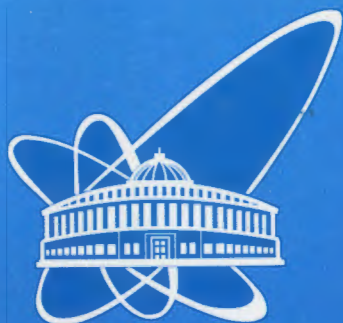


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ELECTRONIC STRUCTURE
FOR THE TWO-BAND HUBBARD MODEL
OF THE LADDER α - NaV_2O_5 COMPOUND

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I. Introduction

Transition-metal oxides which contain degenerate d -level electrons are characterized by strong correlations among them leading to different kinds of mutually competing orders [1]-[4]. One possibility to investigate such systems is to use the well known Hubbard model, where the quantum state of an electron localized on a cell site i can be described with two indexes: spin σ and the type of the occupied orbital α . The normal product of the Fermi operators $a_{i\alpha\sigma}^+ a_{j\beta\sigma'}$ for the d -electrons was replaced with corresponding product of the 1/2-spin \mathbf{S} and 1/2-pseudospin (isospin) τ operators by Kugel and Khomskii [1, 2]. Such spin-pseudospin formalism has been used by many workers who investigated the low dimensional quantum spin systems [5]-[9]. Discovery of the high-temperature superconductivity in lightly doped planar spin 1/2 antiferromagnetic cuprates (see for ex. [10]) initiate also a lot of investigations on the ladder lattice materials because one may expect that 2-leg ladder should be intermediate system between a chain and a plain [11].

A special attention attracted recently the α' -phase ($0 < x < 0.02$) of the $\text{Na}_{1-x}\text{V}_2\text{O}_5$ ladder layer compound with Na deficiency. Isobe and Ueda [12] were the first who found a significant decrease of the macroscopic magnetic susceptibility in a quasi-one-dimensional transition metal oxide compound α' - NaV_2O_5 bellow $T_c \simeq 34$ K, and established the opening of a spin gap in the magnon spectrum. That behavior was attributed to the spin-Peierls (SP) phase transition, where the magnetoelastic coupling of the one-dimensional (1D) spin-1/2 chains with 3D phonons leads to the magnetic lattice dimerization [13, 14].

One of the first theoretical attempts was performed by use of a one-dimensional (1D) dimerized Heisenberg model showing the existence of a low-energy magnon branch separated from the continuum [15]. The authors of the Refs. [16, 17] went beyond the presentation of α' - NaV_2O_5 as a spin-chain compound and included also the charge dynamics in terms of the pseudospin operators. Treating on-site and inter-site Coulomb interactions within the Hartree approximation in the model of single d_{xy} orbital, Seo and Fukuyama [18] found that the inter-site Coulomb interaction induces a zigzag type of charge order (CO) along the ladders of V-ions, resulting in localized spins between neighboring ladders to form a spin gap.

A new view to the electronic structure of vanadate α' - NaV_2O_5 in

centrosymmetric $D_{2h}^{13} - Pmmn$ crystal structure was adopted by Horsch and Mack [19]. They proposed an explanation for the insulating state, which is not based on a charge modulation. Using the Hubbard-type model Hamiltonian they argued that strong correlations, together with the Heitler-London character of the relevant intermediate states, lead to a special kind of antiferromagnetic (AF) Heisenberg chains. In order to investigate the interplay between electron-electron Coulomb repulsion, and electron phonon (or spin-phonon) couplings, a numerical exact diagonalization technique was applied in [20]. For the corresponding set of parameter values of the anisotropic $t - J$ model, it was shown that considered systems undergo instabilities toward the formation of charge density waves, bond order waves, and generalized spin-Peierls modulated structures.

After these theoretical attempts, a lot of experimental work have been done also. Let us mention for example, nuclear magnetic resonance (NMR) [21, 22], inelastic neutron scattering (INS) [23]-[25], angle-resolved photoemission spectroscopy (ARPES)[26], electron paramagnetic resonance (EPR) [27], and Raman spectroscopy [28, 29] measurements.

An important prerequisite, before doing more established theoretical and experimental investigations with the intention of better understanding of low energy electronic properties of the considered compound, is a detailed knowledge of its electronic structure. Several *ab initio* band structure calculations by means of standard density functional methods in the local-density-approximation (LDA), local-spin-density-approximation (LSDA), and more sophisticated LDA+U method, were done [30]-[34]. According to the cited works, the occupied orbitals close to the Fermi level are mostly of vanadium d_{xy} -type. These bands are well separated from lower lying oxygen $2p$ -, and higher lying remaining vanadium $3d$ -, and sodium $3s$ -orbitals. Tight binding fitting of the band structure results showed that intra-ladder next nearest neighbor (n.n.n.) hoppings are much larger than nearest neighbor (n.n.) V-V inter-ladder hopping amplitudes. This makes NaV_2O_5 a quarter filled system of vanadium two-leg ladders (so called Trellis lattice). From the estimated values of the intra-ladder hopping along rung (t_a) and between rungs (t_b), where $2t_a > 4t_b$ relation is fulfilled, one can see that each rung is occupied by a single electron in a bonding state. For the strong on-site Coulomb repulsion, system becomes insulating without involving any CO. Then the

electron state which is delocalized on the ladder rung, can be described by introducing two quantum numbers: spin S and the occupation number of the left or right site of the ends of the chosen rung. As in the well known cases of systems with the orbital degeneracy, it is possible to introduce pseudo-spin operator τ , in order to describe the occupancy of the left (L), or the right (R) site, on the singled out ladder-rung [16],[17],[35]-[37].

Sa and Gros [35] investigated the influence of different inter-site Coulomb repulsion on the exchange couplings and charge orderings. They found that the effective intra-ladder exchange can become ferromagnetic for the case of zigzag CO.

Yushankhai and Thalmeier [36] used molecular orbital representation for intra-rung electronic states, and developed second-order perturbation procedure in order to derive an effective spin-chain model for one ladder. They included possible CO in mean field treatment of inter-rung Coulomb interaction. This results in superexchange integral dependence on the charge ordering (although they found that superexchange is always AF).

Suaud and M.-B. Lepetit [38] performed the numerical *ab initio* evaluations of the hopping and the magnetic exchange integrals in the framework of the n.n. t - J model and also evaluated the relative amplitudes of the underlying extended Hubbard Hamiltonian. They found that the state with an unpaired delocalized electron on each V-O-V rung is energetically more stable, and that the α' - NaV_2O_5 system can be taken as 2D triangular Heisenberg lattice (as in Ref. [19]), where the effective exchange along the ladder-legs direction is antiferromagnetic (AF), while it is ferromagnetic (FM) along the other directions.

After detailed crystal structure determination in [39], bond-valence method was used to determine effective valencies of sodium and the vanadium atoms in both crystal phases of α' - NaV_2O_5 compound. Using Slater-Koster approach, there were estimated the effective V-V hopping and the superexchange integral, and compared with the ones obtained from band structure calculations. Bernert, Thalmeier and Fulde [39] used an extended Hubbard model for vanadium layers with on-site and inter-site Coulomb interactions included. Then they reduce it to an effective low-energy model with Ising chains in transverse field, in terms of the pseudospin operators, and with coupled Heisenberg spin chains. Taking into account that the displacements of the oxygen ions affect superexchange interaction between V spins, in the former Hamiltonian, they added parts describing phonon dispersions of the lattice modes, coupling

between lattice distortions, and additional effective field which can cause CO. Such a model enable them to explain a number of experimental observations, such as the existence of two phase transitions, very close to each other at $T_c \simeq 34$ K, the low-energy magnon dispersion, etc.

