CFEL SCIENCE

SEMINAR

14th November 2018 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Using collocation methods to solve the Schrödinger equation

Chemists typically use a variational method to solve the Schrödinger equation. This requires computing many, and in some cases, high-dimensional integrals. In this talk, I present new ideas for using collocation methods to solve the Schrödinger equation. Collocation has some important advantages: 1) it obviates integrals and quadratures; 2) it facilitates the use of complicated kinetic energy operators; 3) it can be used with any (the best possible) coordinates and basis functions; 4) it is not necessary to have points everywhere where wavefunctions have significant amplitude; 5) as the basis improves, the choice of the points becomes irrelevant.

Host: Robin Santra – CFEL-DESY Theory Division