Isospin model for suppression of charge order in hole-doped NaV$_2$O$_5$

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The layered perovskite compound NaV$_2$O$_5$ exhibits charge ordering (CO) and spin gap formation which is driven by inter-site Coulomb forces and exchange dimerisation. Experimentally it was found that the CO transition is rapidly reduced by doping. Charge ordering in NaV$_2$O$_5$ has a quasi 1D character due to inter-ladder frustration in the Trellis lattice. Based on an extended pseudospin (T=1) approach for hole doped NaV$_2$O$_5$ ladders we construct an Ising like model that explains qualitatively the destruction of the CO phase as function of hole doping $\delta$ and show how the CO parameter depends on $\delta$ and the ratio of Coulomb and hopping energies.

I. INTRODUCTION

The layered perovskite NaV$_2$O$_5$ shows an interesting interplay between charge ordering (CO) of 3d-electrons on the rungs of V-V ladders and a spin-Peierls transition associated with spin gap formation first observed in$^1$ below $T_c=34$ K. This transition is associated with a distortion of the high temperature orthorhombic structure of NaV$_2$O$_5$. The latter can be viewed as Trellis lattice with ab-planes stacked along c. They consist of ladders with V-O-V rungs (inset of Fig. 1) shifted alternatingly along b by half a lattice constant. The precise low temperature structure is still controversial$^{2-6}$ with the proposed models differing in the number of inequivalent V and Na sites and an associated charge ordering on each or only on every second ladder. The slow progress and ambiguity of experimental results has hindered theoretical understanding considerably. However it has become clear now that there is a close connection between charge ordering on the V-V rungs and exchange dimerisation on the ladders$^7$ which leads to the spin gap formation directly seen in inelastic neutron scattering$^8$. It was realized early on$^9$ that the CO on the V-rungs may be described within an Ising model in a transverse field (ITP) where the isospin ($S=\frac{1}{2}$) represents the charge degree of freedom on the V-V rung with inter-site Coulomb forces correspond to Ising interactions and the intra-rung hopping to a transverse field. This is due to the charge transfer (CT) gap of $\sim 0.4-0.5$ eV$^{11,12}$ which leads to an insulating state of NaV$_2$O$_5$ despite having only one 3d-electron per rung (quarter-filled ladders). Therefore only singly occupied rungs have to be considered which may be represented by an isospin and the real spin. A detailed model of the combined Ising-spin Peierls system and its phase transitions has been discussed in$^7$.

The charge ordering in a Trellis lattice compound is severely hindered by frustration of inter-site Coulomb forces which is directly obvious in the Ising model representation. In fact on a rigid lattice CO would be prohibited since the lattice of V-V rungs corresponds to a trigonal covering lattice of Ising spins. The simultaneous structural distortion at $T_c$ reduces the frustration by leading to inequivalent adjacent ladders. The driving mechanism for the transition are inter-site Coulomb interactions and exchange-striiction. The gain in Coulomb energy ($V_b$) by complete CO in a rung is in competition with the loss of intra-rung kinetic energy ($t_a$), the control parameter for CO is therefore $\lambda=2t_a/V_b$ (for convenience the inverse definition of$^{13}$ is used here). The very low CO transition temperature suggests that in NaV$_2$O$_5$ one is close to the quantum critical point $\lambda_c=1$ of the corresponding ITP model$^{13}$. The charge ordering is then essentially of 1D Ising type, this means one has long range correlations along the ladder and no correlations between them, this was indeed obtained in exact diagonalisation studies of the ITP$^{14}$. The ordering may then be viewed as arising from Ising like correlations along the chain which lead to a true 2D broken symmetry state at finite T due to a staggered longitudinal Ising field set up by the distortion of the neighboring ladders$^{13,7}$.

