Diagrammatic Monte Carlo

Thomas Hahn

Group Seminar

SS 2020

universität wien
VASP Vienna Ab-initio Simulation Package
VDS VIENNA - DOCTORAL - SCHOOL - PHYSICS
FWF Der Wissenschaftsfonds.

Outline

1. General introduction to Monte Carlo methods
2. DiagMC – A toy example
3. General aspects of DiagMC
4. DiagMC applied to the polaron problem
5. DiagMC in particle physics

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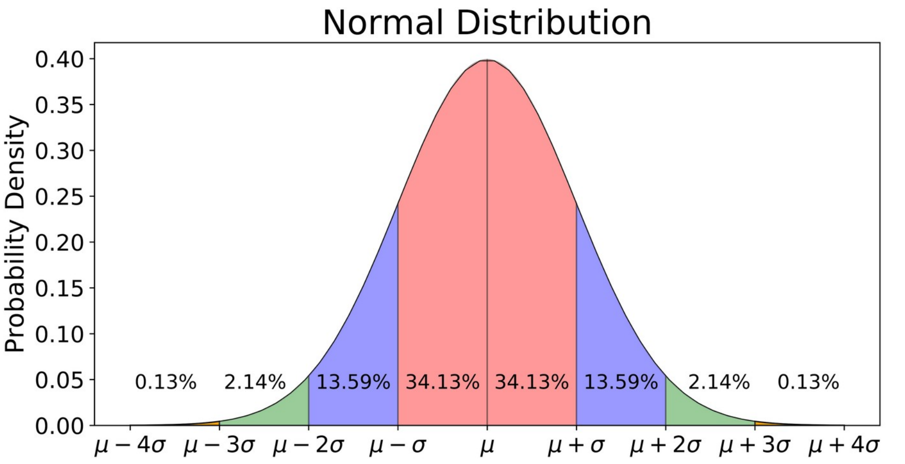
Monte Carlo methods in physics

- huge class of computational algorithms
- common feature $\Longrightarrow$ random numbers
- used when analytical and numerical solutions are not feasible
- 3 main applications:
  - numerical integration (MC integration) $\sigma \propto \frac{1}{\sqrt{N}}$
  - sampling from complicated probability distributions (MCMC)
  - optimization
- classical vs. quantum Monte Carlo

Some statistics notation

- Probability density function $p(x)$:
  - $p(x) \geq 0$
  - $\int_\Omega p(x) dx = 1$

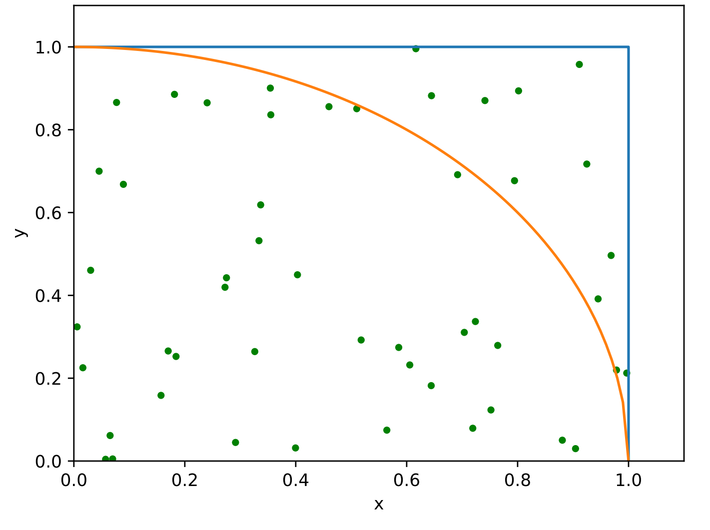


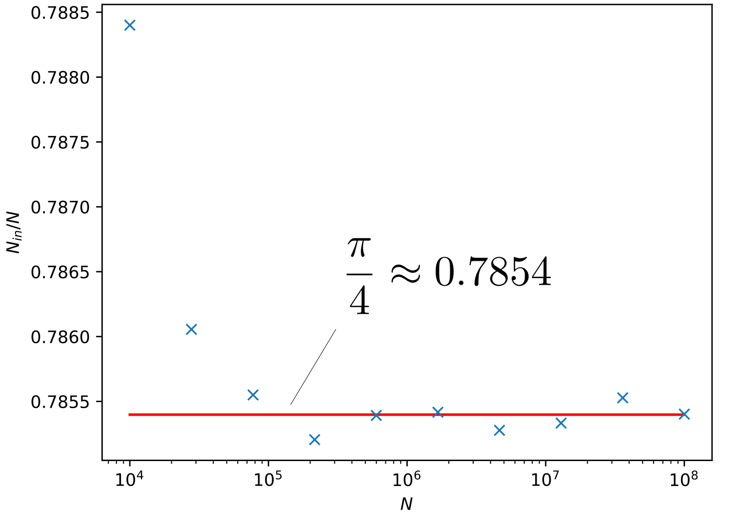
- Expected value:
  - $E\left[X\right] = \langle X \rangle_p = \int_\Omega x p(x) dx \approx \frac{1}{N} \sum_{i=1}^{N} x_i = \overline{X}$

- Variance:
  - $\sigma_X^2 = E[(X - E[X])^2] \approx \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \overline{X})^2 = s_X^2$
  - $\sigma_{\overline{X}}^2 = \frac{\sigma_X^2}{N}$ (only for uncorrelated samples)

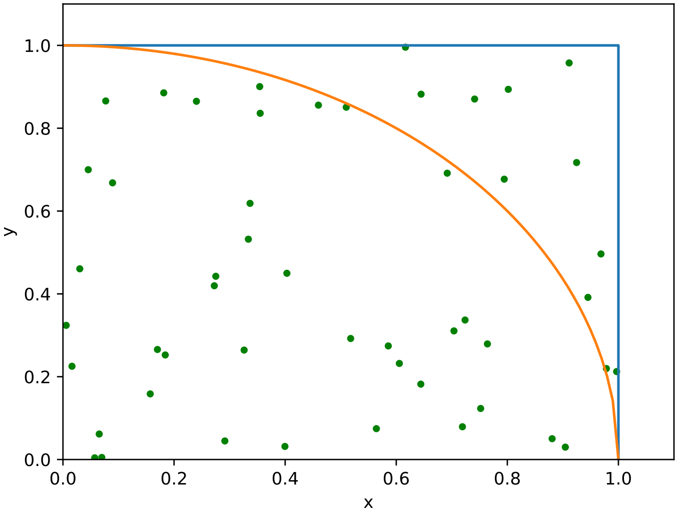
The infamous calculation of π

- **Goal**: calculate π using MC methods
- Standard recipe:
  - produce N points (x_i, y_i) uniformly within the unit square
  - count the points N_{in} within the unit circle
  - apporximate π using: $\frac{\pi}{4} \approx \frac{N_{in}}{N}$
- lean back and observe the convergence for increasing N





