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Finite-temperature investigation of quarter filled ladder systems

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Abstract

We investigate charge ordering in a quarter-filled ladder at finite temperature by determinantal Quantum Monte Carlo. The sign problem is moderate in a wide range of model parameters relevant for NaV_2O_5. The charge order parameter exhibits a crossover as a function of inverse temperature β on finite systems. Above a critical nearest neighbor Coulomb repulsion V_c, the correlation length grows exponentially with β, indicative of the ordered phase at $\beta = \infty$. We find a clear single-particle gap manifesting itself in a flat $n(\mu)$ dependence at large nearest neighbor Coulomb repulsion V.

Keywords: Quarter-filled ladders; Charge ordering; Quantum Monte Carlo

The inorganic ladder compound NaV_2O_5 has attracted great attention in recent years. This interest was triggered by magnetic susceptibility measurements [1], which show a phase transition at $T = 34\,\mathrm{K}$ into a low-temperature spin-gapped phase. This transition is accompanied by charge ordering, as observed in NMR measurements [2], where the valence of the vanadium sites changes from $V^{4.5}$ to $V^{4.5\pm\delta}$, with δ the amount of charge disproportion. This transition has been studied theoretically by several techniques at $T = 0$ [3].

On a microscopic level the system can be described by an extended Hubbard model

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{H.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow} + V\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i, \quad (1)$$

at quarter filling $\langle n\rangle = 0.5$, with hopping matrix elements $t_{ij} = t_x$ along the ladder and $t_{ij} = t_y$ within a rung, and chemical potential μ. We state all energies in units of t_y. These hopping parameters as well as the onsite Coulomb interaction can be extracted from first-principle calculations [4]. The hopping along chains $t_x \simeq 0.5t_y$ is weaker than along rungs. This strongly influences the

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physics of the ladder, for which a spin-gap seems to appear at $t_x \gtrsim t_y$ [3].

We used $t_x = 0.5$ and $U = 8$. Since the non-local Coulomb interaction V cannot be determined properly by band-structure calculations, we used V as a free parameter of the Hamiltonian. The charge order parameter is $\Delta_{\rm co}^2 = \frac{1}{2L\langle n\rangle}\sum_{ij} e^{i\mathbf{Q}(\mathbf{r}_i-\mathbf{r}_j)}(n_i - \langle n\rangle)(n_j - \langle n\rangle)$ with $\mathbf{Q} = (\pi, \pi)$, which is unity for complete ordering.

We performed grand canonical calculations by determinantal quantum Monte Carlo. These are often very difficult for doped systems because of a sign problem. Fortunately, the average sign is favorably large in the relevant parameter range of $t_x/t_y = 0.5$ and large V (Fig. 1). In the opposite case of isotropic $t_x = t_y$ at small V, $\langle$sign$\rangle$ becomes very small. The charge order parameter exhibits similar behavior, but it is less strongly dependent on t_x/t_y. Charge order grows with increasing V.

Fig. 2 shows the charge correlation length $\xi_{\rm cc}$. At small interactions, $V = 1.5$ and 2.0, the correlation length seems to saturate, but for $V = 2.5$ and 3.0 it increases exponentially with β, with a V-dependent slope. This behavior is consistent with the 1D Ising model in a transverse field (IMTF) [5], which is equivalent to Eq. (1) in the limit of one spinless electron per rung. For large V, the transverse field goes to zero, and $\xi_{\rm IMTF} = |\ln\tanh(\beta)|^{-1}$. This is exponential behavior with slope 2 at large β, which the data in Fig. 2 appear to approach. There is long-range order in the thermodynamic limit only at $\beta = \infty$. For weaker interactions, $V < 2t_y$, the correlation length $\xi_{\rm IMTF}$ remains finite even in the limit $\beta \to \infty$, showing a disordered phase at all temperatures. The results in Fig. 2 are nicely consistent with recent DMRG calculations [6] which show that at $T = 0$ the system has a quantum phase transition to an ordered phase at $V_{\rm c} = 2.1(1)$.

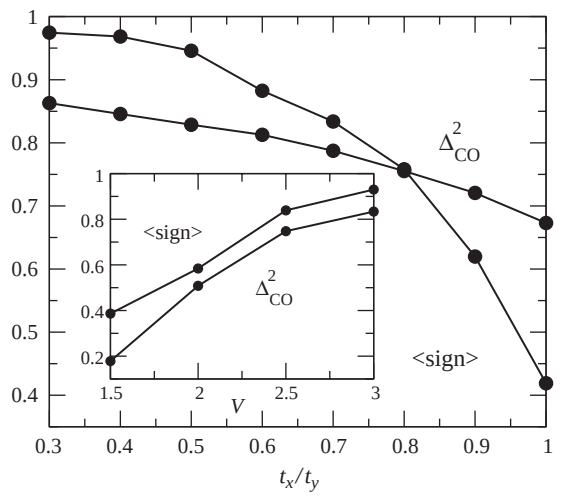

Fig. 1. Mean value of sign and order parameter $\Delta_{\rm co}^2$ as functions of t_x/t_y at $V = 3$, $\beta = 6$, $L = 16$, $\langle n\rangle = 0.5$, and as functions of V at $\beta = 6$ (inset).