In this context it is suggestive that even small perturbations of the 1D Ising correlations might reduce or destroy the CO state in NaV$_2$O$_5$. This can be achieved by reducing the filling factor n of the 1D ladders below $\frac{1}{2}$ by doping with holes. This introduces “empty” rungs into the ladder which cut the Ising bonds. The ensuing destruction of long range 1D correlations should then strongly reduce $T_c$, as function of the hole concentration $\delta$ ($n=\frac{1-\delta}{2}$). This has indeed been found by introducing holes in the ladders through Na-deficiency doping$^{18}$ where a few per cent holes are sufficient to destroy the CO state and the associated spin Peierls transition. Rapid suppression of charge order has also been found in various other doping series, i.e. replacing Na by Li and K (isoelectronic) or Ca (electron-doping).$^{15-17}$ This may be observed directly by specific heat measurements$^{16}$ which show a progressive suppression of $\Delta C(T_c)$ with increasing doping. It is also seen in the susceptibility$^{18,15}$ which shows a closing of the CO induced spin gap.

Most importantly in this doping range NaV$_2$O$_5$ remains an insulator which is not easy to understand within a Hubbard like model for the quarter filled ladder$^{5,7}$, possibly 1D localization effects play a role, indeed the conductivity was found to exhibit variable range hopping behaviour$^{18}$ for hole doping. The notion that charge ordering $T_c$ is reduced because doping creates empty rungs...
which cut the Ising bonds along the ladder is however completely static and invokes a disordered state. It lacks the important ingredient of kinetic energy gain due to the hopping of holes between adjacent rungs leading to a homogeneous state. This problem has sofar not been considered theoretically.

In this work we will give a more solid theoretical basis for the influence of hole doping on CO in NaV$_2$O$_5$. This will again be done in the context of an effective isospin approach. In sect. II we give the basics of the electronic structure of NaV$_2$O$_5$ and discuss the isospin model for the undoped case in sect. III. Subsequently in sect. IV we show that even in the doped case the low energy Hamiltonian may be projected to an effective Ising type form, albeit with an Ising spin $T=1$ to accomodate the holes on empty rungs. In sect. V we discuss how order parameter, kinetic energy and chemical potential (doping level) are represented in the isospin formalism and their respective coupled mean field equations in the ground state in sect. VI. They are solved in sect. VII numerically and we discuss the variation of the CO parameter with the control parameter $\lambda$ and the hole doping $\delta$ which leads to the zero temperature CO phase diagram. Finally sect. VIII gives summary and outlook.

II. ELECTRONIC STRUCTURE OF NaV$_2$O$_5$

The electronic structure of the charge transfer insulator NaV$_2$O$_5$ has been investigated$^{10,11}$ within the LDA and LDA+U approach respectively. A mapping of the resulting band structure to an extended tight binding (TB) model involving both V 3d and O 2p orbitals has also been performed$^{11}$ and an excellent fitting of the LDA+U bandstructure was obtained. For our present purpose it is sufficient to use a reduced TB model involving only V 3d$_{xy}$ orbitals. The hopping elements involved in this model are defined in Fig. 1. There are four V atoms in the unit cell resulting in two 3d$_{xy}$ occupied valence and two empty 3d$_{xy}$ conduction bands separated by a charge transfer gap of about 0.3 meV which is largely determined by the effective intra-rung hopping $t_a$. In the effective TB model this gap may be interpreted as bonding-antibonding gap of V 3d$_{xy}$ orbitals of a rung. Furthermore the valence and conduction band are each almost twofold degenerate due to the weak hopping between ladders. The 3d$_{xy}$ bonding bands have a considerable dispersion of order $t_a + t_d$ along the b- direction while the dispersion $t_b - t_d$ of 3d$_{xy}$ antibonding bands is almost zero due to accidental near equality $t_b \approx t_d$.

III. THE ISOSPIN MODEL HAMILTONIAN FOR UNDOPED NaV$_2$O$_5$

The basic many body Hamiltonian describing NaV$_2$O$_5$ is of the single band (3d$_{xy}$) extended Hubbard type$^{9,7}$. As shown in$^9$, due to the presence of a CT gap the charge degrees of freedom may be represented by an effective ITP Hamiltonian ($T=\frac{1}{2}$) which is obtained by projecting the original Hamiltonian to the subspace of singly occupied rungs$^6$. The states $|\downarrow\rangle$, $|\uparrow\rangle$ of the $T=\frac{1}{2}$ isospin describes occupied d$_{xy}$ orbitals on the left and right V atom of each rung respectively. A simplified version of the resulting ITP Hamiltonian for a single ladder is given by$^{13}$