The infamous calculation of π



- Under the hood:
  - 2-dim integral
  - rewritten as an expectation value

$$\frac{\pi}{4} = \iint_0^1 f(x,y)dxdy = \iint_0^1 \frac{f(x,y)}{p(x,y)}p(x,y)dxdy$$

$$\frac{\pi}{4} = \left\langle \frac{f(x,y)}{p(x,y)} \right\rangle_p \approx \frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i,y_i)}{p(x_i,y_i)} = \frac{N_{in}}{N}$$

$$f(x,y) = \begin{cases} 1 & \text{if } x^2+y^2 \leq 1 \\ 0 & \text{otherwise} \end{cases} \qquad p(x,y) = \mathcal{U}(0,1) * \mathcal{U}(0,1) = 1$$

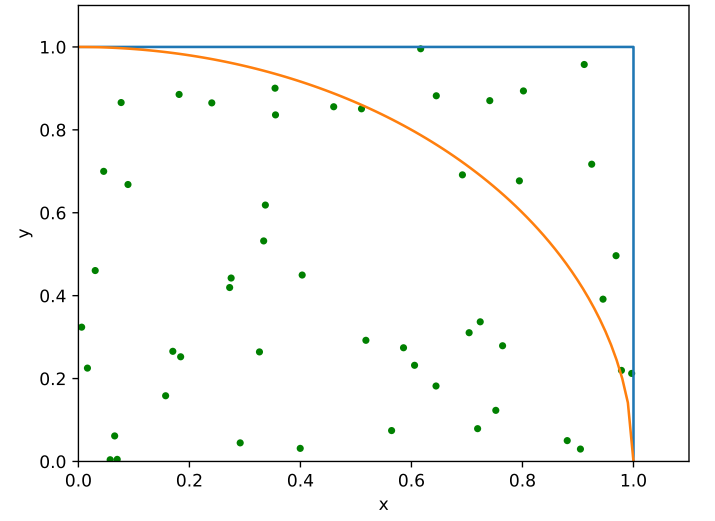
The infamous calculation of π

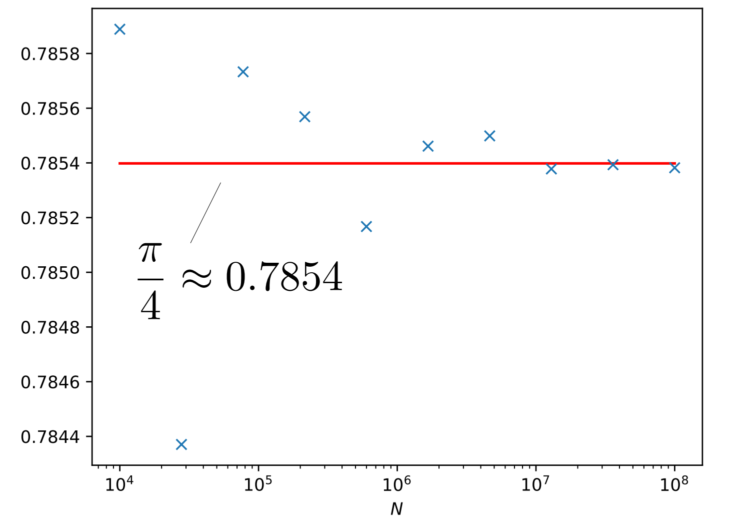
- Alternative way:
  - 1-dim integral
  - rewritten as an expectation value

$$\frac{\pi}{4} = \int_0^1 f(x)dx = \int_0^1 \frac{f(x)}{p(x)}p(x)dx$$

$$\frac{\pi}{4} = \left\langle \frac{f(x)}{p(x)} \right\rangle_p \approx \frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{p(x_i)} = \frac{1}{N}\sum_{i=1}^{N}\sqrt{1-x_i^2}$$

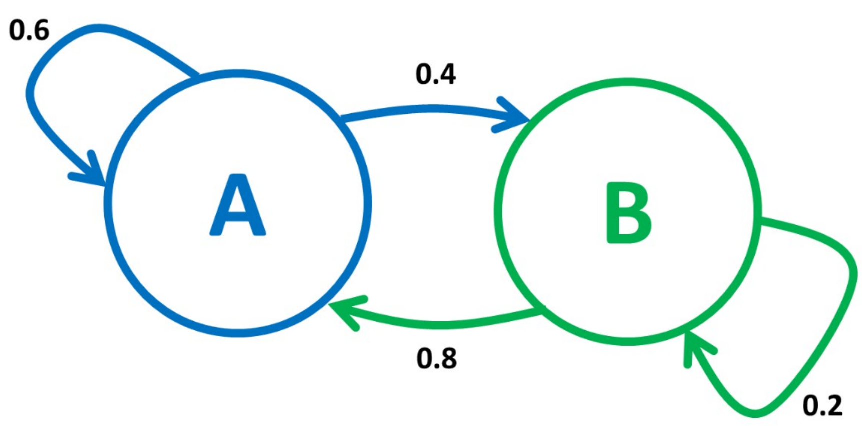
$$f(x) = \sqrt{1-x^2} \qquad p(x) = \mathcal{U}(0,1) = 1$$





Markov Chain Monte Carlo

- algorithms for sampling from complex probability distributions
- generates a Markov chain with the desired distribution as its equilibrium distribution
- Markov chain:
  - state space $\mathcal{S}$ (discrete or continuous)
  - transition probabilities P
- How to choose P such that the visited states represent random samples from the desired distribution?



$\Longrightarrow$ Metropolis-Hastings algorithm

Metropolis-Hastings

Input : initial distribution $\pi^{(0)}$
target distribution $p(X)$
proposal distribution $w_{XX'}$
Output: random samples according to $p(X)$

samples[];
start from initial state $X \sim \pi^{(0)}$;
perform thermalization steps;
while *not enough samples* **do**
    draw a proposal sample X' from $w_{XX'}$;
    calculate $p(X)$ and $p(X')$;
    if $w_{X'X}p(X') \geq w_{XX'}p(X)$ **then**
        $X \leftarrow X'$;
    else
        calculate $R = \frac{w_{X'X}p(X')}{w_{XX'}p(X)}$;
        draw random uniform number r;
        if $r \leq R$ **then**
            $X \leftarrow X'$;
    end
    samples.add(X);
end
return samples;

FIGURE 4.2: Metropolis-Hastings algorithm.

