operator ${}^1\tilde{H}_1^t$.

M) If $-2B < \varepsilon_2 < 0$, then the essential spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of the union of N_1 segments, where $1 \leq N_1 \leq 3$:

$$\begin{aligned} \sigma_{\text{ess}}\left({}^1\tilde{H}_1^t\right) &= [4A - 8B, 4A + 8B] \cup [2A - 4B + z_3, 2A + 4B + z_3] \\ &\cup [2A - 4B + z_4, 2A + 4B + z_4], \end{aligned}$$

and the discrete spectrum of operator ${}^1\tilde{H}_1^t$ is an empty set.

Proof. A) It follows from representation (9), and from Theorem 5, that in one-dimensional case, the continuous spectrum of the operator \tilde{H}_1 is consisted of $\sigma_{\text{cont}}(\tilde{H}_1) = [A - 2B, A + 2B]$, and discrete spectrum of the operator \tilde{H}_1 is consists of unique eigenvalue z . Therefore, the essential spectrum of the operator ${}^1\tilde{H}_1^t$ consists of the union of no more than eight segments:

$$\begin{aligned} \sigma_{\text{ess}}\left({}^1\tilde{H}_1^t\right) &= [4A - 8B, 4A + 8B] \cup [3A - 6B + z, 3A + 6B + z] \\ &\cup [2A - 4B + 2z, 2A + 4B + 2z] \cup [A - 2B + 3z, A + 2B + 3z] \\ &\cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ &\cup [A - 2B + z + z_3, A + 2B + z + z_3] \\ &\cup [A - 2B + z + z_4, A + 2B + z + z_4], \end{aligned}$$

and discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists is the no more than three eigenvalues:

$$\sigma_{disc}({}^1\tilde{H}_1^t) = \{4z, 2z + z_3, 2z + z_4\},$$

This is given to the proof of statement A) from Theorem 6.

The statements B), C), D), E), F) from Theorem 6 are proved similarly.

We now is proved the statement K) from Theorem 6. It can be seen from Theorem 5 (statement K) in a one-dimensional case the operator \tilde{H}_1 has exactly two eigenvalues z_1 and z_2 outside the domain of continuous spectrum of the operator \tilde{H}_1 . Therefore, the set $\sigma_{ess}({}^1\tilde{H}_1^t)$ consists of the union of no more than sixteen intervals:

$$\begin{aligned} \sigma_{ess}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [3A - 6B + z_1, 3A + 6B + z_1] \\ & \cup [3A - 6B + z_2, 3A + 6B + z_2] \cup [2A - 4B + 2z_1, 2A + 4B + 2z_1] \\ & \cup [2A - 4B + z_1 + z_2, 2A + 4B + z_1 + z_2] \cup [2A - 4B + 2z_2, 2A + 4B + 2z_2] \\ & \cup [A - 2B + 3z_1, A + 2B + 3z_1] \cup [A - 2B + 2z_1 + z_2, A + 2B + 2z_1 + z_2] \\ & \cup [A - 2B + z_1 + 2z_2, A + 2B + z_1 + 2z_2] \cup [A - 2B + 3z_2, A + 2B + 3z_2] \\ & \cup [2A - 4B + z_3, 2A + 4B + z_3] \cup [2A - 4B + z_4, 2A + 4B + z_4] \\ & \cup [A - 2B + z_1 + z_3, A + 2B + z_1 + z_3] \cup [A - 2B + z_1 + z_4, A + 2B + z_1 + z_4] \\ & \cup [A - 2B + z_2 + z_3, A + 2B + z_2 + z_3] \cup [A - 2B + z_2 + z_4, A + 2B + z_2 + z_4]. \end{aligned}$$

The discrete spectrum of the operator ${}^1\tilde{H}_1^t$ is consists of no more than eleven eigenvalues:

$$\begin{aligned} \sigma_{disc}({}^1\tilde{H}_1^t) = & \{4z_1, 3z_1 + z_2, 2z_1 + 2z_2, z_1 + 3z_2, 4z_2, 2z_1 + z_3, 2z_1 + z_4, \\ & z_1 + z_2 + z_3, z_1 + z_2 + z_4, 2z_2 + z_3, 2z_2 + z_4\}, \end{aligned}$$

where

$$z_1 = A + \frac{2B(\alpha + E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} < m_1,$$

and

$$z_2 = A + \frac{2B(\alpha - E\sqrt{E^2 - 1 + \alpha^2})}{E^2 - 1} > M_1,$$

and $E = \frac{(B + \varepsilon_2)^2}{\varepsilon_2^2 + 2B\varepsilon_2}$, and real number $|\alpha| < 1$, lying the outside of the essential

spectrum of the operator ${}^1\tilde{H}_1^t$, z_3 and z_4 are the additional eigenvalues of operator ${}^1\tilde{H}_1^t$. This is given to the proof of statement K) from Theorem 6.

We now are proved the statement M) from Theorem 6. It can be seen from Theorem 5 (statement M) in a one-dimensional case the operator \tilde{H}_1 has no eigenvalues outside of the continuous spectrum of the operator \tilde{H}_1 . Therefore, the set $\sigma_{ess}({}^1\tilde{H}_1^t)$ consists of the union of no more than three segment:

$$\begin{aligned} \sigma_{ess}({}^1\tilde{H}_1^t) = & [4A - 8B, 4A + 8B] \cup [2A - 4B + z_3, 2A + 4B + z_3] \\ & \cup [2A - 4B + z_4, 2A + 4B + z_4], \end{aligned}$$

and the operator has no eigenvalues, *i.e.*, $\sigma_{disc}({}^1\tilde{H}_1^t) = \emptyset$. □

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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