

Workshop II: Model Reduction in Quantum Mechanics

Monday April 11, 2022

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*
- 9:00 *Session Chair: Maria Esteban (CNRS and Université Paris-Dauphine)*
- 9:00–9:50 **Volker Bach** (TU Braunschweig)
The Hartree-Fock Approximation and its Generalizations
- 10:00–10:15 *Break*
- 10:15–11:05 **Benjamin Schlein** (University of Zurich)
Virtual Talk: Correlation energy of weakly interacting fermions
- 11:15–11:30 *Break*
- 11:30–12:20 **Garnet Chan** (California Institute of Technology)
Lattice models and ab initio descriptions of correlated materials
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Garnet Chan (Caltech)*
- 2:30–3:20 **Roi Baer** (Hebrew University)
Stochastic Vector Methods for extended systems
- 3:30–3:45 *Break*
- 3:45–4:35 **Qin Li** (University of Wisconsin-Madison)
Multiscale inverse problem, from Schroedinger to Newton to Boltzmann
- 4:45–5:00 *Lightning Poster Presentations*
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday April 12, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Eric Cancès (École Nationale des Ponts-et-Chaussées)*
- 9:00–9:50 **Maria J. Esteban** (CNRS and Université Paris-Dauphine)
Spectral results and open problems for Dirac-Coulomb operators with general charge distributions
- 10:00–10:15 *Break*

(Tuesday schedule continued on next page)



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- 10:15–11:05 **Stefan Teufel** (Eberhard-Karls-Universität Tübingen)
Virtual Talk: Local response in bulk-gapped interacting systems
- 11:15–11:30 *Break*
- 11:30–12:20 **Mathieu Lewin** (CNRS and Université Paris-Dauphine)
Virtual Talk: Recent results in Density Functional Theory
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Volker Bach (TU Braunschweig)*
- 2:30–3:20 **Marco Bernardi** (California Institute of Technology)
Precise quantum mechanical calculations of electron interactions and dynamics in condensed matter
- 3:30–4:00 *Break*
- 4:00–4:50 **Francesco Evangelista** (Emory University)
Many-electron effective Hamiltonians from the similarity renormalization group

Wednesday April 13, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Carlos Garcia-Cervera (UC Santa Barbara)*
- 9:00–9:50 **Giovanni Vignale** (University of Missouri-Columbia)
Quantum continuum mechanics for many-body systems
- 10:00–10:15 *Break*
- 10:15–11:05 **Eric Séré** (Université de Paris IX (Paris-Dauphine))
Virtual Talk: The ground state of the Dirac-Fock energy for molecules and crystals
- 11:15–11:30 *Break*
- 11:30–12:20 **Andreas Savin** (Sorbonne Université)
Getting beyond density functional approximations by using lessons from density functional theory
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: David Ceperley (Univ. Illinois)*
- 2:30–3:20 **Lukas Muechler** (Penn State University)
Quantum embedding methods for correlated excited states of point defects: Case studies and challenges
- 3:30–4:00 *Break*
- 4:00–4:50 **Guido Falk von Rudorff** (University of Vienna)
Systematically improvable models from alchemical perturbations

Thursday April 14, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Francois Gygi (UC Davis)*
- 9:00–9:50 **Steve White** (University of California, Irvine (UCI))
Model reduction using localized bases and DMRG
- 10:00–10:15 *Break*
- 10:15–11:05 **Paola Gori-Giorgi** (Vrije Universiteit Amsterdam)
Virtual Talk: Large-coupling strength expansion in DFT and Hartree-Fock adiabatic connections
- 11:15–11:30 *Break*
- 11:30–12:20 **Feliciano Giustino** (University of Texas at Austin)
Virtual Talk: Methods and software for electron-phonon physics
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Steve White (UC Irvine)*
- 2:30–3:20 **Nandini Ananth** (Cornell University)
Virtual Talk: Quantum dynamics from classical trajectories
- 3:30–4:00 *Break*
- 4:00–4:50 *Moderated Discussion*

Friday April 15, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Andreas Savin (Sorbonne)*
- 9:00–9:50 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)
Some mathematical and numerical results on monolayer and twisted bilayer graphene
- 10:00–10:15 *Break*
- 10:15–11:05 **Anil Damle** (Cornell University)
Localization methods: perspectives on initialization and optimization
- 11:15–11:30 *Break*
- 11:30–12:20 **Eun-Ah Kim** (Cornell University)
Virtual Talk: Machine Learning for Quantum Simulation
- 12:30 *Conclusion*

