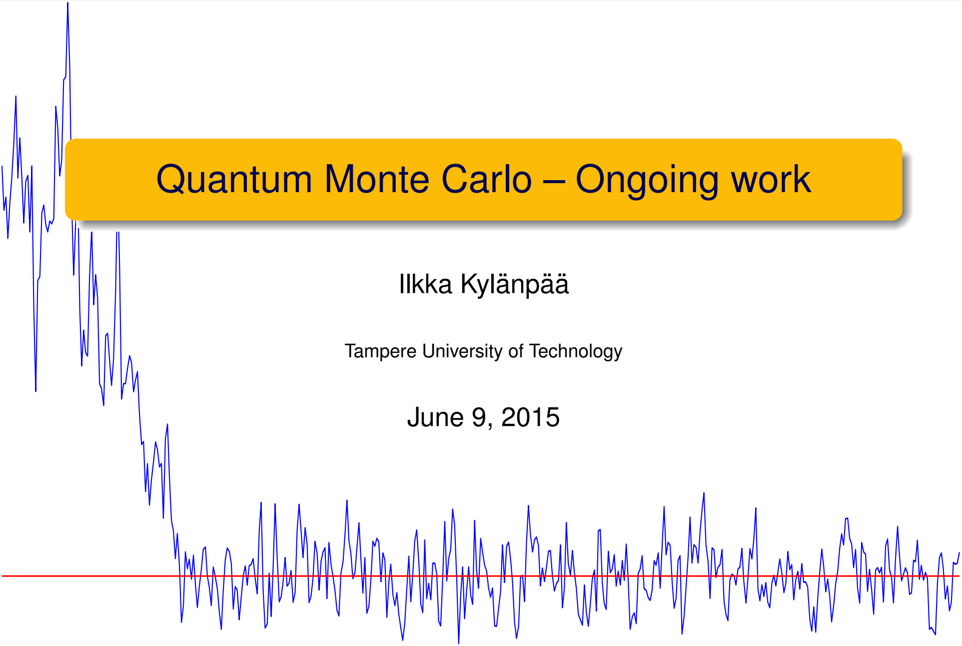
Quantum Monte Carlo – Ongoing work



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June 9, 2015


Path integral Monte Carlo
Diffusion Monte Carlo
Variational Monte Carlo
Reptation Monte Carlo
Auxiliary field Monte Carlo
Path integral ground state
World-line quantum Monte Carlo

Many-body

$H\Psi = E\Psi$

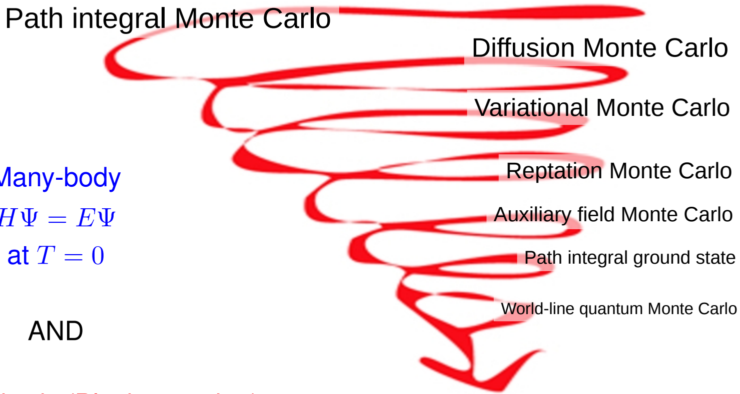
at $T = 0$

AND

Many-body (Bloch equation)

$$\frac{\partial \rho}{\partial \beta} = -H\rho$$

at $T > 0$ ($\beta = 1/k_{\mathrm{B}}T$)



Exact correlations

Path integral Monte Carlo

Diffusion Monte Carlo

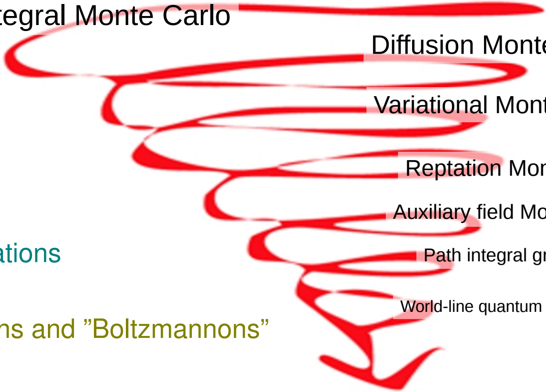
Variational Monte Carlo

Reptation Monte Carlo

Auxiliary field Monte Carlo

Path integral ground state

World-line quantum Monte Carlo



Exact correlations

Exact for Bosons and ”Boltzmannons”