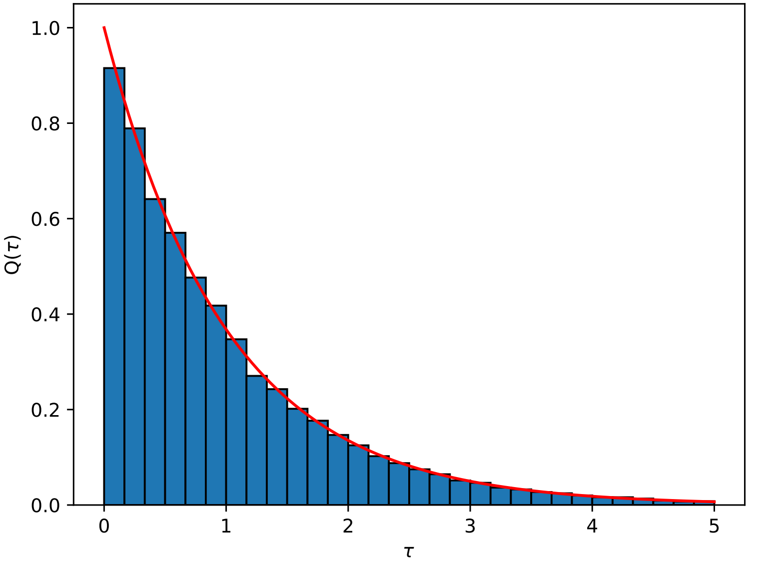
Reconstructing a function

- **Goal**: Reconstruct the function $Q(\tau) = e^{-\alpha\tau}$ for $\alpha = 1, \tau \in [0, 5]$
- Recipe:
  - interpret $Q(\tau)$ as a distribution and draw samples from it with MCMC
  - put the samples in a histogram to reconstruct $Q(\tau)$
- Histogram: discretize τ-space into N bins β_i of size $\Delta\tau_i$ with center τ_i

$$Q(\tau_i) \approx \frac{1}{\Delta\tau_i}\int_{\beta_i} Q(\tau)d\tau = \frac{C}{\Delta\tau_i}\int_0^5 \frac{Q(\tau)}{C}\chi_{\beta_i}(\tau)d\tau$$

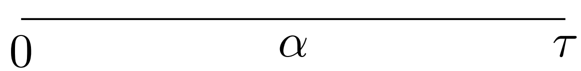
$$Q(\tau_i) \approx \frac{C}{\Delta\tau_i}\langle\chi_{\beta_i}(\tau)\rangle_{Q/C}$$

$$Q(\tau_i) \approx \frac{C}{\Delta\tau_i}\frac{1}{N}\sum_{i=1}^{N}\chi_{\beta_i}(\tau_i)$$



A first glimpse at DiagMC

- view $Q(\tau) = e^{-\alpha\tau}$ as a (Feynman) diagram

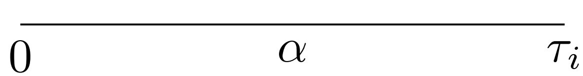


$$= D_0^{\xi_0}(\tau) = e^{-\alpha\tau}$$

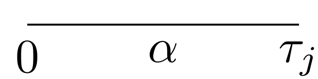
weight of diagram

- perform MCMC in the space of all diagrams
- use updates to propose a new diagram

$D_0^{\xi_0}(\tau_i) =$



$\longleftrightarrow$



$= D_0^{\xi_0}(\tau_j)$

- accept the proposed diagram with probability

$$P_{acc} = \min\left\{1, \frac{D_0^{\xi_0}(\tau_p)p(\tau_c|\tau_p)}{D_0^{\xi_0}(\tau_c)p(\tau_p|\tau_c)}\right\}$$

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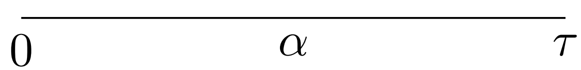
DiagMC – A toy example

- **Goal**: Calculate the function $Q(\tau)$ for $\alpha = 1, \tau \in [0,5], V = 0.5, \beta \in \{0.25, 0.75\}$

$$Q(\tau) = e^{-\alpha\tau} + \sum_{\beta} \int_0^{\tau} d\tau_2 \int_0^{\tau_2} d\tau_1 e^{-\alpha\tau_1} V e^{-\beta(\tau_2-\tau_1)} V e^{-\alpha(\tau-\tau_2)}$$

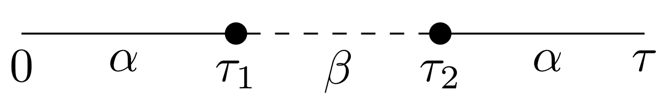
$$= D_0^{\xi_0}(\tau) + \sum_{\beta} \int_0^{\tau} d\tau_2 \int_0^{\tau_2} d\tau_1 D_2^{\xi_2}(\tau, \tau_1, \tau_2, \beta) = Q_0(\tau) + Q_2(\tau)$$

- 0th order diagram:



$$= D_0^{\xi_0}(\tau) = e^{-\alpha\tau}$$

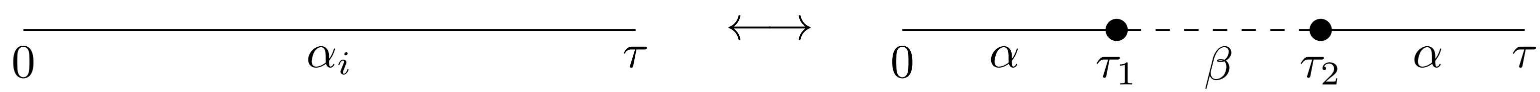
- 2nd order diagram:



$$= D_2^{\xi_2}(\tau, \tau_1, \tau_2, \beta) = e^{-\alpha\tau_1} V e^{-\beta(\tau_2-\tau_1)} V e^{-\alpha(\tau-\tau_2)}$$

DiagMC – A toy example

- change-τ update: same as before
- add-β and remove-β updates:



$$P_{0\to 2} = \min\left\{1, \frac{p_{rem}}{p_{add}} \frac{D_2^{\xi_2}(\tau,\tau_1,\tau_2,\beta)}{D_0^{\xi_0}(\tau)p(\tau_1,\tau_2,\beta)}\right\}$$

$$P_{2\to 0} = \min\left\{1, \frac{p_{add}}{p_{rem}} \frac{D_0^{\xi_0}(\tau)p(\tau_1,\tau_2,\beta)}{D_2^{\xi_2}(\tau,\tau_1,\tau_2,\beta)}\right.$$

- proposal distribution $p(\tau_1,\tau_2,\beta)$:
  - $p(\tau_1,\tau_2,\beta) = p_1(\tau_1)p_2(\tau_2|\tau_1)p_3(\beta)$
  - $p_1(\tau_1) = \mathcal{U}(0,5)$
  - $p_2(\tau_2|\tau_1) = \mathcal{U}(\tau_1,5)$
  - $p_3(\beta) = \mathcal{U}\{0.25, 0.75\}$

DiagMC – A toy example

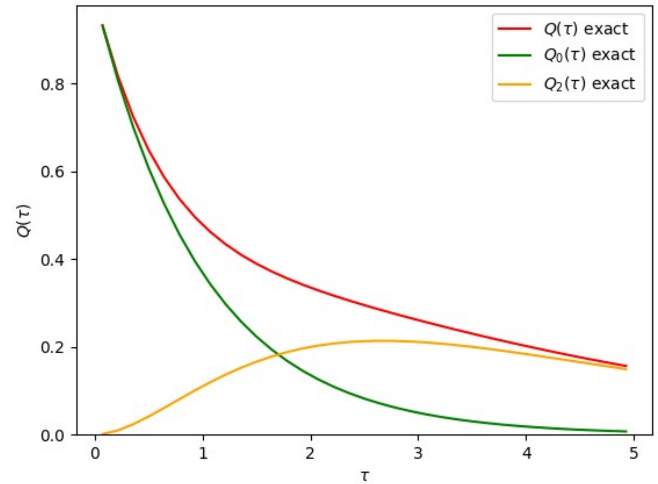
- Step-by-step solution:
  1. Generate initial diagram, e.g. $\mathcal{D}_0^{\xi_0}(\tau)$ with $\tau \sim \mathcal{U}(0,5)$
  2. Choose update U from {change-τ, add-β, remove-β}
  3. Propose new diagram with U and accept/reject
  4. Make measurments
  5. Go back to 2
- Measurements: Histogram, avg. diagram order, etc.

