EFFECTIVE DIMENSIONALITY AND BAND STRUCTURE OF $\alpha'$–NaV$_2$O$_5$ COMPOUND: 1D OR 2D?

V. A. Ivanov$^1$, Z. V. Popovic$^2$, O. P. Khuong$^3$, V. V. Moshchalkov

Laboratorium voor Vaste-Stoffysica en Magnetisme, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Leuven, BELGIUM

Abstract

The AV$_n$O$_{2n+1}$ mixed valence compounds ($n = 1, A = Na$) are classified as dimerized layered system with strongly interacting $d$–electrons of vanadium ions. The derived band gaps, energy dispersion relations and density of electronic states are in a good agreement with available experimental and theoretical data. The correlated band gap provides the insulating state of the high-temperature $\alpha'$–NaV$_2$O$_5$ phase whereas the state, earlier misrepresented as the spin-Peierls state, is governed, in fact, by opening of the Coulomb gap.

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The spin-Peierls phase transition was first observed in one-dimensional organic salts [1]. Since its discovery in quasi-1D material CuGeO$_3$ [2, 3], there were a lot of efforts to find out a spin-Peierls behavior in other inorganic materials. The AV$_n$O$_{2n+1}$ family (A stands for alkali or alkali earth element) has been quite perspective in that respect. In the best studied $\alpha'$-phase of NaV$_2$O$_5$, the opening of a spin gap $\Delta_0 \sim 80 - 110K$ was observed at $T_c \approx 34 - 36K$ [4 - 6]. But at present it has become evident, that the spin-Peierls scenario can not adequately describe the properties of $\alpha' - NaV_2O_5$ oxide. A summary of controversies is given in Ref.[7]: the enlarged entropy of the transition, an enhanced value $2\Delta_0/T_c$, weak dependence of $T_c$ on magnetic field, significant increase of the thermal conductivity below $T_c$ in contrast with the conventional spin-Peierls transition.

The $\alpha' - NaV_2O_5$ crystal with a stable $P_{mmn}(D_{2h}^{13})$ symmetry contains the quarter-filled dimers $V^{4+}(3d^1) - V^{5+}(3d^0)$ ($T < T_c$) or $V^{4.5+} - V^{4.5+}$ ($T > T_c$), forming rungs of two-leg ladders in the ($ab$) plane (Fig.1). Pyramids VO$_5$ are arranged in alternating layers made by vanadium ions and basal oxygens separated by layers formed by Na and apical oxygens. For lattices compressed along the $c$-axis ($\alpha' - NaV_2O_5$ is indeed the case) the crystal field lifts the $t_{2g}$-degeneracy of the vanadium 3$d$-levels with the lowest energy of the single $d_{xy}$-orbital. Theoretical models usually used for $\alpha' - NaV_2O_5$ [8-11] are based on fascinating features of a quasi-1D spin ladder picture beyond the discussion about the electronic structure. Local density analyses [12, 13] have shown that eigenstates near the Fermi energy are constructed mainly from the $d_{xy}$ orbitals of V atoms and revealed the split character of the 3d-band with pronounced peaks in the density of electronic states. But the computations could not establish the character of the peaks in the band structure: do they have 1D, 2D or 3D character? According to them the Fermi level lies inside the conducting band providing the metallic phase, which is in a disagreement with experimental observations.

In this letter we analyze the electronic structure of $\alpha' - NaV_2O_5$. The phase transition at $T_c$ is shown to be not a pure spin-Peierls type but rather it is connected with the opening of the Coulomb gap in the electronic spectrum. The character of the high-temperature insulating phase has been identified via strong electron interactions. Our approach is based on the hypothesis that the $\alpha' - NaV_2O_5$ properties are governed by the electron-electron correlations $U, t_a$ (intrarung/intradimer electron hopping integral), $t_b$ (the amplitude of an electron hopping along legs in crystallographic $b$-direction),
t_d (the hopping along ladder diagonals), t_{xy} (interdimer hoppings between vanadium ions on nearest ladders) (Fig.1).

