Variational cluster study of the phase diagram of κ-BEDT-TTF organic superconductors

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Layered organic conductors κ-$(ET)_2X$, where ET stands for BEDT-TTF and X is an anion, show quasi-two dimensional behavior. Some of these materials exhibit transition from antiferromagnetism to an unconventional superconductivity state upon applying pressure[1]. Experimental studies strongly suggest that the superconductivity gap in these compounds has d-wave nodes. The proximity of antiferromagnetism (AF) and d-wave superconductivity (dSC) in these materials and the transition between them has been a challenging subject in strongly correlated systems in recent past years. These compounds consist of aligned ET dimers that form conducting layers sandwiched between insulating polymerized anion layers[2]. We studied κ-$(ET)_2X$ layered conductors within the dimer Hubbard model as a function of the diagonal hopping t' and Hubbard repulsion U [cond-mat/0604057]. Antiferromagnetism and d-wave superconductivity are investigated at zero temperature using variational cluster perturbation theory. V-CPT is an extension of Cluster Perturbation Theory (CPT)[3] based on self-energy-functional approach (SFA)[4].

Our results show that for large U, antiferromagnetism exists for $t' < t'_{c2}$, with $t'_{c2} \sim 0.9$. For all values of t' we find a dSC phase ($d_{x^2-y^2}$) at sufficiently low U and is favored over antiferromagnetism when the two overlap. The transition between the antiferromagnetism phase and the superconductivity phase in this region appears to be of the first order. There is a critical value of $t'_{c1} \sim 0.8$ of t' beyond which the antiferromagnetism and d-wave superconductivity phases are separated by a spin liquid phase with a Mott gap in the single particle spectrum. For $t' > t'_{c2}$, the antiferromagnetism phase disappears, leaving the d-wave superconductivity and the spin liquid phases.

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