Introduction to Path Integral Monte Carlo. Part II.

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Outline

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1. Path sampling: local and global moves
2. Fermionic/bosonic density matrix
3. Levy-construction and sampling of permutations
4. Permutations and physical properties

Path sampling: Metropolis probabilities

- Consider a thermal average: $\langle A \rangle = \frac{1}{Z} \int dR\, A(R)\, \rho(R, R.\beta)$.

$$\langle A \rangle = \frac{1}{Z} \int dR dR_1 \dots dR_{M-1}\, A(R)\, e^{-\sum_{m=1}^{M} S^m} = \int D\bar{R}\, A(R)\, P(\bar{R})$$

- For direct sampling of microstates $\{\bar{R}\}$ distributed with

$$P(\bar{R}) = e^{-S(\bar{R})}/Z \equiv e^{-\sum_{m=1}^{M} S^m}/Z$$

we need normalization factor Z - partition function.
<u>Solution</u>: use Metropolis algorithm to construct a sequence of microstates

$$\frac{T(\bar{R}_i, \bar{R}_f)}{T(\bar{R}_f, \bar{R}_i)} = \frac{P(\bar{R}_f)}{P(\bar{R}_i)} = \frac{P(R', R'_1, \dots, R'_{M-1})}{P(R, R_1, \dots, R_{M-1})} = \frac{e^{-\sum_{m=1}^{M} S(R'_m)}/Z}{e^{-\sum_{m=1}^{M} S(R_m)}/Z}$$

- Transition probability depends on change in the action between initial and final state

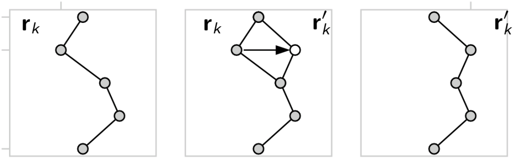
$$T(\bar{R}_i, \bar{R}_f) = min[1, e^{-[S(\bar{R}_f) - S(\bar{R}_i)]}] = min[1, e^{-\Delta S_{kin} - \Delta S_v}]$$

Path sampling: local moves

- We try to modify a path and accept by change in kinetic and potential energies

$$T(\bar{R}_i, \bar{R}_f) = min[1, e^{-\Delta S_{kin} - \Delta S_v}]$$

- Change of a single trajectory slice, $\mathbf{r}_k \rightarrow \mathbf{r}'_k$, involves two pieces $\{\mathbf{r}_{k-1}, \mathbf{r}_k\}$ and $\{\mathbf{r}_k, \mathbf{r}_{k+1}\}$ (for the i-trajectory: $\mathbf{r}_k \equiv \mathbf{r}_i^k$)



$$\Delta S_{kin} = \frac{\pi}{\lambda_D^2(\tau)} \left[(\mathbf{r}_{k-1} - \mathbf{r}'_k)^2 - (\mathbf{r}_{k-1} - \mathbf{r}_k)^2 + (\mathbf{r}'_k - \mathbf{r}_{k+1})^2 - (\mathbf{r}_k - \mathbf{r}_{k+1})^2 \right],$$

$$\Delta S_v = \tau \sum_{i<j} \left[V(\mathbf{r}'^{\,k}_i, \mathbf{r}'^{\,k}_{ij}) - V(\mathbf{r}_i^k, \mathbf{r}_{ij}^k) \right]$$

Problem: local sampling is stacked to a position of two fixed end-points $\Rightarrow$ Exceedingly slow trajectory diffusion and large autocorrelation times.

General Metropolis MC

- We split transition probability $T(\bar{R}_i, \bar{R}_f)$ into sampling and acceptance:

$$T(\bar{R}_i, \bar{R}_f) = P(\bar{R}_i, \bar{R}_f)\, A(\bar{R}_i, \bar{R}_f)$$
$$P(\bar{R}_i, \bar{R}_f) = \text{sampling probability, now } \neq P(\bar{R}_f, \bar{R}_i)$$
$$A(\bar{R}_i, \bar{R}_f) = \text{acceptance probability}$$

- The detail balance can be fulfilled with the choice

$$A(\bar{R}_i, \bar{R}_f) = min\left[1, \frac{P(\bar{R}_f, \bar{R}_i)\, P(\bar{R}_f)}{P(\bar{R}_i, \bar{R}_f)\, P(\bar{R}_i)}\right] = min\left[1, \frac{P(\bar{R}_f, \bar{R}_i)}{P(\bar{R}_i, \bar{R}_f)}\, e^{-\Delta S_{kin} - \Delta S_v}\right]$$

Once again normalization of $P(\bar{R})$ is not needed or used.