Nonspherical angular part $d_{xy}$ of the 3$d$-electron wave-functions $\Psi(\vec{r})$ provides the hopping anisotropy and a layered structure of $\alpha' - NaV_2O_5$ with crystallographic $(ab)$ planes. The small parameter $r_B/a$ ($a$ is a lattice constant and $r_B$ is a vanadium ionic radii) enables us to evaluate the direct $V - V$ hopping integral $t_{xy}$ for $d$-electrons with $\Psi(\vec{r}) = f(r) d_{xy}$. The Gaussian radial part $f(r)$ allows to calculate hopping integrals with any required accuracy as power series of $(r_B/a)^2$ [14]. The estimates show the strong influence of the $V^{4+}/5+$ ion core on an electron hopping. Therefore we will distinguish the $t_{xy}$ magnitudes especially in ordered valence state (Fig.1) as $t^{bc}_{xy} > t^{bm}_{xy} > t^{qm}_{xy}$. The enhanced values of indirect $t_{a, b, d}$ hoppings are influenced by intermediate oxygens. Since the present evaluations of the indirect hopping $t_b$ lead to a substantial ambiguity [8, 10, 12, 13], the recent infrared reflectance studies of $\alpha' - NaV_2O_5$ [15, 16] are more suitable to extract the intradimer hopping amplitude as $t_a \simeq 0.35 eV$. The order of magnitude estimate of the other electron hoppings gives $t_b \sim t_d \sim t_a/2$. As for on-site $d_{xy}-d_{xy}$ interactions, they are taken to be infinite (the value of the Anderson-Hubbard on-site parameter is believed to be $U = 4 - 6$ eV) and somewhat weaker Coulomb interactions between neighbors simply shift on-site one particle energies in the charge ordered phase.

In such a way the present approach is based on the energy scale $U >> t_a > t_b > t_d > t_{xy}$ and we classify the $\alpha' - NaV_2O_5$ oxide as a strongly correlated dimerized electron system. For vanadium $d_{xy}$-electrons one can carry out the simplest fermion mapping to projected X-operators [17, 18] describing intra-vanadium transitions between the one-particle ground and an empty polar states. Applying the X-operator machinery [19], one can derive the tight-binding energy bands for strongly correlated carriers. Neglecting scattering effects, calculations have been done in the first order of the perturbative hopping energy, namely the correlated energy bands $\xi(p)$ have been extracted from zeros of the inverse Green’s function $D^{-1}(i\omega, p) = D^{(0)-1}(i\omega) + \frac{\leftrightarrow t}{\rightarrow t}(p)$ ($i\omega \to \xi + i\delta$), where $\leftrightarrow t(p)$ is the corresponding matrix of hopping integrals. The arrangement of dimers in $\alpha' - NaV_2O_5$ is closer to a triangular lattice. So, our main strategy is based on the assumption that the $V_{2\Sigma}$ rungs form an ideal triangular lattice. Below $T_c$ the $\alpha' - NaV_2O_5$ is in an ordered valence phase whereas above $T_c$ it is in a mixed valence state.

At $T < T_c$ vanadiums are packed in eight sublattices $a, b, c, d, m, n, p, q$.
In a zigzag charge/spin order $d_{xy}$-electrons acquire on-site energy shifts $\varepsilon_{a,d,q,m} = -\varepsilon_{b,c,n,p} \equiv -\varepsilon$, influenced by neighboring Coulomb repulsion $V: \varepsilon = V\Delta n$ ($\Delta n$ is the charge disproportionation on nearest neighbors $V^{4+}\Delta n / 5 - \Delta n$). At positions $a, b, m, n$ and $p, q, c, d$ the $d_{xy}$-electrons have spin projections down and up, respectively. This situation, in parallel with $U = \infty$, allows to consider spinless electrons. The resulting energy dispersions are plotted in Fig.2. The flatness of an antibonding band is caused by the diagonal intraladder hopping $t_d$. Four electrons from the $V^{4+} - V^{5+}$ dimers of a monoclinic unit cell occupy bonding branches completely. The insulating charge (Coulomb) gap $\Delta C$ is provided by the zigzag ordered one-particle energies, $\varepsilon_{c,} = \varepsilon_{a,} - \varepsilon_{b,}$ in $\alpha'-NaV_2O_5$, one can conclude that in low-temperature phase the $\Delta C = 1eV$ (Fig.2). Of special interest is the role of unequal interladder hoppings $t_{xy}$ for $t_{xy}^{bc} = t_{xy}^{bm} + \delta$ and $t_{xy}^{qm} = t_{xy}^{bm} - \delta$ we have revealed the nonmonotonic $\Delta C$ dependence on parameter $\delta$. For $t_{xy} \neq 0$ a finite energy threshold, $\varepsilon_c$, is necessary to produce the zigzag order. The critical Coulomb magnitude $V_c \sim 0.2 eV$ given in Ref.[11], corresponds to our $\varepsilon_c = 28.56meV$ for $t_{xy} = 0.06eV$; $\delta = 0.01eV$. Note worthy that for these parameters the Coulomb gap value coincides with the critical temperature of the so called "spin-Peierls" transition: $\Delta C (\varepsilon_c) = 35K$. Neglecting interladder hoppings the gap in an electronic spectrum can be approximated explicitly as

$$\Delta C = \sqrt{\varepsilon^2 + (t_a + 2t_b)^2} + \sqrt{\varepsilon^2 + (t_a - 2t_b)^2} - 4t_d.$$  