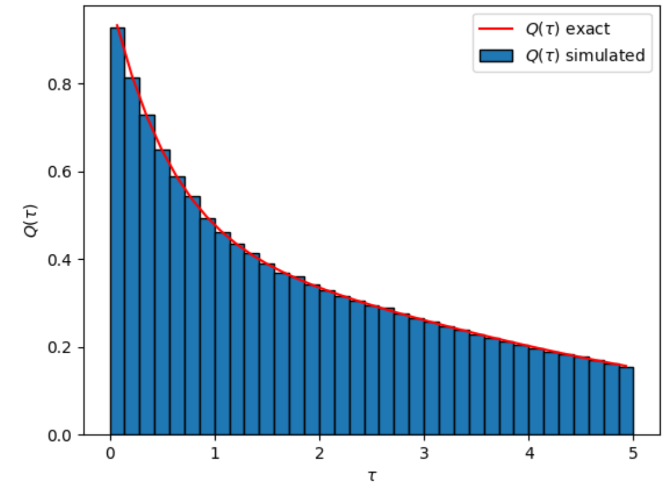
$$Q_0(\tau_i) \approx \frac{C}{\Delta\tau_i}\frac{1}{N}\sum_{i=1}^{N}\chi_{\beta_i}(\tau_i)\chi_0(n_i)$$

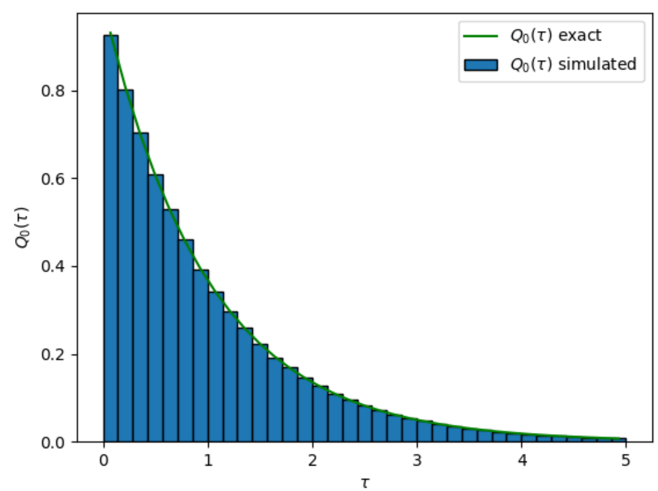
$$Q(\tau_i) \approx \frac{C}{\Delta\tau_i}\frac{1}{N}\sum_{i=1}^{N}\chi_{\beta_i}(\tau_i)$$

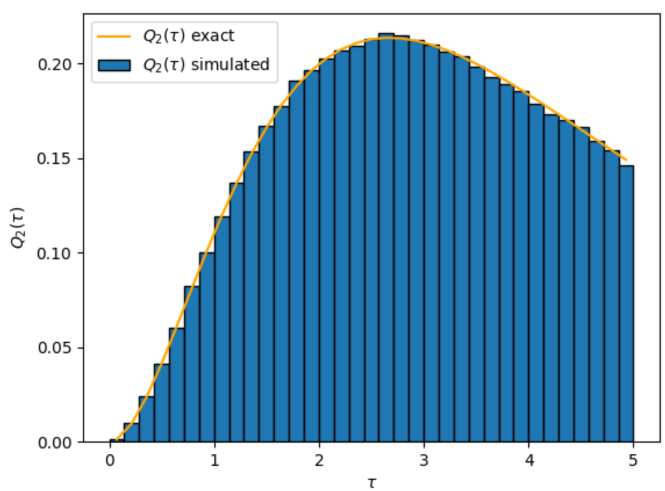
$$Q_2(\tau_i) \approx \frac{C}{\Delta\tau_i}\frac{1}{N}\sum_{i=1}^{N}\chi_{\beta_i}(\tau_i)\chi_2(n_i)$$

DiagMC – A toy example









Outline

DiagMC - Diagrammatic Series

$$Q(\{y\}) = \sum_{n=0}^{\infty} \sum_{\xi_n} \int \mathcal{D}_n^{\xi_n}(\{y\}; x_1, ..., x_n) dx_1 ... dx_n$$

- function of interest $Q(\{y\})$ depending on a set of parameters $\{y\}$
- n is the running index of the series or the order of the diagram
- ξ_n indexes different diagrams of the same order
- $\mathcal{D}_n^{\xi_n}(\{y\}; x_1, ..., x_n)$ represents an actual Feyman diagram
- $x_1, ..., x_n$ are integration variables

How can we evaluate this series? $\Longrightarrow$ DiagMC

DiagMC – How does it work?

$$Q(\{y\}) = \sum_{n=0}^{\infty} \sum_{\xi_n} \int \mathcal{D}_n^{\xi_n}(\{y\}; x_1, ..., x_n) dx_1 ... dx_n$$

- interpret $Q(\{y\})$ as a distribution function for $\{y\}$
- interpret $\mathcal{D}_n^{\xi_n}(\{y\}; x_1, ..., x_n)$ as a distribution function for $(\{y\}; n, \xi_n, x_1, ..., x_n)$
- simulate $Q(\{y\})$ using a MCMC algorithm by sampling the diagrams stochastically
- $\mathcal{D}_n^{\xi_n}(\{y\}; x_1, ..., x_n)$ is the statistical weight of a diagram
- collect statistics for $\{y\}$
- updates that can change the order n, the topology ξ_n , integration variables $x_1, ..., x_n$ and external variables $\{y\}$ of a diagram

DiagMC - Workflow

Input: initial diagram $\mathcal{D}^{(0)} \leftarrow (\{y^{(0)}\}; x_1^{(0)}, \ldots, x_n^{(0)}, n^{(0)}, \xi_n^{(0)})$,
update procedures $\{U_1, \ldots, U_k\}$,
update probabilities $\{p(U_1), \ldots, p(U_k)\}$;
Output: histogram of $Q(\{y\})$;

initialize histogram[];
initialize diagram $\mathcal{D}_{cur} \leftarrow \mathcal{D}^{(0)}$;
while not converged **do**
  choose an update U_i from $\{U_1, \ldots, U_k\}$ with probability $p(U_i)$;
  propose a new diagram $\mathcal{D}_{new} \leftarrow (\{y'\}; x'_1, \ldots, x'_{n'}, n', \xi'_{n'})$ according to U_i;
  calculate acceptance ratio R;
  draw random uniform number r;
  if $R \geq r$ **then**
    accept the proposed diagram: $\mathcal{D}_{cur} \leftarrow \mathcal{D}_{new}$;
  else
    reject the proposed diagram: $\mathcal{D}_{cur} \leftarrow \mathcal{D}_{cur}$;
  end if
  histogram[$\{y\}$]$\leftarrow$ histogram[$\{y\}$]+1;
end while
return histogram;

