

## III Quantum Monte Carlo (QMC) simulations

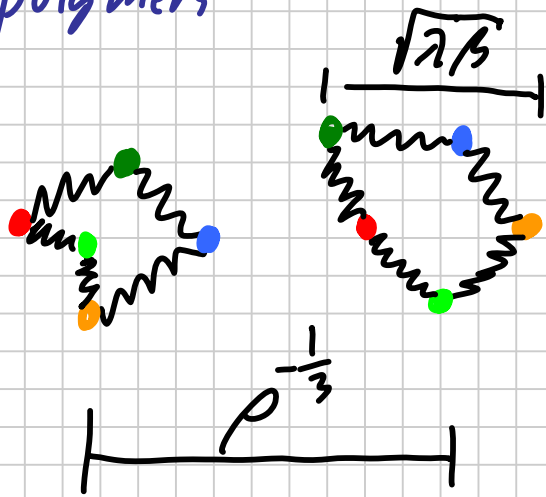
There are many different QMC methods; common feature: Monte Carlo evaluation of high-dimensional integrals relevant for quantum systems.

### 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 bosons, 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)

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**Foundation:** quantum statistical mechanics

In terms of **eigen** states  $|\phi_i\rangle$ , 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

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

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

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

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

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

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

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

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

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

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

Now choose 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  $R = \{\vec{r}_1, \dots, \vec{r}_N\}$ .

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

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

$$\text{with } Z = \int dR \rho(R, R, \beta)$$

*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  $\leadsto$  *convolution*

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

## Discrete path integrals

Now consider  $\hat{H} = \hat{T} + \hat{V}$  with the usual kinetic contribution (nonrelativistic, no magnetic field):

$$\hat{T} = \sum_{n=1}^N -\frac{1}{2m} \hat{p}_n^2 \quad (\hat{p}_n = -i\hbar \vec{\nabla}_n \text{ in position basis})$$

and the potential contribution  $\hat{V} = \int dR \overset{=V(\hat{R})}{V(R)} |R\rangle\langle R|$

The fundamental problem in quantum mechanics is that we know eigen basis and density matrix only for either the kinetic **or** the potential part of the Hamiltonian, not both:

$$e^{-\beta \hat{H}} \neq e^{-\beta \hat{T}} e^{-\beta \hat{V}} \quad (\text{for general } \beta)$$

$\uparrow$  needed, unknown       $\uparrow$  known (see below)       $\uparrow$  known (see below)

**But:** asymptotic factorization at high temperatures (classical limit), i.e. small  $\beta$ . More generally: good high- $T$  approximations for density matrix!

**Notation:** imaginary time step  $\Delta\tau = \frac{\beta}{M}$  ( $M \in \mathbb{N}$ )

Exact discrete path integral ( $M$  equal steps):

$$\rho(R_0, R_M, \beta) = \int dR_1 \int dR_2 \dots \int dR_{M-1} \rho(R_0, R_1; \Delta\tau) \rho(R_1, R_2; \Delta\tau) \dots \rho(R_{M-1}, R_M; \Delta\tau)$$

We will now derive an explicit approximation for this path integral.

Campbell - Baker - Haussdorf formula:

$$\exp\left[-\Delta\tau(\hat{T} + \hat{V}) + \underbrace{\frac{1}{2}\Delta\tau^2[\hat{T}, \hat{V}] + \mathcal{O}(\Delta\tau^3)}_{\text{negligible in limit of small } \Delta\tau}\right] = e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}}$$

→ Trotter formula

$$e^{-\beta(\hat{T} + \hat{V})} = \lim_{M \rightarrow \infty} \left[ e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}} \right]^M; \quad \Delta\tau = \frac{\beta}{M}$$

$$\approx \left[ e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}} \right]^M \text{ for } \Delta\tau \text{ "small"}$$

Primitive approximation in position space for single time step:

$$\rho(R_0, R_2; \Delta\tau) = \int dR_1 \langle R_0 | e^{-\Delta\tau\hat{T}} | R_1 \rangle \langle R_1 | e^{-\Delta\tau\hat{V}} | R_2 \rangle$$

Potential operator is diagonal, therefore:

$$\langle R_1 | e^{-\Delta\tau\hat{V}} | R_2 \rangle = e^{-\Delta\tau V(R_1)} \delta(R_1 - R_2) \quad (*)$$

For kinetic energy operator, introduce eigen function expansion in a cube with side length  $L$  and pbc, denoted by integer vector  $\vec{n} \in \mathbb{R}^{3N}$ ,

$$\phi_{\vec{n}}(\vec{R}) = \langle \vec{n} | \vec{R} \rangle = L^{-3N/2} e^{i\vec{k}_{\vec{n}} \cdot \vec{R}}; \quad \vec{k}_{\vec{n}} = \frac{2\pi\vec{n}}{L} \quad \text{plane waves}$$

$$\text{with eigen values} \quad \frac{\hbar^2}{2m} \vec{k}_{\vec{n}}^2 \equiv \mathcal{E} \vec{k}_{\vec{n}}^2$$

$$\begin{aligned}
\Rightarrow \langle R_0 | e^{-\Delta\tau \hat{T}} | R_1 \rangle &= \sum_{\vec{n}} \langle R_0 | \vec{n} \rangle \langle \vec{n} | e^{-\Delta\tau \hat{T}} | \vec{n} \rangle \langle \vec{n} | R_1 \rangle \\
&= \sum_{\vec{n}} L^{-3N/2} e^{-i\vec{k}_n \cdot \vec{R}_0} e^{-\Delta\tau \lambda \vec{k}_n^2} L^{-3N/2} e^{+i\vec{k}_n \cdot \vec{R}_1} \\
&= \sum_{\vec{n}} L^{-3N} \exp[-\Delta\tau \lambda \vec{k}_n^2 - i\vec{k}_n \cdot (\vec{R}_0 - \vec{R}_1)] \\
&\approx (4\pi\lambda \Delta\tau)^{-3N/2} \exp\left[-\frac{(\vec{R}_0 - \vec{R}_1)^2}{4\lambda\Delta\tau}\right] \quad (A)
\end{aligned}$$

$\sum_{\vec{n}} \rightarrow \int d^3n$ , good for  $\lambda\Delta\tau \ll L^2$   
 then Gauss integral

(exact kinetic density matrix:  $\Theta_3(z, q) \dots$ )

Insert (lowest order) Trotter approximation, using  $*$  and  $\Delta$ , into general discrete path integral:

$$\rho(\vec{R}_0, \vec{R}_M; \beta) = \int d\vec{R}_1 \int d\vec{R}_2 \dots \int d\vec{R}_{M-1} (4\pi\lambda\Delta\tau)^{-3NM/2} \exp\left[-\sum_{m=1}^M \left( \frac{(\vec{R}_{m-1} - \vec{R}_m)^2}{4\lambda\Delta\tau} + \Delta\tau V(\vec{R}_m) \right)\right] \geq 0$$

primitive approximation for density matrix

$Z = \int d\vec{R} \rho(\vec{R}, \vec{R}; \beta)$  corresponds to classical partition function of ring polymers with ideal springs within each polymer and interpolymer interaction only at equal times ( $\cong$  color).