$$H_{ITP} = 2V_b \sum_{ij} [T_{zi}T_{zj} + \frac{1}{4}] - 2t_a \sum_i T_{ix}$$

$$-h_s^0 \sum_i (-1)^iT_{zi} \quad (1)$$

Here $t_a$ is the hopping across the rung and $V_b$ the Coulomb interaction along the leg of a ladder. The last term is due to a staggered longitudinal isospin field $h_s = (\downarrow)$. This simulates the influence of the neighboring ladders$^{13}$. For $\lambda = 2t_a/V_b < \lambda_c=1$ one obtains an AF ordering of isospins which corresponds to the zig-zag ordering of 3d- electrons on the ladder as illustrated in Fig. 1. It was shown$^7$ that the interaction parameters in Eq. 1 are renormalized by virtual processes via doubly occupied rungs or sites which depends on the spin state. This leads to a coupling of isospin (charge) and spin degrees of freedom whose contribution is neglected here.

The zig-zag CO in a ladder is characterized by the order parameter $\langle T_{zi} \rangle = (-1)^i x$ at zero temperature with $\lambda \leq 1$

$$x = \left[ 1 - \left( \frac{\lambda}{\lambda_c} \right)^2 \right]^{\beta} \quad (2)$$

The exact solution of the 1D ITF model has the exponent $\beta = \frac{1}{8}$ and $\lambda_c=1$. It is understood that an infinitesimal staggered field $h_s$ has to be applied to lift the twofold degeneracy of the ordered ground state. A truncated mean field (mf) approximation suppressing double counting of bonds in the molecular field leads to a critical value $\lambda_c=1$. This is the same quantum critical point that separates the CO $(\lambda < 1)$ phase from the disordered phase $(\lambda > 1)$ as for the exact solution$^{13}$. Naturally the mf critical OP exponent $\beta = \frac{1}{2}$ is different.

IV. T=1 ISOSPIN MODEL FOR DOPED NaV$_2$O$_5$

The charge ordering described by the ITP model and its implications for the (spin-) superexchange have been described in detail in$^{13,7}$. In the present work we want to investigate whether the convenient and physically appealing isospin approach for CO in NaV$_2$O$_5$ can also be applied to the hole doped compound to study the suppression of CO. For this purpose the hole states, that is empty V-V rungs with zero 3d- occupation, also have to
be represented by an isospin degree of freedom. As in the stoichiometric case\(^{13,7}\) doubly occupied rung states either have a large charge transfer energy \((t_a)\) or a large on-site Coulomb repulsion and therefore contribute only as intermediate states by renormalizing the interaction parameters of the effective Hamiltonian. Thus the model has to incorporate three basis states, two singly occupied and one empty rung state which suggests to use a \(T=1\) isospin instead of \(T=\frac{1}{2}\) for the stoichiometric \((\delta=0)\) case. The mapping of electronic states to isospin states for rung \(i\) is then defined as

\[
|T_z = -1\rangle_i = |00\rangle_i = 0_i = e_i^\dagger |0\rangle_i
\]

\[
|T_z = 0\rangle_i = |01\rangle_i = e_i^\dagger |1\rangle_i
\]

\[
|T_z = 1\rangle_i = |10\rangle_i = e_i^\dagger |2\rangle_i
\]

\[
(3)
\]

where \(P_0+P_1=1\) and \(P_1=P_L+P_R\) holds. The other projector properties \(P_0P_1=P_1P_0=0\) and \(P^2 = P_0\) \((\lambda=0,L,R)\) are easily verified. Using these projection operators the intra-ladder Coulomb interactions \(V_b\) between adjacent rungs \(i,j\) may be represented by the Hamiltonian

\[
H_C(i,j) = \frac{1}{2} (V_b + V_d) T_i^2 T_{ij}^2 + \frac{1}{2} (V_b - V_d) T_i T_{ij}
\]

\[
(5)
\]

