



THE UNIVERSITY OF CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS COLLOQUIUM

LIN LIN

Department of Mathematics
University of California, Berkeley

Grassmann Manifold, Gauge, and Quantum Chemistry

THURSDAY, November 29, 2018, at 4:00 PM
Jones 226, 5747 South Ellis Avenue

ABSTRACT

The Grassmann manifold $Gr(m,n)$ is the set of n -dimensional subspaces in R^m (assuming $m>n$), and is used in many science and engineering applications. A point in $Gr(m,n)$ can be represented by an orthogonal matrix of size m by n , multiplied by another arbitrary orthogonal matrix of size n by n . In quantum chemistry and in particular the widely used density functional theory (DFT), this arbitrary orthogonal matrix is referred to as the gauge. Physical quantities such as energies and electron densities should be independent of the gauge choice. In this talk, I am going to discuss the interplay between gauge-dependent and gauge-independent quantities in quantum chemistry along three recent directions: time-dependent density functional theory, electron localization, and self-consistent field iteration. In each case, the focus on the gauge-independent representation of the Grassmann manifold brings surprising numerical benefits.

Organizers:

Daniel Sanz-Alonso, Department of Statistics, sanzalonso@uchicago.edu
CAM Colloquium URL: <https://cam.uchicago.edu/seminars/colloq/index.shtml>.

For further information and inquiries about building access for persons with disabilities, please contact Zellencia Harris, zellenciah@uchicago.edu. If you wish to subscribe to our email list, please visit the following website: https://lists.uchicago.edu/web/subscribe/cam_colloquium/.