Path integral estimation of complex-time correlation functions

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In collaboration with: R. Rota, G. Ferré, F. Mazzanti, and J. Casulleras

Outline

- Introduction. Complex-time correlation function
- The PIGS method for the ground state
- PIGS estimation of response in complex time
- Results for 1D HO and x^4
- Results for $N > 1$
- Other approaches: CBF/QMC for $T = 0$ and imaginary-time data at $T > 0$
- Remarks

Introduction

- In Quantum Monte Carlo methods we do not have real-time but imaginary-time dynamics.

- Dynamics in real time is therefore not achievable.

- To access to the dynamic structure function $S(q,\omega)$ from imaginary-time correlation functions requires of inverse Laplace transform $\Longrightarrow$ Ill-posed problem,

$$S(q,\omega) = \int d\tau \; e^{\tau\omega} S(q,\tau)$$

with $S(q,\tau)$ the imaginary-time correlation function computed with QMC.

- Is it possible to go beyond ? We are trying to do it ...

Complex-time correlation function

The imaginary-time correlation correlation function $S(q,\tau)$ is a smooth function with *few* information on excitations.

To get more insight our goal is to calculate the correlation function in complex time,

$$S(q,t_c) = \langle \Psi_0 | e^{it_c \hat{H}/\hbar} \hat{\rho}_q e^{-it_c \hat{H}/\hbar} \hat{\rho}_{-q} | \Psi_0 \rangle \ ,$$

with $\hat{\rho}_q = \sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r}}$ and where the time $t_c = t_m e^{-i\delta}$ is a complex number.

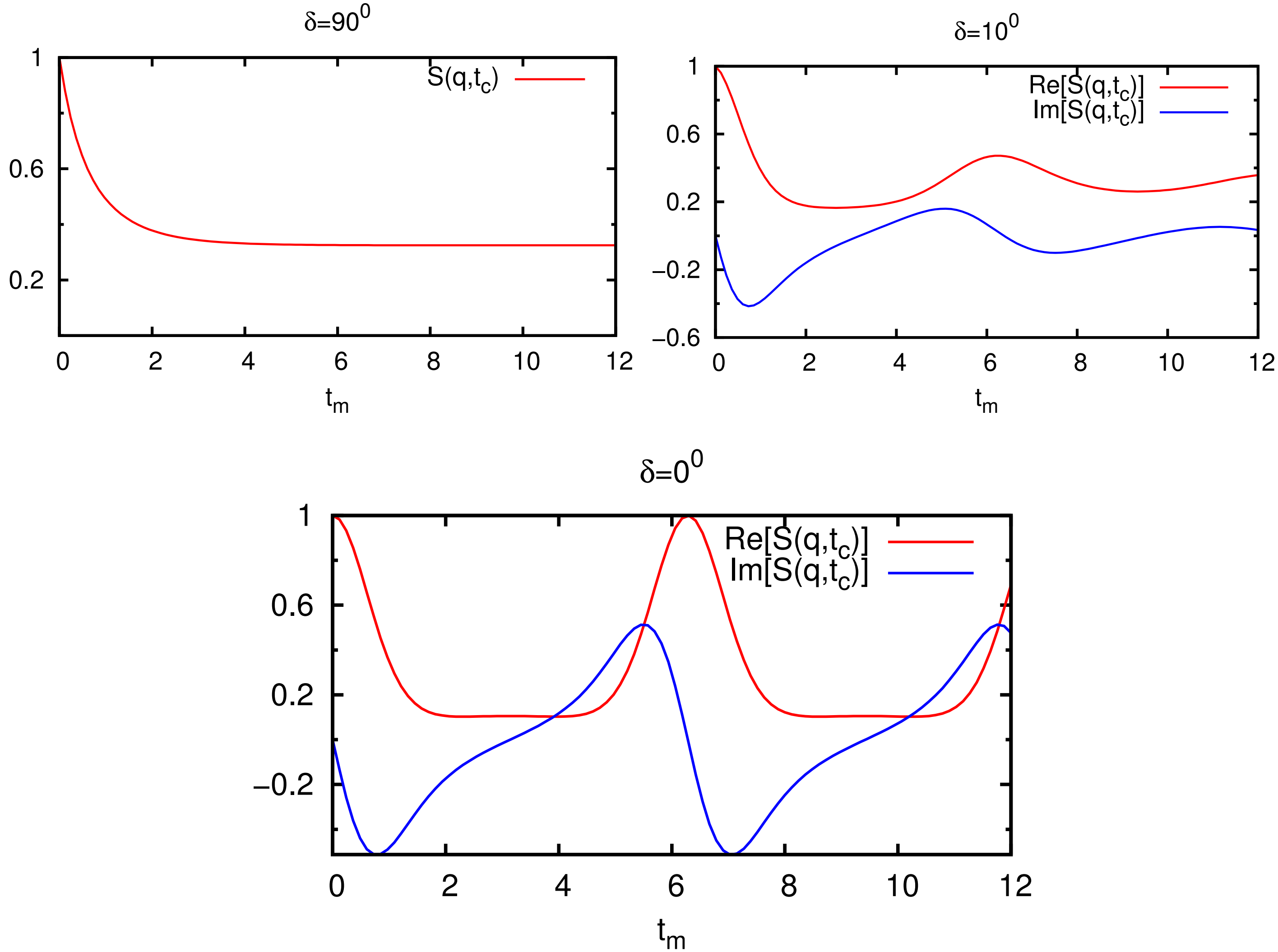
$$\delta = 0 \Longrightarrow \text{Real time}$$

$$\delta = \pi/2 \Longrightarrow \text{Imaginary time}$$

Here, we restrict our estimation to $T=0$. Access to the ground-state wave function Ψ_0 provided by QMC (Path Integral Ground State (PIGS) method).

Behavior with δ

Exact results for one particle in 1D harmonic potential

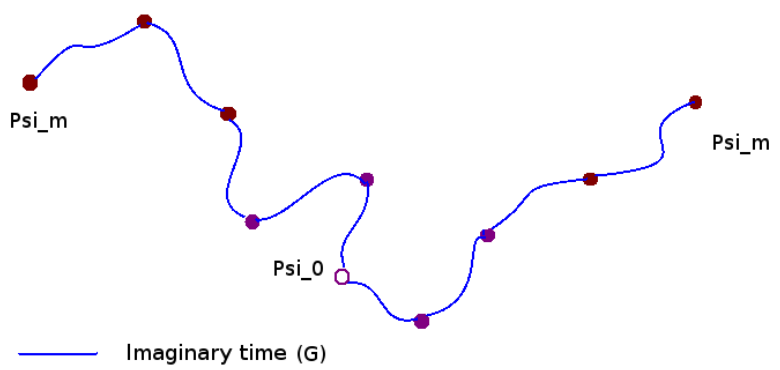


Ground state: PIGS method

To sample complex-time correlation factors we need to know the ground-state wave function Ψ_0. For that we use the PIGS method (A. Sarsa *et al.*, JCP **113**, 1366 (2000); R. Rota *et al.*, PRE **81**, 016707 (2010))

$$\Psi_0(\boldsymbol{R}) = \int d\boldsymbol{S}\; G(\boldsymbol{R},\boldsymbol{S};\tau)\Psi_{\mathrm{m}}(\boldsymbol{S})$$

Assuming an approximation for $G(\boldsymbol{R},\boldsymbol{S};\tau)$, when $\tau \to 0$, and convoluting until convergence one arrives to the ground state



Ground state: PIGS method

Green's function $G(\boldsymbol{R},\boldsymbol{S};\tau)$ is accurate to fourth order in τ (S. A. Chin and C. R. Chen, JCP **117**, 1409(2002)

$$e^{-\tau\hat{H}} = e^{-v_1\tau\,\hat{W}_1} e^{-t_1\tau\,\hat{T}} e^{-v_2\tau\,\hat{W}_2} e^{-2t_0\tau\,\hat{T}} e^{-v_2\tau\,\hat{W}_2} e^{-t_1\tau\,\hat{T}} e^{-v_1\tau\,\hat{W}_1}$$

with $\hat{W}_i = \hat{V} + u_0/(3v_i)\tau^2\,[\hat{V},[\hat{T},\hat{V}]]$ and t_0 a parameter to optimize.

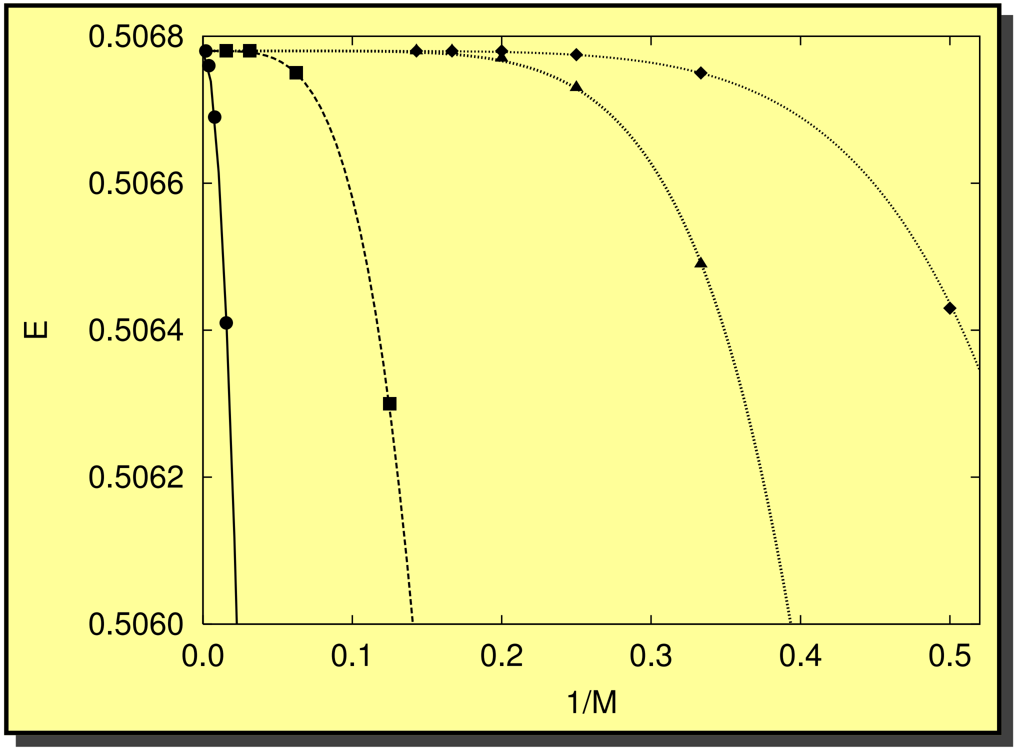
Unbiased (pure) estimations of *any* operator $\hat{O}$ can be calculated in the center of the chain,

$$\langle\hat{O}\rangle = \mathcal{N}^{-1}\langle\Psi_{\mathrm{m}}|G(\varepsilon/2)\hat{O}G(\varepsilon/2)|\Psi_{\mathrm{m}}\rangle$$

- Results are independent of Ψ_{m}; convergence to the ground state are not.
- Cheaper than PIMC in computer time.

Performance of different actions

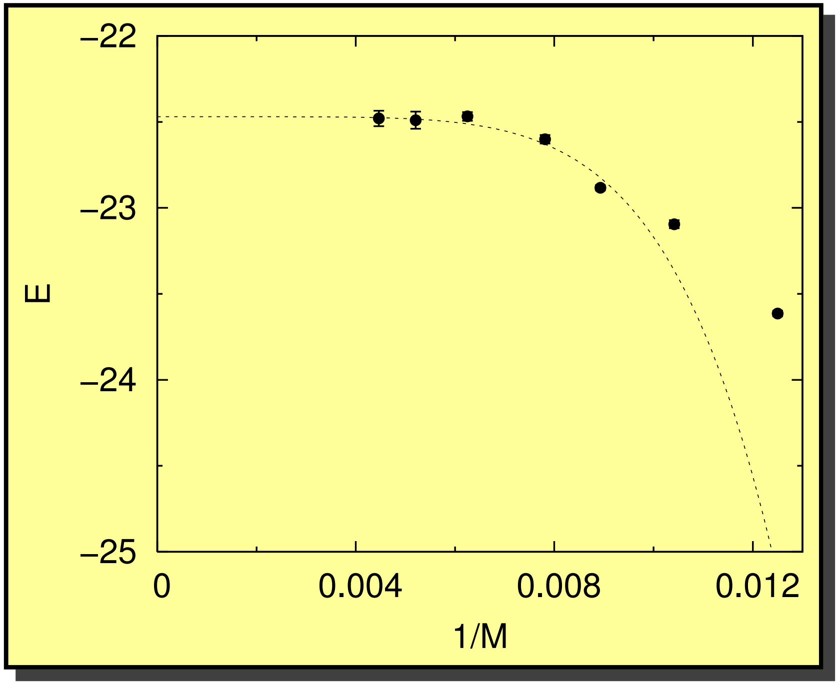
Harmonic oscillator $(T = 0.2)$

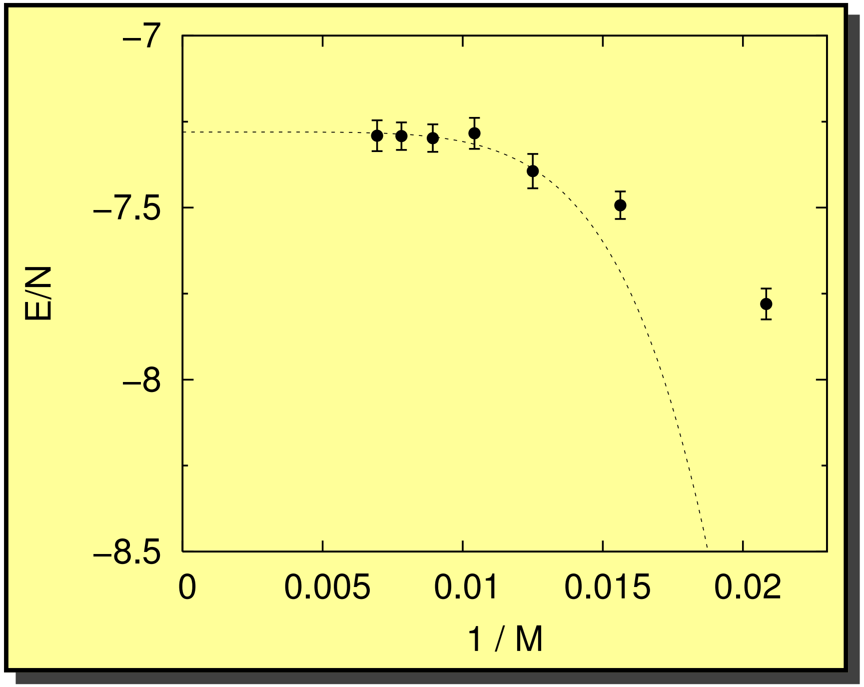


● $\rightarrow$ PA $(M = 512)$ ■ $\rightarrow$ TIA $(M = 128)$

▲ $\rightarrow$ Chin-t_0 $(M = 6)$ ♦ $\rightarrow$ Chin-(t_0,a_1) $(M = 4)$

Performance of different actions





H_2 drop with 22 molecules

$T = 1.0$ K

Liquid ^{4}He

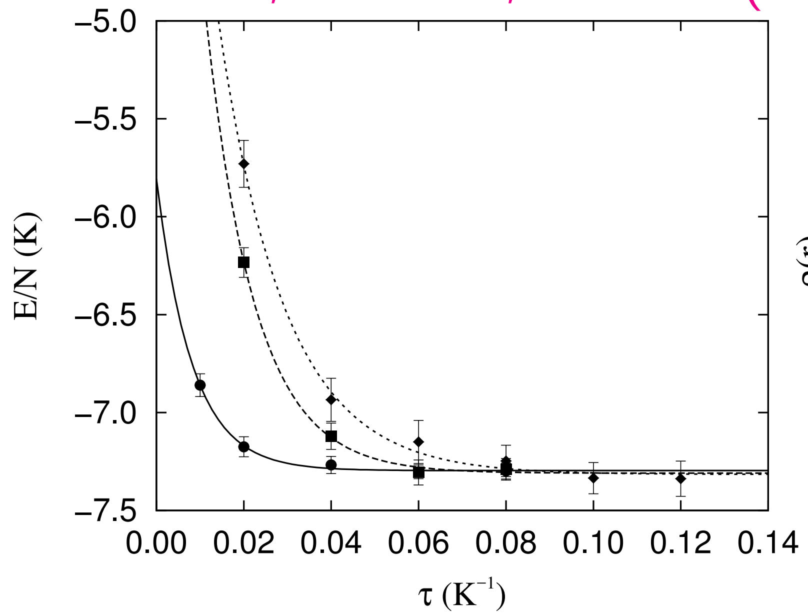
$T = 0.8$ K

The lines correspond to 6th order fits:

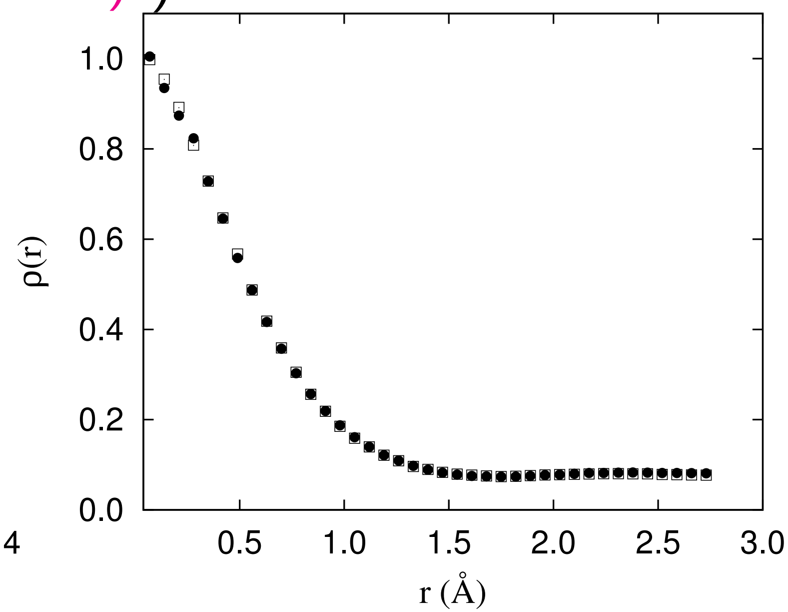
$$E/N = (E/N)_0 + A(1/M)^6$$

Ground state: PIGS method

Results for the ground state of liquid ^{4}He at zero temperature (R. Rota *et al.*, PRE **81**, 016707 (2010))



Energy



One-body distribution function

- Fast convergence: $N_b < 12$
- Pure estimation, even for non-diagonal operators $\rho(r)$

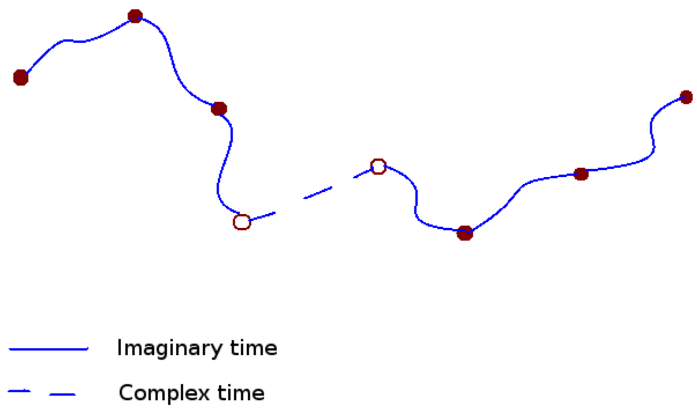
PIGS and complex time

- Our goal is to estimate the complex-time function

$$S(q,t_c) = \int dR_0 dR_M \, e^{it_c E_0} \langle \Psi_0 | R_M \rangle \langle R_M | \hat{\rho}_q e^{-it_c \hat{H}} \hat{\rho}_{-q} | R_0 \rangle \langle R_0 | \Psi_0 \rangle$$
$$= \int dR_0 dR_M \, \Psi_0(R_M) \rho_q(R_M) G(R_0, R_M; t_c) \rho_{-q}(R_0) \Psi_0(R_0) \; ,$$

with $G(R_0, R_M; t_c) = \langle R_M | e^{-it_c(\hat{H}-E_0)} | R_0 \rangle$ using PIGS.

- Use of a combined strategy: imaginary-time until the ground-state Ψ_0 and complex-time estimation of length $t_m = |t_c|$ in the center



PIGS and complex time

- Convolution in complex time

$$G(R_0, R_M; t_c) = \int dR_1 \ldots dR_{M-1} \prod_{k=1}^{M} G\left(R_k, R_{k-1}; \frac{t_c}{M}\right)$$

- We build the path using importance sampling, with a product of free propagators in imaginary time with step τ_s

$$p_{\mathsf{path}}(R_0, R_1, \ldots, R_M) = \prod_{k=1}^{M} G_{\mathsf{free}}(R_k, R_{k-1}; \tau_s) \ ,$$

- The complex-time propagator to be sampled is given by

$$G(R_0, R_M; t_c) \quad = \quad \int dR_1 \ldots dR_{M-1} \prod_{k=1}^{M} \frac{G(R_k, R_{k-1}; \varepsilon_c)}{\exp\left(-\frac{(R_k - R_{k-1})^2}{4\lambda\tau_s}\right)} \times$$
$$p_{\mathsf{path}}(R_0, R_1, \ldots, R_M)$$

PIGS and complex time

- Easiest approximation for the propagator: primitive action (PA)

$$G_{\mathsf{PA}}(R_k, R_{k-1}; \varepsilon_c) = \exp\left(-\frac{(R_k - R_{k-1})^2}{4\lambda\, i\varepsilon_c}\right) \exp\left(-i\frac{V(R_k) + V(R_{k-1})}{2\hbar}\varepsilon_c\right)$$

- Writing $\varepsilon_c = \varepsilon_m e^{-i\delta}$,

$$\prod_{k=1}^{M} \frac{G_{\mathsf{PA}}(R_k, R_{k-1}; \varepsilon_c)}{G_{\mathsf{free}}(R_k, R_{k-1}; \tau_s)} \sim \exp(C_{\mathsf{PA}}) \exp(iA_{\mathsf{PA}})$$

with

$$C_{\mathsf{PA}} = \sum_{k=1}^{M} \left[-\frac{(R_k - R_{k-1})^2}{4\lambda} \left(\frac{\sin\delta}{\varepsilon_m} - \frac{1}{\tau_s} \right) - \varepsilon_m \frac{V(R_k) + V(R_{k+1})}{2\hbar} \sin\delta \right]$$

and

$$A_{\mathsf{PA}} = \sum_{k=1}^{M} \left[\frac{(R_k - R_{k-1})^2}{4\lambda\varepsilon_m} \cos\delta - \varepsilon_m \frac{V(R_k) + V(R_{k+1})}{2\hbar} \cos\delta \right]$$

PIGS and complex time

- PA is not a good choice due to its low convergence; in case of Chin action (CA) and one bead (ε_m),

$$
\begin{aligned}
C_{\mathsf{CA}} \;=\; & \sum_{j=1}^{4} \Bigg[\left(- \frac{(R_{k,j+1} - R_{k,j})^2}{4\lambda t_j} \right) \left(\frac{\sin\delta}{\varepsilon_m} - \frac{1}{\tau_s} \right) + \\
& \left(-\varepsilon_m v_j \frac{V(R_{k,j+1}) + V(R_{k,j})}{2\hbar} \right) \sin\delta + \\
& \left(\varepsilon_m^3 \frac{u_0}{3} \frac{W(R_{k,j+1}) + W(R_{k,j})}{2\hbar} \right) \sin(3\delta) \Bigg]
\end{aligned}
$$

and

$$
\begin{aligned}
A_{\mathsf{CA}} \;=\; & \sum_{j=1}^{4} \Bigg[\left(\frac{(R_{k,j+1} - R_{k,j})^2}{4\lambda t_j \varepsilon_m} \right) \cos\delta + \\
& \left(-\varepsilon_m v_j \frac{V(R_{k,j+1}) + V(R_{k,j})}{2\hbar} \right) \cos\delta + \\
& \left(\varepsilon_m^3 \frac{u_0}{3} \frac{W(R_{k,j+1}) + W(R_{k,j})}{2\hbar} \right) \cos(3\delta) \Bigg]
\end{aligned}
$$

PIGS and complex time

CA is a better action than PA but in complex time introduces a divergence in the term $\exp(C_{\mathsf{CA}})$,

$$\varepsilon_m^3 \frac{u_0}{3} \frac{W(R_{k,j+1}) + W(R_{k,j})}{2\hbar} \sin(3\delta)$$

when $\delta < 60^0$

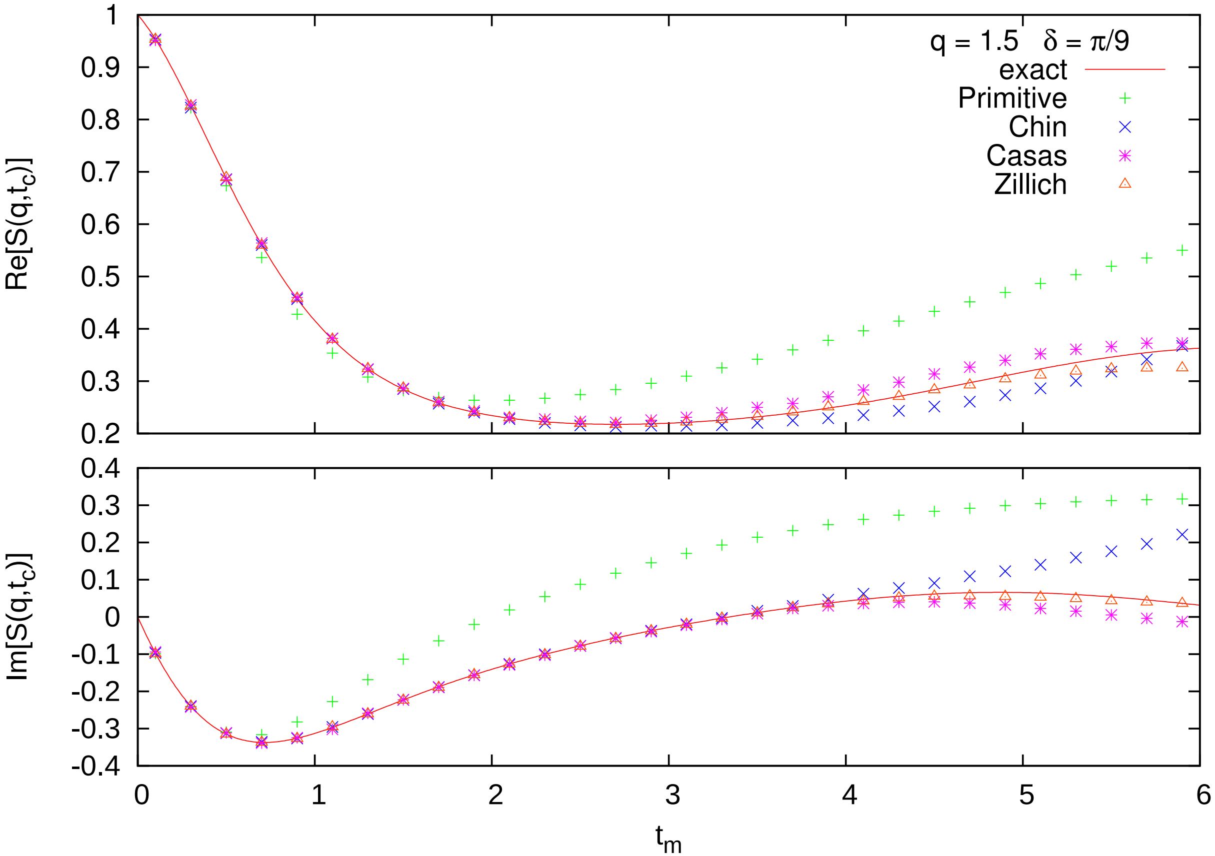
To circumvent this problem we have worked with other expansions

- Sixth-order expansion (Zillich *et al.*, JCP **132**, 044103 (2010))

$$\frac{64}{45} e^{-t_c \hat{V}/8} e^{-t_c \hat{K}/4} e^{-t_c \hat{V}/4} e^{-t_c \hat{K}/4} e^{-t_c \hat{V}/4} e^{-t_c \hat{K}/4} e^{-t_c \hat{V}/4} e^{-t_c \hat{K}/4} e^{-t_c \hat{K}/8}$$
$$-\frac{4}{9} e^{-t_c \hat{V}/4} e^{-t_c \hat{K}/2} e^{-t_c \hat{V}/2} e^{-t_c \hat{K}/2} e^{-t_c \hat{V}/4} + \frac{1}{45} e^{-t_c \hat{V}/2} e^{-t_c \hat{K}} e^{-t_c \hat{V}/2}$$

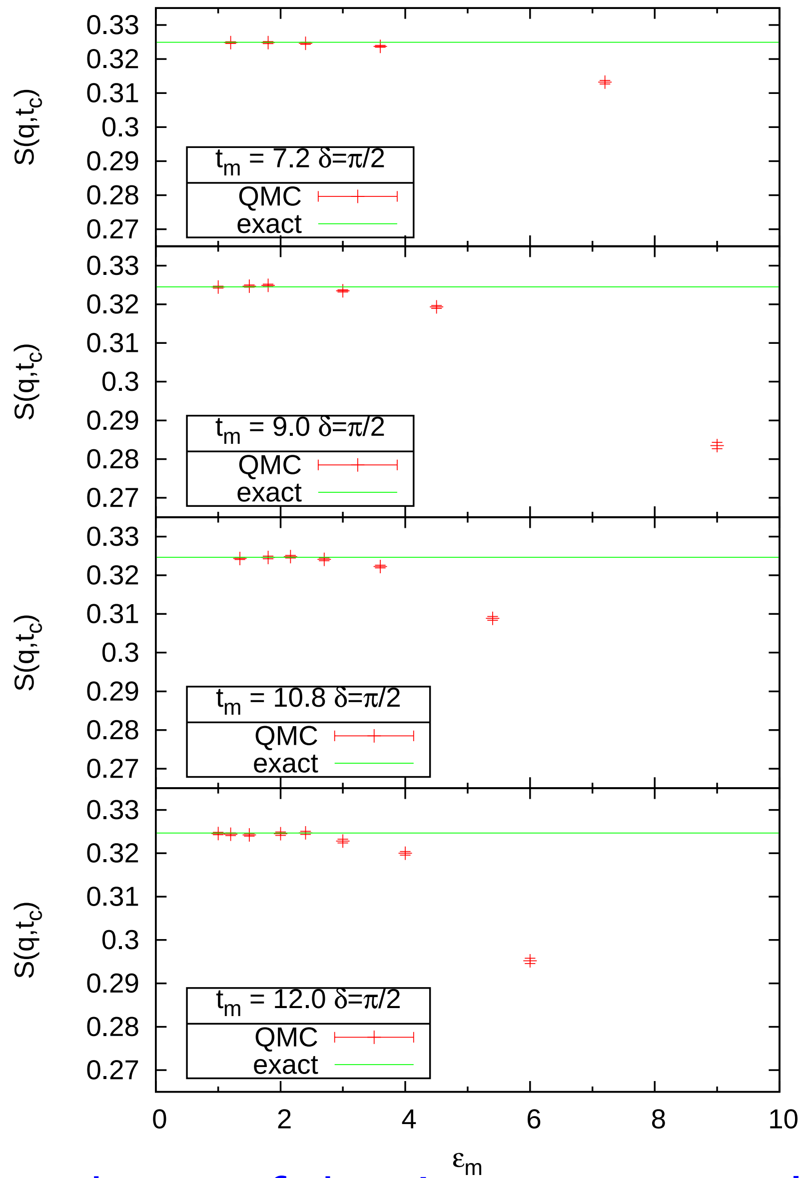
In some cases we verified that it is better to reduce the order of the expansion ($N > 1$)

PIGS and complex time



$S(q, t_c)$ with complex time $t_c = t_m e^{-i\delta}$ when $\delta = \pi/9$: the red lines are the exact analytical results, the symbols are QMC results obtained with $M = 1$ bead and with different approximation schemes for the complex-time propagator.