Compared to the \(T=\frac{1}{2}\) case of Eq. (1) \(H_C\) also contains now biquadratic terms in the isospin. Similarly we construct the intra-rung kinetic energy responsible for the charge transfer gap. Since the R,L-occupation of each rung is now described by \(|T_z = \pm 1\) respectively the intra-rung hopping term must change the isospin by \(\pm 2\) units. The corresponding rung Hamiltonian then reads

\[
H_K(i) = -\frac{1}{2} t_a (T^2_{i+1} + T^2_{i-1}) = -t_a (T^2_{zi} - T^2_{yi})
\]

\[
(6)
\]

which should be compared to the second term in Eq. (1) for \(T=\frac{1}{2}\). Finally there has to be an additional term describing the hole kinetic energy, i.e. when the empty rung (Fig.1) is shifted along the ladder direction. Such processes are described by inter-rung terms like

\[
H'_K(i,j) = 2t_a \left[ O_{zy}(i) O_{zy}(j) + O_{zy}^\dagger(i) O_{zy}(j) \right]
\]

\[
+ 2t_a \left[ O_{zx}(i) O_{zx}^\dagger(j) + O_{zx}^\dagger(i) O_{zx}(j) \right]
\]

\[
(7)
\]

with \(i,j\) denoting rungs along the ladder. Here \(t_a = \frac{1}{2}(t_{oa}+t_{od})\) and \(O_{zy}=iT_z T_y\) and \(O_{zx}=T_z T_x\) may be interpreted as a quadrupolar operator in the \(T=1\) isospin space. In the following we consider only the special case \(t_0 \approx t_\pm\) which is appropriate for \(\text{NaV}_2\text{O}_5\).\(^{11}\) Then the second term above vanishes and the total \(T=1\) model Hamiltonian for the doped ladder now reads

\[
H = \sum_i [T^2_{zi} + t_a (T^2_{zi} - T^2_{yi}) - h_o T_{zi}]
\]

\[
+2t_a \sum_{\langle ij \rangle} \left[ O_{zy}^\dagger(i) O_{zy}(j) + O_{zy}(i) O_{zy}^\dagger(j) \right]
\]

\[
+V_+ \sum_{\langle ij \rangle} T_{zi} T_{zj} + V_- \sum_{\langle ij \rangle} T^2_{zi} T^2_{zj}
\]

\[
(8)
\]

Here \(\epsilon\) is the on-site orbital energy and \(h_o(i) = h_o(\pm 1)\) is again a staggered field due to the influence of neighboring ladders, \(\langle ij \rangle\) denotes n.n. rungs along the ladder. Furthermore we have defined \(V_\pm = \frac{1}{2}(V_b \pm V_d)\). If we neglect the ladder diagonal Coulomb interaction \((V_d \equiv 0)\) then \(V_\pm = \frac{1}{2} V_b\) leading to a single control parameter \(\lambda = 2t_a/V_b\). Although we expect the isospin model a convenient framework to discuss the energetics of charge ordering as function of doping it can however not give answer to the question why the doped system stays an insulator, for this problem one also has to include the doubly occupied rung states. It was argued in\(^{13,7}\) that even under a finite charge transfer between ladders, i.e. deviations

\[
\text{FIG. 1. Mean field eigenvalues (full lines) } E_\kappa (\kappa=0-2) \text{ of Eq. (14) and 'chemical potential' } \mu \text{ (dashed line) as function of the control parameter } \lambda. \text{ Arrow indicates CO transition. Inset shows the NaV}_2\text{O}_5 \text{ ladder along b with effective V-V rungs along a. Closed and open circles correspond to occupied and empty d}_{xy}-\text{orbitals. Hole doped rung has two empty d}_{xy}-\text{orbitals. Only the ground state (}\kappa = 0\text{) is occupied for each rung with a hole count given by Eq. 17. Hopping and interaction parameters are indicated. We used } t_a = 0.380 \text{ eV}, b = 0.170 \text{ eV; for numerical reasons the latter is twice the value used in}^{13}.
\]

with \(|00\rangle_i\) denoting the empty rung state. We first express the inter-rung Coulomb energy already present in Eq. (1) in the above extended isospin basis. The projectors to this basis may be written in terms of the \(T=1\) isospin operators \(T = (T_x,T_y,T_z)\) as

\[
P_L = \frac{1}{2} T_0 T_z + T_0
\]

\[
P_R = \frac{1}{2} T_0 (T_z - 1)
\]

\[
P_0 = 1 - T^2_z
\]

\[
(4)
\]
from quarter-filling, an insulating state can be expected for the relevant hopping and interaction parameters realised in NaV$_2$O$_5$.

