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**Inhomogeneous CDMFT and nonmagnetic impurities in graphene**[1] M. CHARLEBOIS, D. SÉNÉCHAL, A.-M. GAGNON, A.-M.S. TREMBLAY, Université de Sherbrooke — In cluster dynamical mean-field theory (CDMFT), we usually apply the self-consistency condition on an infinite superlattice of identical clusters. However, in some problems a large unit cell is required, for instance in the presence of a periodically repeated impurity. Since the impurity solver (exact diagonalization) can only treat small clusters, we break the unit cell into multiple small clusters that can be solved individually. This new technique is called inhomogeneous CDMFT (1) and is analogous to inhomogeneous DMFT (2). In this presentation, we will explain both the CDMFT and inhomogeneous CDMFT self-consistency loops within a unified, simple picture. We then apply this technique to a nonmagnetic impurity in graphene and study the emerging magnetism. Our results take into account dynamical correlations; nevertheless they qualitatively agree with previous mean-field and density functional theory studies.
(1) Charlebois, M. et al., Phys. Rev. B 91, 035132 (2015).
(2) Snoek, M. et al., New J. Phys. 10, 093008 (2008).

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