Quantum Monte Carlo estimation of complex-time correlations for the study of ground-state spectral functions

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Motivation

- Quantum Monte Carlo methods: stochastic propagation in imaginary time $\Rightarrow$ accurate results for static properties
- Attempts to infer spectral functions from the inversion of Laplace transform: reliable results for the low-energy dynamics
- At finite temperature, real-time correlation function written in terms of a propagator in complex time:

$$C_{AB}(t) = \mathrm{Tr}\left(e^{-\beta\hat{H}}\, e^{it\hat{H}/\hbar}\,\hat{A}\, e^{-it\hat{H}/\hbar}\,\hat{B}\right)$$

Possibility to improve the calculation of the spectral functions

Objective of the work

Extend the formalism of complex-time correlation functions to ground-state calculations

- At $T = 0$, the complex time has no physical meaning
- Introduction of an **adjustable parameter**, i.e. the phase of complex time

Outline

1. Numerical Approach
   - Importance Sampling
   - Approximation for the time propagator
2. Results for model systems
   - Harmonic Oscillator
   - Anharmonic Oscillator
3. Conclusions and Perspectives

Complex-time correlation function

$$C_{AB}(t_c) \;=\; \langle \Psi_0 |\, e^{it_c \hat{H}/\hbar}\, \hat{A}\, e^{-it_c \hat{H}/\hbar}\, \hat{B}\, | \Psi_0 \rangle$$

Ground-state average of the product of the observable $\hat{A}$ at time t_c and the observable $\hat{B}$ at time 0

- The time $t_c = t_m e^{-i\delta}$ is considered as a **complex number**:
  - For $\delta = 0$, we recover the real time of Nature: correlation functions are inaccessible with QMC (dynamical sign-problem)
  - For $\delta = \pi/2$, we recover the imaginary time of usual QMC methods: ill-posed inversion procedure to get spectral functions
- Between these two cases, we can find an **optimal values** of δ

Complex-time correlation function

$$C_{AB}(t_c) = \mathcal{N} \int dx_0 dx_M \, A(x_M) \, G(x_0, x_M; t_c) \, B(x_0) \times \Psi_0(x_M) \, \Psi_0(x_0)$$

$C_{AB}(t_c)$ in coordinate space (assuming $\hat{A}$ and $\hat{B}$ diagonal):

- Ψ_0 is the ground state wave function
- $\mathcal{N}$ is a normalization constant
- $G(x_0, x_M; t_c) = \langle x_M | e^{-it_c \hat{H}} | x_0 \rangle$ is the time propagator, known only for small $t_m = |t_c| \Rightarrow$ Convolution property:

  $$G(x_0, x_M; t_c) = \int dx_1 \dots dx_{M-1} \prod_{k=1}^{M} G\left(x_k, x_{k-1}; \varepsilon_c\right)$$

  with $\varepsilon_c = t_c / M$.

Complex-time correlation function

$$C_{AB}(t_c) = \mathcal{N} \int dx_0 \dots dx_M \, A(x_M) \prod_{k=1}^{M} G(x_k, x_{k-1}; \varepsilon_c) \, B(x_0) \times \Psi_0(x_M) \, \Psi_0(x_0)$$

- Only if ε_c is purely imaginary, $G(x_0, x_M; \varepsilon_c)$ is real and positive definite
- In the general case, need to define a probability distribution p_{path} to sample the whole path $\{x_1, \dots, x_{M-1}\}$ from x_0 to x_M

Complex-time correlation function

$$C_{AB}(t_c) = \mathcal{N} \int dx_0 \ldots dx_M \; A(x_M) \, \frac{\prod_{k=1}^{M} G(x_k, x_{k-1}; \varepsilon_c)}{p_{path}(x_0, \ldots, x_M)} \, B(x_0) \times \Psi_0(x_M) \, \Psi_0(x_0) \, p_{path}(x_0, \ldots, x_M)$$

Complex-time correlation function

$$C_{AB}(t_c) = \mathcal{N} \int dx_0 \dots dx_M \, \underbrace{A(x_M) \frac{\prod_{k=1}^{M} G(x_k, x_{k-1}; \varepsilon_c)}{p_{path}(x_0, \dots, x_M)} B(x_0)}_{\text{Estimator}} \times \underbrace{\Psi_0(x_M)\,\Psi_0(x_0)\,p_{path}(x_0, \dots, x_M)}_{\text{Probability distribution}}$$