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- Example (2D Ising model): Address (M) number of down-spins and $(N-M)$ up-spins as two different species. Choose probability $p_\pm = 1/2$ to update up- or down-spins. Probability to select a spin for update: for the up-spins $P_s(N-M) = 1/(N-M)$, for down-spins $P_s(M) = 1/M$.
  Acceptance to increase by one number of down-spins:

$$A(M \rightarrow (M+1)) = \frac{p_- P_s(M+1)}{p_+ P_s(N-M)} = \left(\frac{p_-}{p_+}\right)\left(\frac{N-M}{M+1}\right)\, e^{-\beta(E_{M+1} - E_M)}$$

  At low temperatures: $N \gg M \approx N\, e^{-4J\beta\Delta s_i} \Rightarrow \frac{N-M}{M+1} \gg 1.$

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Once again normalization of $P(\bar{R})$ is not needed or used.

- Similar idea: choose the sampling probability to fulfill

$$\frac{P(\bar{R}_f, \bar{R}_i)}{P(\bar{R}_i, \bar{R}_f)} = e^{+\Delta S_{kin}}$$

Then an ideal or weakly interacting systems $A(\bar{R}_i, \bar{R}_f) \to 1$.

Path sampling: multi-slice moves

- Consider a trajectory $\bar{r}$, for a free particle ($V = 0$), moving from $\mathbf{r}$ to $\mathbf{r}'$ by time $p\tau$.

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$$T[\bar{r}(\mathbf{r}, \mathbf{r}', p\tau)] = \prod_{m=0}^{p-1} \rho_F(\mathbf{r}^m, \mathbf{r}^{m+1}, \tau), \quad \rho_F(\mathbf{r}^m, \mathbf{r}^{m+1}, \tau) = \frac{1}{\lambda_\tau^d} e^{-\pi(\mathbf{r}^m - \mathbf{r}^{m+1})^2/\lambda_\tau^2}$$

with $\mathbf{r}^0 = \mathbf{r}$ and $\mathbf{r}^p = \mathbf{r}'$.

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  with $\mathbf{r}^0 = \mathbf{r}$ and $\mathbf{r}^p = \mathbf{r}'$.
- Now consider the probability to sample an arbitrary trajectory $\bar{r}$

$$P(\bar{r}) = \frac{T[\bar{r}(\mathbf{r}, \mathbf{r}', p\tau)]}{N} = \frac{T[\bar{r}(\mathbf{r}, \mathbf{r}', p\tau)]}{\rho_F(\mathbf{r}, \mathbf{r}', p\tau)}$$

  where the normalization N reduces to a free-particle density matrix

$$\sum_{\bar{r}} T[\bar{r}(\mathbf{r}, \mathbf{r}', p\tau)] = \int d\mathbf{r}^1 \ldots d\mathbf{r}^{p-1} T[\bar{r}(\mathbf{r}, \mathbf{r}', p\tau)] = \rho_F(\mathbf{r}, \mathbf{r}', p\tau)$$

Path sampling: multi-slice moves (continued)

Normalized sampling probability (of any trajectory) can be identically rewritten as

$$P(\bar{r}) = \frac{T[\bar{r}(\mathbf{r}, \mathbf{r}', p\tau)]}{\rho_F(\mathbf{r}, \mathbf{r}', p\tau)} = \frac{\rho_F(\mathbf{r}, \mathbf{r}^1, \tau)\rho_F(\mathbf{r}^1, \mathbf{r}', (p-1)\tau)}{\rho_F(\mathbf{r}, \mathbf{r}', p\tau)}$$