However, starting from extended Hubbard model [35]-[37], it seems favorable to use Hubbard operators formalism as in [36] (but without reducing the problem to one band model). The occupancy of the left or right rung site is included as corresponding index on the X operator, which at the same time describes certain transition between low energy electronic states. Due to the fact that the technique of operating with Hubbard operators is well elaborate (see for ex. [42]) it is much easier to follow the physical meaning of approximations which should be introduced during the calculations.

In order to describe low energy electronic spectrum of α' - NaV_2O_5 compound, we consider an extended two band Hubbard model. To get possible low temperature charge orderings, in the main part of the tight binding Hamiltonian for d_{xy} -vanadium orbitals obtained by use of band structure calculations [30]-[34], on-site and inter-site Coulomb interactions are added (like in Refs. [35] and [37]). To take into account rigorously the projected character of electron operators, we employ the Hubbard operator technique as in [36]. Using the cell perturbation method [19, 36, 40], we reduce considered Hamiltonian to effective one-particle and singlet two-band asymmetric Hubbard model, without further reduction to corresponding one-band t - J model [38],[36]. Further reduction to a corresponding one band t - J model has some disadvantages. For example, it neglects completely the charge fluctuations between the two particle and the one-particle states. This modifies the spectrum in a considerable way and can be serious shortcoming. The t - J model may not reproduce in a correct way the spectral weight changes which occur with doping. To avoid these shortcomings we present in this paper an effective Hubbard model for one-particle and two-particle singlet states. That keeps the possibility to describe the dynamical effects of the exchange interaction in terms of Green's functions [42].

The appearance of singlet quasiparticle states inside the d -charge transfer gap can be expected and should be proved by different methods based on exact diagonalization, cluster calculations, projection technique and other calculations. It should be noted that the commonly used local density approximation cannot describe such a singlet band formation due

to the insufficient accuracy in the treatment of electronic correlations.

The main purpose of the present work consists in the presentation of a new Hamiltonian to describe low-energy physics in the α' - NaV_2O_5 compound similarly to the two-band singlet-hole model proposed for the copper-oxide plane [42]. Contrary to the usual Hubbard model, one ends up with an asymmetric model, with different hopping integrals for the singlet and the one-particle bands. Using such Hamiltonian has some practical advantages since several well established techniques are for the Green's functions decoupling schemes can be exploited here [42].

We also apply the projection technique for the two-time matrix GF in terms of Hubbard operators. We ends up with the Dyson equation, where the zero-order GF in a generalized mean-field approximation (GMFA) is introduced. Zero-order GF is defined through the frequency matrix. Its components are determined by the energy shifts and by the renormalized hopping parameters. Both contain the correlation functions which take care of many body effects in systems with pronounced electronic correlation effects. Additional work should be done in order to obtain the self-consistent system of the equations for the one-particle GF, whose numerical solutions will give the electronic structure and the density of states for the α' - NaV_2O_5 compound.

The paper is organized as follows: after presenting the reduction procedure from the $V\text{-}d_{xy}$ two bands model to an effective two-subband Hubbard model in Sect. II. we define the one-particle GF in Sect. III. In Sect. IV. we discuss results of obtained energy shifts and the renormalized hopping parameters. The self-consistent system of equations and the results of a numerical calculation will be presented elsewhere. Finally, in Sect. V. we summarize the results and briefly describe our further intentions.

II. Two-band model Hamiltonian

Taking into account band structure calculations [30]-[34], experimental [12][21]-[29], and theoretical results [15]-[20] and [35]-[37], we consider an effective electronic Hamiltonian for the quarter-filled two-leg ladder vanadate α' - NaV_2O_5 compound, which has a general form of an extended two-band Hubbard model already applied in [35],[36]-[37]. This Hamiltonian takes into account strong electronic correlations at the vanadium

sites and strong Coulomb interactions between them, and has the form:

$$H = H_0 + H_v + H_t . \quad (1)$$

First part H_0 describe intra-cell (intra-rung) interactions

$$H_0 = t_a \sum_{im\sigma} (R_{im\sigma}^+ L_{im\sigma} + H.c.) + U \sum_{im} (n_{im\uparrow}^R n_{im\downarrow}^R + n_{im\uparrow}^L n_{im\downarrow}^L) + V_a \sum_{im\sigma\sigma'} n_{im\sigma}^R n_{im\sigma'}^L , \quad (2)$$

where t_a is the hopping integral between left and right sites on the same ladder-rung, $R_{im\sigma}^+$ is the creation operator of an electron in d_{xy} vanadium state on the right site of unit cell im (i denotes rung of the ladder m) and $L_{im\sigma}$ is the corresponding one-particle annihilation operator on the left site of the unit cell im (cf. Fig.1).

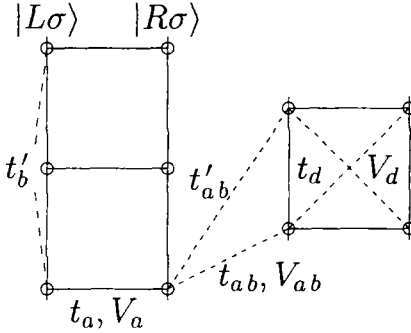


Fig. 1. Part of schematic ladder structure

Electron density operators at these sites are $n_{im\sigma}^R$ and $n_{im\sigma}^L$, with spin $\sigma = (\uparrow, \downarrow) = (+, -)$, and U and V_a are the on-site and inter-site Coulomb repulsion in a rung, respectively. The inter-rung Coulomb interactions H_v can be divided in the intra-ladder parts $H_v(V_b)$ - along ladder-legs, and $H_v(V_d)$ - along the diagonal connecting different ends of the neighboring rungs of the same ladder, and the inter-ladders part $H_v(V_{ab})$ as follows:

$$H_v = H_v(V_b) + H_v(V_d) + H_v(V_{ab}) , \quad (3)$$

$$H_v(V_b) = V_b \sum_{\langle i,j \rangle m\sigma\sigma'} (n_{im\sigma}^L n_{jm\sigma'}^L + n_{im\sigma}^R n_{jm\sigma'}^R) , \quad (4)$$

$$H_v(V_d) = V_d \sum_{\langle i,j \rangle m \sigma \sigma'} (n_{im\sigma}^L n_{jm\sigma'}^R + n_{im\sigma}^R n_{jm\sigma'}^L), \quad (5)$$

$$H_v(V_{ab}) = V_{ab} \sum_{\langle i,j \rangle m \sigma \sigma'} n_{im\sigma}^R n_{j,m+1,\sigma'}^L, \quad (6)$$

where $n = m + 1$ and the summation is performed over n.n. sites $\langle i, j \rangle$, ladder m and spins σ, σ' , correspondingly. Corresponding Coulomb terms are estimated phenomenologically by taking into account electron screening interactions [35]: $V_a \simeq 0.37$ eV, $V_b \simeq 0.36$ eV, $V_d \simeq 0.26$ eV and $V_{ab} \simeq 0.43$ eV. We also adduce values of inter-site Coulomb repulsive interactions, used in different works (cf. Table 1).