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Highly accurate (if not exact)
for Fermions

Exact correlations

Exact for Bosons and "Boltzmannons"

Highly accurate (if not exact)

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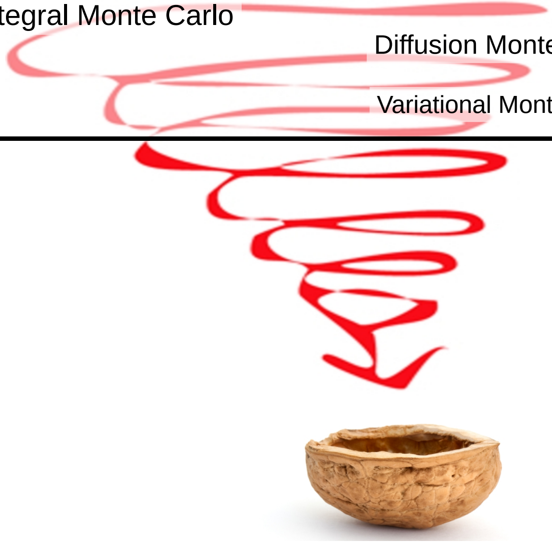
$\longrightarrow$ Fermion sign-problem

Straightforward to go beyond the Born–Oppenheimer approximation!

Path integral Monte Carlo

Diffusion Monte Carlo

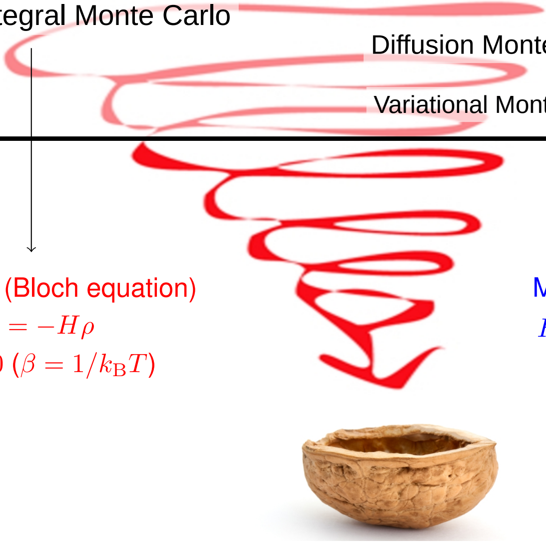
Variational Monte Carlo



Path integral Monte Carlo

Diffusion Monte Carlo

Variational Monte Carlo



Many-body (Bloch equation)

$$\frac{\partial \rho}{\partial \beta} = -H\rho$$

at $T > 0$ ($\beta = 1/k_{\mathrm{B}}T$)

Many-body

$$H\Psi = E\Psi$$

at $T = 0$

Path integral Monte Carlo method

Partition function

$$Z = \mathrm{Tr}\ \hat{\rho}(\beta) = \int \mathrm{dR}_0 \langle \mathrm{R}_0 | \hat{\rho}(\beta) | \mathrm{R}_0 \rangle = \int \mathrm{dR}_0\, \underbrace{\rho(R_0, R_0; \beta)}_{\text{density matrix}},$$

where $\hat{\rho}(\beta) = e^{-\beta \hat{H}}$ and $\beta = 1/k_{\mathrm{B}} T$.

$$\hat{\rho}(\beta) = \underbrace{e^{-\beta \hat{H}/M} e^{-\beta \hat{H}/M} \cdots e^{-\beta \hat{H}/M}}_{M \text{ factors}} \quad \text{and} \quad \int \mathrm{d}R\, |R\rangle\langle R| = \mathbf{I}$$

