III Quantum Monte Carlo (QMC) simulations

There are many different QMC methods; common feature: Monte Carlo evaluation of high-dimensional integrals relevant for quantum systems.

III.1 Classification of QMC methods

a) Systems:
- continuum systems (in real space)
- lattice systems (in particular: electrons)
- single-impurity model (relevant for DMFT)
- quantum Heisenberg model ...

b) regime:
- finite temperatures (canonical ensemble)
- ground state (projective QMC)
- variational MC (upper bound on E_{GS})

c) approach:
- wave function
- density matrix
- auxiliary field

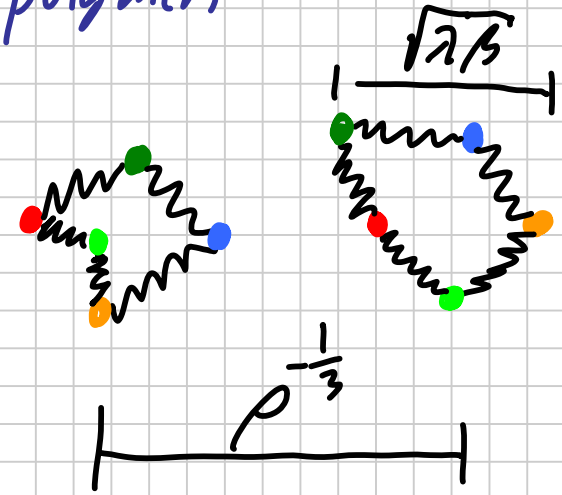
d) statistics:
- „boltzmannons" (distinguishable particles)
- bosons
- fermions

III.2 Path integral Monte Carlo (PIMC)

Characterization: • continuum system • finite T • based on density matrix • works best for boltzmannons, good for bosons; fermions require fixed-node approximation

• employs analogy between path integrals and polymers

$$\lambda = \frac{\hbar^2}{2m}$$



• beads connected by springs

• interactions only between beads of different ring polymers at "equal time" (equal color)

Foundation: quantum statistical mechanics

In terms of eigenstates $|\phi_i\rangle$, thermal expectation values of observables may be written as

$$\langle \hat{O} \rangle = Z^{-1} \sum_i \langle \phi_i | \hat{O} | \phi_i \rangle e^{-\beta E_i}$$

where $\beta = \frac{1}{k_B T}$, the partition function is

$$Z = \sum_i e^{-\beta E_i}$$

and $E_i = \langle \phi_i | \hat{H} | \phi_i \rangle$.

Compare classical case: every state is eigen state

$$Z_{class} \propto \int d^{3N}r \int d^{3N}v \; e^{-\beta E(\{r\},\{v\})}$$

$$E = E_{pot} + E_{kin};\; E_{kin} = \sum_{i=1}^{3N} \frac{1}{2} m_i v_i^2;\; E_{pot} = E_{pot}(\{r\})$$

$$Z_{class} \propto \left(\int d^{3N}r \, e^{-\beta E_{pot}(\{r\})}\right)\left(\int dv \, e^{-\beta \frac{1}{2} m v^2}\right)^{3N}$$

$$= Z_{pot} \left(\frac{2\pi}{\beta m}\right)^{3N/2}$$

Kinetic part has trivial solution $\rightsquigarrow$ MC for static problem

For an arbitrary basis (in which the Hamiltonian is in general not diagonal):

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_{\alpha} \langle \alpha | \hat{O} e^{-\beta \hat{H}} | \alpha \rangle = \frac{1}{Z} tr(\hat{O} e^{-\beta \hat{H}})$$

$$= \frac{1}{Z} \sum_{\alpha} \sum_{\alpha'} \langle \alpha | \hat{O} | \alpha' \rangle \langle \alpha' | e^{-\beta \hat{H}} | \alpha \rangle$$

with $$Z = \sum_{\alpha} \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle = tr(e^{-\beta \hat{H}})$$

Central operator: **density matrix** $e^{-\beta \hat{H}}$

Now <u>choose</u> position basis with labeled particles.

Advantage: in this basis, all matrix elements are real and positive (proof: later).

Position-space density matrix:

$$\rho(R, R'; \beta) = \langle R | e^{-\beta \hat{H}} | R' \rangle = \sum_i \phi_i^*(R) \phi_i(R') e^{-\beta E_i}$$

with position representations of the eigen states

$$\phi_i(R') = \langle i | R' \rangle \; ; \quad \phi_i^*(R) = \langle R | i \rangle = \langle i | R \rangle^*$$

and position vectors $R = \{\vec{r}_1, \ldots, \vec{r}_N\}$.

In $d=3$ dimensions, ρ is a function of $6N+1$ variables. In position basis, the expectation values become:

$$\langle \hat{O} \rangle = Z^{-1} \int dR dR' \; \rho(R, R', \beta) \langle R' | O | R \rangle$$

with $$Z = \int dR \; \rho(R, R, \beta)$$

Note: the product of two density matrices is a density matrix (all for the same Hamiltonian!):

$$e^{-\beta_1 \hat{H}} \; e^{-\beta_2 \hat{H}} = e^{-(\beta_1 + \beta_2)\hat{H}}$$

- in this case, operators can be treated like numbers since $[\hat{H}, \hat{H}] = 0$
- the product matrix is associated with a lower temperature

Written for positions $\rightsquigarrow$ convolution

$$\rho(R_1, R_3; \beta_1 + \beta_2) = \int dR_2 \; \rho(R_1, R_2, \beta_1) \, \rho(R_2, R_3; \beta_2)$$