Table 1: Values (in eV) of the inter-site Coulomb interactions used in different works.

| Ref. | V_a | V_b | V_d | V_{ab} | Ref. | V_a | V_b | V_d | V_{ab} |
|----------|-------|-------|-------|------------|----------|-------|-------|-------|----------|
| [30, 33] | | | | | [19, 34] | | | | |
| [18] | 1 | 1 | | $\sqrt{2}$ | [35] | 0.37 | 0.36 | 0.26 | 0.43 |
| [39] | | 0.344 | | | [38] | | 1.076 | | |

The hopping interactions H_t can be divided in the intra- and inter-ladder hopping. Both of them contain parts with n.n. and the next nearest neighbor (n.n.n.) interacted sites. The hopping parameters of the n.n. parts are t_b, t_d and t_{ab} and for the n.n.n., they are t'_b and t'_{ab} . Respectively, the intra- (b, d) and inter-ladder (ab) with (n.n.) and (n.n.n.) parts are according to the sense given in the following Eqs.

$$H_t = H_t(t_b) + H_t(t'_b) + H_t(t_d) + H_t(t_{ab}) + H_t(t'_{ab}), \quad (7)$$

$$H_t(t_b) = t_b \sum_{\langle i,j \rangle m \sigma} (R_{im\sigma}^+ R_{jm\sigma} + L_{im\sigma}^+ L_{jm\sigma} + H.c.), \quad (8)$$

$$H_t(t'_b) = t'_b \sum_{\langle\langle i,j \rangle\rangle m \sigma} (R_{im\sigma}^+ R_{jm\sigma} + L_{im\sigma}^+ L_{jm\sigma} + H.c.), \quad (9)$$

$$H_t(t_d) = t_d \sum_{\langle i,j \rangle m \sigma} (R_{im\sigma}^+ L_{jm\sigma} + L_{im\sigma}^+ R_{jm\sigma} + H.c.), \quad (10)$$

$$H_t(t_{ab}) = t_{ab} \sum_{\langle i,j \rangle m \sigma \sigma'} (R_{im\sigma}^+ L_{j,m+1,\sigma'} + H.c.), \quad (11)$$

$$H_t(t'_{ab}) = t'_{ab} \sum_{\langle\langle i,j \rangle\rangle m\sigma\sigma'} (R_{im\sigma}^+ L_{j,m+1,\sigma} + H.c.), \quad (12)$$

where $\langle i, j \rangle$ and $\langle\langle i, j \rangle\rangle$ respectively mean the summation over n.n. and n.n.n. corresponding sites. The hopping parameters t_α and on-site Coulomb interactions U obtained by use of various band structure methods are presented in the Table 2.

Table 2: Values (in eV) of the hopping parameters t_α and on-site Coulomb interaction U , obtained on the basis of band-structure calculations .

| Ref. | t_a | t_b | t'_b | t_d | t_{ab} | t'_{ab} | U |
|----------|--------|--------|--------|-------|----------|-----------|------|
| [30, 35] | -0.38 | -0.17 | | | 0.012 | | 2.8 |
| [18, 19] | -0.35 | -0.15 | | | -0.3 | | 4.0 |
| [38] | 0.5382 | 0.1246 | | | -0.0442 | | 6.8 |
| [33] | | -0.085 | | 0.085 | | | 4.1 |
| [39] | 0.172 | 0.049 | | 0.062 | -0.110 | | 4.0 |
| [34] | -0.35 | -0.09 | -0.03 | -0.15 | 0.02 | 0.03 | 6.82 |

To derive the singlet band one can apply cell-perturbation method following mainly ([19, 36, 40]) and references cited therein. Firstly, one should diagonalize the intra-rung (intra-cell) hamiltonian (2) in the one-particle and two-particle sectors, which acts in the manifold of the following set of states:

- vacuum - $|0\rangle$,
- one-particle states: $|R\sigma\rangle = R_\sigma^+|0\rangle$ and $|L\sigma\rangle = L_\sigma^+|0\rangle$,
- two-particle states:

singlets

$$\begin{aligned} - |\psi_1\rangle &= R_\uparrow^+ R_\downarrow^+ |0\rangle, \\ - |\psi_2\rangle &= L_\uparrow^+ L_\downarrow^+ |0\rangle, \\ - |\psi_3\rangle &= \frac{1}{\sqrt{2}}(R_\uparrow^+ L_\downarrow^+ - R_\downarrow^+ L_\uparrow^+) |0\rangle, \end{aligned}$$

and triplets

$$\begin{aligned}
- |\xi_1\rangle &= R_{\uparrow}^+ L_{\uparrow}^+ |0\rangle, \\
- |\xi_2\rangle &= \frac{1}{\sqrt{2}}(R_{\uparrow}^+ L_{\downarrow}^+ + R_{\downarrow}^+ L_{\uparrow}^+) |0\rangle, \\
- |\xi_3\rangle &= R_{\downarrow}^+ L_{\downarrow}^+ |0\rangle.
\end{aligned}$$

One can propose that the low energy excitations in the system can be described taking into account only transitions inside the manifold, constructed with upper intra-cell states. Because of shortness, cell ladder indexes will be omitted any time when it could not leads to cumberosomes.

The action of the upper Fermi operators can be expressed as a sum of the transition operators, or Hubbard X-operators $X^{\alpha,\beta} \equiv |\alpha\rangle\langle\beta|$:

$$R_{\sigma}^+ \simeq X^{R\sigma,0} + \frac{\sigma}{\sqrt{2}} X^{\psi_3,L\bar{\sigma}} + \delta_{\uparrow,\sigma} X^{\xi_1,L\uparrow} + \frac{1}{\sqrt{2}} X^{\xi_2,L\bar{\sigma}} + \delta_{\downarrow,\sigma} X^{\xi_3,L\downarrow} + \sigma X^{\psi_1,R\bar{\sigma}}, \quad (13)$$

$$L_{\sigma}^+ \simeq X^{L\sigma,0} - \frac{\sigma}{\sqrt{2}} X^{\psi_3,R\bar{\sigma}} - \delta_{\uparrow,\sigma} X^{\xi_1,R\uparrow} - \frac{1}{\sqrt{2}} X^{\xi_2,R\bar{\sigma}} - \delta_{\downarrow,\sigma} X^{\xi_3,R\downarrow} + \sigma X^{\psi_2,L\bar{\sigma}}. \quad (14)$$

Using this representation, intra-cell Hamiltonian can be represented as a sum of distinct (non-overlapping) sectors, i.e.:

$$H_0 = H_0(R, L) + H_0(\psi_1, \psi_2, \psi_3) + H_0(\xi_1) + H_0(\xi_2) + H_0(\xi_3), \quad (15)$$

where

$$H_0(R, L) = t_a \sum_{im\sigma} (X_{im}^{R\sigma,L\sigma} + H.c.), \quad (16)$$

$$H_0(\psi_1, \psi_2, \psi_3) =$$

$$\sum_{im} \{U(X_{im}^{\psi_1,\psi_1} + X_{im}^{\psi_2,\psi_2}) + V_a X_{im}^{\psi_3,\psi_3} + t_a \sqrt{2}(X_{im}^{\psi_3,\psi_2} - X_{im}^{\psi_1,\psi_3} + H.c.)\}, \quad (17)$$

$$H_0(\xi_1) = V_a \sum_{im} X_{im}^{\xi_1,\xi_1}, H_0(\xi_2) = V_a \sum_{im} X_{im}^{\xi_2,\xi_2}, H_0(\xi_3) = V_a \sum_{im} X_{im}^{\xi_3,\xi_3}. \quad (18)$$