The Eq.(1) is the extension of the splitting in terms of the "charged-magnon" scenario for a single $V^{4+} - V^{5+}$ rung ($t_{bd} = 0$) used in Refs.[10,16]. We have established also, that an often discussed chain-type order for $\alpha' - NaV_2O_5$, $\varepsilon_{a,p,c,m} = -\varepsilon_{b,q,n,d} \equiv -\varepsilon$ (c.f., Fig.1), does not cause the $\Delta C$ formation below $T_c$, to trigger the phase transition of interest.

At $T > T_c$ a quarter-filled highly dimerized compound $\alpha' - NaV_2^{4.5+}O_5$ can be described by a half-filled Hubbard like model for bonding electrons with two dimers/sites in a orkhorhombic unit cell (Fig.1). For $U = \infty$ an effective Anderson-Hubbard parameter of this model is simply the gain of the intradimer kinetic energy: $2t_a$. Then the energy bands are formed by the four one-particle branches

$$\frac{\xi^+_p}{t_b + t_d} = \varepsilon^+_p + \sqrt{(\frac{t_a}{t_b + t_d})^2 + (\varepsilon^+_p)^2}, \quad \frac{\xi^-_p}{t_b + t_d} = \varepsilon^-_p - \sqrt{(\frac{t_a}{t_b + t_d})^2 + (\varepsilon^+_p)^2}$$
where dimensionless tight-binding non-correlated energies are

$$
\epsilon_p^\pm = -\cos p_y \pm 2t \cos \frac{p_x \sqrt{3}}{2} \left( t = \frac{t_{xy}}{2(t_b + t_d)} \right).
$$

(3)

So, the standard energies (3) are split by the electron interactions. The lower, $\xi_p^-$, and the upper, $\xi_p^+$, bands are split due to the presence of a pair of $V^{4.5+}$ dimers/sites in a high-temperature unit cell. The two $d_{xy}$-electrons from a unit cell occupy the lower pair $\xi_p^-$ of the correlated energy bands.

The non-correlated energy dispersions, Eq.(3), reflect the main peculiarities of the reported "spaghetti" pictures [12, 13] rather well. They are in the ranges $-1 - 2t \leq \epsilon_p^- \leq 1$ and $-1 \leq \epsilon_p^+ \leq 1/2 + t$. The upper bonding branch, $\epsilon_p^+$, has a hyperbolic metric in a proximity of the $\Gamma (0,0)$-point of the Brillouine zone. The electrons with these energies have a 2D character of motion. The electrons with bonding energies, $\epsilon_p^-$, posses 1D features. If it were metallic carriers, the $\epsilon_p^-$ and $\epsilon_p^+$ would have provided the quasi-2D saddle and the quasi-1D saddleless portions of the Fermi surface, respectively.

Above $T_c$ the electron density of states is positioned in the ranges of correlated energies $\xi_p^\alpha$ ($\alpha = \pm$). For dimensionless energies, $\omega_\alpha = \xi_p^\alpha / (t_b + t_d)$ (Eqs.(2)), it is given analytically by equations

$$
\rho^\alpha (-1 - 2t - S + T_\alpha \leq \omega_\alpha \leq -1 + 2t - S + P_\alpha) =
$$

(4)

$$
\frac{1}{\pi^2 \sqrt{k_\alpha t}} [1 + \frac{q_\alpha^2}{4 (\alpha |\omega| + S)^2}] K(q_\alpha);
$$

$$
\rho^\alpha (-1 + 2t - S + P_\alpha \leq \omega_\alpha \leq 1 + S + Q_\alpha) =
$$

