Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Theory of the carrier concentration-dependent behavior in layered cobaltates HONGTAO LI, University of Arizona, R. TORSTEN CLAY, Mississippi State University, SUMIT MAZUMDAR, University of Arizona — Layered cobaltates — anhydrous $\text{Na}_x\text{CoO}_2$, $\text{Li}_x\text{CoO}_2$ and the “misfit” cobaltates $[\text{Bi}_2\text{A}_2\text{O}_4] : [\text{CoO}_2]_m$, where A = Ba, Sr or Ca — have attracted wide attention for their 2D layered structure and metallicity (both reminescent of 2D cuprates), and the tunability of the carrier concentration over a wide range. The Co ions form a 2D triangular lattice, and their formal charge in $\text{Na}_x\text{CoO}_2$ and $\text{Li}_x\text{CoO}_2$ can be tuned from $\text{Co}^{3+}$ at $x = 1$ to $\text{Co}^{4+}$ at $x = 0$. Charge carriers in all cases are holes, with the carrier concentration given by the fraction of Co-ions that are in the $S = 1/2$ $\text{Co}^{4+}$ state. Experiments have indicated remarkable carrier concentration dependent magnetic susceptibility and thermoelectric power that remains unexplained to date. Specifically, all three systems show weakly correlated behavior at small nonzero $x$ (large carrier concentration), and strongly correlated behavior at large $x$ (small carrier concentration). In this talk we give clear theoretical explanation of the observed carrier concentration dependence within an $a_{1g}$-only one-band extended Hubbard Hamiltonian. The key to understanding the $x$-dependence is to have realistic finite on-site correlation $U$ and significant intersite Coulomb interaction $V$. We present exact numerical results for triangular lattices upto 20 sites, and make detailed comparisons to experiments.

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Date submitted: 19 Nov 2010
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