PIGS and complex time

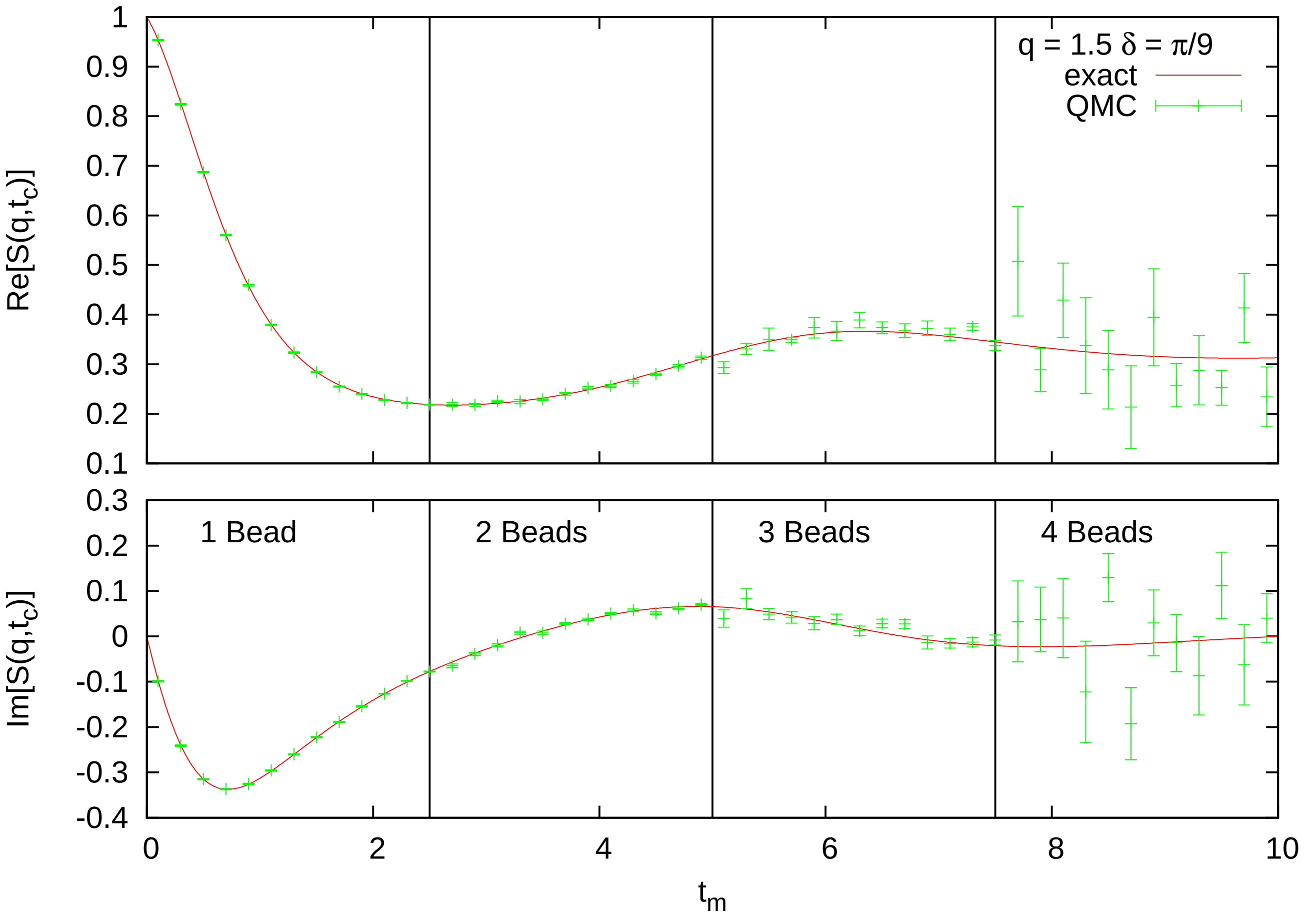


Time-step dependence of density response calculation (HO)

PIGS and complex time

- For this action (ZC) we can take an optimal time per bead of $\varepsilon_m^* = 2.5$
- The number of beads in complex time is determined with the condition $\varepsilon_m = |t_c|/M \leq \varepsilon_m^*$
- The time step τ_s for importance sampling is taken as $\tau_s \simeq \varepsilon_m / \sin\delta$
- Statistical errors increase with the number of beads in complex time. In practice, there is a maximum t_c attainable which decreases with δ

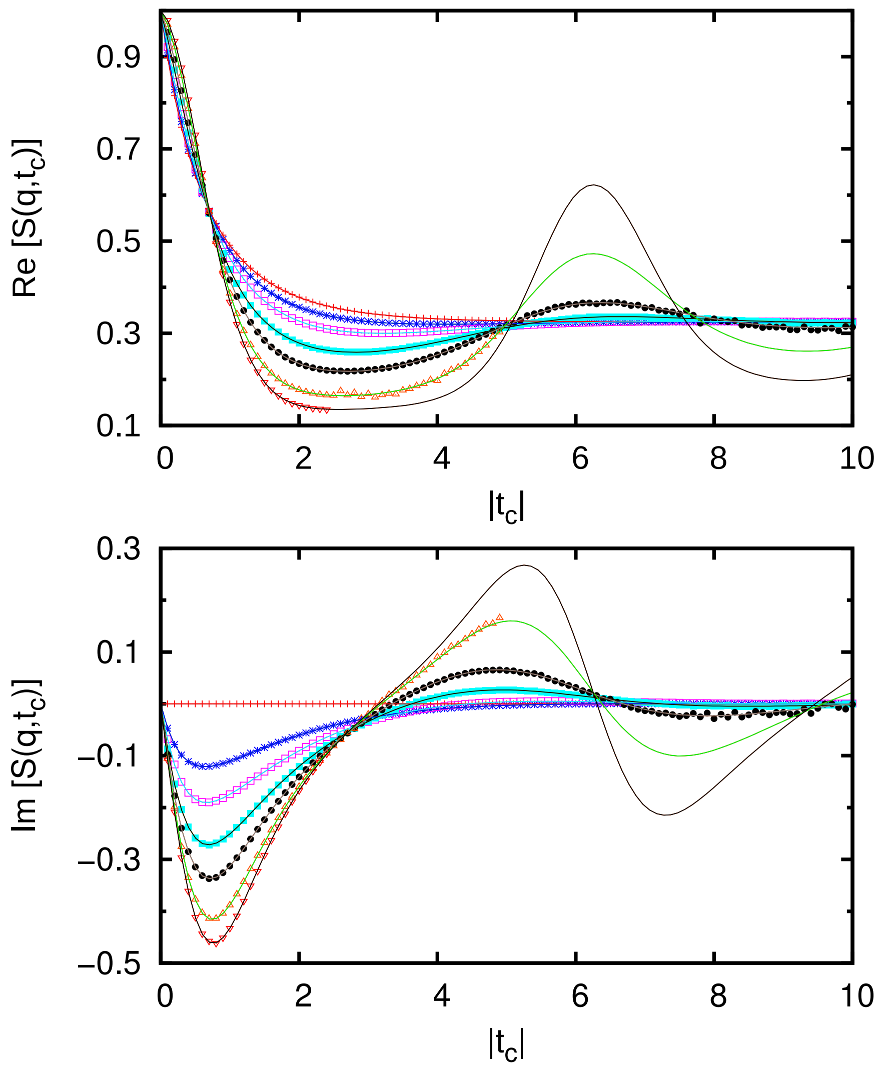
PIGS and complex time



PIGS HO results with different number of beads in complex time

$$S^{\text{exact}}_{\text{HO}}(q,t_c) = \exp\left[\frac{q^2}{2}\left(e^{-it_c} - 1\right)\right]$$

HO Results



R. Rota *et al.*, JCP **142**, 114114 (2015)

Extracting $\mathbf{S(q,\omega)}$

The complex-time response obtained with PIGS is the transform of the dynamic response

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

with $t_c = t_m e^{i\delta}$

When $\delta = 0$ one recovers the Fourier transform

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

If $\delta = \pi/2$ one has to solve the Laplace transform

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

Extracting $\mathbf{S(q,\omega)}$

In practice, one assumes a simple model for $S(q,\omega)$ such as

$$S(q,\omega) = \sum_i \xi_i \, \delta(\omega - \omega_i)$$

or

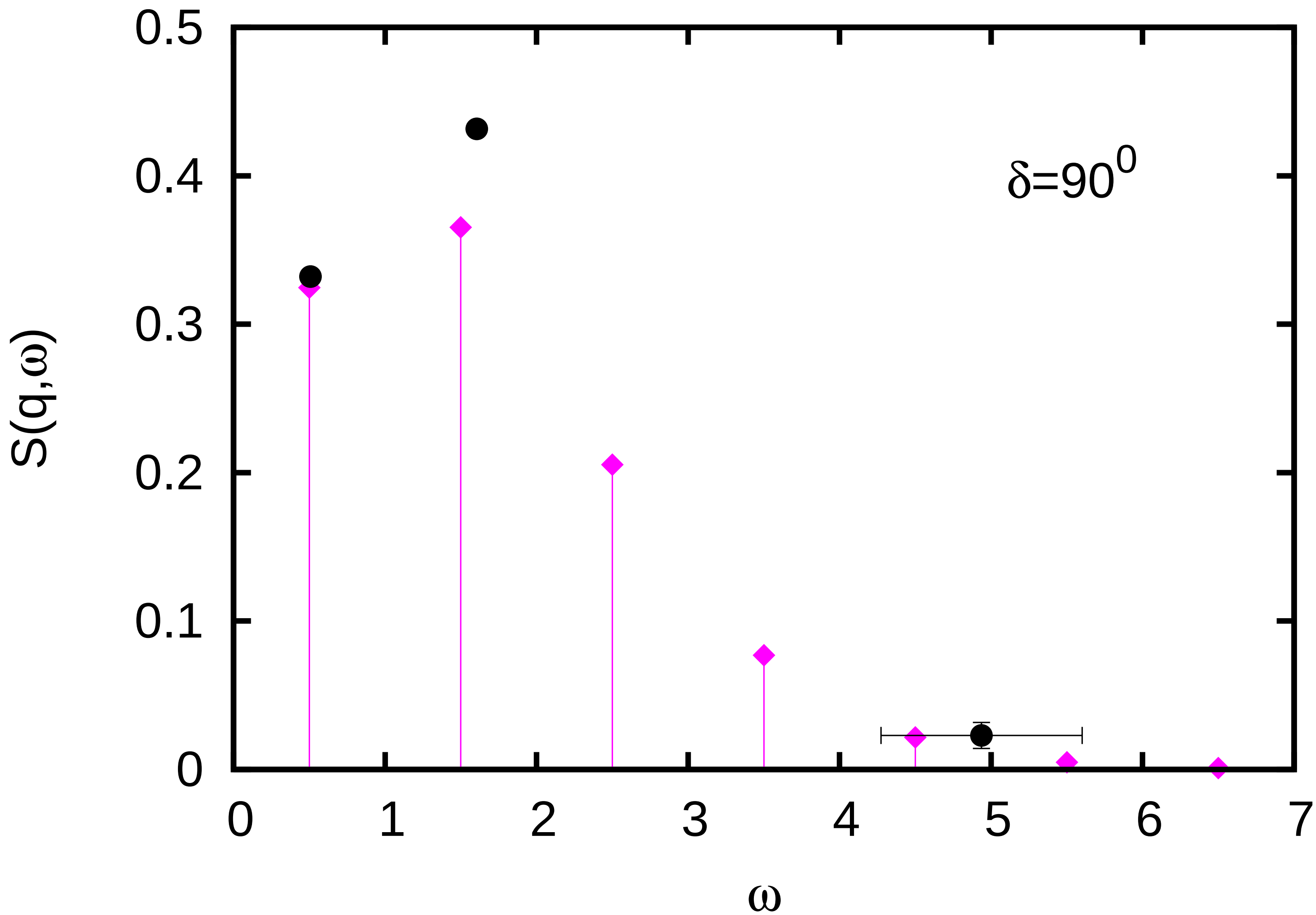
$$S(q,\omega) = \sum_i \xi_i \, \Theta(\omega - \omega_i)\Theta(\omega_{i+1} - \omega)$$

Optimal values for ξ_i and ω_i are obtained using different methods

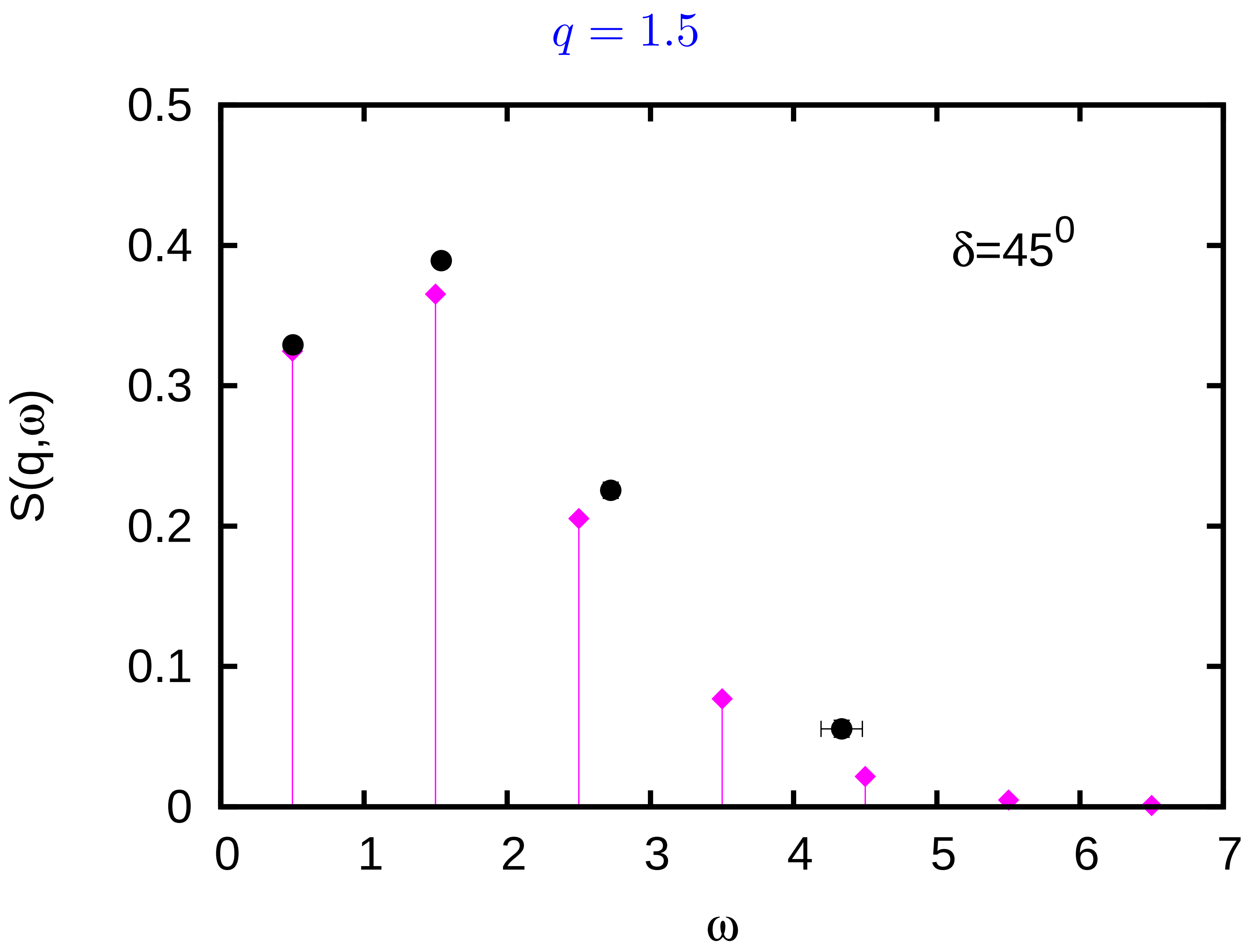
- Stochastic optimization methods: simulated annealing, genetic algorithm
- A regularization method; Tikhonov approximation