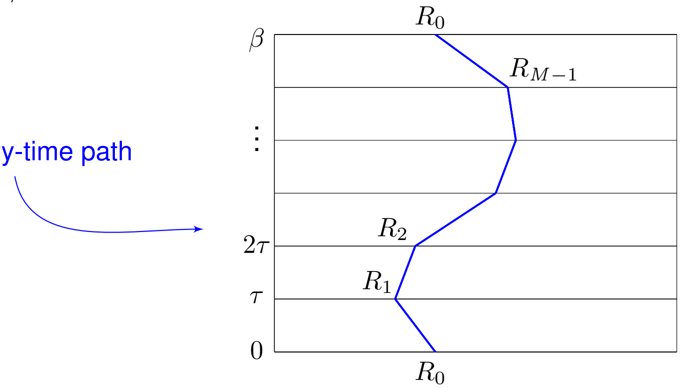
Path integral Monte Carlo method

Feynman's formulation of quantum statistics

$$Z = \int \mathrm{dR_0 dR_1 \ldots dR_{M-1}} \rho(\mathrm{R_0}, \mathrm{R_1}; \tau) \rho(\mathrm{R_1}, \mathrm{R_2}; \tau) \cdots \rho(\mathrm{R}_{M-1}, \mathrm{R_0}; \tau),$$

where $\tau = \beta/M$.

Imaginary-time path



Path integral Monte Carlo method

Feynman's formulation of quantum statistics

$$Z = \text{Tr}\ \hat{\rho}(\beta) = \int \mathrm{dR_0 dR_1} \ldots \mathrm{dR}_{M-1} \prod_{\mathrm{i=0}}^{M-1} \mathrm{e}^{-\mathrm{S(R_i,R_{i+1};\tau)}},$$

where $e^{-S(R_i,R_{i+1};\tau)} = \rho(R_i, R_{i+1}; \tau)$, $R_M = R_0$ and the action

$$S(R_i, R_{i+1}; \tau) = \underbrace{K(R_i, R_{i+1}; \tau)}_{\text{kinetic part}} + \underbrace{U(R_i, R_{i+1}; \tau)}_{\text{interaction part}}.$$

$$K(R_i, R_{i+1}; \tau) = \frac{3N}{2} \ln\left(4\pi\lambda\tau\right) + \frac{(R_i - R_{i+1})^2}{4\lambda\tau}.$$

$$U(R_i, R_{i+1}; \tau) = \underbrace{\frac{\tau}{2}\left[V(R_i) + V(R_{i+1})\right]}_{\text{primitive approximation}} + \mathcal{O}(\tau^2).$$

Path integral Monte Carlo method

Feynman's formulation of quantum statistics

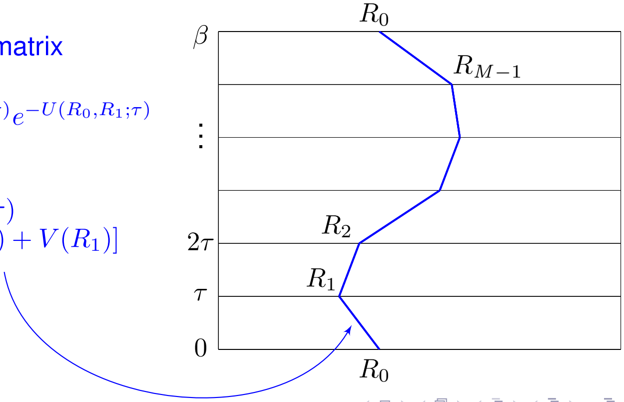
$$Z = \int \mathrm{dR}_0 \mathrm{dR}_1 \ldots \mathrm{dR}_{M-1} \rho(\mathrm{R}_0, \mathrm{R}_1; \tau) \rho(\mathrm{R}_1, \mathrm{R}_2; \tau) \cdots \rho(\mathrm{R}_{M-1}, \mathrm{R}_0; \tau),$$