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Polarons - Historical view

- 1930s: introduction by Lev Landau
  - semiclassical calculations by Landau and Pekar
- 1950s: Fröhlich derives Hamiltonian
  - perturbational and variational calculations
- 1955: Feynman's path integral solution
- Since then:
  - testing ground for numerical methods
  - generalization of polaron concept

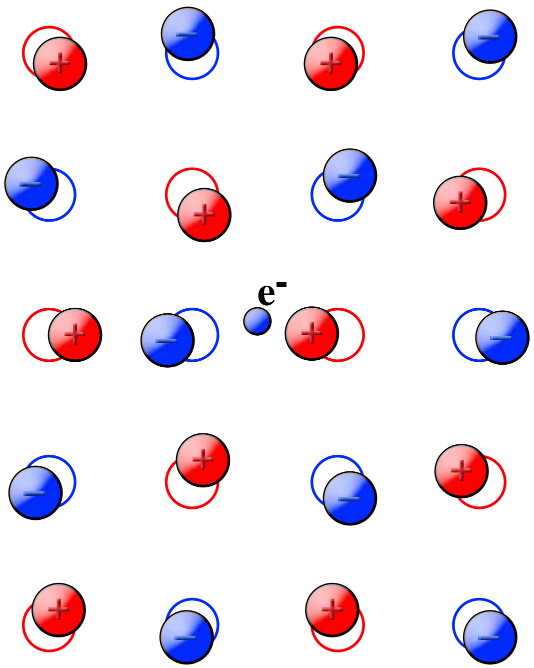


Image: Devreese, J. T. arXiv preprint arXiv:1611.06122 (2016).

Polarons – Modern view

- Particle interacting with its environment:
  - Magnetic polaron
  - Fermi polaron
  - BEC-impurity polaron
  - Piezoelectric polaron
  - Ripplonic polaron
  - Angulon

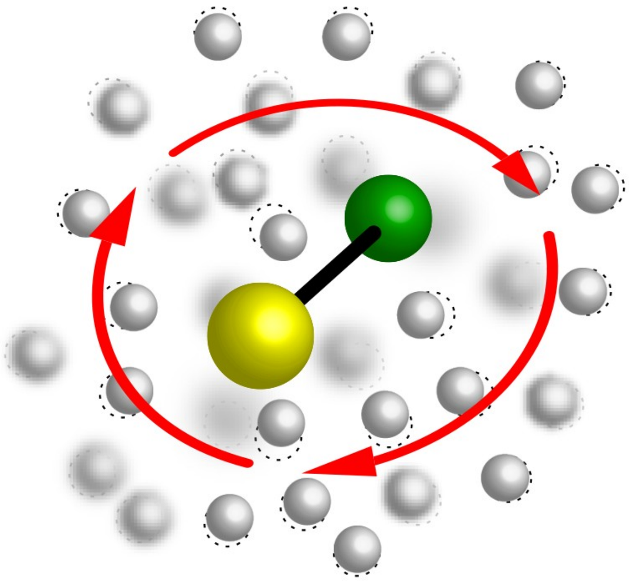


Image: Lemeshko, Mikhail, and Richard Schmidt. arXiv preprint arXiv:1703.06753 (2017).

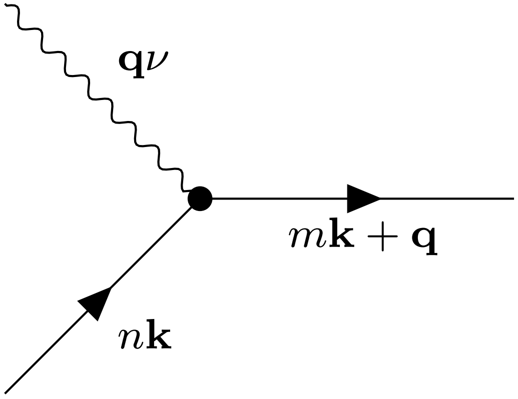
Polaron Hamiltonian

$$H = \sum_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} \hat{c}^{\dagger}_{n\mathbf{k}} \hat{c}_{n\mathbf{k}} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} \hat{a}^{\dagger}_{\mathbf{q}\nu} \hat{a}_{\mathbf{q}\nu} + \sum_{\substack{\mathbf{k},\mathbf{q} \\ mn\nu}} g_{mn\nu}(\mathbf{k},\mathbf{q}) \hat{c}^{\dagger}_{m\mathbf{k}+\mathbf{q}} \hat{c}_{n\mathbf{k}} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}^{\dagger}_{-\mathbf{q}\nu} \right)$$

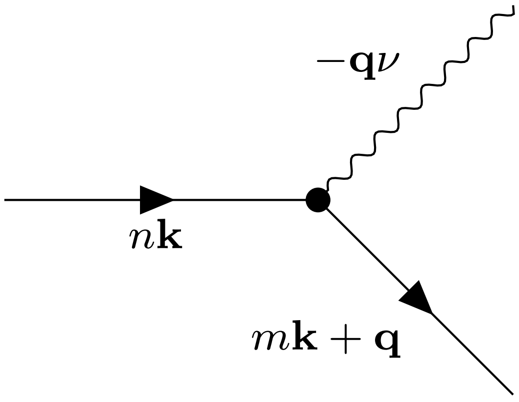
- electronic band structure $\varepsilon_{n\mathbf{k}}$
- phonon dispersion $\omega_{\mathbf{q}\nu}$
- electron-phonon matrix elements $g_{mn\nu}(\mathbf{k},\mathbf{q})$

Electron-phonon interaction

$$g_{mn\nu}(\mathbf{k},\mathbf{q})\hat{c}^{\dagger}_{m\mathbf{k}+\mathbf{q}}\hat{c}_{n\mathbf{k}}\hat{a}_{\mathbf{q}\nu}\ :$$



$$g_{mn\nu}(\mathbf{k},\mathbf{q})\hat{c}^{\dagger}_{m\mathbf{k}+\mathbf{q}}\hat{c}_{n\mathbf{k}}\hat{a}^{\dagger}_{-\mathbf{q}\nu}\ :$$



DiagMC – Green‘s function

Imaginary time, one-electron Green‘s function at T=0:

$$G(\mathbf{k},\tau) = \langle \mathrm{vac}|\, \hat{c}_{\mathbf{k}}(\tau)\hat{c}^{\dagger}_{\mathbf{k}}(0)\, |\mathrm{vac}\rangle$$

Diagrammatic expansion of $G(\mathbf{k},\tau)$:

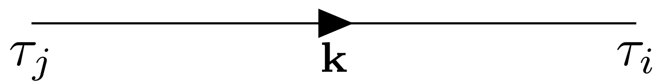
$$G(\mathbf{k},\tau) = \sum_{n=0}^{\infty} \sum_{\xi_n} \int \mathcal{D}_n^{\xi_n}\left(\mathbf{k},\tau;\{\tau_n\},\{\mathbf{q}\}\right) \prod_i^n d\tau_i \prod_j^{n/2} \mathbf{q}_j$$