One should diagonalize the first two terms:

$$\begin{aligned}
H_0(R, L) &= |R\sigma\rangle t_a \langle L\sigma| + |L\sigma\rangle t_a \langle R\sigma| \\
&= (|R\sigma\rangle |L\sigma\rangle) \begin{pmatrix} 0 & t_a \\ t_a & 0 \end{pmatrix} \begin{pmatrix} \langle R\sigma| \\ \langle L\sigma| \end{pmatrix} \\
&= |\underline{R}\sigma\rangle t_a \langle \underline{R}\sigma| - |\underline{L}\sigma\rangle t_a \langle \underline{L}\sigma|, \quad (19)
\end{aligned}$$

where

$$\begin{pmatrix} |\underline{R\sigma}\rangle \\ |\underline{L\sigma}\rangle \end{pmatrix} = T^{-1} \begin{pmatrix} |R\sigma\rangle \\ |L\sigma\rangle \end{pmatrix} \quad (20)$$

are new molecular diagonalizing one-particle intra-cell states. Corresponding transformation (20) realize the following orthogonal ($T^{-1} = T^T$) matrix

$$T^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & t_a \\ t_a & 0 \end{pmatrix}. \quad (21)$$

For the singlet sector, one has

$$\begin{aligned} H_0(\psi_1, \psi_2, \psi_3) &= (|\psi_1\rangle |\psi_2\rangle |\psi_3\rangle) \begin{pmatrix} U & 0 & -t_a\sqrt{2} \\ 0 & U & t_a\sqrt{2} \\ -t_a\sqrt{2} & t_a\sqrt{2} & V_a \end{pmatrix} \begin{pmatrix} \langle\psi_1| \\ \langle\psi_2| \\ \langle\psi_3| \end{pmatrix} \\ &= |\underline{\psi_1}\rangle E_{\underline{\psi_1}} \langle\underline{\psi_1}| + |\underline{\psi_2}\rangle E_{\underline{\psi_2}} \langle\underline{\psi_2}| + |\underline{\psi_3}\rangle E_{\underline{\psi_3}} \langle\underline{\psi_3}|, \end{aligned} \quad (22)$$

where

$$\begin{pmatrix} |\underline{\psi_1}\rangle \\ |\underline{\psi_2}\rangle \\ |\underline{\psi_3}\rangle \end{pmatrix} = S^{-1} \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \\ |\psi_3\rangle \end{pmatrix}. \quad (23)$$

Here $\underline{\psi_\alpha}$ and $E_{\underline{\psi_\alpha}}$ are new molecular diagonalizing intra-cell singlet states and corresponding energies, which are obtained after diagonalizing square matrix in (23) using corresponding orthogonal transformation matrix $S^{-1} = S^T$. One can calculate their values as a function the model parameters t_a , U , and by use of $V_a = 0.37$ eV (V_a is taken from Ref. [35]). The corresponding values of the singlet energies $E_{\underline{\psi}}$ are given in the Table 3. One should note that the matrix elements of \overline{S} transformation matrix (which transform $|\underline{\psi_\alpha}\rangle \rightarrow |\psi_\beta\rangle$) satisfy the following relation $s_{13} = -s_{23}$.

Band structure calculations [30]-[34] indicate that α' - NaV_2O_5 can be considered as quarter filled ladder compound with. In order to investigate physical characteristics caused by the low-energy electron excitations in the considered system, one can propose that it is enough to consider a restriction to the manifold constructed with the lowest one-particle and two-particle states. As one can see, the bonding state $|\underline{R\sigma}\rangle$ has about $2|t_a| \simeq 0.7$ eV lower energy then antibonding one-hole state $|\underline{L\sigma}\rangle$ which can be neglected in the subspace of one-hole states. The singlet states $|\underline{\psi_3}\rangle$ are the lowest among the two-hole states, and have to be filled first

Table 3: Values (in eV) of the corresponding energy eigenvalues for diagonalized singlet states, calculated by using the parameter values obtained in different cited works and with $V_a = 0.37$ eV ([35]). Only in [18], there proposed value $V_a = 1$ eV, is used.

| Ref. | E_{ψ_1} | E_{ψ_2} | E_{ψ_3} | Ref. | E_{ψ_1} | E_{ψ_2} | E_{ψ_3} |
|------|--------------|--------------|--------------|------|--------------|--------------|--------------|
| [30] | 3.01 | 2.8 | 0.15 | [35] | 6.97 | 6.8 | 0.19 |
| [19] | 4.13 | 4.0 | 0.24 | [39] | 4.03 | 4.0 | 0.34 |
| [18] | 4.15 | 4.0 | 0.84 | [34] | 6.89 | 6.82 | 0.29 |

with doping. Other singlet states, $|\psi_1\rangle$ and $|\psi_2\rangle$ with very high energies $E_{\psi_{1,2}}$ of about few eV (cf. Table 3), and the triplet states with the energy level $|t_a| + V_a \simeq 0.7$ eV, are above the referent one-particle bonding level at $t_a \simeq -0.35$ eV. At small doping levels we can also neglect the higher singlet states. This is permitted due to the expectation that the mixing between lower singlet and higher singlet and triplet bands is rather small.

Intra-cell (intra-rung) Hamiltonian can be written as

$$\tilde{H}_0 \simeq t_a \sum_{im\sigma} X_{im}^{\underline{R\sigma}, \underline{R\sigma}} + E_{\psi_3} \sum_{im} X_{im}^{\psi_3, \psi_3}. \quad (24)$$

Here, and further on, i will denote site of the chain m . Recall that after diagonalization of the intra-cell Hamiltonian, and after projecting it to the subspace (or manifold) of the low energy states, ladder 'compress' to a chain.

The products of Fermi operators with different cell indexes, which are contained in the inter-cell interaction parts H_v and H_t , can be presented in terms of the Hubbard operator products with corresponding indexes. That Hubbard X operators describe transition between states inside reduced low-energy manifold builded with vacuum $|0\rangle$ and molecular diagonalizing intra-cell states $|\underline{R\sigma}\rangle$ and $|\psi_3\rangle$, which are associated to all rung. It becomes superfluous further to take care of left/right rung side (site). However, it does not mean that the corresponding inter-chain ('inter-ladder') Coulomb interactions between one chain-site and the neighboring sites on left and right neighbor chains, should be the same as in the charge ordered phase ($T \leq 34$ K).