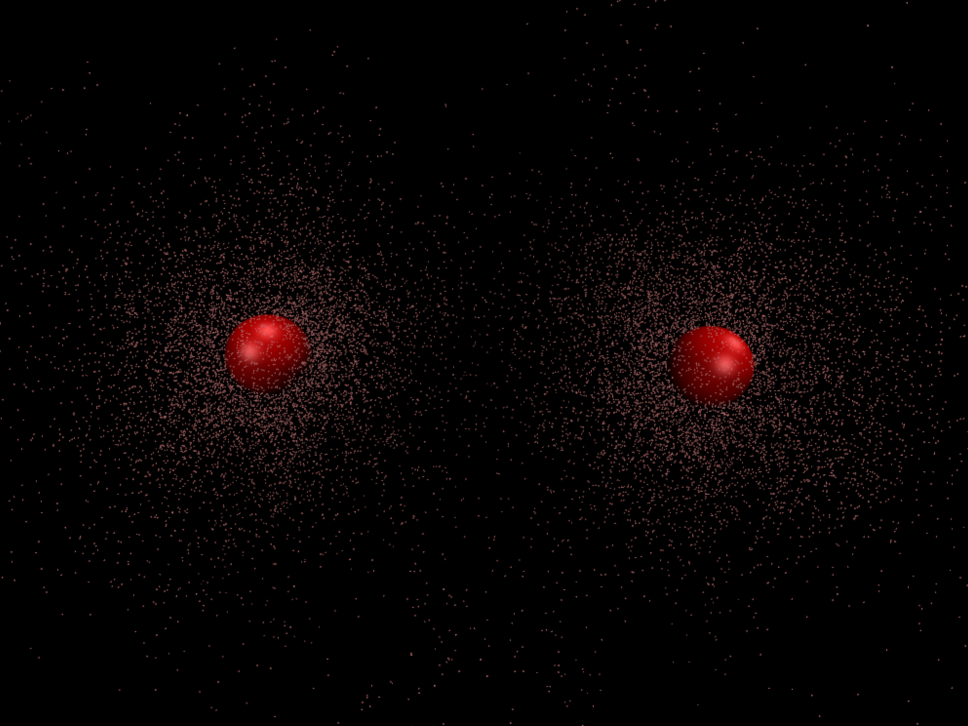
where $\tau = \beta/M$.

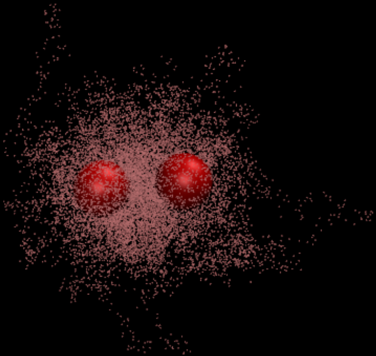
High-T density matrix

$$\rho(R_0, R_1; \tau) = e^{-K(R_0,R_1;\tau)} e^{-U(R_0,R_1;\tau)}$$

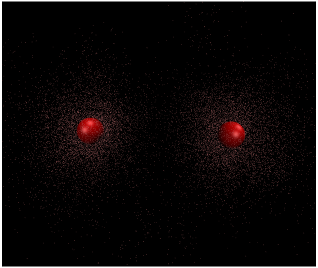
$$U(R_0, R_1; \tau) \approx \frac{\tau}{2} \left[V(R_0) + V(R_1)\right]$$