\[
\lambda = 2t_a/V_b
\]

\[
\delta = 0.0 \quad 0.03 \quad 0.06 \quad 0.09
\]

\[
\delta = 0.03 \quad 0.06 \quad 0.09
\]

\[
\langle T_x \rangle = \langle T_z \rangle
\]

\[
\delta = 0
\]

\[
\delta = 0.01
\]

FIG. 2. zig-zag charge order parameter \(\langle T_z \rangle\) as function of control parameter \(\lambda\) for small and moderate hole doping \(\delta\) (full lines). Dashed lines represent average hole hopping energy \(\langle T_x \rangle\) (units: \(t_b\)) for \(\delta = 0\): \(\langle T_z \rangle \equiv 0\)

V. CHARGE ORDER PARAMETER, DOPING AND 'CHEMICAL POTENTIAL'

It is obvious that the model defined by eq. 8 is much more complex due to the additional hole state \((T_z = 0)\) and has no exact 1D solution like the \(T=\frac{1}{2}\) ITF model. As mentioned previously the truncated mf approximation for the charge order parameter of the ITF model has the same quantum critical point \(\lambda_c = 1\) as the exact solution. It is therefore plausible that a mf treatment of Eq. 8 in the doped case still gives a qualitatively correct picture for the conditions of charge ordering. As in the ITF case the order parameter for \(V_b > V_d\) should be staggered, i.e zig-zag CO should be realized, then for the two sublattices we have

\[
x = \langle T_{zA} \rangle = -\langle T_{zB} \rangle
\]

Now \(x\) not only depends on the control parameter \(\lambda = 2t_a/V_b\) but also on the number of holes or unoccupied rungs. The representation of the hole number operator in fermionic and isospin language is given by

\[
\hat{\delta}_t = 1 - \hat{n}_t = 1 - c^\dagger_{L}c_{L} - c^\dagger_{R}c_{R}
\]

\[
\hat{\delta}_t = 1 - \hat{P}_{L} - \hat{P}_{R} = 1 - T^2_{z1}
\]

so that the hole concentration is obtained as

\[
\delta = 1 - \langle T^2_z \rangle
\]

Since it is externally fixed by the level of doping the local orbital energy has to be adjusted selfconsistently for each parameter set such that \(\delta\) is obtained. This can be done by adding a 'chemical potential', i.e. replacing \(\epsilon \rightarrow \epsilon - \mu\). For each microscopic parameter set and order parameter \(x\), the chemical potential \(\mu\) has to be adjusted appropriately to obtain the physical hole number.

FIG. 3. upper panel: melting of CO with hole doping \(\delta\) for various \(\lambda\) given in decreasing order. The absolute slope value \(-(dx/d\delta)\) increases strongly when approaching the quantum critical point \(\lambda_c = 1\) of CO; this is shown in the inset. lower panel: Hole kinetic energy \(\langle T_x \rangle\) (in units of \(t_b\)) as function of \(\delta\) in the complete doping range, plotted for five values of \(\lambda\) corresponding to curves in increasing order. Downward arrows indicate CO transition \((x=0)\) where the curves for different \(\lambda\) merge.