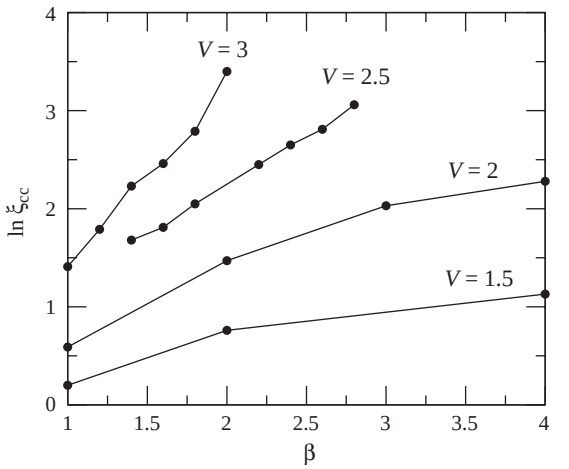

Fig. 2. Logarithm of the charge correlation length $\xi_{\rm cc}$ as a function of β for different interactions V ($L = 32$ for $V = 1.5$ and 2; $L = 44$ for $V = 2.5$ and 3).

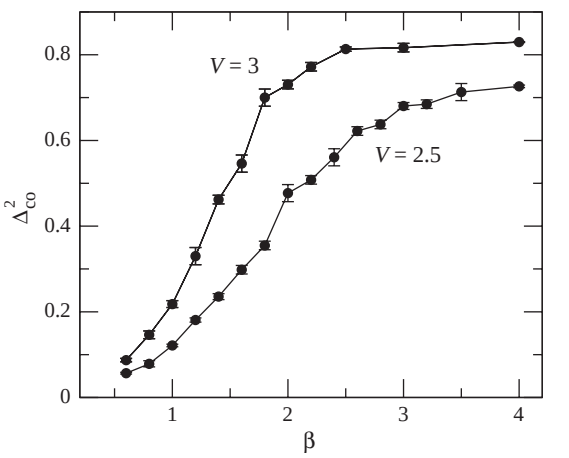

Fig. 3. Charge order parameter as a function of β for $V = 3.0$ and $V = 2.5$ with $L = 32$ rungs.

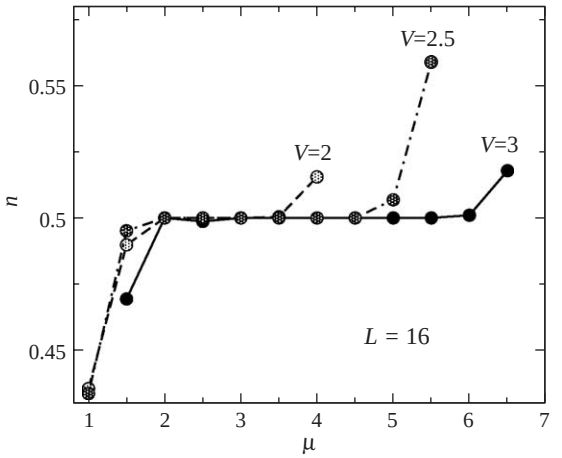

Fig. 4. Mean electron density as a function of the chemical potential μ at $\beta = 6$, L = 16.

However, the behavior of finite size systems is different from the IMTF in the thermodynamic limit. As a function of inverse temperature, the charge order parameter exhibits a crossover at large V (Fig. 3). For the single ladder, this crossover is a finite size effect. It appears since at some β, the charge order correlation length will exceed the system size, resulting in apparent long-range order. For a three-dimensional system of coupled ladders, this crossover can become a phase transition. The order parameter at $V = 3$ and different β scales well as a function of $\xi(L)/L$.

The onset of charge order at large V is most clearly visible in the single particle gap shown in Fig. 4. It manifests itself as a plateau in the $n(\mu)$ dependence where $\langle n \rangle = 0.5$ remains constant in a region $\mu_{\min} < \mu < \mu_{\max}$. At large V, the upper boundary $\mu_{\max}$ shifts with V as approximately $3V$, which is the same value as in the atomic limit at full ordering.

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