(5)

$$
= \frac{1}{\pi^2 q_\alpha \sqrt{k_\alpha t}} [1 + \frac{q_\alpha^2}{4 (\alpha |\omega| + S)^2}] [K(\frac{1}{q_\alpha}) \theta(1 - S + Q_\alpha - \omega_\alpha) +
+F(\arcsin \frac{1}{a_\alpha}; \frac{1}{q_\alpha}) \theta(1/2 + t - S + R_\alpha)],
$$
where \( \vartheta \) is a Heaviside step function, \( \mathcal{S} = \sqrt{\tau^2 + (1 + 2t)^2} - \sqrt{\tau^2 + 1 - t} \), \( T_\alpha = \alpha \sqrt{\tau^2 + (1 + 2t)^2} \), \( P_\alpha = \alpha \sqrt{\tau^2 + (1 - 2t)^2} \), \( Q_\alpha = \alpha \sqrt{\tau^2 + 1} \), \( R_\alpha = \alpha \sqrt{\tau^2 + (1/2 + t)^2} \), \( (\tau \equiv t_o/(t_b + t_d)) \). In Eqs.(4, 5) the elliptic integrals \( F \) and \( K \) have modulus \( q_\alpha = \sqrt{[2t(t + k_\alpha) + 1 - (\omega_0^\alpha)^2]/k_\alpha t/2} \) and argument \( a_\alpha = \sqrt{k_\alpha(1 + \omega_0^\alpha)(t + k_\alpha)/[2t(t + k_\alpha) + 1 - (\omega_0^\alpha)^2]} \) with \( k_\alpha = \sqrt{2(1 - \omega_0^\alpha) + t^2} \), \( \omega_0^\alpha = [(\alpha |\omega| + S)^2 - \tau^2]/[2(\alpha |\omega| + S)] \). The Eqs.(4, 5) are valid if the \( \varepsilon_p^\pm \)-band, Eq.(3), is inside the energy interval of the \( \varepsilon_p^- \)-band, \( i.e. \) at the hopping parameters obeying the realistic for \( \alpha' - NaV_2O_5 \) constraint \( t_{xy} < t_b + t_d \). The main panel of Fig.3 displays the density of correlated electron states with a gapped electronic structure at \( T > T_c \). In a limiting non-correlated case, the density of states (inset) reproduces the essentials of the first principle computations [12]. The overlap of the energy ranges for the electronic dispersions, Eqs.(2, 3), leads in Fig.3 to peculiarities of the electronic structure at \( T > T_c \) in inset. Logarithmic divergencies inside the band at \( \varepsilon = -1 + 2t \) and \( \varepsilon = 1 \) (inset), and at \( L_2 = -1 + 2t + P_\alpha - S \) and \( U_2 = -1 + 2t + P_\alpha + S \) (main panel) are clear manifestations of the 2D electronic structure of \( \alpha' - NaV_2O_5 \) compound. We would like to emphasize that in the one-dimensional limit \( (t_{xy} \rightarrow 0) \) the electron density of states is taking features of a single spin-ladder without any logarithmic peaks, the divergencies are becoming square-root like with positions at the band edges. Under the strong electron interactions the lower correlated bands, Eqs.(2), are completely occupied by the electron pair from an orthorhombic unit cell (Fig.1). Finally it results in the appearance of the correlated band gap (Fig.3):

\[
\Delta_g = \min \xi_p^+ (\varepsilon_p^-) - \max \xi_p^- (\varepsilon_p^+) = \sqrt{t_a^2 + (t_b + t_d)^2} + \sqrt{t_a^2 + (t_b + t_d + t_{xy})^2} - 2(t_b + t_d) - t_{xy}. \quad (6)
\]

Substituting to Eq.(6) the realistic values of hopping parameters, \( t_a = 0.35eV \), \( t_b = 0.15eV \), \( t_d = 0.1eV \), \( t_{xy} = 0.06eV \), one can derive the numerical value of the high-temperature gap in \( \alpha' - NaV_2O_5 \) as \( \Delta_g = 0.34eV \).

In summary, the \( \alpha' - NaV_2O_5 \) band structure has been analyzed. The analysis of derived \( \xi_p^\pm \) curves and density of electronic states in an explicit form leads to the conclusion about pronounced 2D features. At \( T < T_c \) the zigzag order redistributes large \( V^{4+} \) and small \( V^{5+} \) ions and it is accompanied...
by the Coulomb gap $\Delta_C$ (see Fig.2 and Eq.(1)). Its estimated magnitude $\Delta_C \simeq 1\text{eV}$ (for $\Delta n = 0.8$, $V = 0.8\text{eV}$ [20], $t_a = 0.35\text{eV}$, $t_b = 0.15\text{eV}$, $t_d = 0.1\text{eV}$) corresponds to the observed strong absorption of the light [17]. At $T > T_c$ the correlated band gap (6) provides an insulating state of $\alpha' - \text{NaV}_2\text{O}_5$. The studies, reported in Ref.[21], give an experimental evidence of the clear semiconducting behaviour of $\alpha' - \text{NaV}_2\text{O}_5$ below and above $T_c$ with the increased dimensionality of an electron transport.