Probability distribution

Estimator

How to make QMC works

- Ψ_0 obtained with standard ground-state QMC techniques (e.g. PIGS method)
- Choice of the importance sampling for the paths
- Choice of the approximation for the time propagator

Importance Sampling

$$C_{AB}(t_c) = \mathcal{N} \int dx_0 \dots dx_M \; A(x_M) \frac{\prod_{k=1}^{M} G(x_k, x_{k-1}; \varepsilon_c)}{p_{path}(x_0, \dots, x_M)} B(x_0) \times \Psi_0(x_M)\, \Psi_0(x_0)\, p_{path}(x_0, \dots, x_M)$$

- Best choice: $p_{path}(x_0, \dots, x_M) = \left| \prod_{k=1}^{M} G(x_k, x_{k-1}; \varepsilon_c) \right|$
- For smooth potentials, a simple and flexible option for p_{path} is the product of M free propagators in imaginary time
- **The good choice for p_{path} depends on the value of t_c**

Approximation for the complex-time propagator

$$C_{AB}(t_c) = \mathcal{N} \int dx_0 \ldots dx_M \; A(x_M) \, \frac{\prod_{k=1}^{M} G(x_k, x_{k-1}; \varepsilon_c)}{p_{path}(x_0, \ldots, x_M)} \, B(x_0) \times \Psi_0(x_M) \, \Psi_0(x_0) \, p_{path}(x_0, \ldots, x_M)$$

- The accuracy of the results increases as ε_c decreases
- The statistical noise increases as the number M of convolutions increases

High-order approximations are needed to keep ε_c large and M small (Zillich *et al.*, J. Chem. Phys. (2010))

Harmonic Oscillator: complex-time correlations

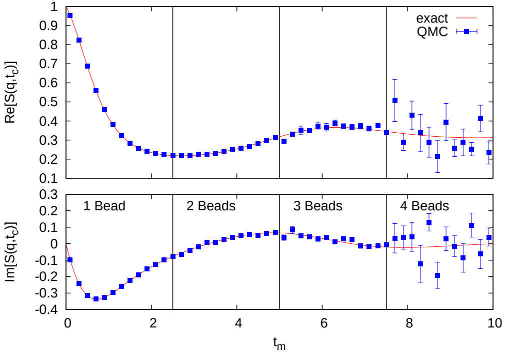
1D Harmonic oscillator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Density-density correlations

$$S(q,t_c) = \langle \Psi_0 | \hat{\rho}_q(t_c)\hat{\rho}_{-q}(0) | \Psi_0 \rangle$$
$$\hat{\rho}_q(t) = \sum_{i=1}^{N} e^{iqx_i(t)}$$

$S(q,t_c)$ with $t_c = t_m e^{-i\delta}$, $\delta = \pi/9$, $q = 1.5$



The whole range of t_m is divided in intervals $[(M-1)\varepsilon_m^*, M\varepsilon_m^*]$, each of which is calculated with M beads (ε_m^* is the maximum time reachable with a single bead)

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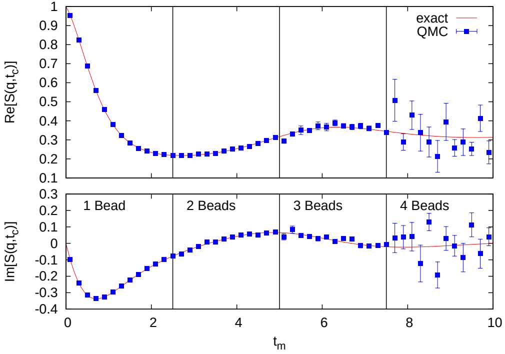
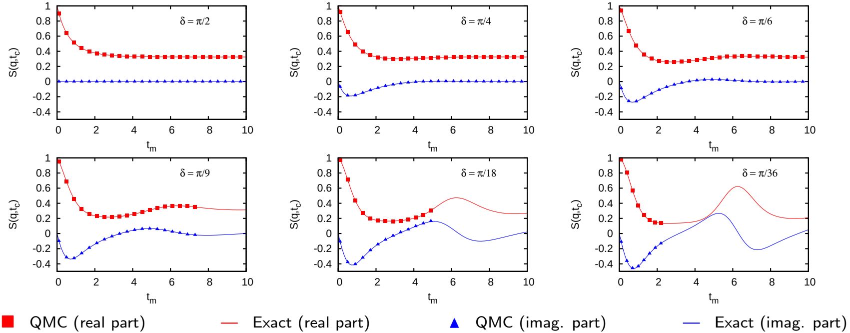