$\Longrightarrow$ $G(\mathbf{k},\tau\to\infty) \to Z_0(\mathbf{k})e^{-E_0(\mathbf{k})\tau}$

$\Longrightarrow$ $\mathcal{D}_n^{\xi_n}$ is a product of free electron Green's functions $G^0(\mathbf{k},\tau)$, free phonon Green's functions $F^0(\mathbf{q},\tau)$ and electron-phonon matrix elements

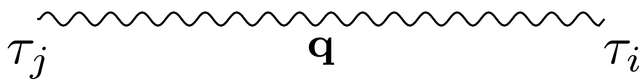
DiagMC – Feynman rules

free electron Green‘s functions are drawn as solid lines:



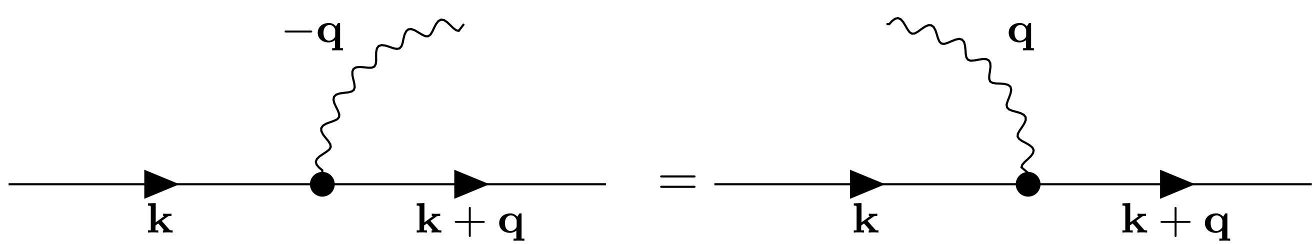
$$= G^0(\mathbf{k}, \tau_i - \tau_j) = e^{-\varepsilon_{\mathbf{k}}(\tau_i - \tau_j)}$$

free phonon Green‘s functions are drawn as wiggly lines:



$$= F^0(\mathbf{q}, \tau_i - \tau_j) = e^{-\omega_{\mathbf{q}}(\tau_i - \tau_j)}$$

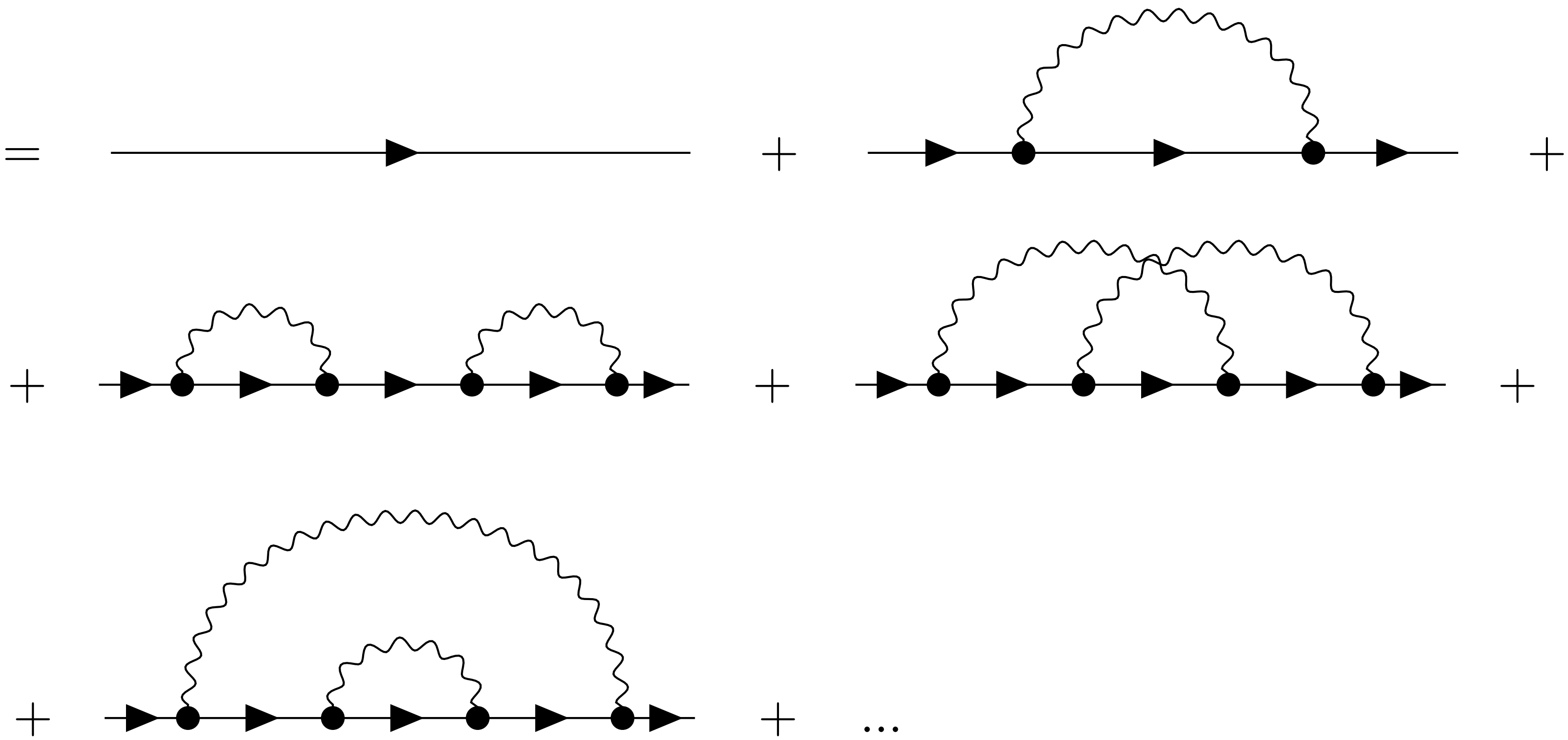
electron-phonon matrix elements are drawn as vertices:



