CMP Seminar

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Quantum Molecular Dynamics Simulations of Strongly Correlated Materials

I will present a new formulation of quantum molecular dynamics that includes electron correlation effects via the Gutzwiller method. Our novel scheme enables the study of the dynamical behavior of atoms and molecules with strong electron interactions. The Gutzwiller approach goes beyond the conventional mean-field treatment of the intra-atomic electron repulsion and captures crucial correlation effects such as band narrowing and electron localization. We use Gutzwiller quantum molecular dynamics to investigate the Mott metal-insulator transition in the liquid Hubbard model, which can be viewed as a toy model of hydrogens under high pressures. Moreover, using this new quantum MD method, we have conducted the first-ever microscopic dynamical simulation of the thermal Mott transition in the Hubbard model. Finally, I will also discuss how modern machine learning can be trained to emulate the many-body Gutzwiller calculation, offering the prospect of large-scale MD simulations with the accuracy of quantum calculations.

Monday, September 30th, 2019 at 4:10 p.m.
Room 1400 BPS Bldg.
Host: S.D. Mahanti