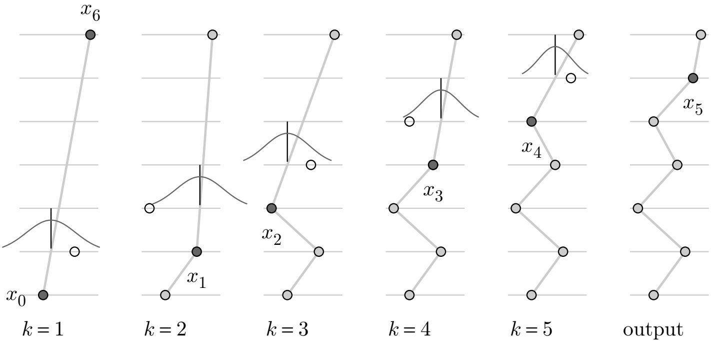
$$\times \frac{\rho_F(\mathbf{r}^1, \mathbf{r}^2, \tau)\rho_F(\mathbf{r}^2, \mathbf{r}', (p-2)\tau)}{\rho_F(\mathbf{r}^1, \mathbf{r}', (p-1)\tau)} \cdots \frac{\rho_F(\mathbf{r}^{m-2}, \mathbf{r}^{m-1}, \tau)\rho_F(\mathbf{r}^{m-1}, \mathbf{r}', \tau)}{\rho_F(\mathbf{r}^{m-2}, \mathbf{r}', 2\tau)}$$

Path sampling: multi-slice moves (continued)

$$P(\bar{r}) = \frac{\rho_F(x_0, x_1, \tau)\rho_F(x_1, x_6, 5\tau)}{\rho_F(x_0, x_6, 6\tau)} \cdot \frac{\rho_F(x_1, x_2, \tau)\rho_F(x_2, x_6, 4\tau)}{\rho_F(x_1, x_6, 5\tau)} \cdots \frac{\rho_F(x_4, x_5, \tau)\rho_F(x_5, x_6, \tau)}{\rho_F(x_4, x_6, 2\tau)}$$

Each term represents a normal (Gaussian) distribution around the mid-point $\bar{x}_m$ and variance σ_m^2, $m = 1, \ldots, p-1$ $(p = 6)$

$$\alpha = \frac{p-m}{p-m+1}, \quad \bar{x}_m = \alpha\, x_{m-1} + (1-\alpha)\, x_p, \quad \sigma_m = \sqrt{\frac{\alpha}{2\pi}}\lambda_\tau$$



Outline

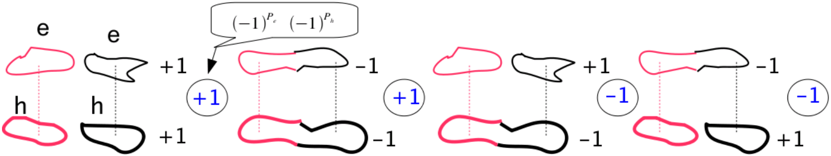
Fermionic/bosonic density matrix

- For quantum systems only two symmetries of the states are allowed:
  – density matrix is antisymmetric/symmetric under arbitrary exchange of identical particles (e.g. electrons, holes, bosonic atoms): $\hat{\rho} \longrightarrow \hat{\rho}^{A/S}$ for fermions/bosons.
- We use permutation operator $\hat{P}$ to project out the correct states: construct $\hat{\rho}^{A/S}$ as superposition of all $N!$ permutations
- Diagonal density matrix: only *closed* trajectories → periodicity with $T = n \cdot \beta$

$$\rho^{S/A}(R(0), R(\beta); \beta) = \frac{1}{N!} \sum_{P=1}^{N!} (\pm 1)^{\delta P} \rho(R(0), \hat{P}R(\beta); \beta)$$

Example: pair exchange of two electrons and holes

$$\hat{P}_{12}(\mathbf{r}_1(\beta), \mathbf{r}_2(\beta), ..) = (\mathbf{r}_{\hat{P}1}(\beta), \mathbf{r}_{\hat{P}2}(\beta), ..) = (\mathbf{r}_2(\beta), \mathbf{r}_1(\beta), ..) = (\mathbf{r}_2(0), \mathbf{r}_1(0), ..).$$



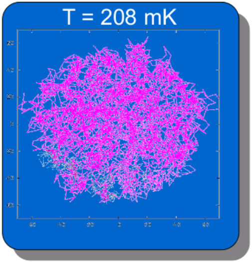
Antisymmetric density matrix: multi-component systems