$$= g(\mathbf{k}, \mathbf{q})$$

DiagMC – Feynman diagrams

$$G(\mathbf{k},\tau) =$$

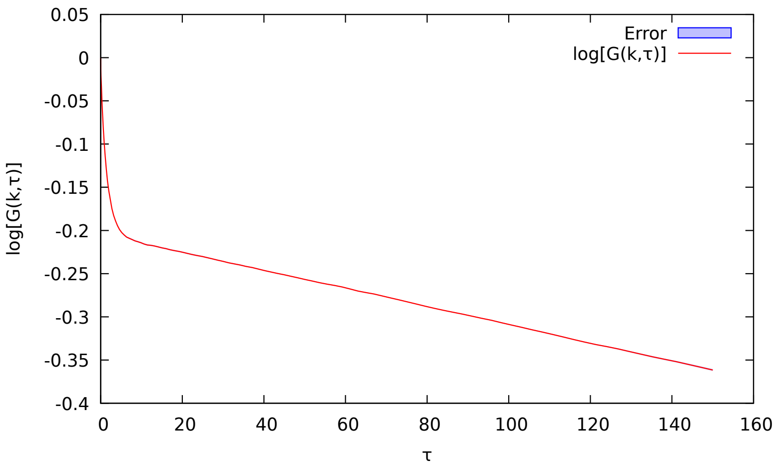


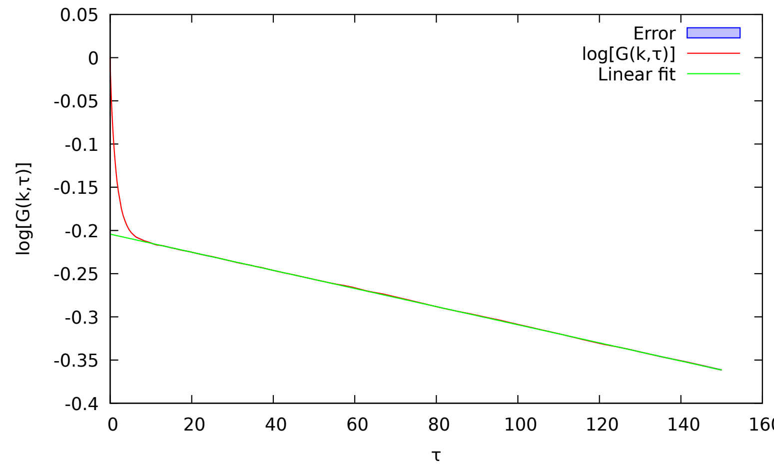
DiagMC - Summary

Goal: Calculate ground state energy and quasiparticle weight $E_0(\mathbf{k}), Z_0(\mathbf{k})$ from the one-electron Green‘s function:

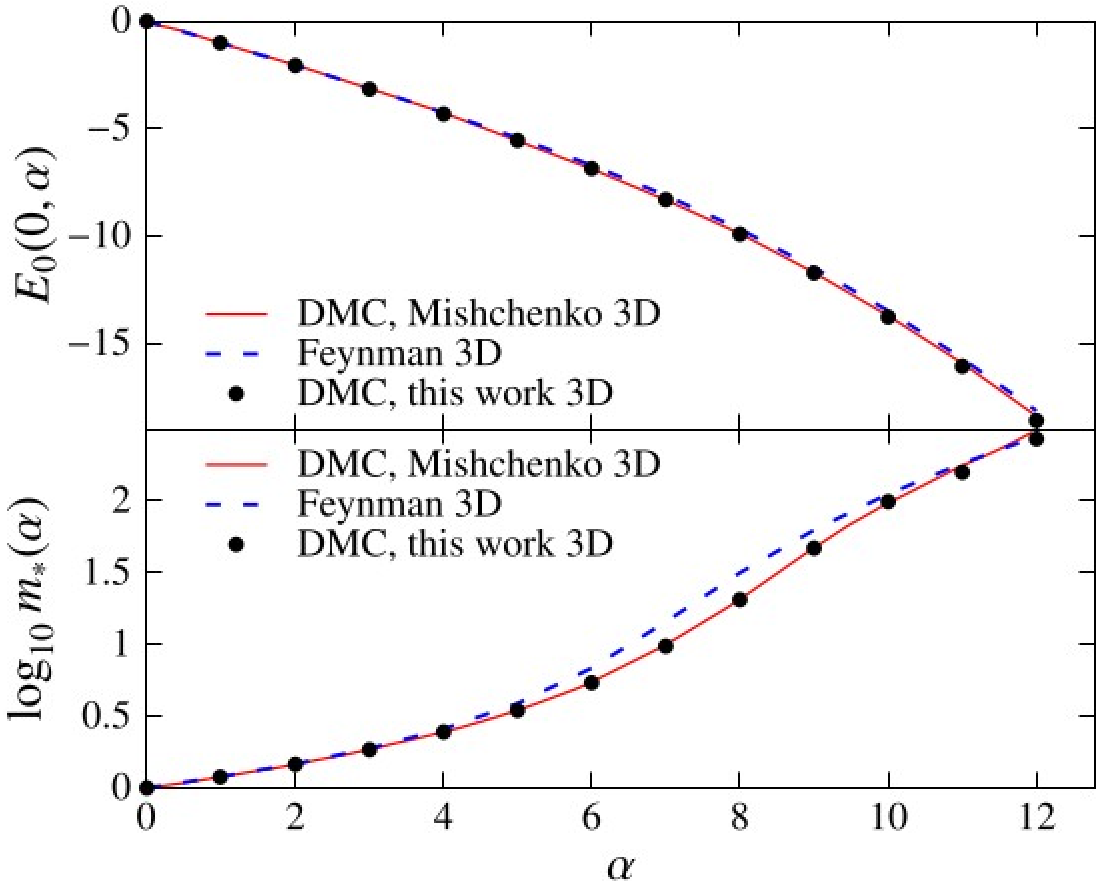
$$G(\mathbf{k}, \tau \to \infty) \to Z_0(\mathbf{k}) e^{-E_0(\mathbf{k})\tau}$$

- Requirements:
  - Diagrammatic expansion of Green‘s function
  - Updates to sample the whole space of Feynman diagrams