HO $S(q,\omega)$

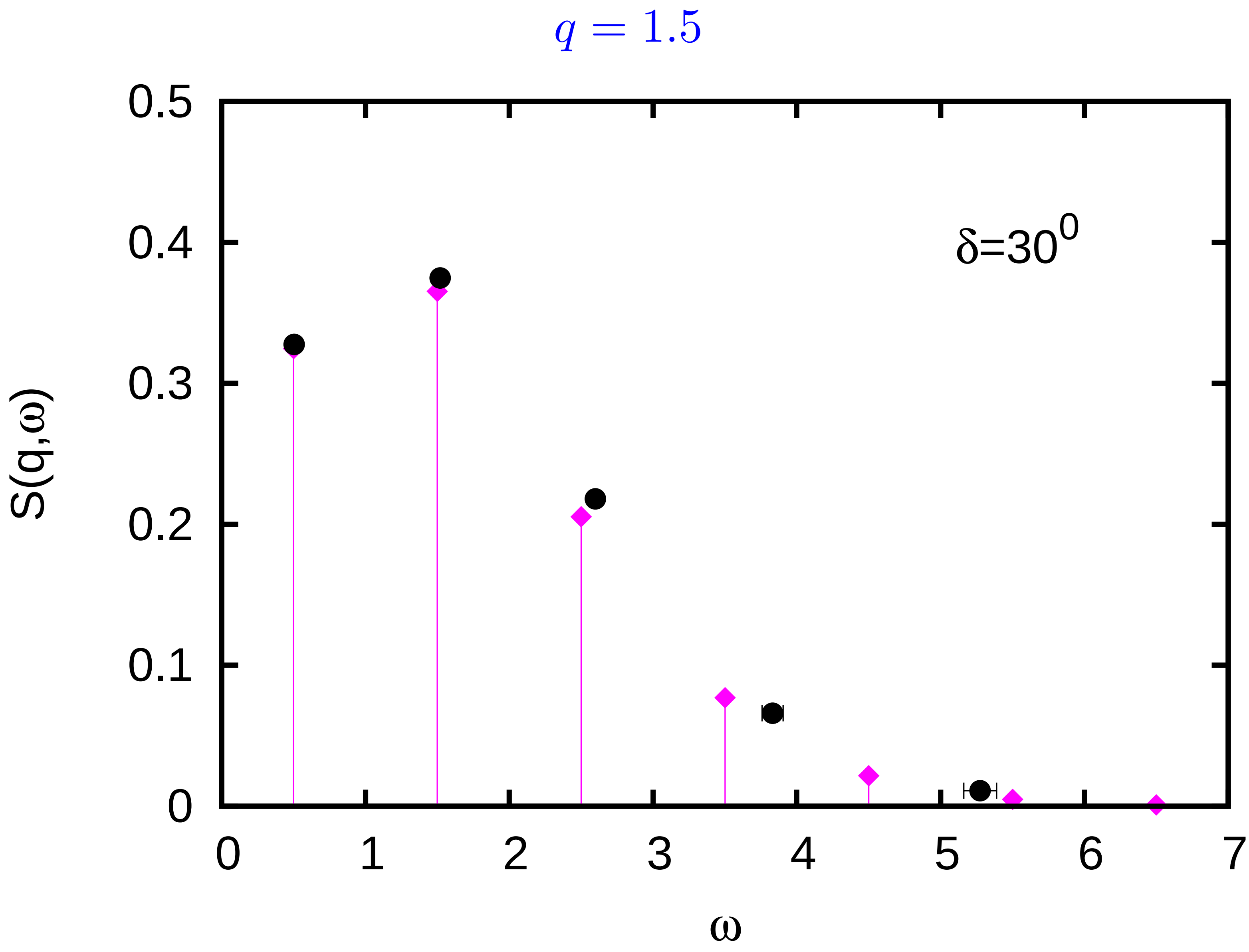
$q = 1.5$



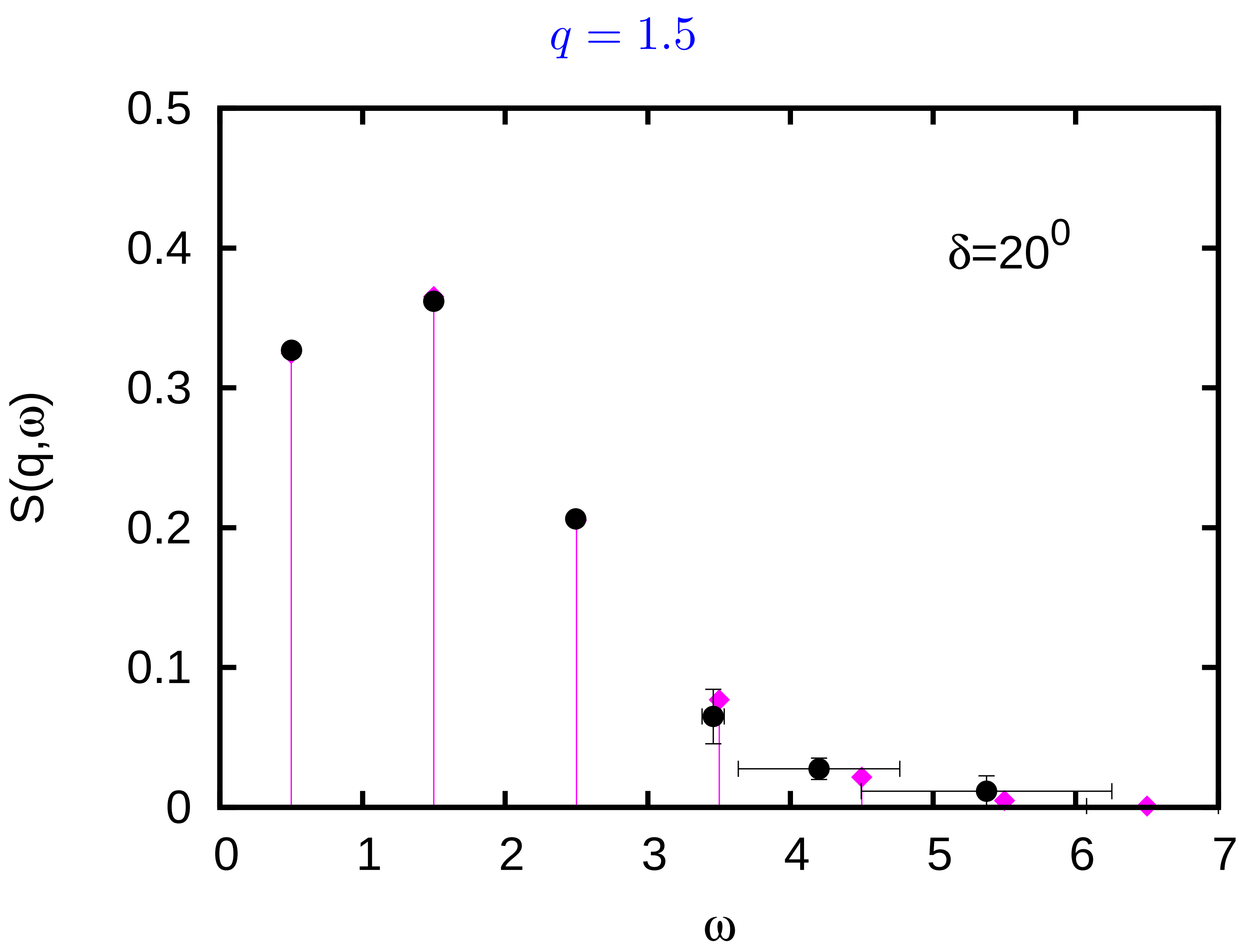
HO $S(q,\omega)$



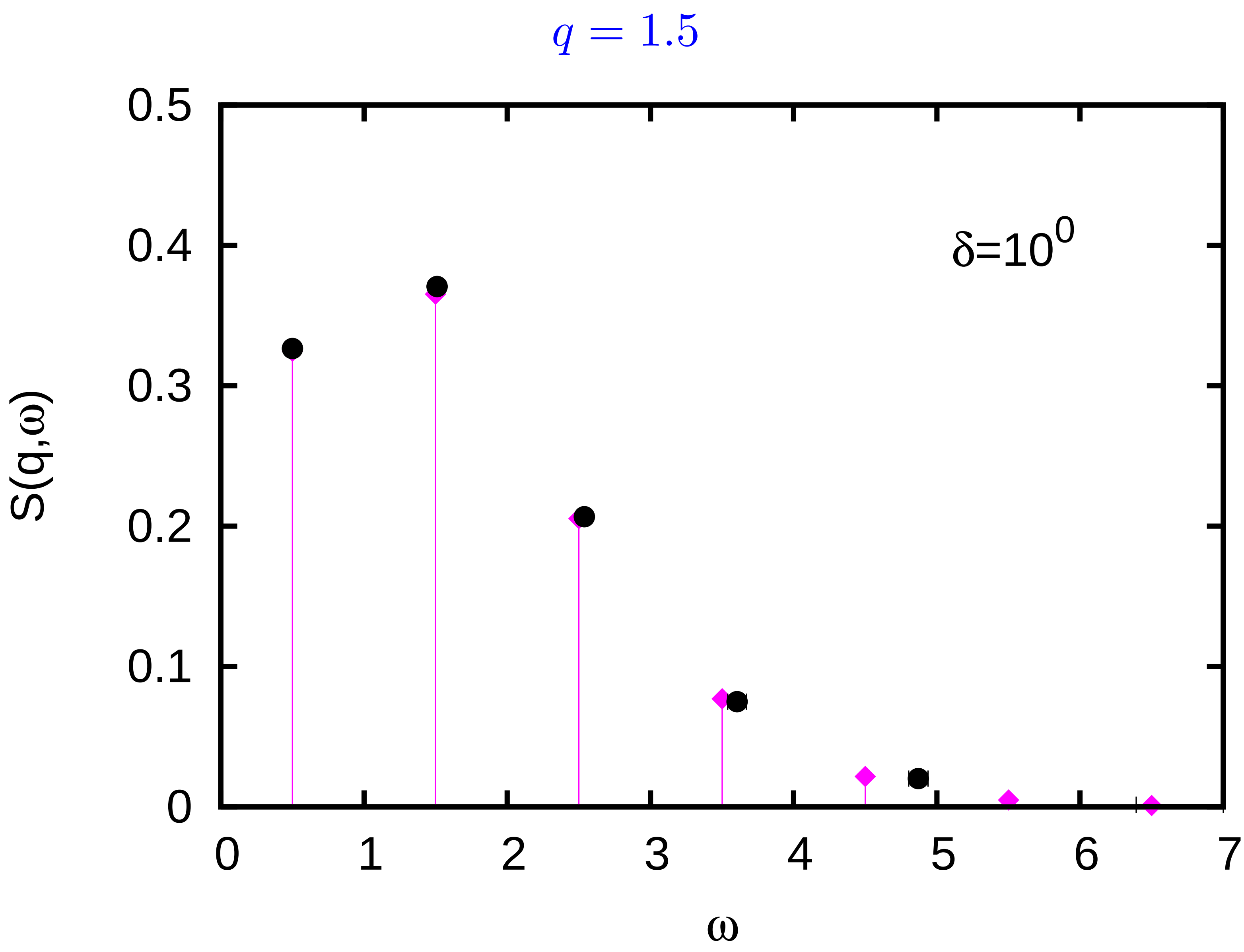
HO $S(q,\omega)$



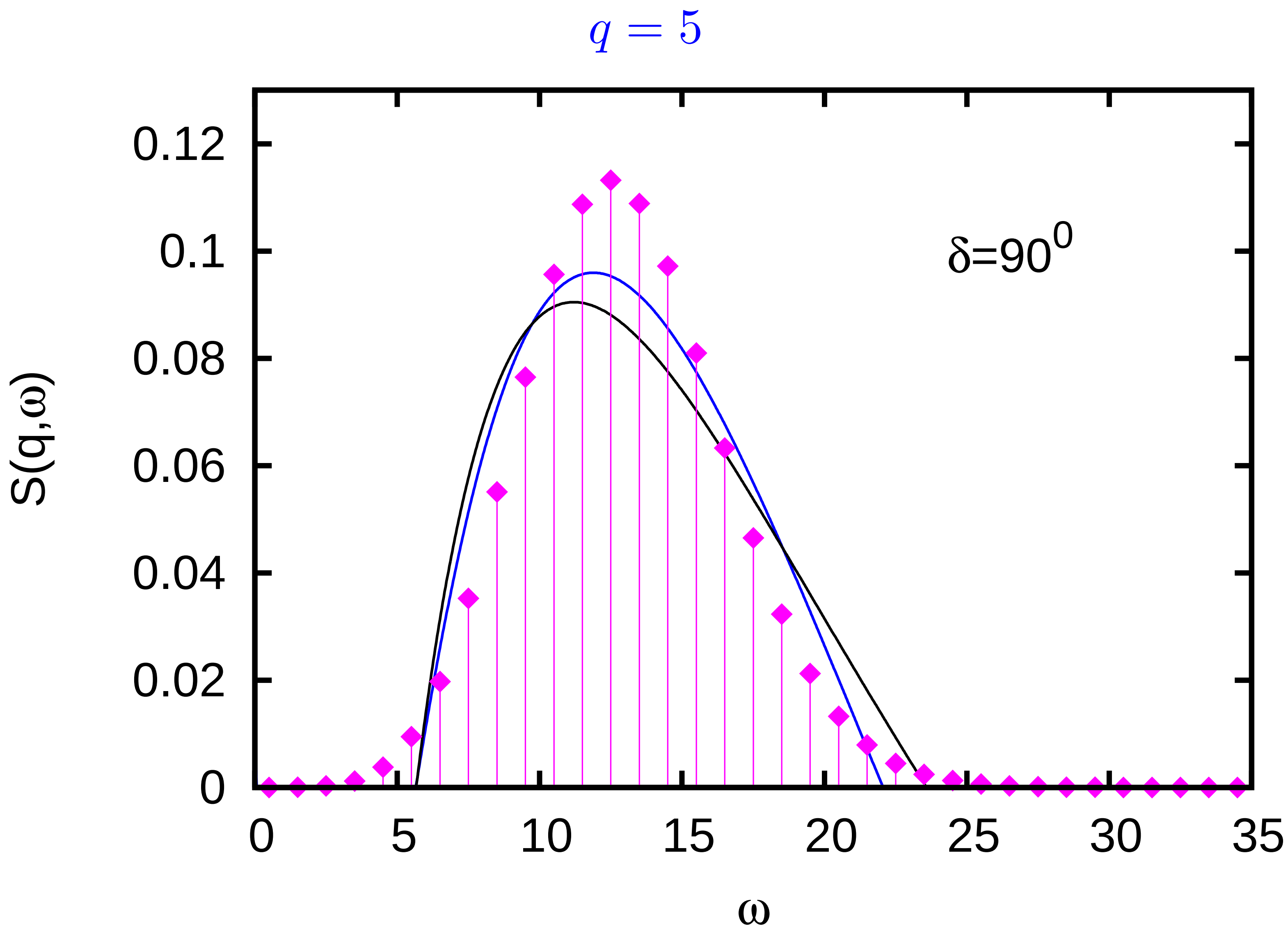
HO $\mathbf{S(q,\omega)}$



HO $\mathbf{S}(\mathbf{q},\omega)$