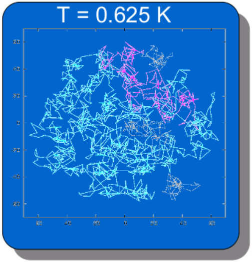
- Two-component system: spin polarized electrons and holes with particle numbers N_e and N_h

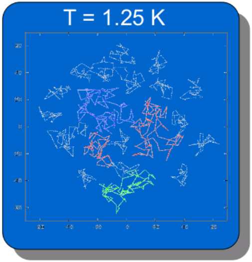
$$\rho^A(R_e, R_h, R_e, R_h; \beta) = (N_e! N_h!)^{-1} \sum_{P_e, P_h=1}^{N_e!\, N_h!} (-1)^{\delta P_e} (-1)^{\delta P_h} \rho(R_e, R_h, \hat{P}_e R_e, \hat{P}_h R_h; \beta)$$

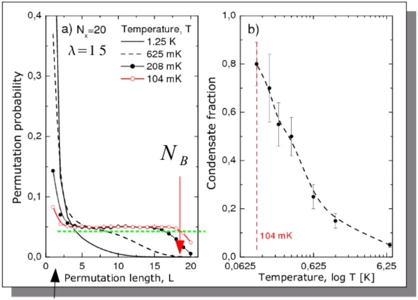
  Total number of permutations: $N = N_e! \times N_h!$.
- We try to reconnect the paths in different ways to form larger paths: form multi-particle exchange.
- This corresponds to sampling of different permutations in the sum $\sum_{P=1}^{N!}$
- Number of permutations is significantly reduced using the Metropolis algorithm and the importance sampling.

Permutation-length distribution: T -dependence





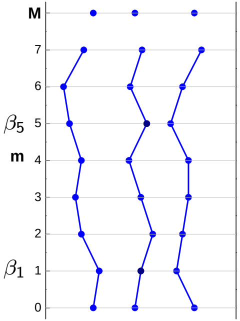




- System: Fully spin polarized N electrons (or bosons) in 2D parabolic quantum dot.
- Classical system: only identity permutations.
- Low temperatures $T \rightarrow 0$: equal probability of all permutation lengths.
- Ideal bosons: threshold value estimates condensate fraction.

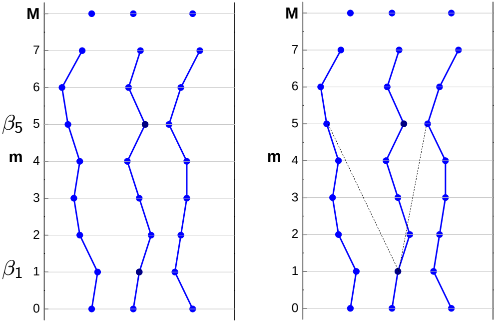
Outline

Levy-construction and pair exchange



- Select at random a path "i"
- Select a time interval (β_1, β_5) along the time axis $\beta = M\tau$.

Levy-construction and pair exchange



- Select at random a path "i"
- Select a time interval (β_1, β_5) along the time axis $\beta = M\tau$.
- Choose a particle "j" (green path) from all neighbours N_f within a distance of $\lambda_{4\tau}$.

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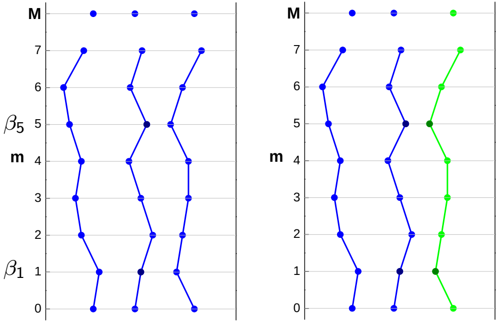

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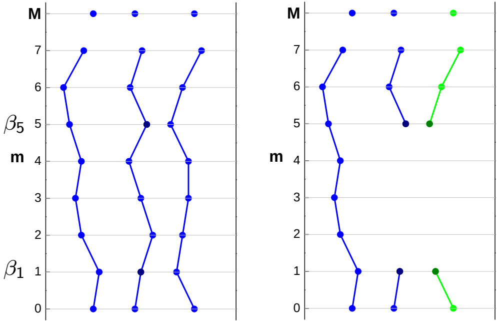