In $\alpha' - \text{NaV}_2\text{O}_5$ the strong interplay between charge, spin and lattice degrees of freedom should be forthcoming [22]. The electron-lattice interactions renormalize an energy scale. Starting from ideas about on-site [23] and inter-site [24] electron pairs it is possible to show that the $V^{4+} - V^{4+}$ dimers are the shortest ($S$), whereas $V^{5+} - V^{5+}$ones are the longest ones ($L$) (c.f.,Fig.1). This conclusion is also consistent with the X-ray and neutron diffraction data [25] indicating the presence of the low-temperature modulated sequence $S - L - L - L - S - L...$ in $\alpha' - \text{NaV}_2\text{O}_5$.

According to Eqs.(3) there are two periodicities along $b$-axis in agreement with ARPES data [26]. At $T < T_c$ the charge order has been obtained without invoking the exchange $J$-terms. However, as a consequence of charge order the alternative exchange antiferromagnetic interactions open the spin-gap [7]. Diagonal hopping parameters $t_d$, $t_{bm}^{xy}$, $t_{qm}^{xy}$ cause exchange interactions, responsible for splitting of magnon modes observed in inelastic neutron scattering [27–29]. If $J$ constants are much smaller than electron hopping, the spin-dependent terms can be treated as a perturbation resulting in a spin-charge separation for 1D Hubbard or $t - J$ models [30]. From that point of view it is interesting to consider an interpretation of a strong temperature induced modification of the spectral intensity seen by the ARPES in $\text{NaV}_2\text{O}_5$ [26,31]. In terms of the 1D $t - J$ model the authors [31] described the experiment as an evidence of availability of spinon and holon Fermi surfaces. Our study of electronic structure has revealed an importance of interladder couplings in $\alpha' - \text{NaV}_2\text{O}_5$.

Let us also note that the $A^+\text{V}_2\text{O}_5$-family can be treated as an electron counterpart of striped layered cuprates. An angular symmetry of $d_{x^2-y^2}$-wave function of copper holes in layered high-$T_c$ cuprates has a similarity with the $d_{xy}$ - wave function of vanadium electrons. However, in vanadates the role of $d - p$ hybridization is diminished but the role of electron correlations is enhanced in contrast to cuprates.

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On leave from:

1 N. S. Kurnakov Institute of the General and Inorganic Chemistry of the Russian Academy of Sciences, Leninskii prospect 31, 117 907 Moscow, RUSSIA