VI. MEAN FIELD APPROXIMATION AND SOLUTION FOR CO

The usefulness of a simple mf solution relies on the Ising type nature of the present model. In this approximation the doping term \(\sim t_b\) in Eq. 8 simplifies considerably using \(O_{xy}^* + O_{xy} = T_x\) and \(O_{xy}O_{xy}^* = iT_y\), we obtain
\[
H_{K,mf}(i) = -2t_b[O_{yz}(O_{yz} + O_{yz}(O_{zy})]
\]
\[
= -t_b(T_x(i) + (T_y)T_y(i))
\]
\[
= -t_b(T_x)cos(\phi T_x + sin \phi T_y)
\]

where \((T_x) = \sqrt{(T_x)^2 + (T_y)^2} \text{ and } \phi \text{ which is given by}
\[
tan^{-1}(\phi / T_y / T_x) \text{ is an arbitrary angle which may be chosen as } \phi = 0.\text{ Then only } (T_x) \text{ appears and the quantity } W = t_b(T_x) \text{ may be interpreted as the average inter-rung hopping amplitude of the hole. Together with the remaining terms in Eq. 8 we get the following rung mf Hamiltonian for A,B sublattices:
\[
H_{mf}^{A,B} = [\epsilon + V_+(1 - \delta) - \mu]T_x^2 - t_a(T_x^2 - T_y^2)
\]
\[
= -(h_s^0 + V_+)T_x - WT_x
\]

The effective mf orbital energies and staggered fields are then given by
\[
\hat{\epsilon} = \epsilon - \mu + V_+(1 - \delta)
\]
\[
h_s = h_s^0 + V_+ x
\]

In the T=1 isospin space the mf Hamiltonian for A,B sublattices can explicitly be written as
\[
H_{mf}^{A,B} = \begin{pmatrix}
\hat{\epsilon} + h_s & -W/\sqrt{2} & -t_a \\
-W/\sqrt{2} & 0 & -W/\sqrt{2} \\
-t_a & -W/\sqrt{2} & \hat{\epsilon} + h_s
\end{pmatrix}
\]

where A,B corresponds to upper and lower signs respectively. These equations have to be selfconsistently solved for the charge order parameter x, keeping the hole concentration fixed by varying the chemical potential \(\mu\). Only the T=0 case is considered, then the expectation values \(<X> = \langle \psi_{mf}^{0} | X | \psi_{mf}^{0} \rangle\) are obtained from the ground state \(\psi_{mf}^{0}\) of solution of Eq. 14. For the actual calculation, in addition to assuming \(t_b \approx t_d\) which has been justified in ref. 11, we take for simplicity \(V_d \approx 0\). If we suppress the hole hopping described by the matrix elements \(-W\) for the moment, the \(T_x=0\) and \(T_x = \pm 1\) subspaces disconnect and the mf ground state and its energy of the isolated rungs can be written explicitly as
\[
E_0 = \hat{\epsilon} - \frac{1}{2}\sqrt{(\Delta \epsilon)^2 + (2t_a)^2}
\]
\[
|\psi_{mf}^{0}\rangle_i = u_{1i}(1) + u_{2i}| - 1\)

where \(\Delta \epsilon = V_{d}X\) is the splitting of L,R orbital energies and the staggered mf coefficients are given by
\[
u_{1,2i} = \frac{1}{2} \left[ 1 \pm \frac{(1) \Delta \epsilon_i}{\sqrt{(\Delta \epsilon)^2 + (2t_a)^2}} \right]
\]

When the effect of hole hopping along the legs \((W > 0)\) is now included the mf eigenstates will be mixtures of the isolated rung states \(|\psi_{mf}^{0}\rangle_i\) and the hole state \(|0\rangle_i\). The hole concentration is then given by
\[
\delta = 1 - \langle \psi_{0}^{mf} | T_x^2 | \psi_{0}^{mf} \rangle
\]

The new mf ground state energy, its wave function and associated expectation values of \(T_x, T_z\) and \(T_z^2\) then have to be calculated selfconsistently from Eq. 14. The numerical results will be discussed in the next section.

VII. NUMERICAL SOLUTION, DOPING DEPENDENCE OF CO AND PHASE DIAGRAM

In this section the numerical results for the above model will be presented. The main goal is the determination of the charge parameter \(x(\delta, \lambda)\) as function of the hole concentration \(\delta\) and the control parameter \(\lambda = 2t_a/V_b\). To achieve a given hole number \(\delta = 1 - (T_z^2)\) the ‘chemical potential’ \(\mu\) has to be adjusted selfconsistently together with the determination of the order parameter \(x = (T_z)\) and the normalized kinetic energy \(\langle T_x \rangle = W/t_b\). Physically \(\mu\) corresponds to an orbital energy shift of the empty and singly occupied rung states. This energy shift together with the mf eigenvalues of Eq. 14 as function of the control parameter \(\lambda\) is shown in Fig. 1 for \(\delta = 0.09\).