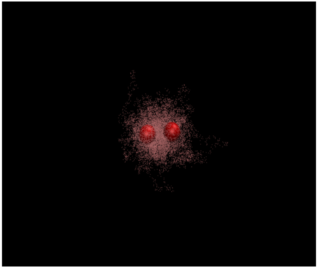




Formation of H_2



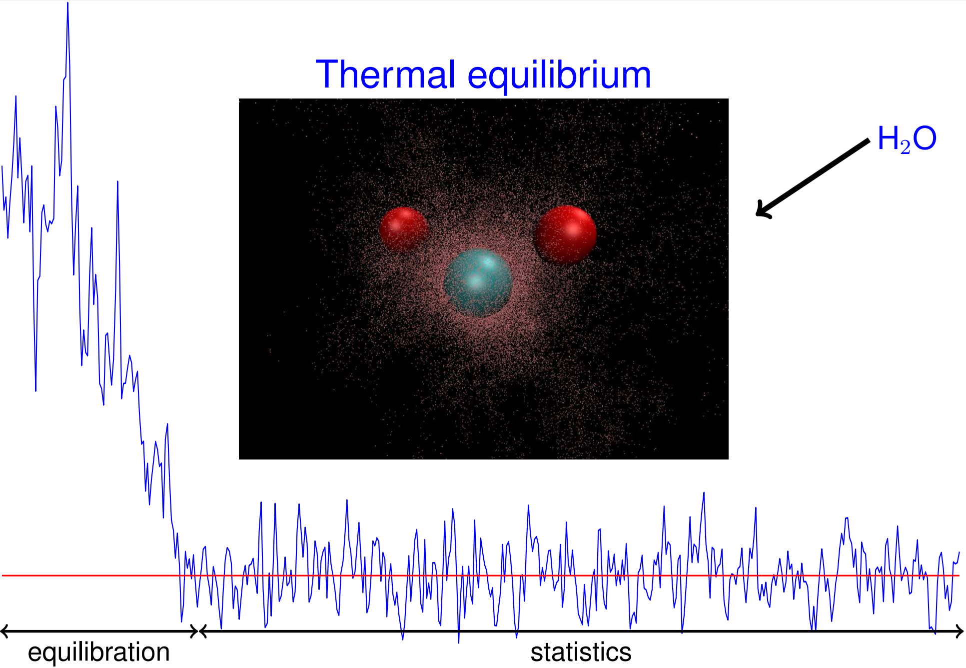
Dissociation of H_2

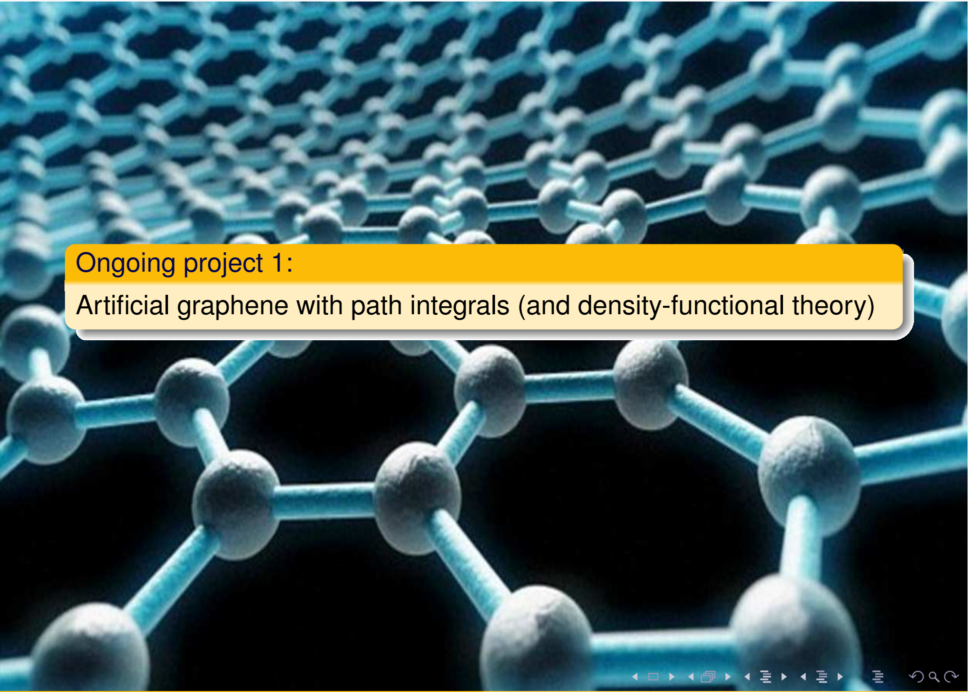


Low T

High T

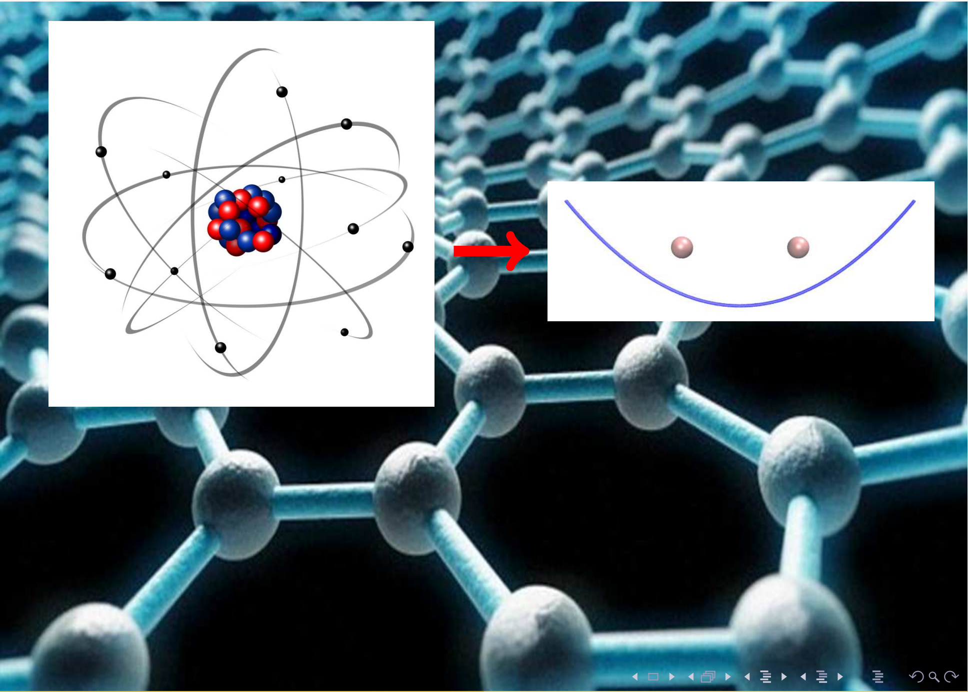
Thermal equilibrium



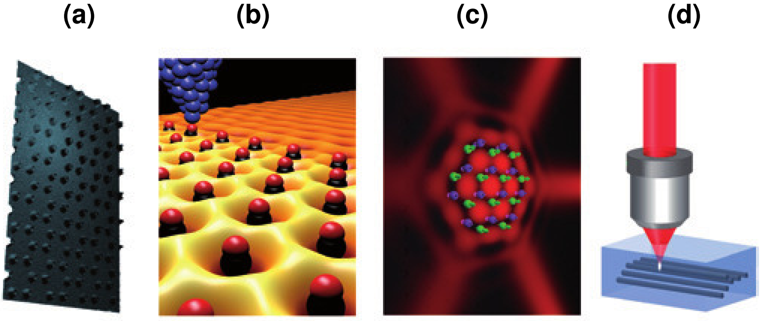


Ongoing project 1:

Artificial graphene with path integrals (and density-functional theory)



Experimental setups



M. Polini *et al.*, Nature Nanotechnology 8, 625 (2013)

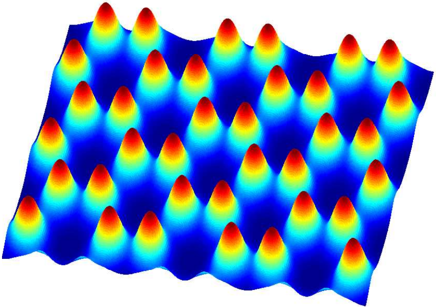
(a) Scanning electron micrograph (GaAs heterostructure).

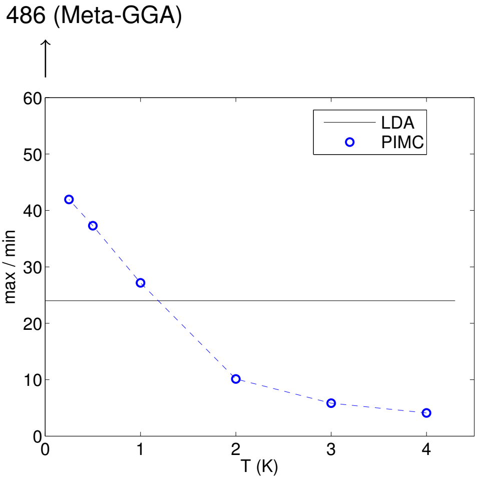
(b) Molecular graphene system.

(c) Optical lattices for cold atoms.