The results are **reliable up to a maximum value** of t_m, above which the statistical error explodes

From imaginary to real times

$S(q, t_c)$ for different phases δ ofthe complex time ($q = 1.5$)



Approaching the real axis (i.e. decreasing δ), $S(q, t_c)$ contains more information on the dynamics of the system, but the maximum time estimable with QMC gets smaller

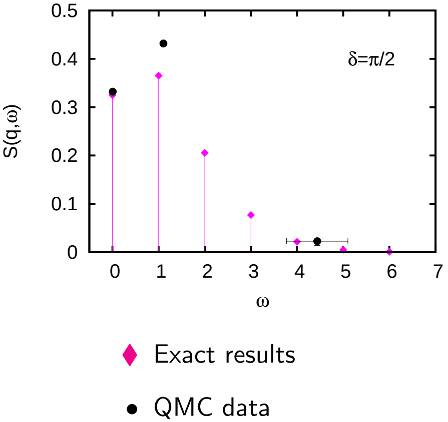
Dynamic structure factor $S(q, \omega)$

Dynamic structure factor vs. time correlation function

$$S(q, t_c) = \int d\omega \, e^{-it_c\omega} S(q, \omega)$$

- Inversion technique: Tikhonov regularization of the psuedo-inverse matrix
- Decreasing δ, the ill-posed nature of the inversion is reduced $\Rightarrow$ QMC data in better agreement with exact results

$q = 1.5$



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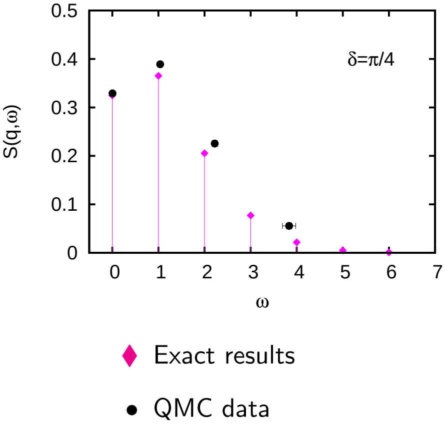

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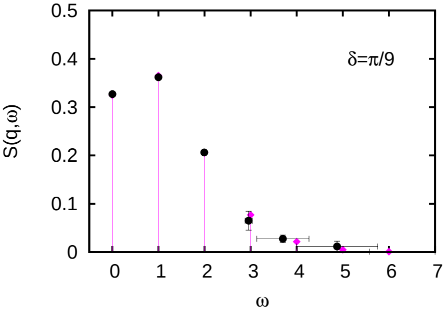

Exact results

QMC data

Dynamic structure factor $S(q, \omega)$

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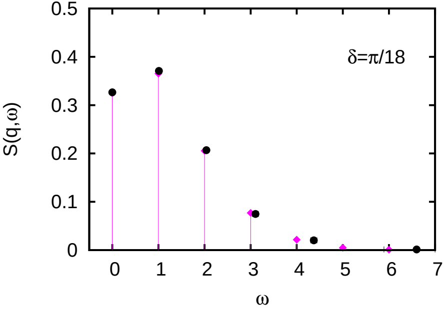
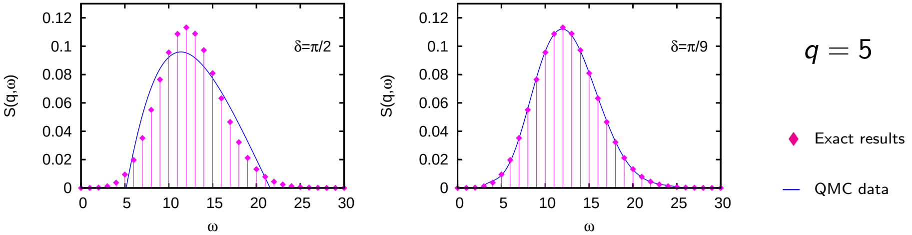