![Fig. 4. CO/MV phase diagram in the \(\delta, \lambda\) plane. Contour lines for CO phase with \(\delta = (T_z)\) for \(x = 0.01, 0.25, 0.5, 0.75\) (moving to lower left corner) are also shown. MV denotes the disordered homogeneus mixed valent phase.](image)

The corresponding variation of the charge order parameter \(x\) for several hole concentrations is shown in Fig. 2. As the hole concentration increases our results show the expected qualitative behaviour: i) the CO even for large \(V_b\) (small \(\lambda\)) is no longer complete due to the presence of empty rung states and its variation with \(\lambda\) becomes essentially flat. ii) the critical value \(\lambda_c\) for the CO transition to appear is reduced from the value \(\lambda_c = 1\)
of the undoped ITF model. In addition the kinetic energy $\langle T_z \rangle$ is shown. It increases almost linearly with $\lambda=2t_z/V_b$ and rapidly with the hole concentration.

The complementary reduction of charge order as function of the hole concentration for constant $\lambda$ is shown in Fig. 3. Most significantly for small $\delta$ one observes a rapid reduction of the CO- parameter with increasing hole concentration. The slope of this reduction increases even further when $\lambda$ approaches the quantum critical point $\lambda_c=1$ of CO from below. This is shown in more detail in the inset of Fig. 3. The origin of this drastic reduction of CO for small $\delta$ lies in the rapid increase of hole kinetic energy with doping as can been seen in the lower panel of Fig. 3.

Our results shown in Fig. 3 describe qualitatively correct the experimental situation, namely a destruction of the CO state in NaV$_2$O$_5$ by a few percent hole doping$^{16}$. For example assuming a value $\lambda=0.95$ close to $\lambda_c=1$ one obtains a critical concentration $\delta=0.03$. The maximum size of CO at $\delta=0$ for this $\lambda$- value is already considerably reduced to $x_0 \approx 0.3$. The experimental value of the nominal hole concentration for suppression of CO in Na-deficient NaV$_2$O$_5$ is indeed about $\delta=0.03$.$^{15}$

Finally we summarize the results of our calculations in Fig. 4 which shows the phase diagram of CO in the $(\delta, \lambda)$-plane and the size of the charge order parameter $x$ as a contour plot in the ordered regime.

VIII. SUMMARY AND OULOOK

In this work we have proposed an extended isospin approach proposed in$^9$ to the charge ordering transition in Na- deficient (hole-doped) NaV$_2$O$_5$. The additional hole (empty rung) state can be accommodated within a $T=1$ isospin as the $T_z=0$ component whereas the (left and right) occupied rung states are represented by the $T_z=\pm 1$ components. The effective isospin Hamiltonian for the doped system is of more complex type than the simple $T=\pm 1$ ITF model in the undoped case due to the existence of biquadratic terms. Contrary to the ITF model there is no exact solution. However it was argued that a mf treatment of the extended model for the doped ladder still gives a qualitatively correct description of charge order and its destruction by doping.

Indeed it was found that the CO ground state is rapidly destroyed by hole doping and the size of the slope of the order parameter reduction $-dx/d\delta$ increases strongly when one approaches the quantum critical point ($\lambda \leq 1$) which corresponds qualitatively to the observed behaviour in NaV$_2$O$_5$. A phase diagram in the doping$(\delta)$- control parameter $(\lambda)$ plane was derived showing the evolution of the charge order parameter.

Naturally the present model should be investigated beyond the present mf approximation. As shown in the case of the ITF model for pure NaV$_2$O$_5$ the exact diagonalisation Lanczos approach of finite ladders or clusters with the Trellis lattice structure is a powerful method to gain more insight into the appearance of charge order. It can also be used for the present extended $T=1$ isospin model of hole- doped NaV$_2$O$_5$.

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