2 Institute of Physics, 11080 Belgrade, P.O. Box 68, YUGOSLAVIA

3 Institute of Engineering Physics, Hanoi University of Technology, 10 000 Hanoi, VIETNAM
References

[1] T. Ishiguro, K. Yamaji and G. Saito, Organic Superconductors (Springer Series in Solid-State Sciences, v.88, Springer, 1998) and Refs. the re.
[2] G. Petrakovskii et al., JETP 71, 772 (1990) - we note that their analysis had been done in terms of the antiferromagnetic phase transition.
[3] M. Hase, I. Terasaki, and K. Uchinokura, Phys. Rev. Lett. 70, 3651 (1993).
[4] M. Isobe and Y. Ueda, J. Phys. Soc. Jpn. 65, 1178 (1996).
[5] M. Weiden et al., Z. Phys. B 103, 1 (1997).
[6] T. Ohama et al., J. Phys. Soc. Jpn. 66, 3008 (1997); Phys. Rev.B 59, 3299 (1999).
[7] M.V. Mostovoy and D.I. Khomskii, cond-mat/9806217 (1998).
[8] P. Horsch and F. Mack, Eur. Phys. J. B 5, 367 (1998).
[9] P. Thalmeier and P. Fulde, cond-mat/9805231 (1998).
[10] S. Nishimoto and Y. Ohta, J. Phys. Soc. Jpn. 67, 3679 (1998).
[11] H. Seo and H. Fukuyama, J. Phys. Soc. Jpn., 67, 2602 (1998).
[12] H. Smolinskii et al., Phys. Rev. Lett. 80, 5164 (1998).
[13] Z.S. Popovic and F.R. Vukailovic, Phys. Rev. B 59, 5333 (1999).
[14] V.A. Ivanov, J. Phys.: Condens. Matter 6, 2065 (1994); Physica C 185-189, 1635 (1991).
[15] D. Smirnov et al., Physica B 259-261, 992 (1999).
[16] A. Damascelli et al., cond-mat/9906042 (1999); A. Damascelli et al., Phys. Rev. Lett. 81, 918 (1998).
[17] S. Okubo, Prog. Theor. Phys., 27, 949 (1962).
[18] J. Hubbard, Proc Roy. Soc. A 276, 238 (1963), ibid. 277, 237 (1964).
[19] V.A. Ivanov, Physica B 186-188, 921 (1993); Physica C 271, 127 (1996); in Studies of High Temperature Superconductors, edited by A. Narlikar, Vol. 11 (Nova Science Publishers, New York, 1993 ), p.331.
[20] M. Cuoco, P. Horsch, and F. Mack, cond-mat/9906169 (1999).
[21] J. Hemberger et al. Europhysics Lett. 42, 661 (1998); M. Lohmann et al. Physica B 259-261, 983 (1999).
[22] J. Riera and D. Poilblanc, Phys. Rev. B 59, 2667 (1999).
[23] P.W. Anderson, Phys. Rev. Lett. 34, 953 (1975).
[24] B.K. Chakraverty et al., Phys. Rev. B 17, 3781 (1978).
[25] T. Chatterji et al., Solid State Commun. 108, 23 (1999).
[26] K. Kobayashi et al., Phys. Rev. Lett. 80, 3121 (1998).
[27] T. Yoshihama et al., J. Phys. Soc. Jpn. 67, 744 (1998).
[28] C. Gros and R. Valenti, Phys. Rev. Lett. 82, 976 (1999).
[29] P. Thalmeier and A.N. Yareshko, cond-mat/9904443 (1999).
[30] S. Sorella and A. Parola, J. Phys.: Condens. Matter 4, 3589 (1992); H. Suzuura and N. Nagaosa, Phys. Rev. B 56, 3548 (1997).
[31] K. Kobayashi et al., Phys. Rev. Lett. 82, 803 (1999).
Figure captions

Fig.1.
The schematic view of $\alpha'$ – NaV$_2$O$_5$. Each dimer/rung is replaced by a circle. The inter/intra)dimer hopping $t_b$ ($t_a$) in the $b(a)$-direction is set along the $y$($x$)-axis. The distances at room temperature between the nearest V-ions on neighboring dimers/rungs are 3.04Å and the leg constant is 3.61Å. The dimer size is 3.44Å. Oxygen $p$–wave functions (opened) enhance the hopping $t_d$ along ladder diagonals. For $T > T_c$: the orthorhombic unit cell with two dimers is shown in lower panel. For $T < T_c$: the size of arrows (lower panel) reflects the charge disproportionation $\Delta n = n_{a,d,m,q} - n_{b,c,n,p}$ in the monoclinic unit cell; the shaded portions have a zigzag order.

Fig.2.
The tight-binding energy dispersions for correlated $d_{xy}$-electrons in $\alpha'$ – NaV$_2$O$_5$ below $T_c$ for parameters $t_a = 0.35eV$, $t_b = 0.15eV$, $t_d = 0.1eV$, $t_{xy}^{bm} = 0.06eV$, $\delta = 0.01eV$ and $\varepsilon = V\Delta n$ ($V = 0.8eV$, $\Delta n = 0.8$). Momenta are given in units $|p_x\sqrt{3}| = |p_y| = \pi$ of the Brillouine zone boundaries, the Fermi energy, $E_F = 0$, is inside the Coulomb gap $\Delta_C = 1$ eV.

Fig.3.
The high-temperature ($T > T_c$) electron density of states as a function of dimensionless energies $\xi / (t_b + t_d)$, $E_F = 0$ (main panel). The inset shows the density of states for non-interacting bonding electrons. The Latin letters denote the energies: $L_1 = -1 - 2t - S + T_-$, $L_2 = -1 + 2t - S + P_-$, $L_3 = 1/2 + t - S + R_-$, $L_4 = 1 - S + Q_-$, $U_1 = -1 - 2t - S + T_+$, $U_2 = -1 + 2t - S + P_+$, $U_3 = 1/2 + t - S + R_+$, $U_4 = 1 - S + Q_+$, where parameters $S$, $T_\pm$, $P_\pm$, $Q_\pm$, $R_\pm$ are done in Eq.(5) and $t = t_{xy}/[2(t_b + t_d)]$. 

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