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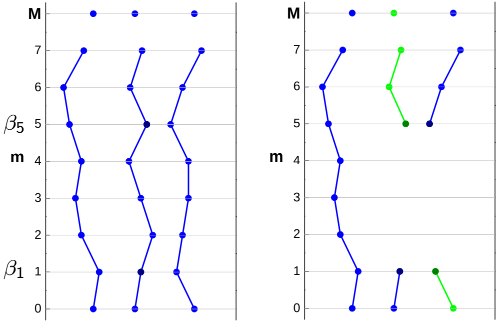

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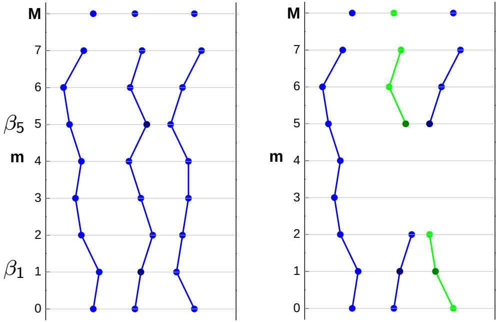
- Sample new path points $(\mathbf{r}^2_{i(j)}, \mathbf{r}^3_{i(j)}, \mathbf{r}^4_{i(j)})$ using the probability $P(\bar{r})$.

Levy-construction and pair exchange



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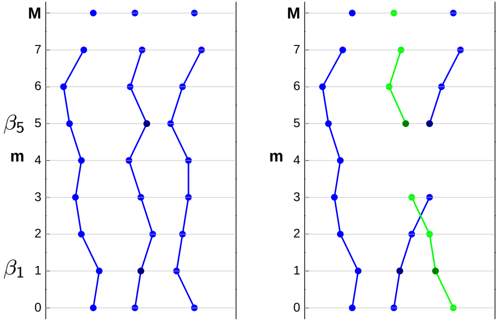

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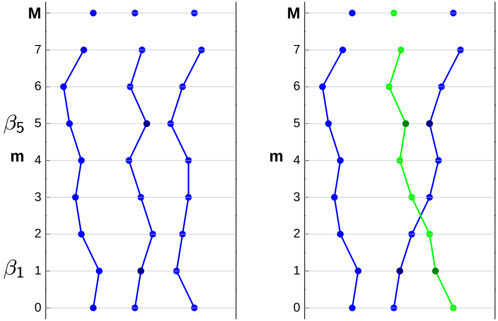

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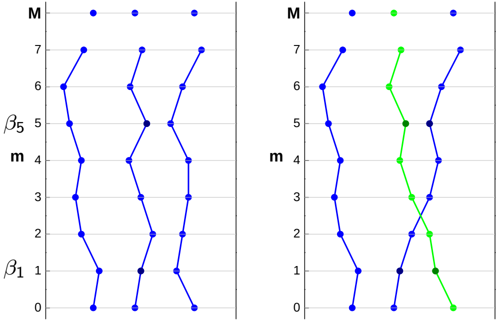

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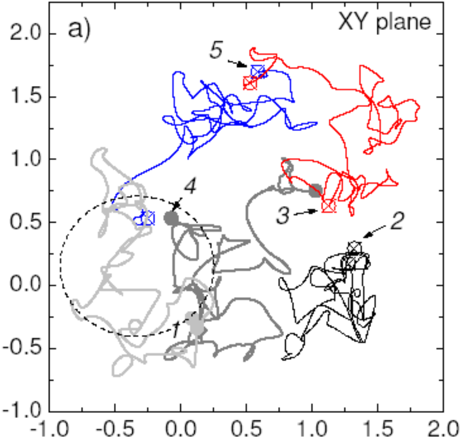
- Sample new path points $(\mathbf{r}^2_{i(j)}, \mathbf{r}^3_{i(j)}, \mathbf{r}^4_{i(j)})$ using the probability $P(\bar{r})$.
- Find number of neighbours for the reverse move N_r and accept or reject

$$A(i \rightarrow f) = min\left[1, \frac{N_r}{N_f} e^{-\Delta S_V}\right]$$

Beyond two-particle exchange



Example: 5 fermions/bosons in 2D

Initial permutation state:

