Mixed Spin-Charge Solitons and the Phase Diagram of $(TMTCF)_2X$, C = S, Se

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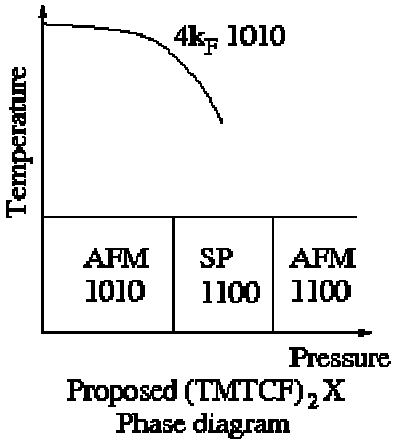
We report results of temperature-dependent calculations of static charge and bond-susceptibilities that give a systematic and complete understanding of the phase diagrams of $(TMTCF)_2X$ and other $\frac{1}{4}$-filled band charge transfer solids[1]. We are able to explain the occurrence of two different antiferromagnetic phases but a single spin-Peierls phase in the $(TMTCF)_2X$. The two antiferromagnetic phases correspond to two different site charge occupancies, Wigner crystal and Bond-Charge-Spin-Density Wave[2]. In contrast, the spin-Peierls state is unique and is a Bond-Charge-Density Wave, independent of whether the high temperature $4k_F$ state is charge- or bond-dimerized. The same spin-Peierls state can therefore evolve into two different $4k_F$ states at high temperature. Based on exact diagonalization calculations[1] we show that this unusual behavior originates from the mixed spin-charge character of soliton excitations from the spin-Peierls state in the interacting $\frac{1}{4}$-filled band. We explain the competition and coexistence between charge-ordered and spin-Peierls phases in $(TMTTF)_2PF_6$ and $(TMTTF)_2AsF_6$ as well as the observed isotope effect with deuteration[3].



[1] R.T. Clay, R.P. Hardikar, S. Mazumdar, http://arxiv.org/abs/0704.1656, submitted to *Phys. Rev. Lett.*, (2007).
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[3] F. Nad et al., *J. Phys. Condens. Matt.* **17,** L399 (2005), K. Furukawa, T. Hara, T. Nakamura, *J. Phys. Soc. Jpn.* **74**, 3288 (2005).