Physics & Astrophysics Colloquium

Electronic Structure of Semiconductor Nanoparticles from Stochastic Evaluation of Imaginary-Time Path Integral

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4:00 PM Friday, May 5, 2023, Room 211, Witmer Hall

Abstract: The fermion sign problem, when severe, prevents the computation of physical quantities of a system of interacting fermions via stochastic evaluation of its path integral defined on discretized space-time due to the oscillatory nature of the integrand exp(-S), where S is the imaginary-time action. However, in the Kohn-Sham orbital basis, which is the output of a Density Functional Theory simulation, the path integral lattice field theory approach for electrons in a semiconductor nanoparticle may have only a mild fermion sign problem and is amenable to evaluation by standard stochastic methods. This is evidenced by our simulations of silicon hydrogen-passivated nanocrystals (NCs), such as $Si_{35}H_{36}$, $Si_{87}H_{76}$, $Si_{147}H_{100}$ and $Si_{293}H_{172}$, which range in size 1.0 - 2.4 nm and contain 176 to 1344 valence electrons, and to a 1.8 nm hetero-structured (Janus-type) NC $Cd_{37}Pb_{31}Se_{68}$with 1582 valence electrons. We find that approximating the fermion action by its leading order polarization term results in a positive-definite integrand and is a very good approximation of the full action. We compute imaginary-time electron propagators and extract the energies of low-lying electron and hole levels. Our quasiparticle gap predictions agree with the results of previous G_0W_0 calculations. This formalism naturally allows calculations of more complex excited states, such as excitons, for which we present some results. Also, the formalism can be extended to the zero-temperature zero-density case suitable to few-body systems, such as light atoms. We present some current results for helium atom.

Refreshments at 3:30 PM in Witmer Hall, Room 215

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