Underline will be omitted in further notations and we will use the following shorthanded designations: $|\underline{R\sigma}\rangle = |\sigma\rangle$ and $|\underline{\psi_3}\rangle = |2\rangle$. Thus, by projecting the original Fermi R and L operators in the inter-cell part of Hamiltonian, onto the subspace of one-particle $|\sigma\rangle$ and two-particle $|2\rangle$ states (22) and (24), one obtains:

$$R_{im\sigma}^+ = \frac{1}{\sqrt{2}}X_{im}^{\sigma 0} + \sigma AX_{im}^{2\bar{\sigma}}, \quad L_{im\sigma}^+ = \frac{1}{\sqrt{2}}X_{im}^{\sigma 0} - \sigma AX_{im}^{2\bar{\sigma}}, \quad (25)$$

with the coefficient

$$A = \frac{1}{2}s_{33} + \frac{1}{\sqrt{2}}s_{13}, \quad (26)$$

and $\sigma = \pm 1$. Now, we can write the inter-cell terms in Eqs. (3) and (7) as a sum of different parts describing Coulomb repulsion H_v and the hopping interactions H_t between intra- and inter-chain sites ('ladder rungs'), in the form of the corresponding Hubbard transition operators between one $|\sigma\rangle$ and two particle $|2\rangle$ states:

$$H = \tilde{H}_0 + H_{int}, \quad \tilde{H}_0 = \tilde{E}_1 \sum_{im\sigma} X_{im}^{\sigma\sigma} + \tilde{E}_2 \sum_{im} X_{im}^{22}. \quad (27)$$

In the intra-cell part of Hamiltonian \tilde{H}_0 the one- and two-particle energies are respectively $E_1 = t_a \simeq -0.38$ eV and $E_2 \simeq 0.15$ eV. The chemical potential μ and the particle number operator are introduced:

$$N = \sum_{im} (2X_{im}^{22} + \sum_{\sigma} X_{im}^{\sigma\sigma}), \quad (28)$$

and the relation $[N, H] = 0$ is valid. Part H_{int} describing inter-cell interactions is given by:

$$H_{int} = H_v + H_t, \quad H_v = \tilde{V}_{11} + \tilde{V}_{12} + \tilde{V}_{22}, \quad H_t = \tilde{T}_{11} + \tilde{T}_{12} + \tilde{T}_{22}, \quad (29)$$

$$\tilde{V}_{11} = \sum_{\langle i,j \rangle \{mn\} \sigma \sigma'} v_{11}^{mn} X_{im}^{\sigma\sigma} X_{jn}^{\sigma'\sigma'}, \quad \tilde{V}_{22} = \sum_{\langle i,j \rangle \{mn\}} v_{22}^{mn} X_{im}^{22} X_{jn}^{22}, \quad (30)$$

$$\tilde{V}_{12} = \sum_{\langle i,j \rangle \{mn\} \sigma} v_{12}^{mn} (X_{im}^{\sigma\sigma} X_{jn}^{22} + X_{im}^{22} X_{jn}^{\sigma\sigma}), \quad (31)$$

where $\sum_{\langle i,j \rangle}$ means summation over n.n. $\langle i, j \rangle$ cell site index i and j and $\sum_{\{mn\}}$ contains two parts $n = m$ and $n = m + 1$, i.e. the same and n.n. chains (ladders). Model parameters for Coulomb interactions H_v are given in the Table 4.

Table 4: The dependence of effective v_α parameters for n.n. Coulomb interactions on corresponding original model parameters.

| | | | | | |
|-----------------|----------------|--------------------|---------------|---------------|---------------|
| v_{11}^{mm} | v_{12}^{mm} | v_{22}^{mm} | v_{11}^{mn} | v_{12}^{mn} | v_{22}^{mn} |
| $(V_b + V_d)/4$ | $C(V_b + V_d)$ | $2C^2(2V_b + V_d)$ | $V_{ab}/4$ | CV_{ab} | $4C^2V_{ab}$ |

The hopping interactions can be summarized as follows:

$$\tilde{T}_{11} = \sum_{[ij],\{mn\}\sigma} t_{11}^{mn}(i,j)(X_{im}^{\sigma 0} X_{jn}^{0\sigma} + H.c.), \quad (32)$$

$$\tilde{T}_{12} = \sum_{[ij],\{mn\}\sigma} t_{12}^{mn}(i,j)\sigma(X_{im}^{\sigma 0} X_{jn}^{\sigma 2} - X_{im}^{2\sigma} X_{jn}^{0\sigma} + H.c.), \quad (33)$$

$$\tilde{T}_{22} = \sum_{[ij],\{mn\}\sigma} v_{22}^{mn}(i,j)(X_{im}^{2\sigma} X_{jn}^{\sigma 2} + H.c.), \quad (34)$$

where $\sum_{[ij]}$ means summing over n.n. $\langle i, j \rangle$ and n.n.n. $\langle\langle i, j \rangle\rangle$ cell site index i and j and where $\sum_{\{mn\}}$ contains two parts $n = m$ and $n = m + 1$, i.e, the same and n.n. chains (ladders). Model parameters for hopping interactions H_t are given in the Table 5.

Table 5: Form of dependence t_α parameters for n.n. and n.n.n. hopping interactions, on corresponding original model parameters.

| | | | | | | |
|--------|---------------|---------------|-------------------|---------------|-----------------------|----------------|
| | t_{11}^{mm} | t_{12}^{mm} | t_{22}^{mm} | t_{11}^{mn} | t_{12}^{mn} | t_{22}^{mn} |
| n.n. | $t_b + t_d$ | 0 | $2A^2(t_b - t_d)$ | $t_{ab}/2$ | $-At_{ab}/\sqrt{2}$ | $-A^2 t_{ab}$ |
| n.n.n. | t'_b | 0 | $2A^2 t'_b$ | $t'_{ab}/2$ | $-A t'_{ab}/\sqrt{2}$ | $-A^2 t'_{ab}$ |

Using values of the model parameters (1-7) which follows from band structure calculations [30] and [34], one can calculate the parameters in the inter-cell interaction part of the hamiltonian H_{int} . Values of the coefficients A and C , which appear in the Eq. (25) and in the Tables 4 and 5, are defined with use of the elements of the orthogonal transformation matrix ($|\psi_\alpha\rangle \rightarrow |\psi'_\alpha\rangle$), $\alpha = 1, 2, 3$. These coefficients express the original Fermi operators in terms of the Hubbard operators with transitions between new diagonalizing states $|\sigma\rangle$ and $|2\rangle$ and they are given in the Table 6.

Table 6: Values (in eV) of the coefficients A and C which appear in the Eq. (25) and in the Tables 4 and 5.

| Ref. | A | C | Ref. | A | C |
|----------|--------|-------|------|-------|-------|
| [30, 35] | 0.345 | 0.497 | [38] | 0.574 | 0.500 |
| [31] | -0.400 | 0.5 | [39] | 0.545 | 0.500 |
| [18] | -0.379 | 0.5 | [33] | 0.44 | 0.49 |

The numerical values for the renormalized Coulomb v_α^β and the hopping t_α^β parameters are given in the Tables 7 and 8.