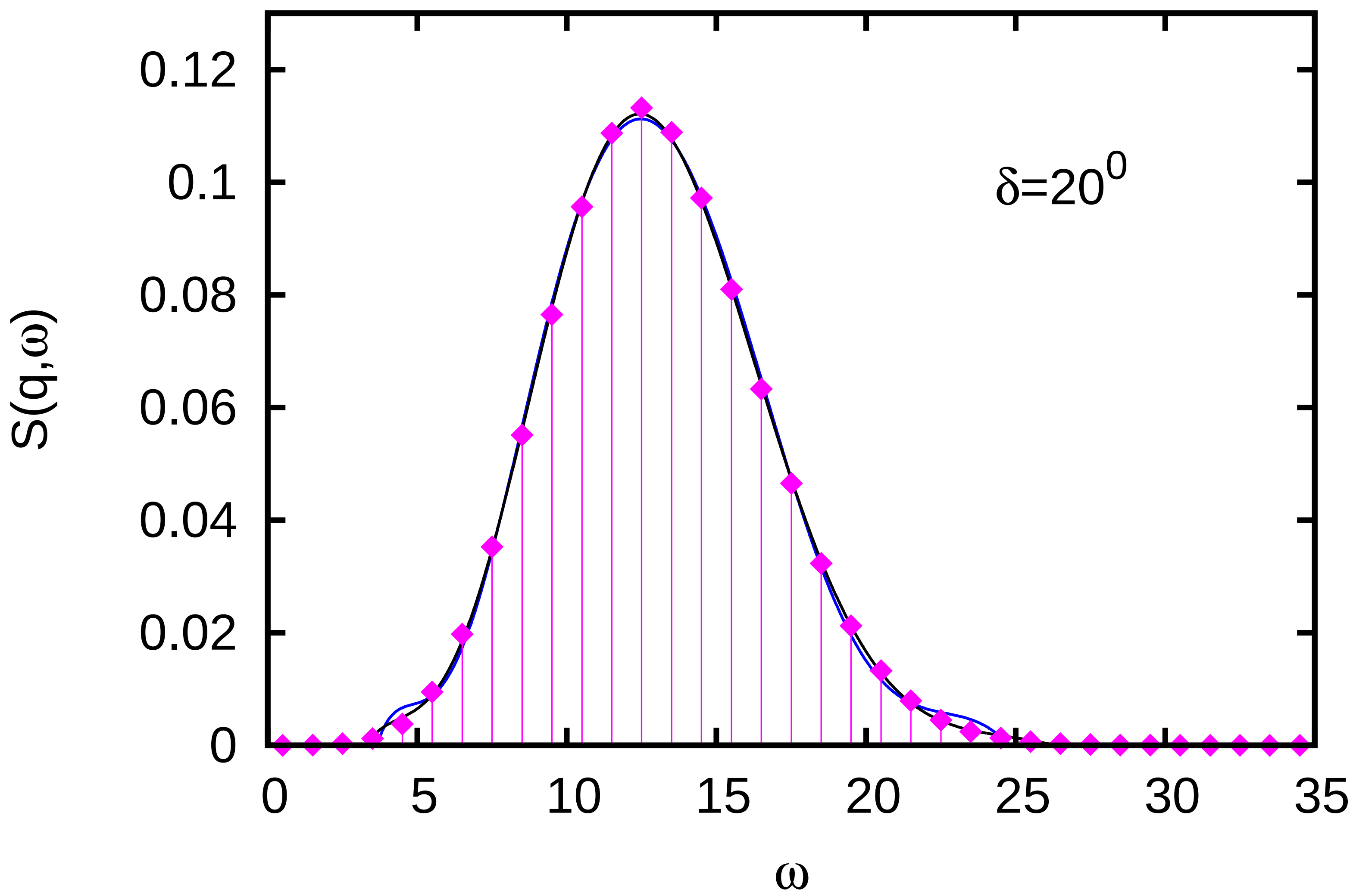


HO $S(q, \omega)$



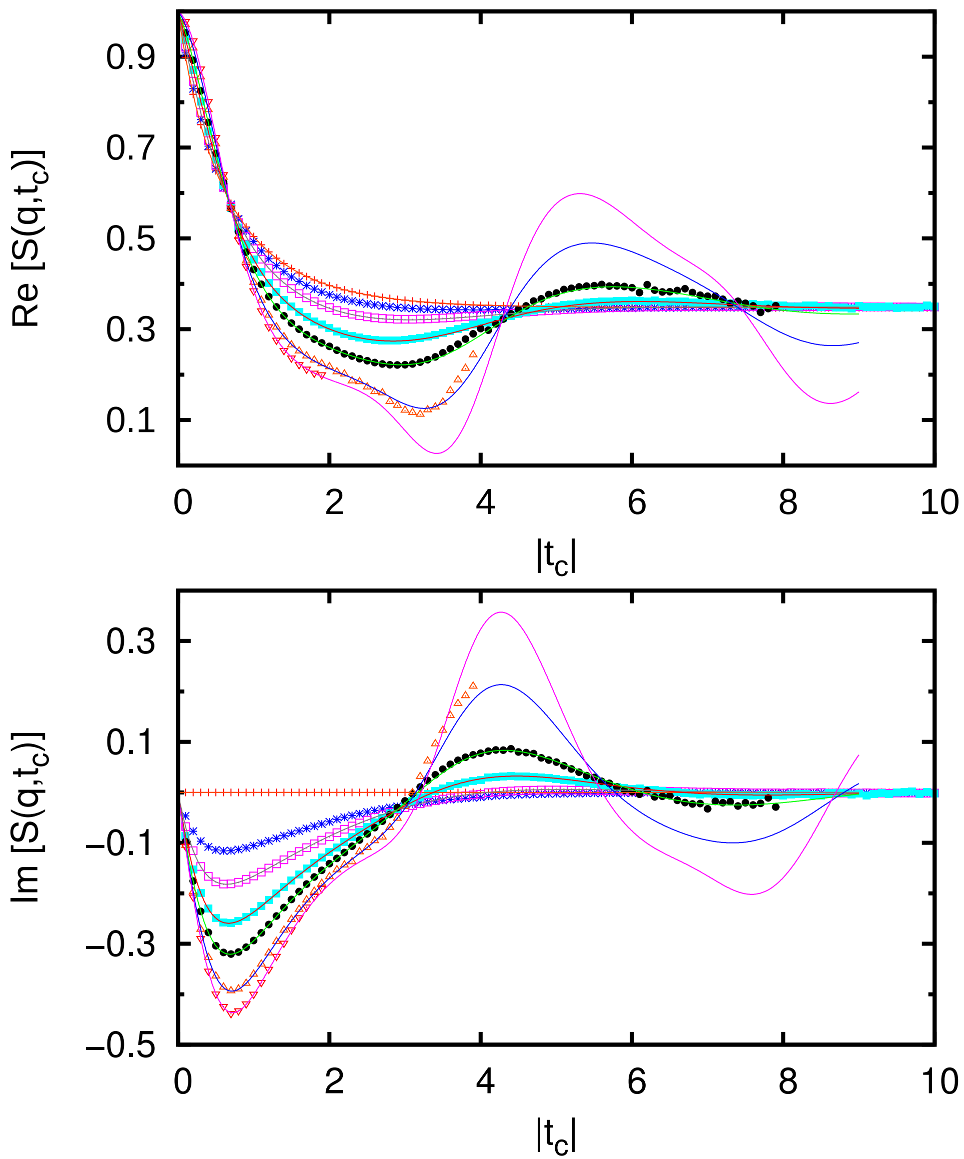
HO $S(q, \omega)$

$q = 5$

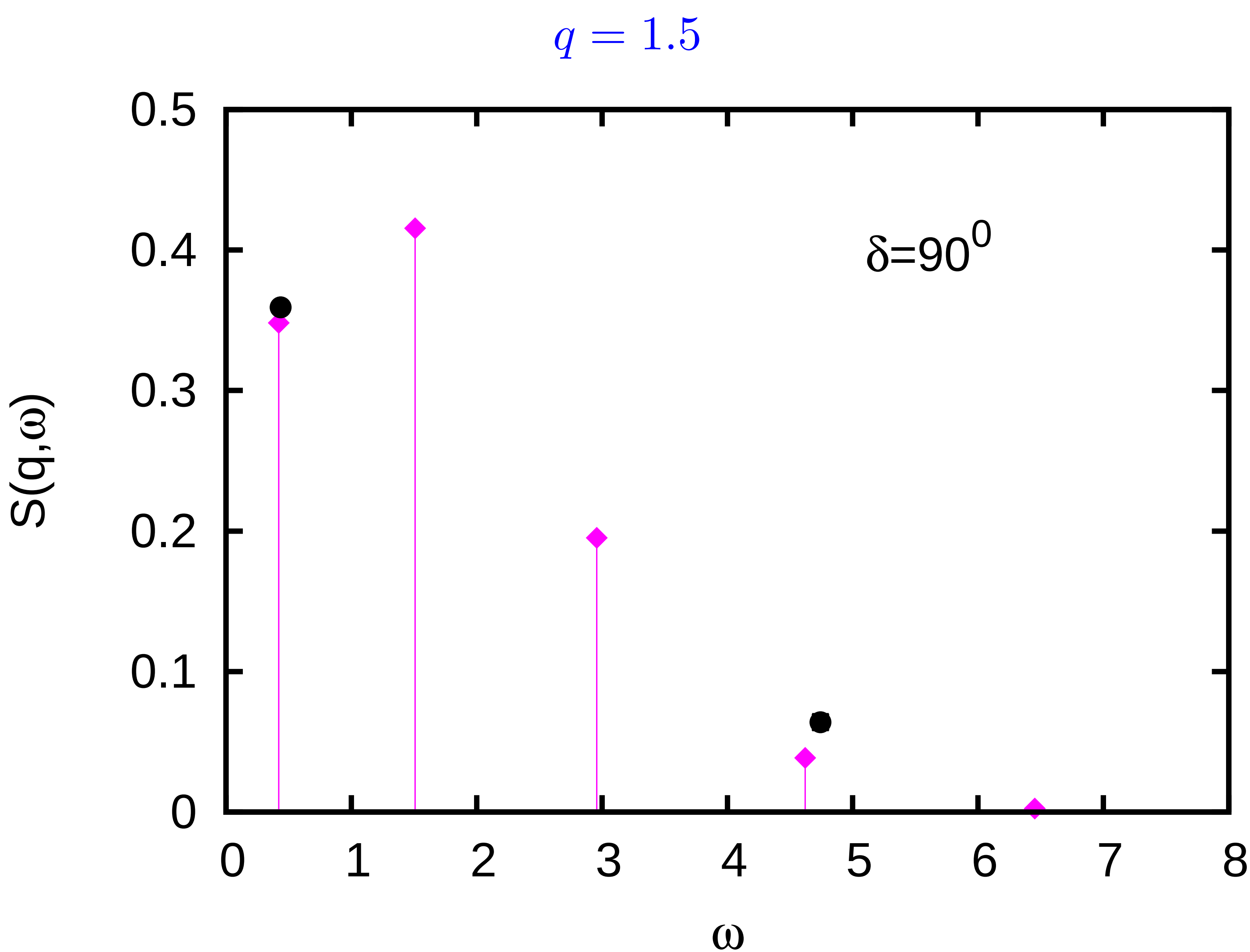


x^4 Results

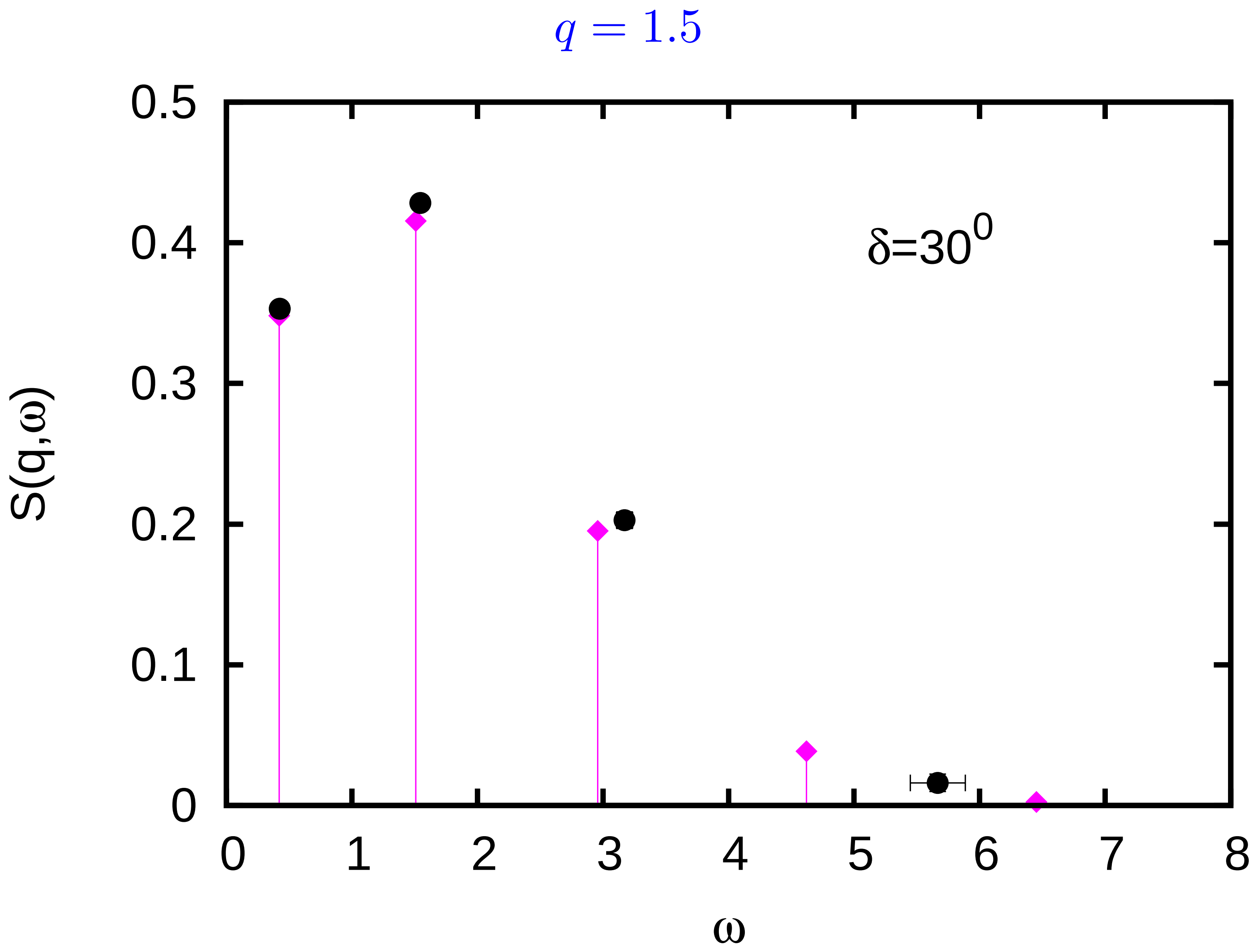
x^4 potential: similar accuracy to the one achieved for HO



x^4 S(q, ω)