Exact results

QMC data

Dynamic structure factors at large momentum

At large q, the number of modes contributing to $S(q, \omega)$ increases

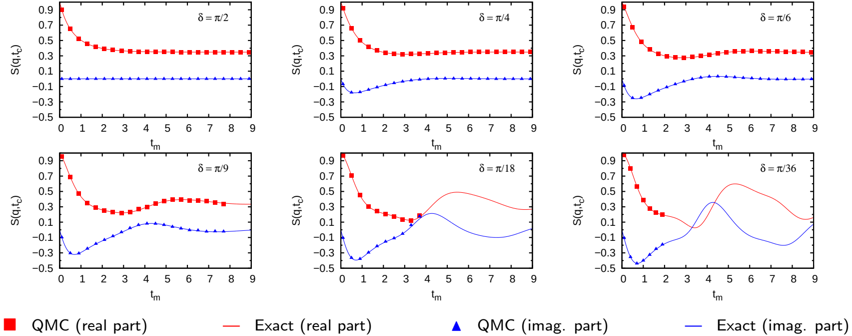


$q = 5$

- Imaginary time: QMC data recover the position and roughly the height of the peak
- Complex time: QMC data reproduce accurately **the shape of the spectrum**

Anharmonic Oscillator: complex-time correlations

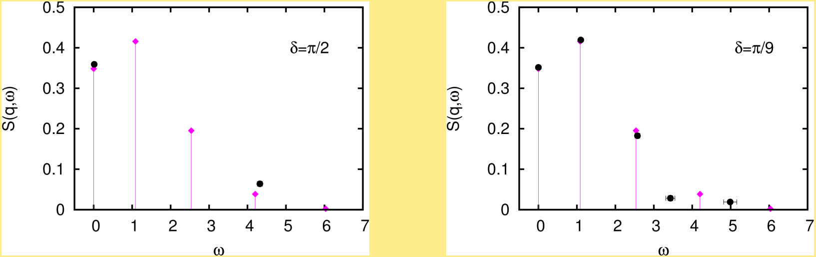
1D Quartic oscillator: $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{4}\lambda x^4$



Same qualitative behavior as HO: QMC data reliable up to a maximum value of t_m which decreases as δ decreases.

Anharmonic Oscillator: dynamic structure factors

Small momentum ($q = 1.5$)

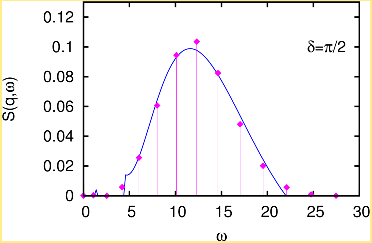


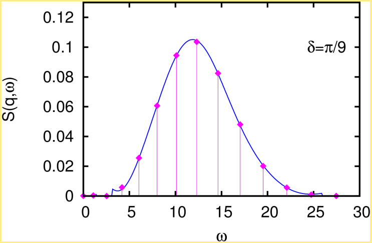
♦ Exact results ● QMC data

Results for the AO confirm the improvement in the calculation of the spectral functions

Anharmonic Oscillator: dynamic structure factors

Large momentum ($q = 5$)





♦ Exact results — QMC data

Results for the AO confirm the improvement in the calculation of the spectral functions

Conclusions and Perspectives

We propose a new QMC strategy to study dynamic response of quantum systems at zero temperature

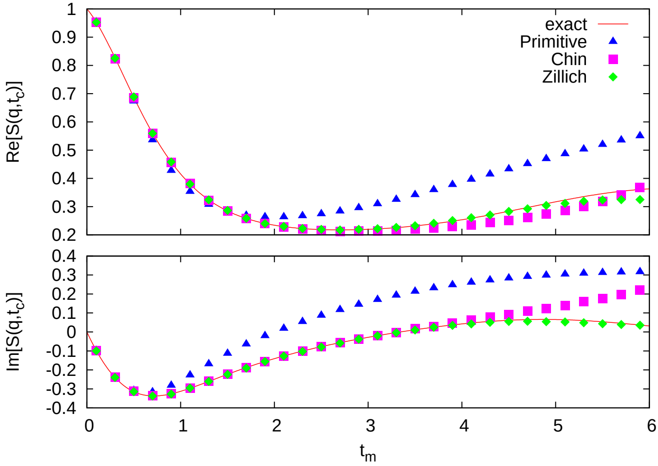
- Calculation of correlation functions for times analytically continued in the complex plane
- Ill-posed nature of the inversion procedure highly reduced: accurate results for the spectral function obtainable with simple regularization techniques
- Use of high-order approximation for the propagator crucial to get reliable data up to large times
- **Future perspectives**: extend the formalism to systems of physical interest (3D many-body systems)