Table 7: Values (in eV) of the intra-chain Coulomb $v_\alpha \equiv v_\alpha^{mm}$ parameters for n.n. and the intra-chain hopping $t_\alpha \equiv t_\alpha^{mm}$ parameters for n.n. and n.n.n. interactions with ($\alpha = 11, 12, 22$) and according to the values given in the Tables 1 and 2 .

| Ref. | v_{11} | v_{12} | v_{22} | t_{11} | t_{22} | t'_{11} | t'_{22} |
|----------|----------|----------|----------|----------|----------|-----------|-----------|
| [30, 35] | 0.31 | 0.62 | 0.97 | -0.17 | -0.041 | | |
| [31] | | | | -0.15 | -0.048 | | |
| [18] | 0.5 | 1 | 2 | -0.15 | -0.048 | | |
| [38] | 0.54 | 1.08 | 2.15 | 0.12 | 0.08 | | |
| [33] | | | | -0.24 | 0.023 | -0.03 | 0.12 |
| [39] | 0.172 | 0.344 | 0.688 | 0.111 | -0.008 | | |

One can see that the hopping parameters t_{12} and t'_{12} are absent in the Table 7 because they are equal to zero. Thus there is no hopping terms between one-particle and singlet band if one do not take into account very small inter-ladder contributions t_{12}^{mn} . From these one can expect insulating behavior of the considered system, if the filling of the band is lower than one half. That corresponds to the original quarter-filled bonding band, before projection.

Table 8: Values (in eV) of the $(n = m + 1)$ inter-chain v_{α}^{mn} for n.n. Coulomb and t_{α}^{mn} for n.n. and n.n.n. hopping parameters with $(\alpha = 11, 12, 22)$ and according to the values given in the Tables 1 and 2 .

| Ref | v_{11}^{mn} | v_{12}^{mn} | v_{22}^{mn} | t_{11}^{mn} | t_{12}^{mn} | t_{22}^{mn} | $t_{11}^{\prime mn}$ | $t_{12}^{\prime mn}$ | $t_{22}^{\prime mn}$ |
|------|---------------|---------------|---------------|---------------|---------------|---------------|----------------------|----------------------|----------------------|
| [35] | 0.11 | 0.21 | 0.42 | 0.006 | 0.003 | -0.001 | 0.015 | 0.007 | -0.003 |
| [31] | | | | -0.15 | 0.085 | 0.048 | | | |
| [18] | 0.35 | 0.705 | 1.41 | -0.15 | 0.08 | 0.04 | | | |
| [38] | | | | -0.06 | -0.04 | 0.03 | | | |
| [33] | | | | 0.01 | 0.006 | -0.004 | 0.015 | 0.009 | -0.006 |

III. Green's functions and Dyson equation

In order to consider the electron excitation spectrum for the two-band model (27-34) we employ the equation of motion method for the two-time Green function (GF). By use of the projection technique we obtain the Dyson equation which will be solved in a GMFA with neglecting the finite lifetime effects. To study the two-band problem we have to introduce the matrix Green's function:

$$\hat{G}_{im,jn,\sigma}(t-t') = \langle\langle \hat{X}_{im\sigma}(t); \hat{X}_{jn\sigma}^+(t') \rangle\rangle, \quad (35)$$

where we have used Zubarev's notations [40] for the anticommutator GF for the two-component operators:

$$\hat{X}_{im\sigma} = \begin{pmatrix} X_{im}^{\sigma 2} \\ X_{im}^{0\sigma} \end{pmatrix}; \quad \hat{X}_{jn\sigma}^+ = \begin{pmatrix} X_{jn}^{2\sigma} & X_{jn}^{\sigma 0} \end{pmatrix}. \quad (36)$$

By differentiating the GF (35) over time t we get for the Fourier component the following equation:

$$\omega \hat{G}_{im,jn,\sigma}(\omega) = \delta_{ij} \delta_{mn} \hat{\chi} + \langle\langle \hat{Z}_{im\sigma} | \hat{X}_{jn\sigma}^+ \rangle\rangle_{\omega}, \quad (37)$$

where the equation of motion for the Hubbard operator $\hat{X}_{im\sigma}$ has the form:

$$i \frac{d}{dt} \hat{X}_{im\sigma}(t) \equiv \hat{Z}_{im\sigma} = [\hat{X}_{im\sigma}, H] = \sum_{kp} \hat{E}_{im,kp,\sigma} \hat{X}_{kp\sigma} + \hat{Z}_{im\sigma}^{(irr)}, \quad (38)$$

with

$$\hat{\chi} = \begin{pmatrix} \chi_\psi & 0 \\ 0 & \chi_D \end{pmatrix}, \quad (39)$$

and the matrix elements representing the averaged anticommutators:

$$\begin{aligned} \chi_\psi &= \langle \{X_{im}^{\sigma 2}, X_{jn}^{2\sigma}\} \rangle = \langle X_{im}^\psi \rangle = \langle X_{im}^{22} + X_{im}^{\sigma\sigma} \rangle, \\ \chi_D &= \langle \{X_{im}^{0\bar{\sigma}}, X_{jn}^{\sigma 0}\} \rangle = \langle X_{im}^D \rangle = \langle X_{im}^{\sigma\sigma} + X_{im}^{00} \rangle. \end{aligned} \quad (40)$$

Here, and in what follows, we consider a spin-singlet state for which the correlation functions (18) do not depend on the spin σ . For the two-band model (27) we have:

$$X_{im}^{00} + \sum_{\sigma} X_{im}^{\sigma\sigma} + X_{im}^{22} = 1, \quad (41)$$

and that implies that: $\chi_D = 1 - \chi_\psi$. The elements of the frequency matrix:

$$\hat{E}_{im,jn,\sigma} = \langle \{[\hat{X}_{im\sigma}, H], \hat{X}_{jn\sigma}^+\} \rangle \hat{\chi}^{-1} \quad (42)$$

are defined by the projection condition:

$$\langle \{[\hat{Z}_{im\sigma}^{(irr)}, \hat{X}_{jn\sigma}^+\} \rangle = 0. \quad (43)$$

Here, $\{A, B\}$ and $[A, B]$ are the anticommutator and the commutator, respectively for A, B operators.

Neglecting finite lifetime effects due to the scattering described by the irreducible part of the equation of motion (38), one can introduce the zero-order GF in the GMFA as:

$$\hat{G}_{im,jn,\sigma}^0(\omega) = \{\omega \hat{\tau}_0 \delta_{ij} \delta_{mn} - \hat{E}_{im,jn,\sigma}\}^{-1} \hat{\chi}, \quad (44)$$

where $\hat{\tau}_0$ is the unity matrix. Performing the same procedure for the GF right-hand side operator $\hat{X}_{jn\sigma}(t')$ and taking into account the projection condition one becomes to the Dyson equation for the GF

$$\hat{G}_{im,jn,\sigma}(\omega) = \hat{G}_{im,jn,\sigma}^0(\omega) + \sum_{kp,lr} \hat{G}_{im,kp,\sigma}^0(\omega) M_{kp,lr,\sigma}(\omega) \hat{G}_{lr,jn,\sigma}(\omega),$$

where the self-energy operator $\hat{M}_{kp,lr,\sigma}(\omega)$ is defined by the equation:

$$\hat{T}_{im,jn,\sigma}(\omega) = \hat{M}_{im,jn,\sigma}(\omega) + \sum_{kp,lr} \hat{M}_{im,kp,\sigma}(\omega) \hat{G}_{kp,lr,\sigma}^0(\omega) \hat{T}_{lr,jn,\sigma}(\omega). \quad (45)$$

The scattering matrix is given by the equation

$$\hat{T}_{im,jn,\sigma}(\omega) = \hat{\chi}^{-1} \langle\langle \hat{Z}_{im\sigma}^{(irr)} | \hat{Z}_{jn\sigma}^{(irr)+} \rangle\rangle_{\omega} \hat{\chi}^{-1}. \quad (46)$$

Equations (44)-(46) give an exact representation for the one-particle GF (35).