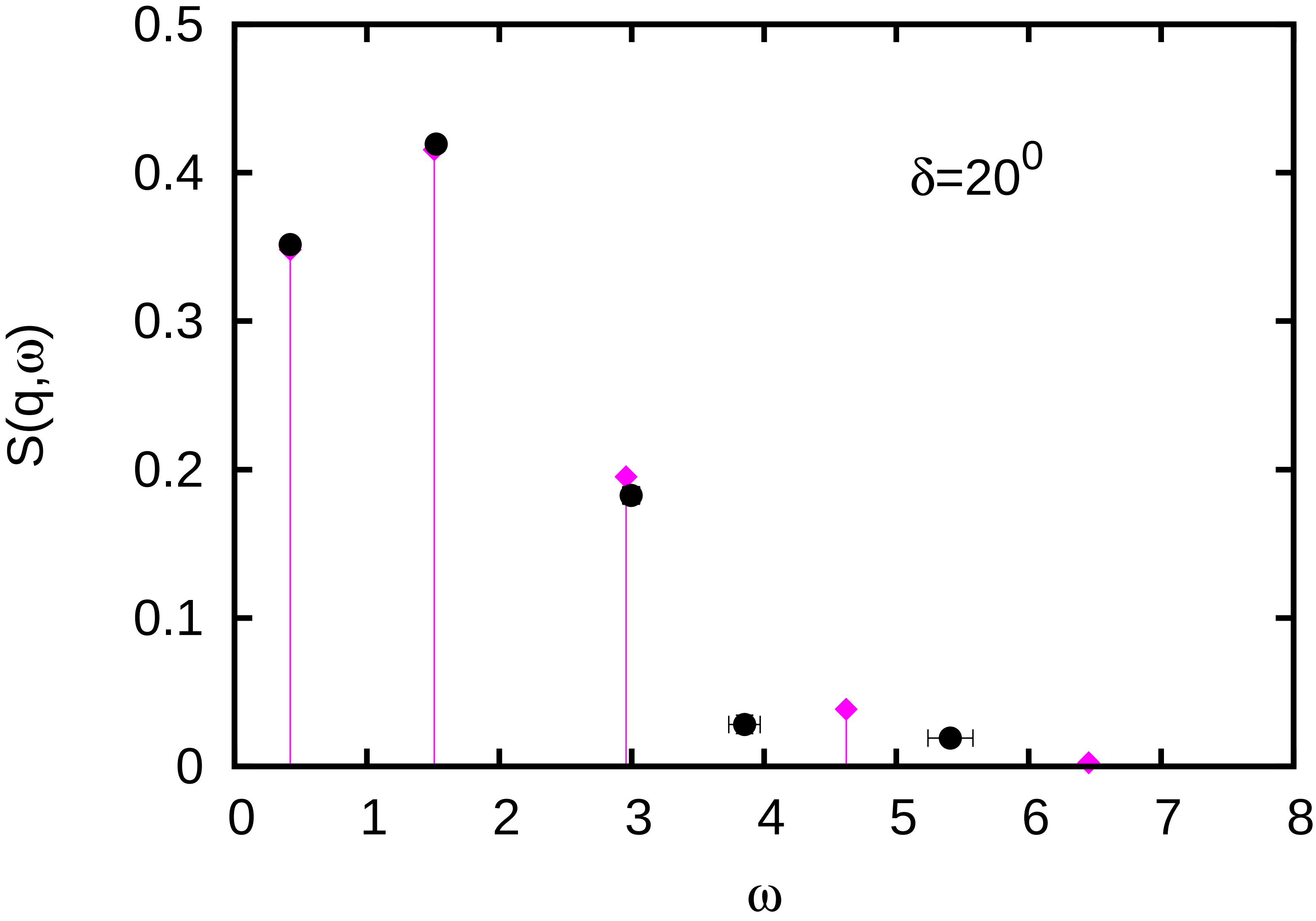


x^4 S(q, ω)

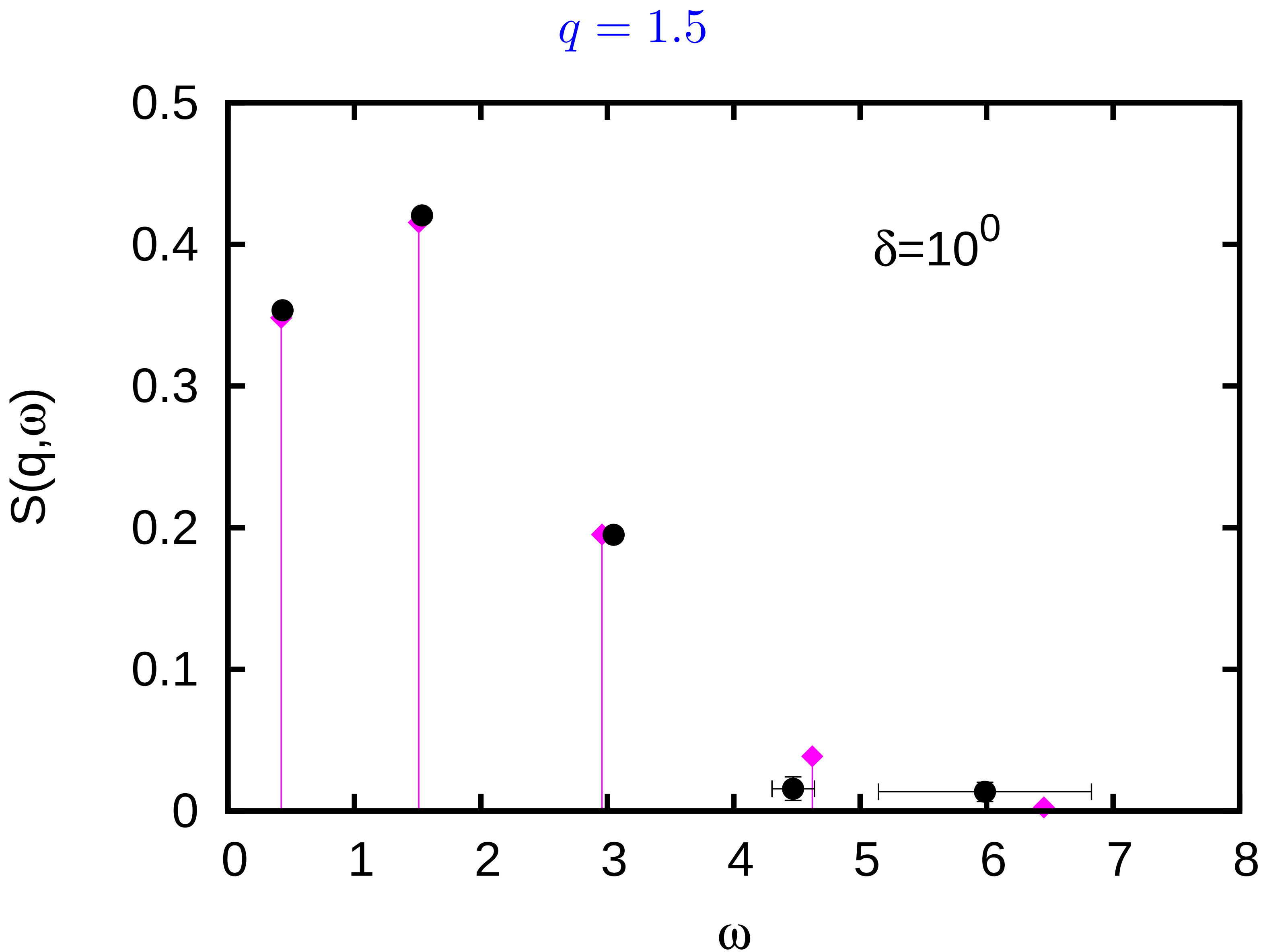


x^4 S(q, ω)

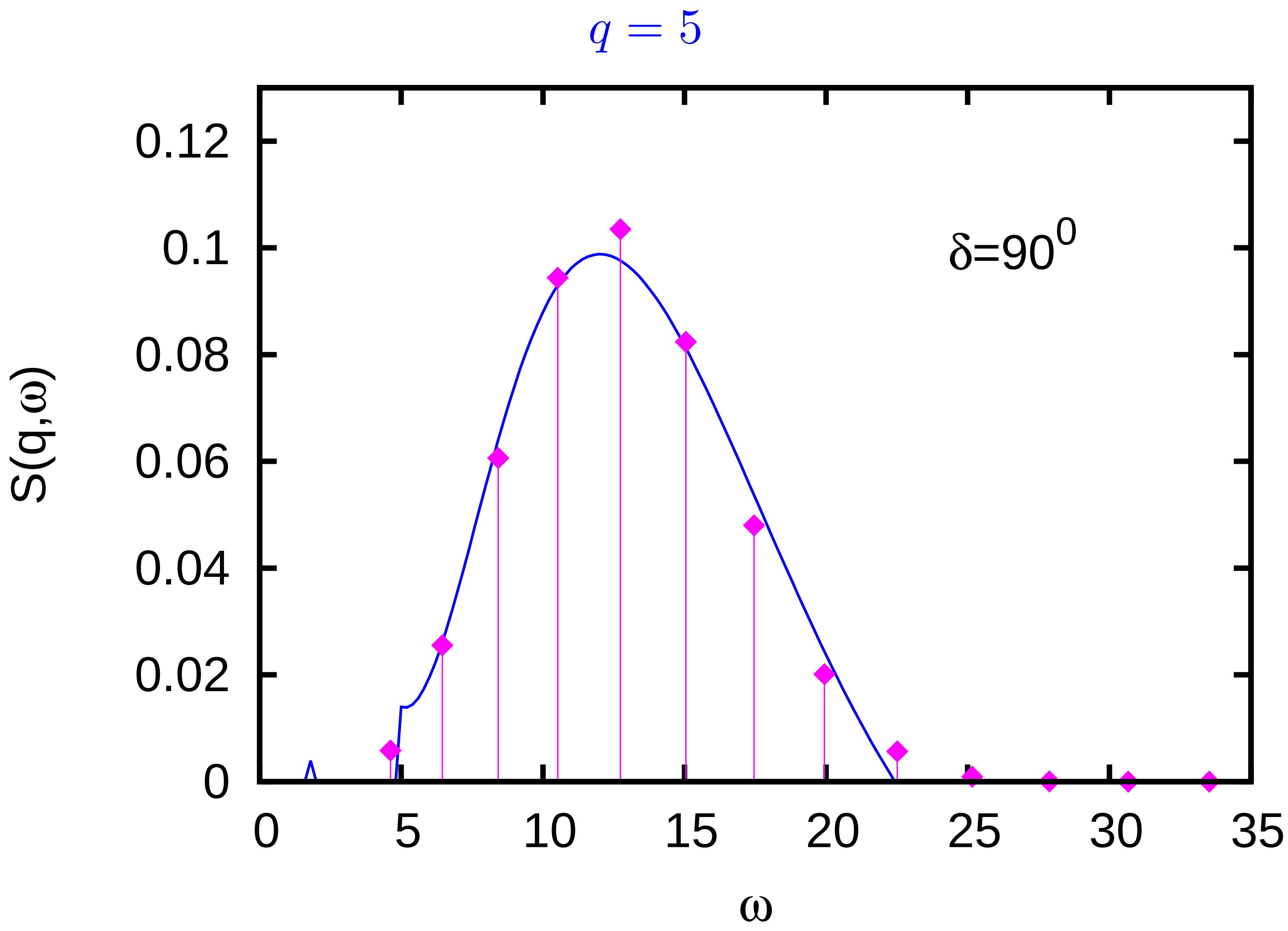
$q = 1.5$



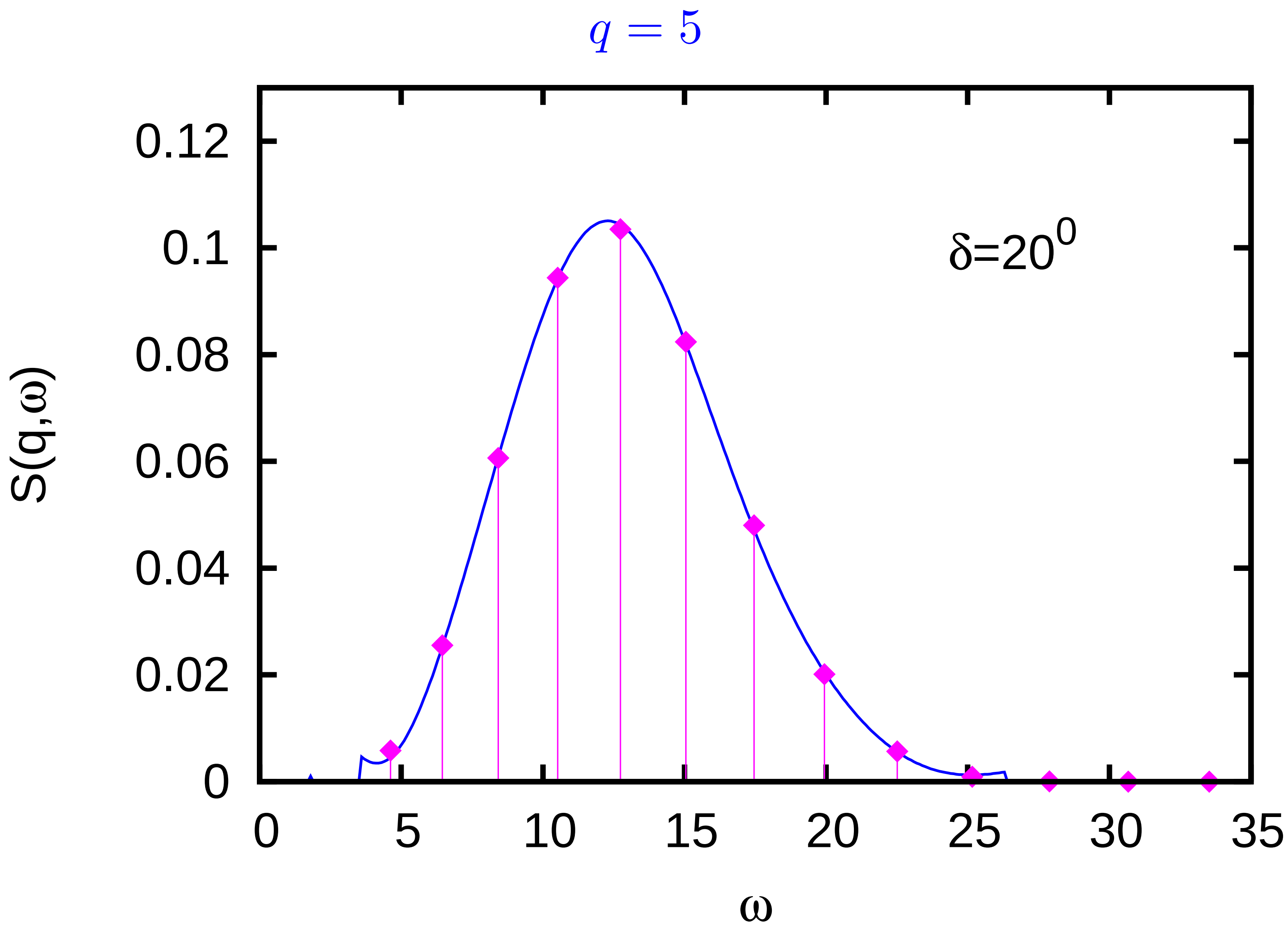
x^4 S(q, ω)



x^4 S(q, ω)