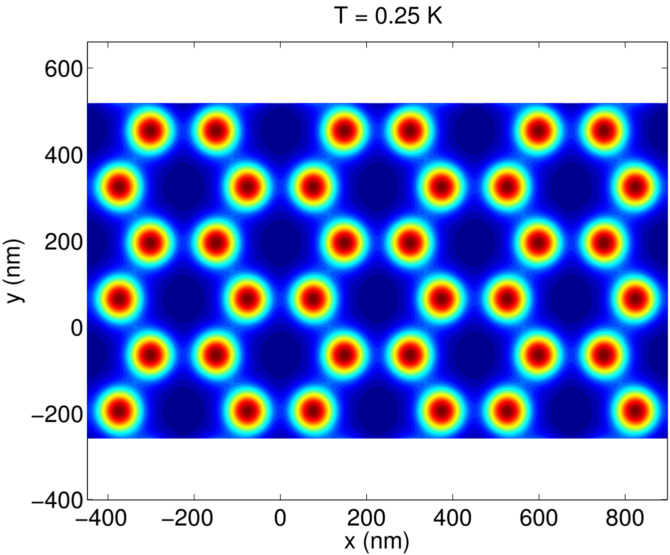
(d) Photonic honeycomb crystals (optical induction methods).

Hexagonal lattice: Density fluctuations



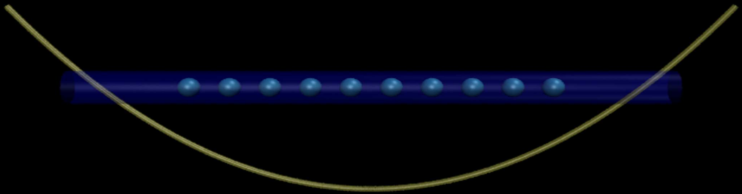


Hexagonal lattice: Finite temperature electron density

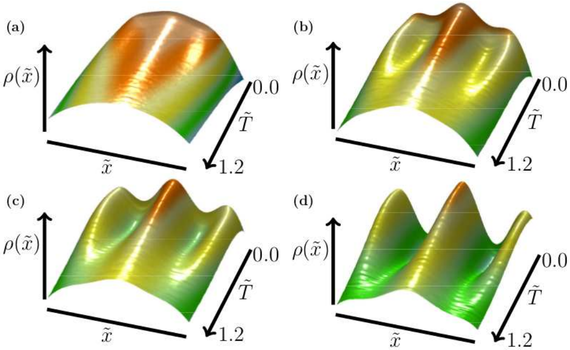


Ongoing project 2:

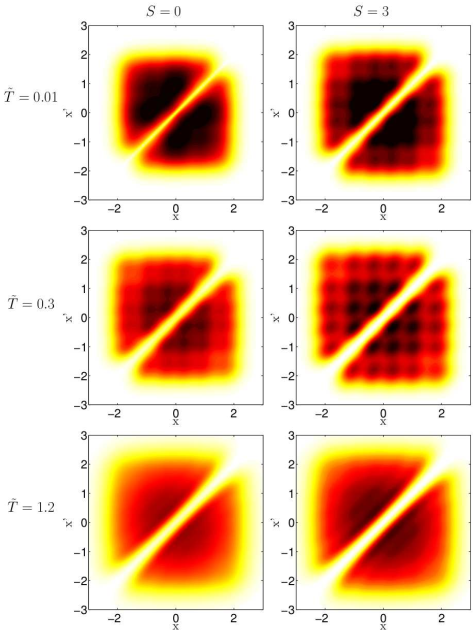
1D quantum wire: Thermal effects



Thermally enhanced localization of electrons



$$V_{e-e}(x) = \frac{c}{\sqrt{x^2+\lambda^2}}$$


S = 0
S = 3
T̃ = 0.01
T̃ = 0.3
T̃ = 1.2
x
x'

Other ongoing QMC-projects

- 2D harmonic dot with upto $N = 80$ strongly interacting electrons (test case)
- Adiabatic and nonadiabatic static polarizabilities of small atoms and molecules
- Ionization and atomization energies without the Born-Oppenheimer approximation (Diffusion Monte Carlo study)
- Positron interacting with homogeneous electron gas
- Calculation of Deuterium Hugoniot (validation of coupled electron-ion Monte Carlo results)
- Pairing and superfluid properties of dilute fermion gases (test case for improving nodes etc.)
- Trions and biexcitons in transition metal dichalcogenides

Thank you!

Acknowledging collaboration with

- Esa Räsänen, Tapio Rantala and Juha Tiihonen at TUT, Finland
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- Hannu-Pekka Komsa at Aalto Univ., Finland
- Ethan Brown at ETH, Zurich
- Michael Aichinger and Stefan Janecek at RICAM, Austria