CMS Colloquium - Sponsored by IMS

A New Approach to Hedin's Many-Body Perturbation Theory Applied to Cuprates

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Abstract: Hedin[1] showed that if we could determine only four functions – the Green's function, the self-energy, the polarization, and the vertex correction – we could exactly solve the many-body perturbation series. This is an extremely difficult task, as all these functions must be determined self-consistently. However, a second issue bedeviled early attempts at a solution: how does one determine the bare hopping and interaction parameters when the experimental parameters are strongly renormalized by the interactions? In recent years a hypothesis has arisen: that an appropriate density-functional theory (DFT) calculation can be used to derive the bare parameters.

This idea lies at the basis of the many recent 'DFT+X' approaches to correlated materials, particularly when X includes self-energy effects, via some GW calculation, or some vertex corrections. In this talk, I discuss the particular version of the model that our group has developed. This involves two self-consistent steps. (1) First, we extend the commonly-used G0W0 self energy to a one-parameter self-consistent quasipqrticle-GW (QPGW) approach, more appropriate when the renormalization parameter Z is significantly less than one.2 (2) While this works well at low temperatures, the phase transitions are treated as mean-field. To improve on this, we incorporate vertex corrections to include the effects of fluctuations3. The resulting model satisfies the Mermin-Wagner theorem, and more importantly includes strong mode-coupling effects. The resulting frustration due to competition between conventional Fermi-surface nesting and Van Hove nesting has many characteristics of the pseudogap phase.

1. *L. Hedin, J. Phys. Condens. Matter 11, R489-R528 (1999).*
2. *Tanmoy Das, R.S. Markiewicz, and A. Bansil, Adv. Phys. 63, 151-266 (2014).*
3. *R.S. Markiewicz, I.G. Buda, P. Mistark, and A. Bansil, arXiv:1505.04770.*

Bio: Bob Markiewicz got his Ph.D. in Berkeley in 1976, studying electron-hole droplets in Ge [Kittel, ISSP, 8th. Ed., Fig. 15.12]. After a two-year Post-Doc, he joined the Research Staff at G.E. in Schenectady, N.Y., where he studied graphite intercalation compounds and localization in ultrathin metal films. In 1980 he moved to Northeastern University in Boston, where he began studying cuprate physics in 1987, concentrating mainly on nanoscale phase separation and the role of the Van Hove singularity.

Around 2000 he began an ongoing collaboration with Arun Bansil at NU, to extend first-principles density-functional theories to study spectroscopies and more strongly-correlated materials. They initially studied ARPES [angle-resolved photoemission spectroscopy], and found that electron-doped cuprates were much simpler to understand, involving only (pi,pi) antiferromagnetism and superconductivity. He developed a form of DFT+GW calculation which could be applied to a variety of spectroscopies, including STM, optical, neutron scattering, and RIXS, and analyzed the competing-order phase diagrams of hole-doped cuprates, finding that LSCO is significantly different from other cuprates. He is now extending these calculations to include vertex corrections necessary to understand pseudogap physics.

He has also worked on SO(8), stripe physics, Fermi surface nesting, edge singularities in RIXS, and negative compressibility.

Hosted By Alexander Balatsky