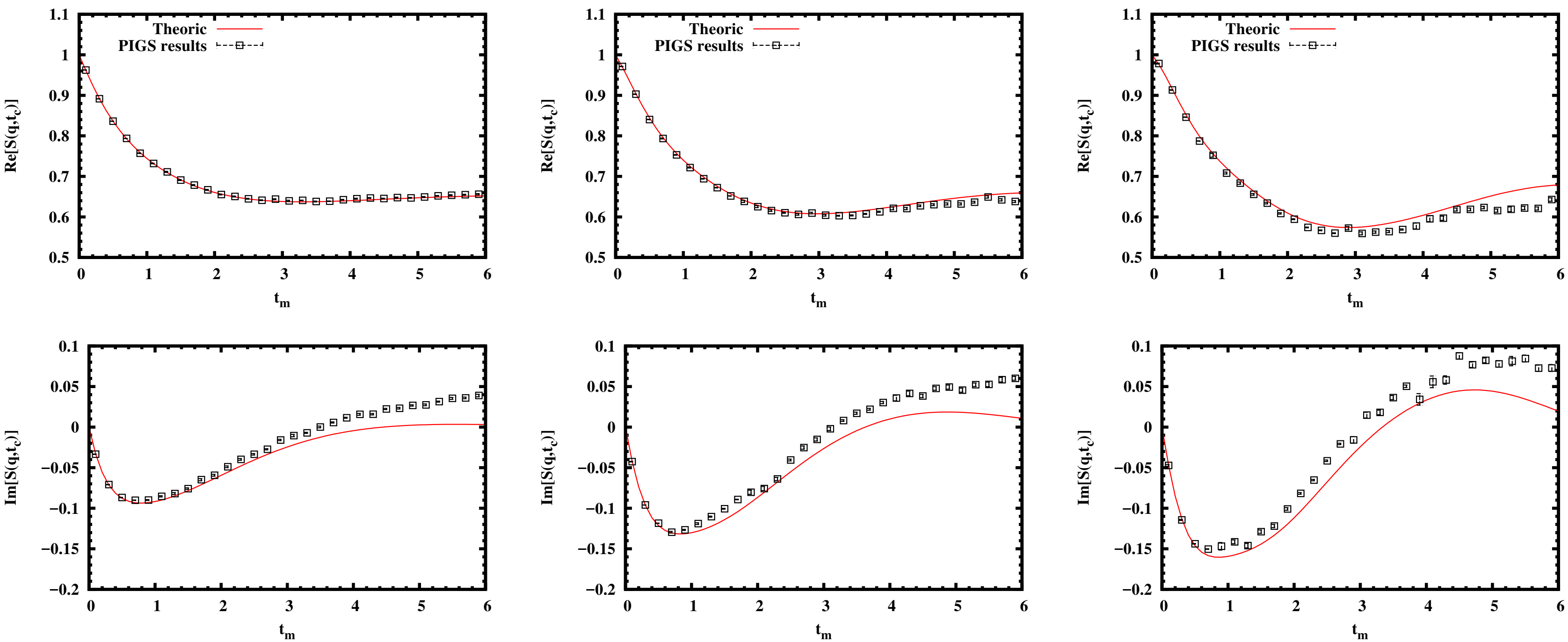
x^4 S(q, ω)



$N > 1$ systems

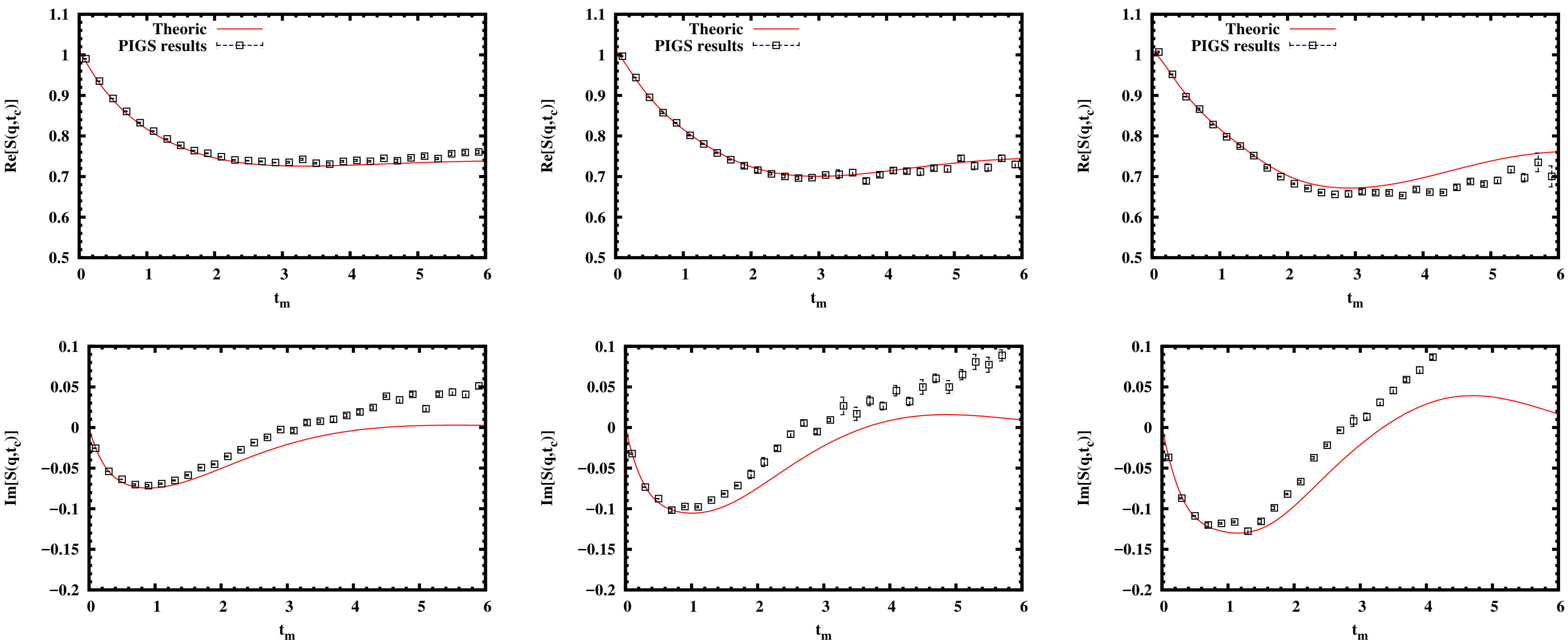
- We are currently trying to calculate complex-time correlation functions for systems with $N > 1$
- We choose harmonic interaction between particles and a confining term ($(\sum_i x_i^2)/N$)
- When $N \leq 4$ we can compare with exact results
- Up to $N = 4$ we have verified that taking all the permutations or just uniform sampling leads to same results
- Calculations become harder since noise increases but still useful information can be drawn

$N = 3$ results



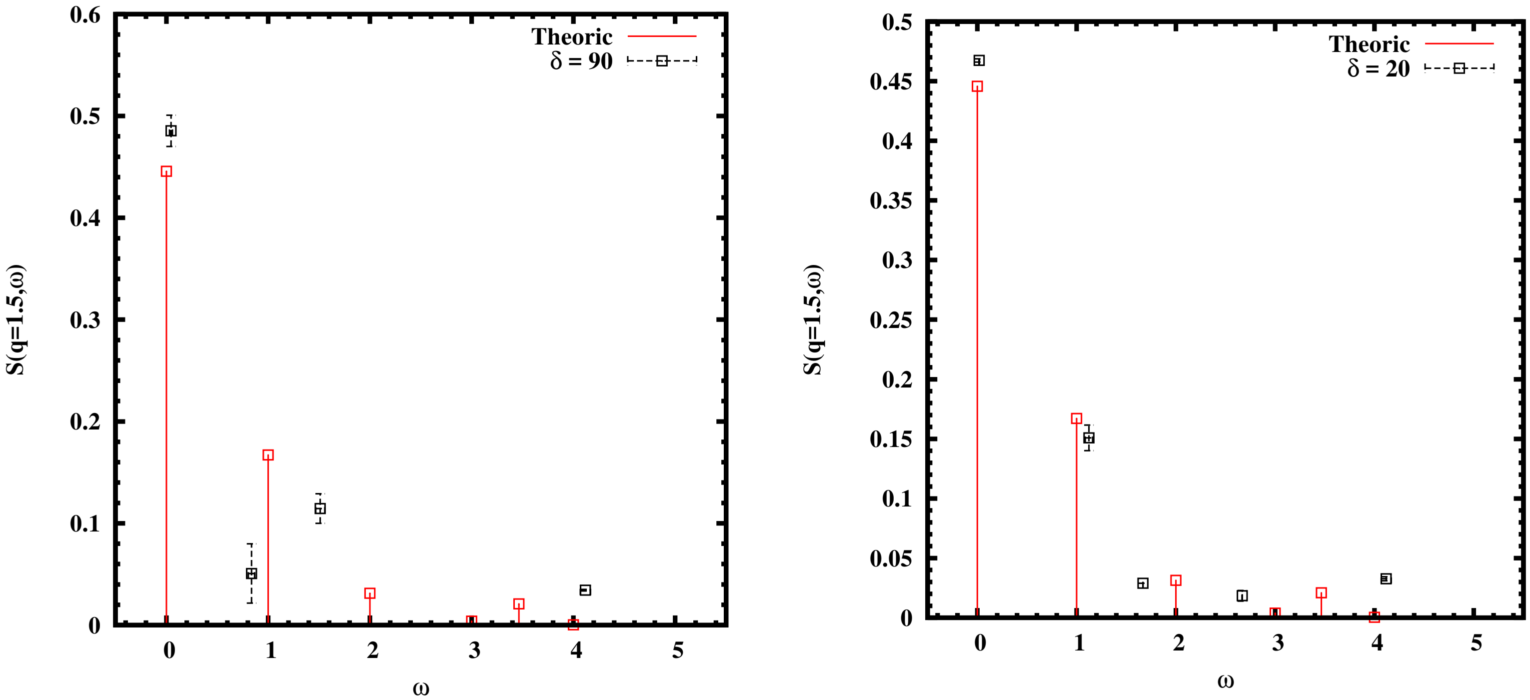
$\delta = 45^\circ$ $\delta = 30^\circ$ $\delta = 20^\circ$

$N = 4$ results



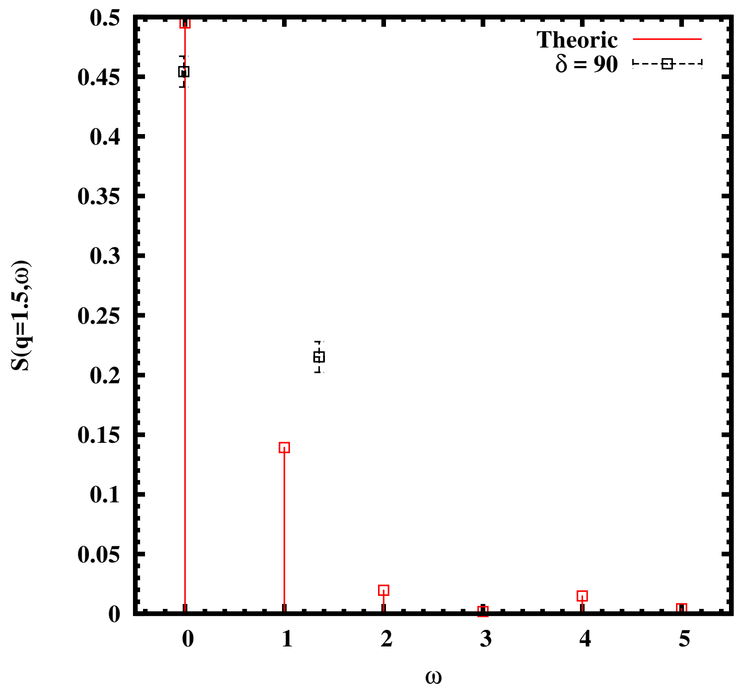
$\delta = 45^\circ$ $\delta = 30^\circ$ $\delta = 20^\circ$

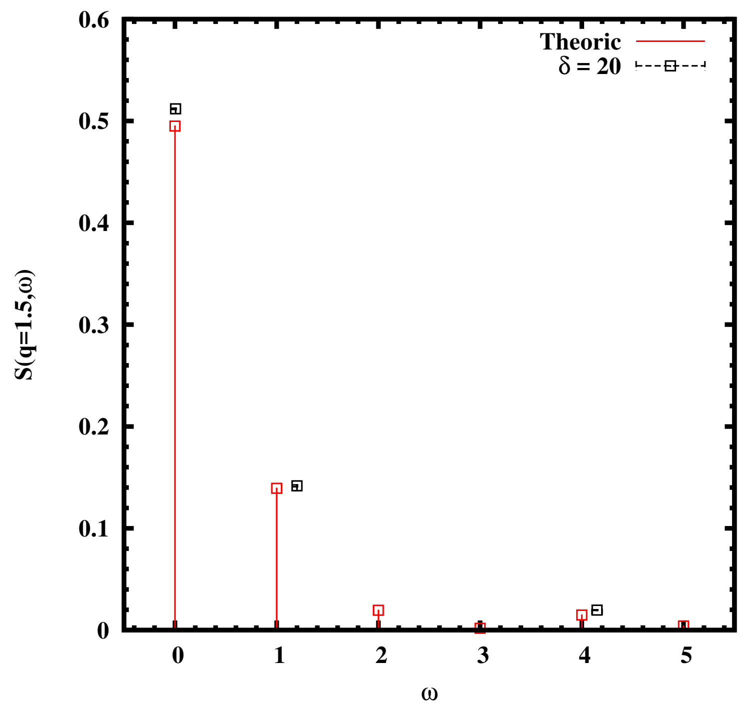
$N = 3 \quad S(q,\omega)$



Results in the frequency domain.
Use of complex time still improves imaginary-time data.

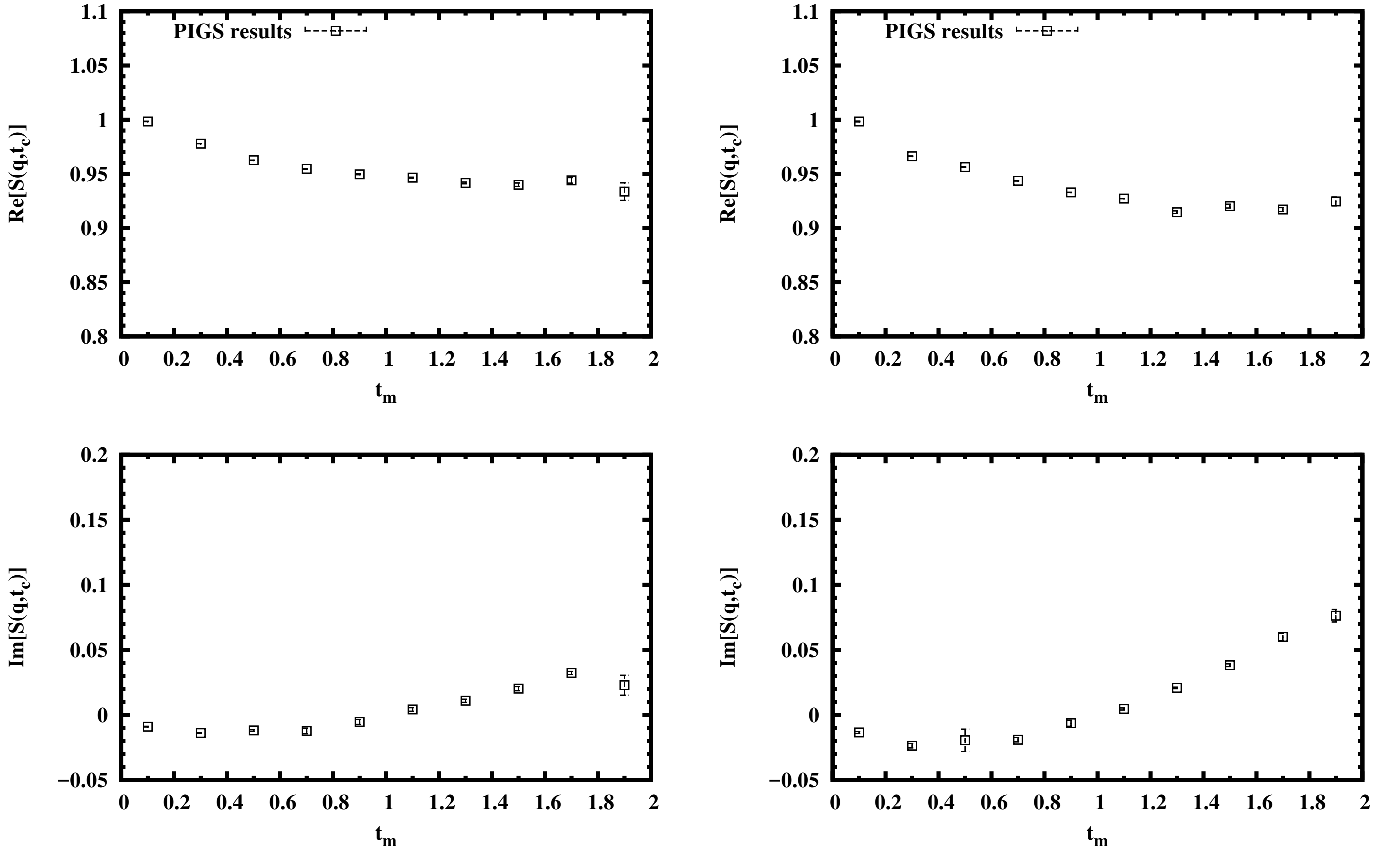
$N = 4 \quad S(q,\omega)$





Results in the frequency domain.
Use of complex time still improves imaginary-time data.