IV. Results and discussion

After performing the necessary commutations of the Hubbard operators with the Hamiltonian (27-34) we obtain the following representation for the frequency matrix (42):

$$\begin{aligned} \hat{E}_{im,jn,\sigma} = & \delta_{ij}\delta_{mn} \begin{pmatrix} E_{\psi} - E_D - \mu + \Delta_{\sigma}^{\psi\psi} & \Delta_{\sigma}^{\psi D} \\ \Delta_{\sigma}^{D\psi} & E_D - \mu + \Delta_{\sigma}^{DD} \end{pmatrix} \quad (47) \\ & + (1 - \delta_{ij}) \delta_{mn} \begin{pmatrix} K_{ij\sigma}^{\psi\psi} & K_{ij\sigma}^{\psi D} \\ K_{ij\sigma}^{D\psi} & K_{ij\sigma}^{DD} \end{pmatrix} + (1 - \delta_{ij}\delta_{mn}) \begin{pmatrix} K_{im,jn,\sigma}^{\psi\psi} & K_{im,jn,\sigma}^{\psi D} \\ K_{im,jn,\sigma}^{D\psi} & K_{im,jn,\sigma}^{DD} \end{pmatrix}. \end{aligned}$$

The on-site contributions to the frequency matrix components are determined by the following energy shifts:

$$\Delta_{\sigma}^{\psi\psi} = \Delta_{\sigma}^{\psi\psi}(v) + \Delta_{\sigma}^{\psi\psi}(t); \quad \Delta_{\sigma}^{DD} = \Delta_{\sigma}^{DD}(v) + \Delta_{\sigma}^{DD}(t), \quad (48)$$

with $\alpha \equiv ij$ for $m = n$ if sites i and j are in the same chain ($m = n$) and $\alpha \equiv im, jn$ for $n = m + 1$. The corresponding main diagonal matrix elements contain the following singlet energy shifts:

$$\begin{aligned} \Delta_{\sigma}^{\psi\psi}(v)\chi_{\psi} = & 2 \sum_{\langle ki \rangle \{mp\}} \{ (v_{12}^{mp} - v_{11}^{mp}) (\langle \chi_{im}^{\psi} X_{kp}^{\sigma\sigma} \rangle) \\ & + \langle \chi_{im}^{\psi} X_{kp}^{\sigma\bar{\sigma}} \rangle) + (v_{22}^{mp} - v_{12}^{mp}) (\langle \chi_{im}^{\psi} X_{kp}^{22} \rangle) \}, \end{aligned}$$

$$\Delta_{\sigma}^{\psi\psi}(t)\chi_{\psi} = 2 \sum_{[ik] \{mp\}} (t_{22}^{mp} \langle X_{im}^{2\bar{\sigma}} X_{kp}^{\sigma\bar{\sigma}} \rangle) \quad (49)$$

and the following one-particle state energy shifts:

$$\Delta_{\sigma}^{DD}(v)\chi_D = \sum_{\langle ik \rangle \{mp\}} \{ 2v_{11}^{mp} (\langle \chi_{im\bar{\sigma}}^D X_{kp}^{\sigma\sigma} \rangle + \langle \chi_{im\bar{\sigma}}^D X_{kp}^{\sigma\bar{\sigma}} \rangle) + v_{12}^{mp} \langle \chi_{im\bar{\sigma}}^D X_{kp}^{22} \rangle \},$$

$$\Delta_{\sigma}^{DD}(t)\chi_D = -2 \sum_{[ik]\{mp\}} (t_{22}^{mp} \langle X_{im}^{\bar{\sigma}2} X_{kp}^{2\bar{\sigma}} \rangle + t_{11}^{mp} \langle X_{im}^{\sigma 0} X_{kp}^{0\sigma} \rangle). \quad (50)$$

The skew diagonal frequency matrix elements contain the energy shifts:

$$\Delta_{\sigma}^{\psi D} \chi_D = -2 \sum_{[ik]\{mp\}} (t_{11}^{mp} \langle X_{im}^{\bar{\sigma}2} X_{kp}^{\sigma 0} \rangle + t_{22}^{mp} \langle X_{im}^{\sigma 0} X_{kp}^{\bar{\sigma}2} \rangle), \quad (51)$$

and for the skew diagonal matrix elements the following relation is valid:

$$E_{im,jn,\sigma}^{D\psi} \chi_{\psi} = (E_{im,jn,\sigma}^{\psi D})^+ \chi_D. \quad (52)$$

The frequency-matrix has two terms with different site indexes (second and third term in the Eq. (47)). The second term, which is $\propto (1 - \delta_{ij}) \delta_{mn}$, means that the sites $i \neq j$ are in the same chain. The third term, which is $\propto (1 - \delta_{ij} \delta_{mn})$, means that the sites $i \neq j$ are in the neighboring chains $n = m + 1$. These matrix components are determined by the renormalized hopping parameters:

$$K_{\alpha\sigma}^{\psi\psi} = K_{\alpha\sigma}^{\psi\psi}(v) + K_{\alpha\sigma}^{\psi\psi}(t), \quad K_{\alpha\sigma}^{DD} = K_{\alpha\sigma}^{DD}(v) + K_{\alpha\sigma}^{DD}(t), \quad (53)$$

where the main diagonal matrix elements contain the following singlet state hopping parameters:

$$K_{\alpha\sigma}^{\psi\psi}(v) \chi_{\psi} = 2(v_{11}^{mn} - 2v_{12}^{mn} + v_{22}^{mn}) \langle X_{im}^{\sigma 2} X_{jn}^{2\sigma} \rangle,$$

$$K_{\alpha\sigma}^{\psi\psi}(t) \chi_{\psi} = 2\{t_{22}^{mn} \langle \chi_{im\sigma}^{\psi} \chi_{jn\sigma}^{\psi} \rangle + X_{im}^{\sigma\bar{\sigma}} X_{jn}^{\bar{\sigma}\sigma} \rangle - t_{11} \langle X_{im}^{02} X_{jn}^{20} \rangle\}, \quad (54)$$

and the one-particle state hopping parameters:

$$K_{\alpha\sigma}^{DD}(v) \chi_D = 2v_{11}^{mn} \langle X_{im}^{0\bar{\sigma}} X_{jn}^{\bar{\sigma}0} \rangle, \quad (55)$$

$$K_{\alpha\sigma}^{DD}(t) \chi_D = 2t_{11}^{mn} \langle \chi_{im\bar{\sigma}}^D \chi_{jn\bar{\sigma}}^D \rangle + X_{im}^{\sigma\bar{\sigma}} X_{jn}^{\bar{\sigma}\sigma} \rangle - 2t_{22}^{mn} \langle X_{im}^{02} X_{jn}^{20} \rangle. \quad (56)$$

The corresponding skew diagonal element is:

$$K_{\alpha\sigma}^{\psi D} \chi_D = (v_{12}^{mn} - 2v_{11}^{mn}) \langle X_{im}^{\sigma 2} X_{jn}^{\bar{\sigma}0} \rangle. \quad (57)$$

It should be stressed here that for the contribution connected the addend $\propto (1 - \delta_{ij}) \delta_{mn}$, i.e., for the term whose sites i and j are in the same chain ($m = n$), one should set $\alpha = ij$ and the superscript indexes on the

parameter v should be omitted or set to mm . Similarly, for the parts which are connected with $\alpha (1 - \delta_{ij}\delta_{mn})$, i.e., if the sites $i \neq j$ are from the neighboring chains nm , ($n = m + 1$), one should keep superscript indexes mn as already written there.

