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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 Na_xCoO_2, Li_xCoO_2 and the "misfit" cobaltates $[Bi_2A_2O_4] \cdot [CoO_2]_m$, 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 Na_xCoO_2 and Li_xCoO_2 can be tuned from Co^{3+} at $x = 1$ to 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 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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[X] Prefer Oral Session
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