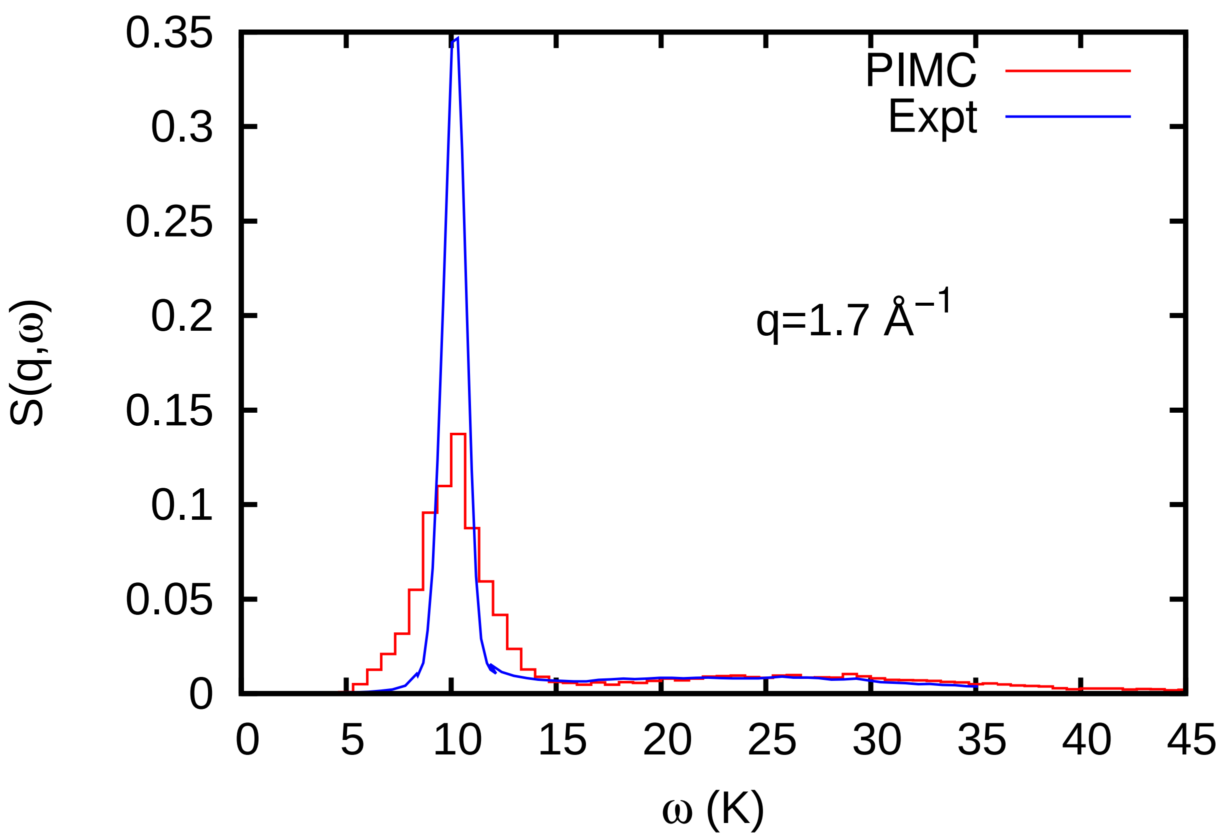
$N = 10$ results



$\delta = 45°$ $\delta = 30°$

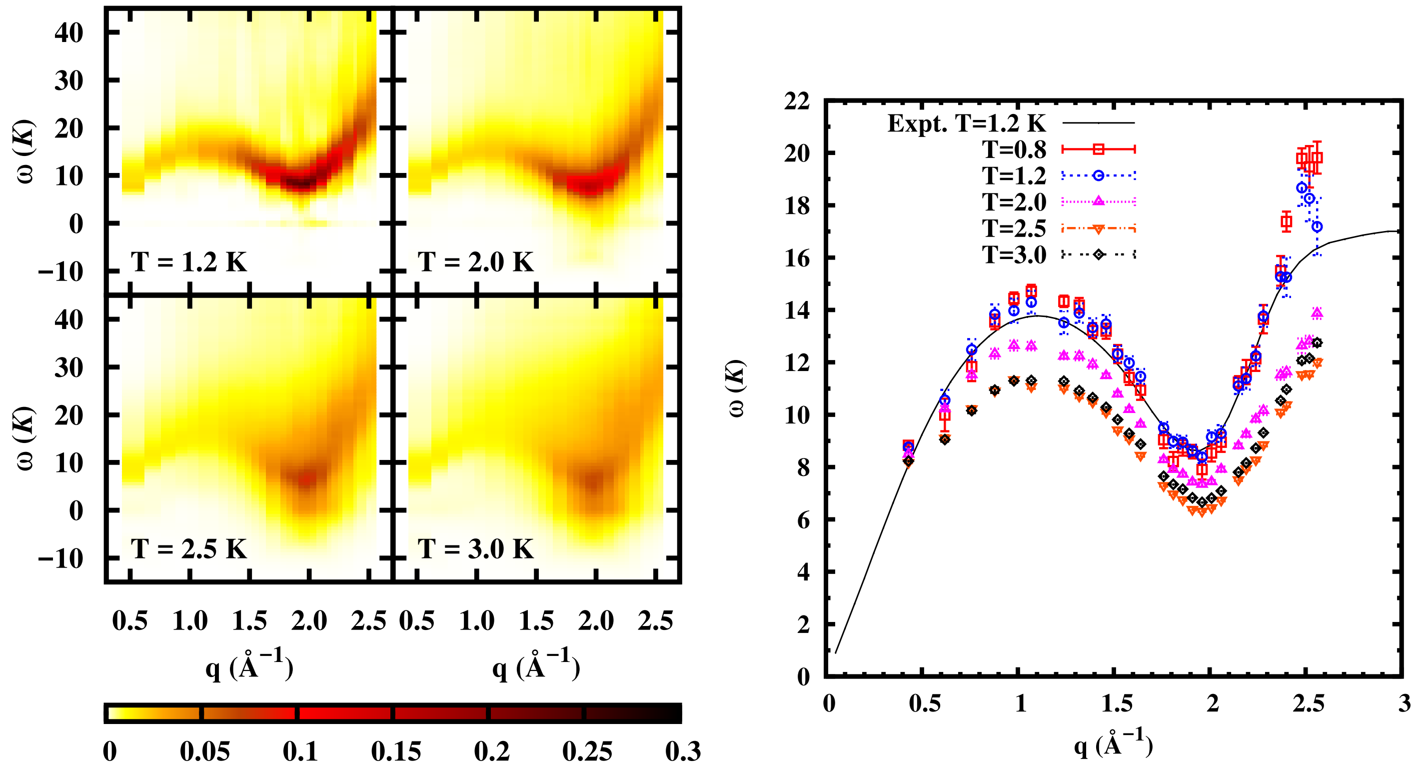
Dynamic structure function ^{4}He

Up to now, at the many-body level we rely only on inverse Laplace transform of the imaginary-time correlation factor $S(q, \tau)$



Dynamic structure function ^{4}He

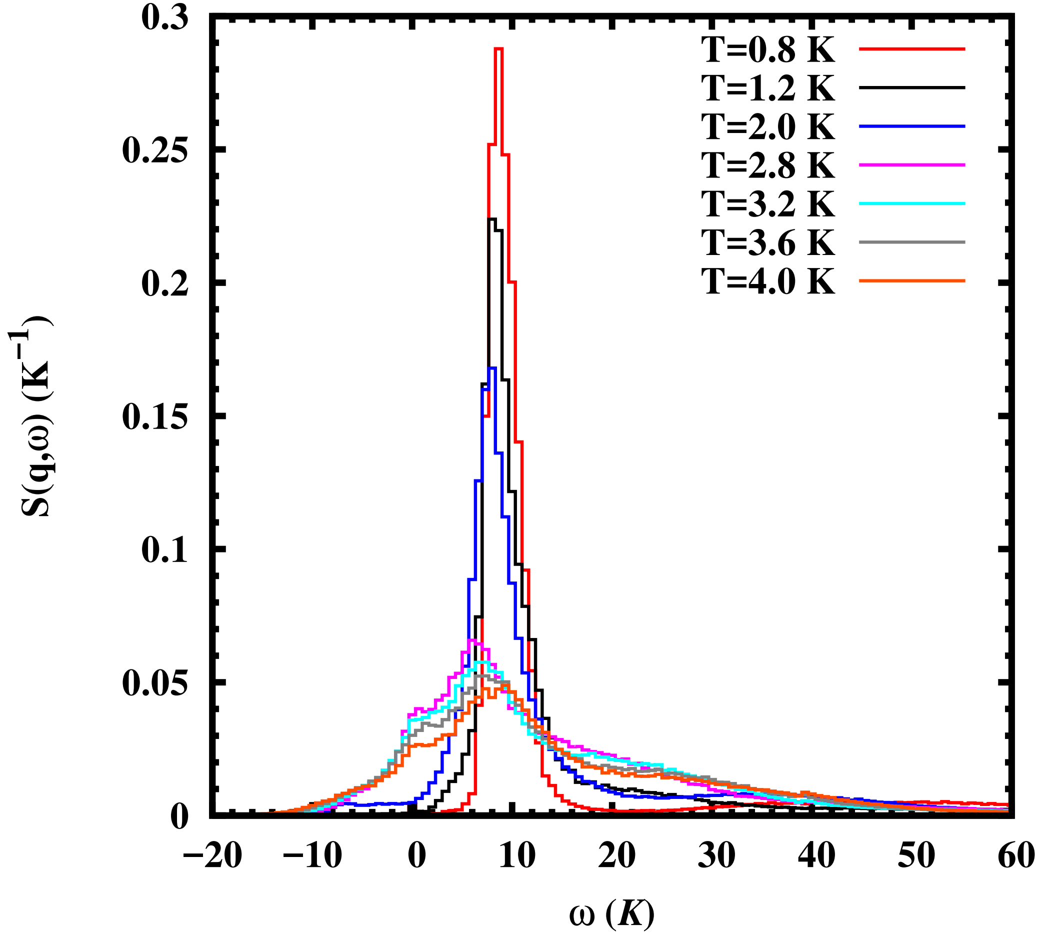
The phonon-roton spectrum is reasonably well described, except Pitaevskii plateau



G. Ferré and J. B., Phys. Rev. B **93**, 104510 (2016)

Dynamic structure function ^{4}He

The behavior with temperature is qualitatively correct. Largest effects in the roton



QMC-CBF approach

Results for $\epsilon(k)$ can be obtained by using CBF theory. More importantly, access to the full dynamic response $S(k,\omega)$.

In CBF,

$$S(k,\omega) = -\frac{1}{\pi}\text{Im}\frac{S(k)}{\hbar\omega - \epsilon_F(k) - \Sigma(k,\omega) + i\eta}$$

Self-energy,

$$\Sigma(k,\omega) = \frac{1}{2}\int \frac{d\mathbf{p}\,d\mathbf{q}}{(2\pi)^3\rho}\,\frac{\delta(\mathbf{k}+\mathbf{p}+\mathbf{q})|V_3(\mathbf{k},\mathbf{p},\mathbf{q})|^2}{\hbar\omega - \epsilon_F(p) - \epsilon_F(q) + i\zeta}$$

with the matrix element

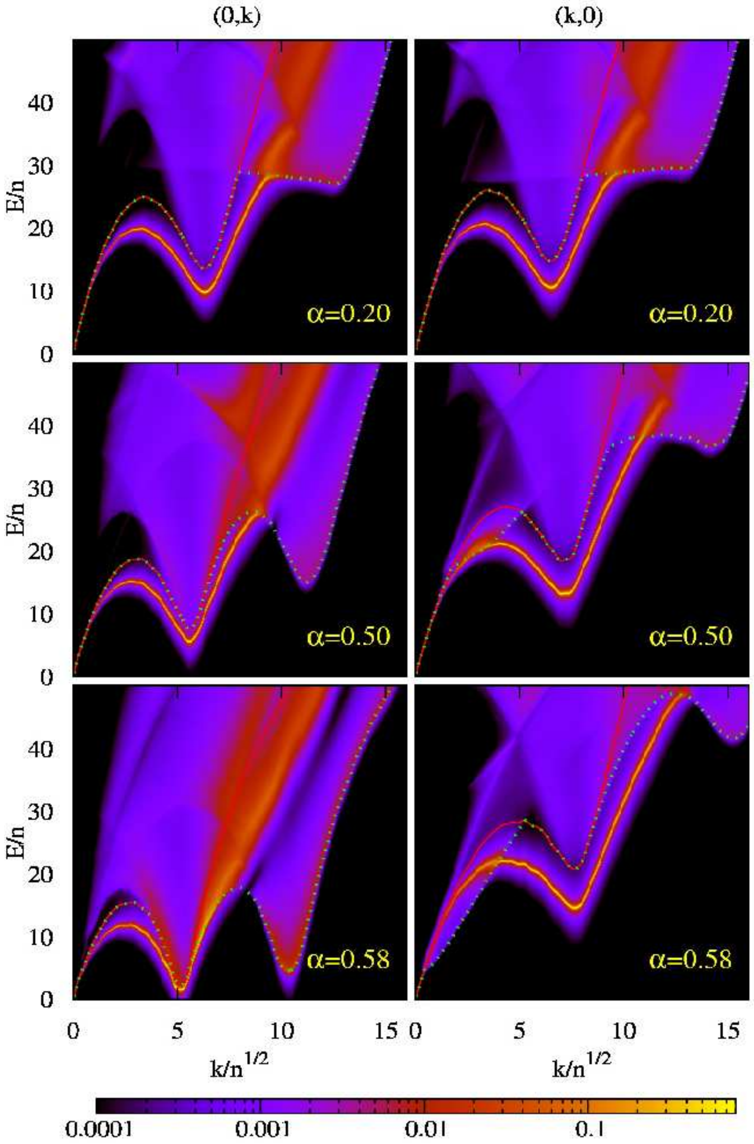
$$V_3(\mathbf{k},\mathbf{p},\mathbf{q}) = \frac{\hbar^2}{2m}\sqrt{\frac{S(p)S(q)}{S(k)}}\left[\mathbf{k}\cdot\mathbf{p}X(p) + \mathbf{k}\cdot\mathbf{q}X(q) - k^2 u_3(\mathbf{k},\mathbf{p},\mathbf{q})\right]$$

written in terms of the direct correlation function $X(k) = 1 - 1/S(k)$.

QMC input for $S(k)$

Example: stripe phase

The dipolar interaction is anisotropic $\Longrightarrow$ the excitation spectrum is also anisotropic, with roton mimima approaching zero in the stripe phase.



CBF results, $n = 128$

(A. Macia *et al.*, Phys. Rev. Lett. **109**, 235307 (2012))

Remarks

- It is possible to calculate complex-time correlation functions using QMC methods with reasonable accuracy
- Inversion towards dynamic response is much less *ill-posed*
- First results for few-body problems show increase of noise but still relevant signals are observed
- Our goal: improve dynamics using QMC without the difficulties of relying only on imaginary-time functions (standard setup up to now !)

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THANKS FOR YOUR ATTENTION !