There are two sorts of the contributions in the expressions for the energy shifts and the hopping parameters. In addition to the terms $\Delta_\alpha(t)$ and $K_\alpha(t)$, which appear due to the hopping interactions H_t as in [42], the $\Delta_\alpha(v)$ and $K_\alpha(v)$ appear due to the Coulomb interactions H_v . One can also see that the energy shifts caused by hoppings $\Delta_\alpha(t)$, and by renormalized hopping parameters determined by Coulomb interactions $K_\alpha(v)$, are defined through the correlation functions of the pairs of the Fermi-like Hubbard operators. On the contrary, the energy shifts $\Delta_\alpha(v)$ and the renormalized hopping parameters $K_\alpha(t)$ are determined through the correlation functions of the pairs of the Bose-like Hubbard operators. The skew diagonal matrix elements $E_\alpha^{\psi D}$ and $E_\alpha^{D\psi}$ contain only $\Delta_\alpha^{\psi D}(t)$ and $K_{\alpha\sigma}^{\psi D}(v)$. One should especially stress that the sign "-" in the interband hopping part of Hamiltonian \tilde{T}_{12} , instead of the "+" sign obtained in [42], cause zero contribution in the energy shifts Δ_α and hopping K_α terms, which contain parameters t_{12}^α . In the Ref. [42] the nonzero contributions appear only in the skew diagonal energy shifts $\Delta^{\psi D}$ and hopping $K^{\psi D}$ parameters. It is also worth noting that in the case of sign "-" one has $\langle \tilde{T}_{12} \rangle = 0$, so hopping between zones give zero contribution to the mean energy $\langle H \rangle = 0$ of the considered system.

Instead of the two addends in the expression for the frequency matrix in [42], here we have three. They describe the energy shifts and renormalized hopping parameters on-site and between sites in the same and in the neighboring chains ('ladders'). The square lattice has been considered in Ref. [42], while here we consider Trellis ladder lattice, which after applying cell-perturbation procedure becomes the lattice of the parallely-shifted chains. Including interactions between the chains, the latter one can be seen as triangular lattice.

Further one can introduce the representation of the spin operator components, for $\sigma = (+, -)$ and $\bar{\sigma} = -\sigma$:

$$\sigma S_i^z = \frac{1}{2}(X_i^{\sigma\sigma} - X_i^{\bar{\sigma}\bar{\sigma}}), \quad S_i^\sigma = X_i^{\sigma\bar{\sigma}},$$

which leads to the form of the Hubbard operators with more obvious

physical meaning:

$$\chi_{im\sigma}^{\psi} = \frac{1}{2} \left(\sum_{\sigma} X_{im}^{\sigma\sigma} + 2X_{im}^{22} \right) + \frac{1}{2} (X_{im}^{\sigma\sigma} - X_{im}^{\bar{\sigma}\bar{\sigma}}) = \frac{1}{2} N_{im} + \sigma S_{im}^z,$$

and

$$\chi_{im\sigma}^D = 1 - \frac{1}{2} N_{im} + \sigma S_{im}^z.$$

As in the [42], we decouple the product $N_{im}N_{jn}$ of the number operators on different lattice sites $im \neq jn$ like in the Hubbard - I approximation, but keep spin correlations $\langle \mathbf{S}_{im} \mathbf{S}_{jn} \rangle$. In such a case, one have

$$\langle \chi_{im\sigma}^{\psi} \chi_{j\sigma}^{\psi} + X_{im}^{\sigma\bar{\sigma}} X_{jn}^{\bar{\sigma}\sigma} \rangle \simeq \chi_{\psi} \chi_{\psi} + \langle \mathbf{S}_{im} \mathbf{S}_{jn} \rangle,$$

$$\langle \chi_{im\sigma}^D \chi_{j\sigma}^D + X_{im}^{\sigma\bar{\sigma}} X_{jn}^{\bar{\sigma}\sigma} \rangle \simeq 1 + \chi_{\psi} (\chi_{\psi} - 2) + \langle \mathbf{S}_{im} \mathbf{S}_{jn} \rangle,$$

$$\langle \chi_{im\sigma}^{\psi} \chi_{j\sigma}^D - X_{im}^{\sigma\bar{\sigma}} X_{jn}^{\bar{\sigma}\sigma} \rangle \simeq \chi_{\psi} (1 - \chi_{\psi}) - \langle \mathbf{S}_{im} \mathbf{S}_{jn} \rangle.$$

By analogy with [42], we can also neglect correlations in the creation and annihilation of pairs, i.e.

$$\langle X_{im}^{02} X_{jn}^{20} \rangle \simeq \langle X_{im}^{02} \rangle \langle X_{jn}^{20} \rangle = 0.$$

V. Conclusions and further intentions

In summary, we derived two-band Hubbard model for the ladder α' - NaV_2O_5 compound. Due to very small inter-band hopping, the corresponding ground state will be insulating. By means of modeling $\{\mathbf{q}\}$ -dependence of the Fourier transform of the diagonal $\langle X_{\mathbf{q}}^{\alpha\alpha} X_{\mathbf{q}}^{\beta\beta} \rangle$ correlation functions, one can obtain some of the possible inter-ladder charge orderings. The influence of the short-range AF spin fluctuations on the electronic spectra can be naturally investigated. In order to do that, one should keep the spin-spin correlation function $\langle \mathbf{S}_{im} \mathbf{S}_{jn} \rangle$ as a parameter and use the experimental results for the spin susceptibility.

The essential differences between the present work and Ref. [42] can be listed as follows:

- Coulomb interactions included;

- Sign "-" in the inter-band \tilde{T}_{12} Hamiltonian which produces that there is no contributions of the hopping $\propto t^{\psi D}$ in the frequency matrix;
- here we have effectively triangular lattice bands.

The diagonal hopping term, which we are taking into account, leads to the widening and shortening of the one-particle $|\sigma\rangle$ and $|\psi\rangle$ zones, respectively (cf. Table 5).

In the future work we intend to express the correlation functions in the frequency matrix through the corresponding GF (like in Ref. [42]) and to derive self-consistent system of equations. Approximate solutions for the zero-order GF should give the two-band spectrum for d -like one - particle and singlet states. We shall consider only the paramagnetic state which may have, however, strong short-range antiferromagnetic correlations (characteristic for the low-dimensional magnetic systems). Evidently, this system of equations have the spin correlation functions as parameters. The main task of our future numerical calculations will be the analysis of the influence of short range antiferromagnetic spin fluctuations, and some of the possible CO, on the properties of the one-particle GF.

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