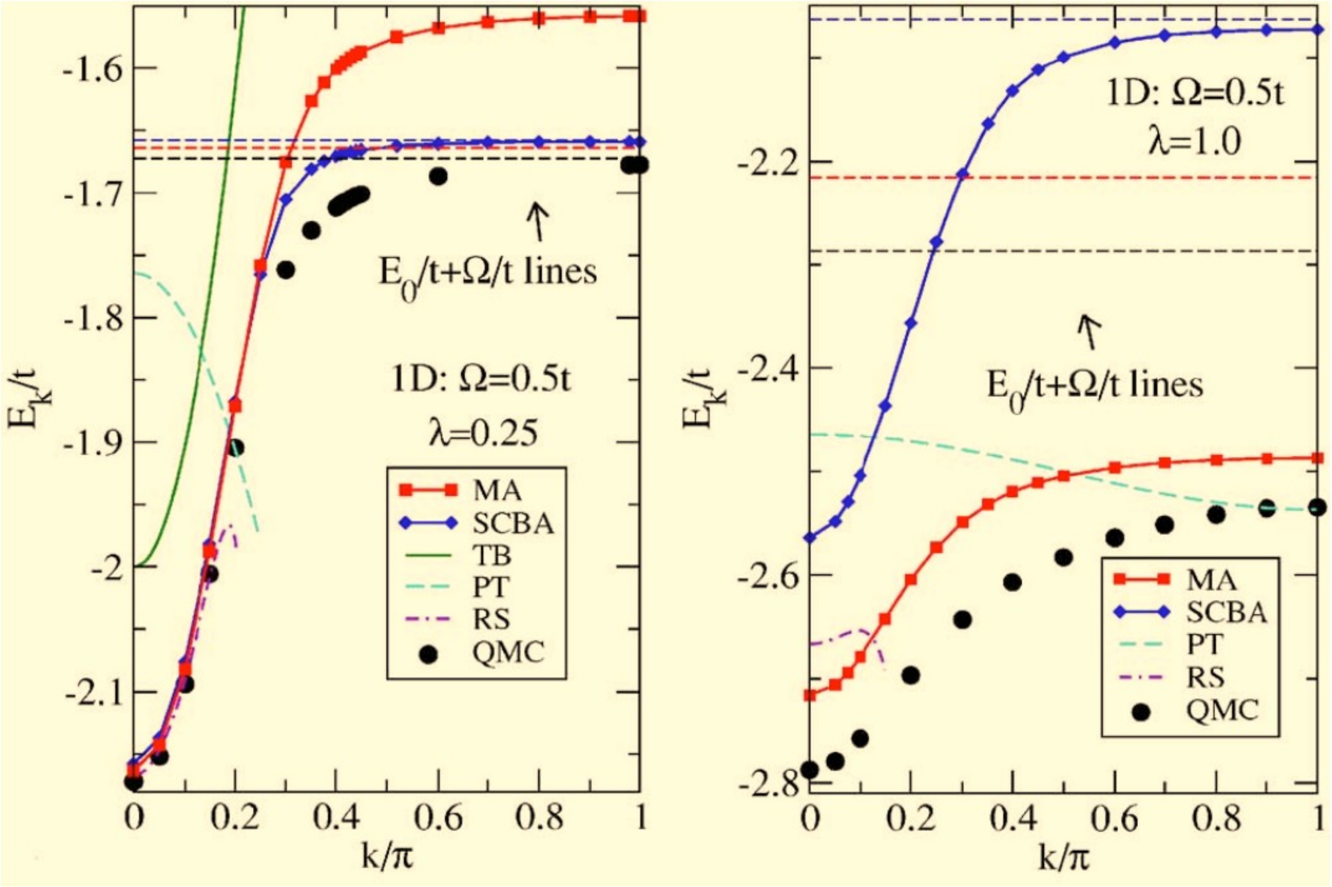


DiagMC – Fröhlich ground state



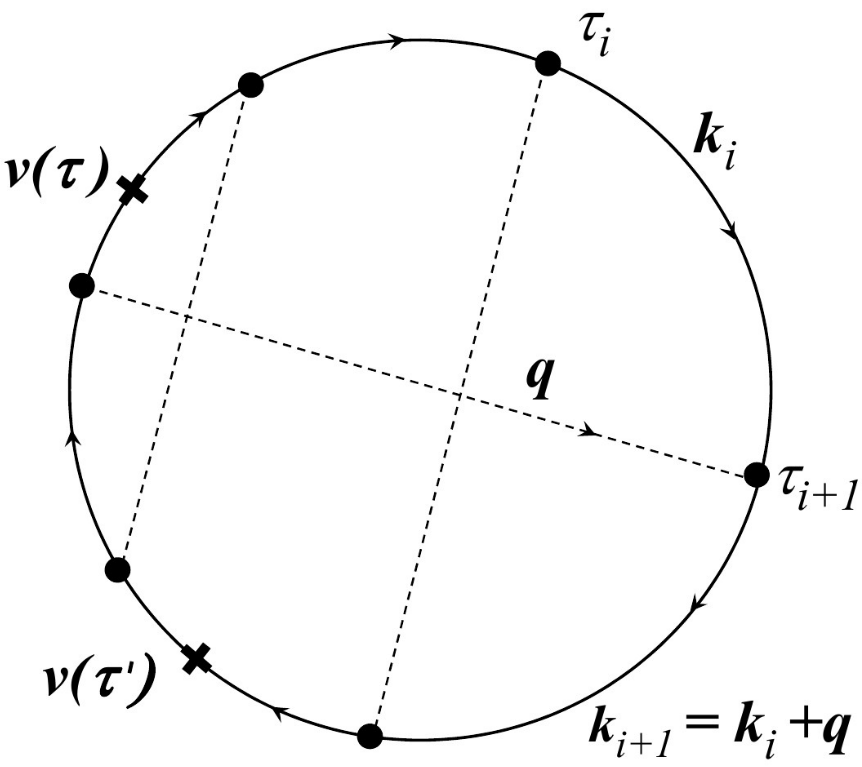
Hahn, Thomas, et al. Physical Review B 97.13 (2018): 134305.

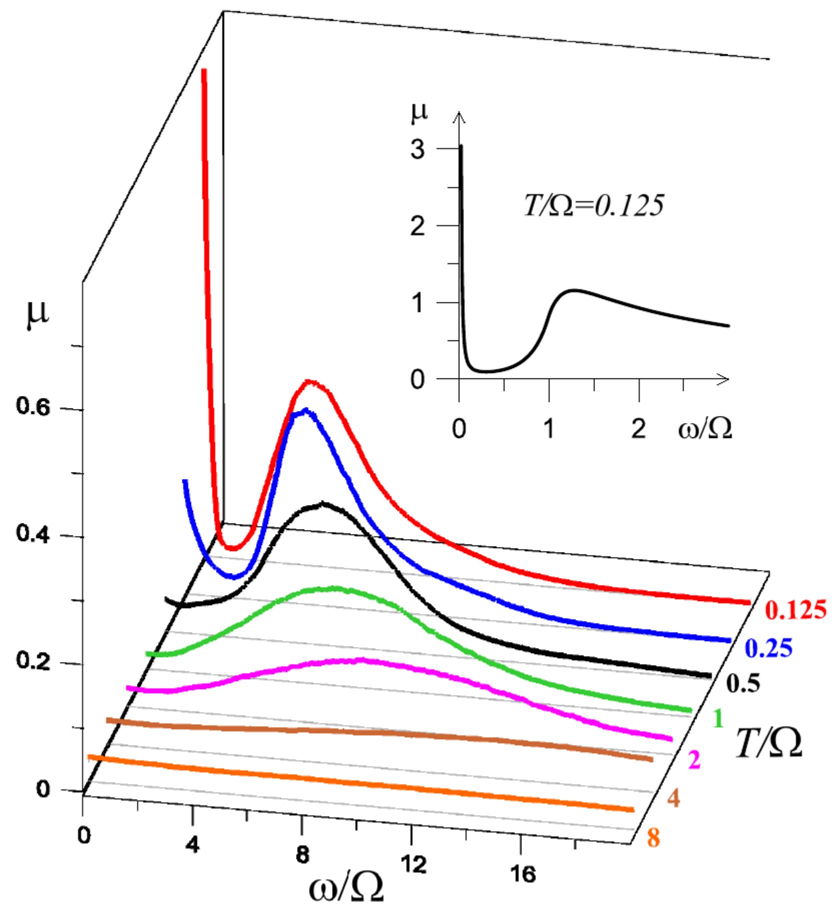
DiagMC – Holstein dispersion



Goodvin, Glen L. et al. Physical Review B 74.24 (2006): 245104.

DiagMC – Fröhlich mobility





Mishchenko, Andrey S., et al. Physical review letters 123.7 (2019): 076601.

Outline

1. General introduction to Monte Carlo methods
2. DiagMC – A toy example
3. General aspects of DiagMC
4. DiagMC applied to the polaron problem
5. DiagMC in particle physics

DiagMC in Particle Physics

- What kind of diagrammatic series?
- Sign problem? → Bold DiagMC
- Divergences?
- Renormalization?
- Combination of analytical methods and DiagMC
- Resummation techniques

References

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- DiagMC:
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