- Two identity permutations (1)(2): $[\mathbf{r}_1(\beta) = \mathbf{r}_1(0), \mathbf{r}_2(\beta) = \mathbf{r}_2(0)]$.
- Three-particle permutation (354): $[\mathbf{r}_3(\beta) = \mathbf{r}_5(0), \mathbf{r}_5(\beta) = \mathbf{r}_4(0)]$, $\mathbf{r}_4(\beta) = \mathbf{r}_3(0)$.

We can restore identity permutations by two successive pair-transpositions:

$$\hat{P}_{34}(1)(2)(354) \longrightarrow (1)(2)(3)(45),$$

$$\hat{P}_{45}(1)(2)(3)(45) \longrightarrow (1)(2)(3)(4)(5)$$

or we can restore the initial permutation state by

$$\hat{P}_{34}\,\hat{P}_{45}(1)(2)(3)(4)(5) = (1)(2)(354)$$

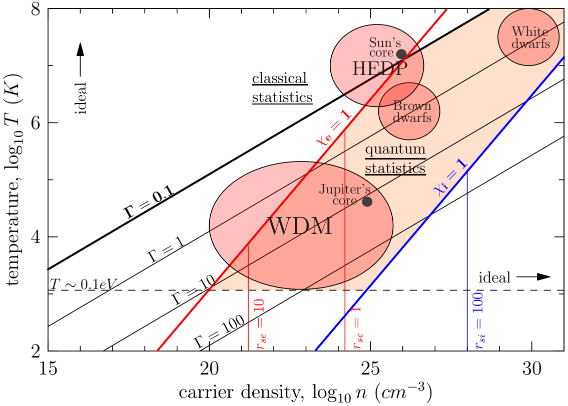
Beyond two-particle exchange

- Any many-particle permutation can be constructed by a successive action of the two-particle permutation operator $\hat{P}_{ij}$:

$$\hat{P}\rho^{dist}(\{\mathbf{r}_1,\ldots\mathbf{r}_N\},\{\mathbf{r}_1,\ldots\mathbf{r}_N\}) = \prod_{ij}\hat{P}_{ij}\,\rho^{dist}(\{\mathbf{r}_1,\ldots\mathbf{r}_N\},\{\mathbf{r}_1,\ldots\mathbf{r}_N\})$$

$$\hat{P}_{ij}\,\rho(\{\mathbf{r}_1,\ldots\mathbf{r}_N\},\{\ldots,\mathbf{r}_i,\ldots,\mathbf{r}_j,\ldots\}) = (\pm 1)\,\rho(\{\mathbf{r}_1,\ldots\mathbf{r}_N\},\{\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_i,\ldots\})$$

Quantum degeneracy effects



Density: $n = 1/\bar{r}^3$

Classical coupling parameter: $\Gamma = \langle V \rangle / k_B T$

Quantum coupling parameter: $r_s = \langle V \rangle / E_0$, zero-point energy $E_0 = \frac{\hbar^2}{m\bar{r}^2}$

Degeneracy parameter: $\chi(n, T) = n\lambda_D^3(T) \geq 1 \quad \Rightarrow \lambda_D(T) \geq \bar{r}$

Outline

Permutations and physical properties

- When system is degenerate permutations are important : $\lambda_D(T) \geq \bar{r}$ (thermal wavelength is comparable with the inter-particle spacing)
- Long permutations: relation to physical phenomena
  - Normal-superfluid phase transition in bosonic systems: He^4, para-hydrogen, cold neutral atomic gases, dipole molecule, excitonic systems, etc.
  - Offdiagonal long-range order – condensation in momentum space
  - Spin effects in fermionic systems: superconductivity, Hunds rules in quantum dots, etc.
- Particles interaction (in "strong coupling" regime) can suppress the degeneracy ⇒ quantum simulations without exchange:
  - He^4 in solid phase
  - Wigner solids in 2D and 3D
  - Protons and ions in degenerate quantum plasmas