THANK YOU
FOR YOUR ATTENTION

Approximations for the complex-time propagators

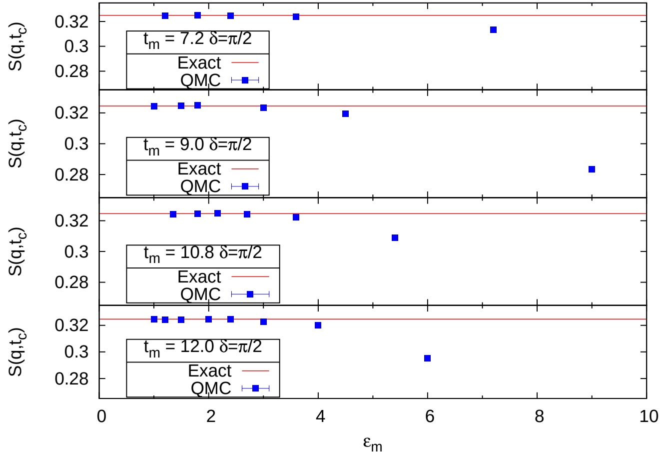
$S(q, t_c)$ with $t_c = t_m e^{-i\delta}$, $\delta = \pi/9$

Results with $M = 1$ bead ($q = 1.5$)



Optimization of ε_m^*

$S(q, t_c)$ for a fixed value of $t_c = t_m e^{-i\delta}$ as a function of $\varepsilon_m = t_m/M$ (M is the number of convlution terms)



ε_m^* does not depend on $\delta \Rightarrow$
optimization performed for purely imaginary times

Tikhonov regularization technique

$$S(q, t_c) = \int d\omega \, e^{-it_c\omega} S(q, \omega)$$

Inversion procedure

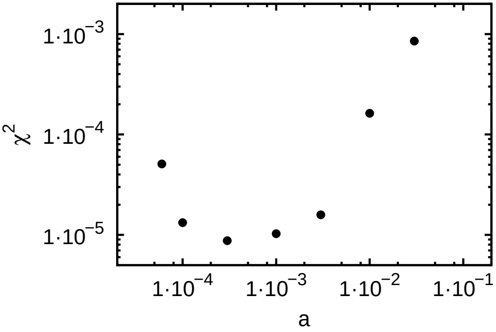
$$y = Ax \quad (1)$$

$$x = A^T(AA^T)^{-1}y \quad (2)$$

$$x = A^T(AA^T + \mathbb{1}a)^{-1}y \quad (3)$$

χ^2 between $C_{QMC}(t_c)$ and $C_{INV}(t_c, a)$

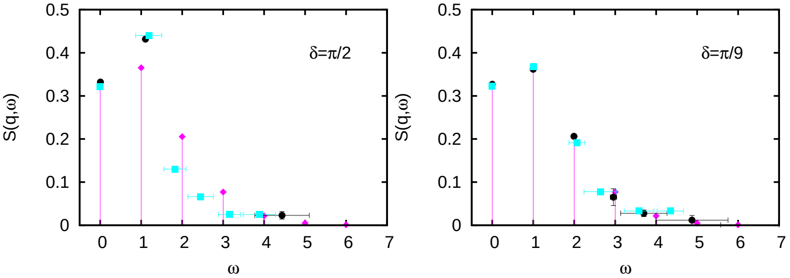
- $C_{QMC}(t_c)$ = QMC data for complex time correlation function
- $C_{INV}(t_c, a)$ = complex time correlation function from the transform of the spectrum obtained from Tikhonov regularization with parameter a



- Small a: unstable inversion procedure
- Large a: regularization technique affects the results

Stability of the inversion technique

$S(q,\omega)$ for HO with $q = 1.5$



- Exact results
- Tikhonov regularization
- Optimization with simulated annealing