

## Semiclassical Origins of Density Functional Approximations

### Wednesday September 4, 2013

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–9:50 **Kieron Burke** (University of California, Irvine (UCI))  
*Semiclassical Origins of Density Functional Approximations*
- 10:00–10:35 **Barry Simon** (California Institute of Technology)  
*The Semiclassical Limit of Thomas Fermi Theory - Forty Years After*
- 10:45–11:15 *Break*
- 11:15–11:50 **Berthold-Georg Englert** (National University of Singapore)  
*Density-potential functionals and Wigner functions*
- 12:00–12:35 **Jan Philip Solovej** (University of Copenhagen)  
*The Scott correction with relativistic and magnetic effects included*
- 12:45–2:00 *Lunch (on your own)*
- 2:00–2:35 **Hardy Gross** (Max Planck Institute of Microstructure Physics)  
*What's the correct classical force on the nuclei: A fresh look at potential energy surfaces and Berry phases in the time domain*
- 2:45–3:15 *Break*
- 3:15–3:50 **William Miller** (University of California, Berkeley (UC Berkeley))  
*Semiclassical Theory of Electronically Non-Adiabatic Dynamics*
- 4:00–4:35 **Qian Niu** (University of Texas at Austin)  
*Berry phase effects on electronic properties*
- 4:45–6:15 *Poster Session & Reception (Hosted by IPAM)*

### Thursday September 5, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:35 **Elliott Lieb** (Princeton University)  
*Current Densities in Density Functional Theory*
- 9:45–10:20 **Ann Mattsson** (Sandia National Laboratories)  
*Improving the Predictive Power of Density Functional Theory Calculations*
- 10:30–11:00 *Break*

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- 11:00–11:35 **Matthias Brack** (Universität Regensburg)  
*Semiclassical approaches to the kinetic-energy functionals  $T_s[\rho]$  and  $\tau[\rho]$*
- 11:45–12:20 **Eric Heller** (Harvard University)  
*Semiclassical statistical mechanics and correlated Thomas Fermi theory*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:35 **Francis Nier** (Université de Rennes I)  
*Phase-space approach to the bosonic mean field dynamics*
- 2:45–3:15 *Break*
- 3:15–3:50 **Jan-Michael Rost** (Max Planck Institute for the Physics of Complex Systems)  
*Dominant Interaction Hamiltonians*
- 4:00–4:20 **Attila Cangi** (Max Planck Institute of Microstructure Physics)
- 4:25–5:00 *Discussion*

### Friday September 6, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:35 **Michael Seidl** (Universität Regensburg)  
*The strong-interaction limit of density functional theory*
- 9:45–10:20 **Paola Gori-Giorgi** (Vrije Universiteit)  
*Kohn-Sham density functional theory for strong-interacting systems*
- 10:30–11:00 *Break*
- 11:00–11:35 **Lin Lin** (Lawrence Berkeley Laboratory)  
*Kantorovich dual solution for strictly correlated electrons in atoms and molecules*
- 11:45–12:20 **Maciej Zworski** (University of California, Berkeley (UC Berkeley))  
*Decay of correlations for normally hyperbolic trapping*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:35 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UC Santa Barbara))  
*Spin-polarized transport in ferromagnetic multilayers*
- 2:45–3:15 *Break*
- 3:15–3:50 **Gero Friesecke** (Technische Universität München)  
*Density functional theory and optimal transport with Coulomb cost*
- 4:00–4:35 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)

