Universit t of Göttingen
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**Methods of omputational Physics**
**WiSe 2019/20**

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## Sheet 3: Quantum Monte- arlo simulation

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- **Diffusion Quantum Monte- arlo (DQM ) simulation for groundstate wavefunction**
  - Consider the one-dimensional harmonic oscillator with mass $m$ and frequency $\omega$. The potential energy takes the form

$$V(x) = \frac{1}{2} m\omega^2 x^2 \tag{1}$$

    Scale all length in units of $x_0 = \sqrt{\frac{}{m}}$ and all energies in units of $\omega$. Express the diffusion propagator and the weight change of the birth-and-death process of the DQMC algorithm in these units. Implement this algorithm in a program that calculates the wavefunction and the energy of the groundstate. Verify your program by comparison to the exact result.
  - How does the estimate for the groundstate energy depend on the imaginary time step, $\omega$ ?
  - If all replicas are initialized at position $x = 0$, how long do you have to propagate the system in imaginary time to converge towards the groundstate. Observe the converges in the DQMC simulation and provide a rational for the result.
  - Consider the double-well potential

$$\frac{V(x)}{\omega} = \frac{\left([x/x_0]^2 \quad d^2\right)^2}{8d^2} \tag{2}$$

    and study the wavefunction and the groundstate energy as a function of $d$. Explain your findings? Why do you have to propagate the longer in imaginary time the larger $d$ is?

- **Quantum Monte- arlo simulation for $T > 0$**
  - Consider again a single particle in one-dimensional space with mass, $m$, subjected to an external potential $V(x)$, according to Equation 1. The particle is in thermal equilibrium with a heat bath at temperature, $T$. s in the previous task, express the density matrix in position representation via a path integral, scaling position by $x_0$ and energies by $\omega$. Show that the only relevant parameters are the number of $N$ slices of the path integral and the ratio, $\omega/k_{\mathrm{B}}T$, of the energy of the oscillator and the thermal energy.
  - Study the world lines of the particle in the harmonic potential by the path-integral Monte-Carlo algorithm, using random local displacement of the positions, $x_i$, in the different slices $i = 1, \cdots, N$. Monte-Carlo Step (MCS) is defined by a set of moves, giving each $x_i$ the chance to be displaced once on average. How many MCS are necessary to generate independent configurations? Measure the potential and kinetic energy, and use known properties of the harmonic oscillator to verify your program.

– Update the conformation of the path integral by proposing $2^k \quad 1$ new sequential positions, $x_i$ with $i = j+1, \cdots, j+2^k \quad 1$ (applying periodic boundary conditions on the index, $i$) in one Monte-Carlo step using the Levy-bridge construction for the free propagator. To this end, use the conditional probability

$$P(x_{j \;\; n} | x_j, x_{j \;\; 2n}) \sim \exp\left( \quad \frac{2}{2b^2 n} \quad x_{j \;\; n} \quad \frac{x_j + x_{j \;\; 2n}}{2} \right]^2 \right) \tag{3}$$

where $b^2 = \langle [x_i \quad x_{i \;\; 1}]^2 \rangle = \frac{}{k_{\mathrm{B}} T N}$ (for the harmonic oscillator) denotes the average, mean-squared distance of positions in neighboring slices of a free particle, and construct the new positions recursively. Formulate the corresponding Monte-Carlo acceptance criterion and implement the Monte-Carlo move in your program. Verify the program by comparison with the previous results. Discuss on which parameters does a suitable choice of the length of the Levy bridge, $2^k$, depend?

– How much faster is this algorithm compared with the local displacement scheme?