A Parameter Free Genetic Algorithm for Estimating the Dynamic Structure Factor at Zero and Finite Temperature

Nathan Nichols
(University of Vermont)

Adrian Del Maestro
(University of Vermont)

Timothy Prisk
(National Institute of Standards and Technology)

Garfield T Warren
(Indiana University Bloomington)

Paul E Sokol
(Indiana University Bloomington)

DMR-1809027 DMR-1808440 OAC-1827314

The University of Vermont

VERMONT ADVANCED COMPUTING CORE
UNIVERSITY OF VERMONT

The problem

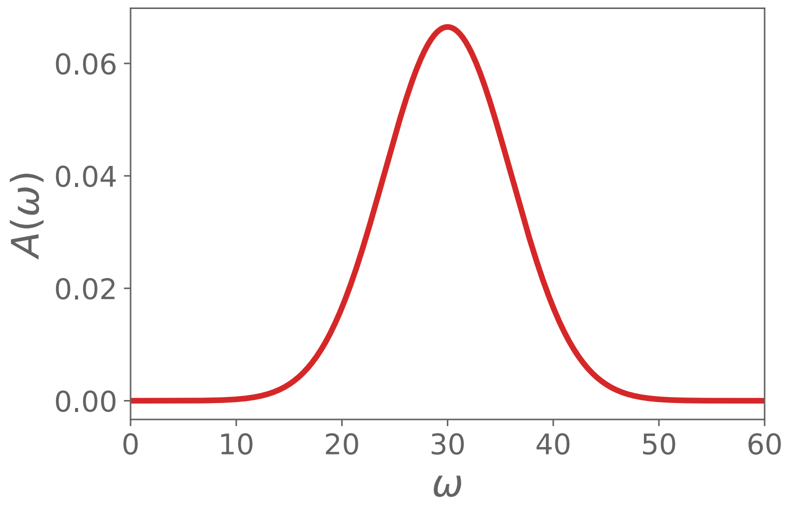
Green function:

$$G(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$

The problem

Green function:

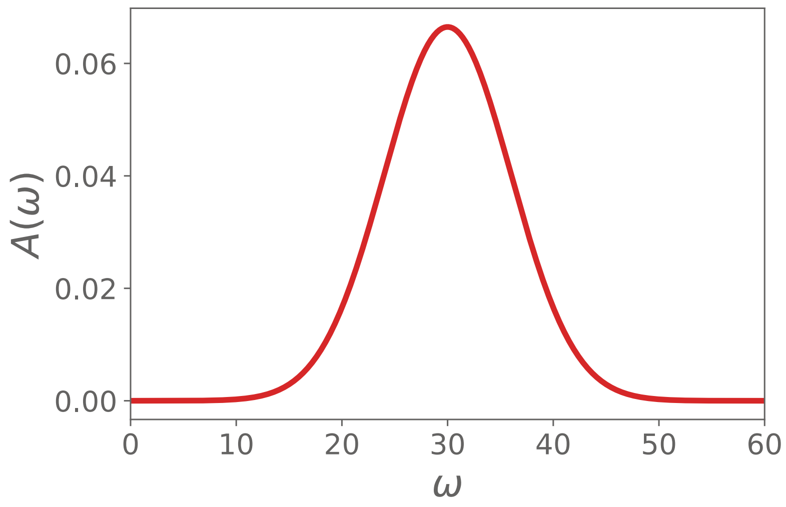
$$G(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$



The problem

Green function:

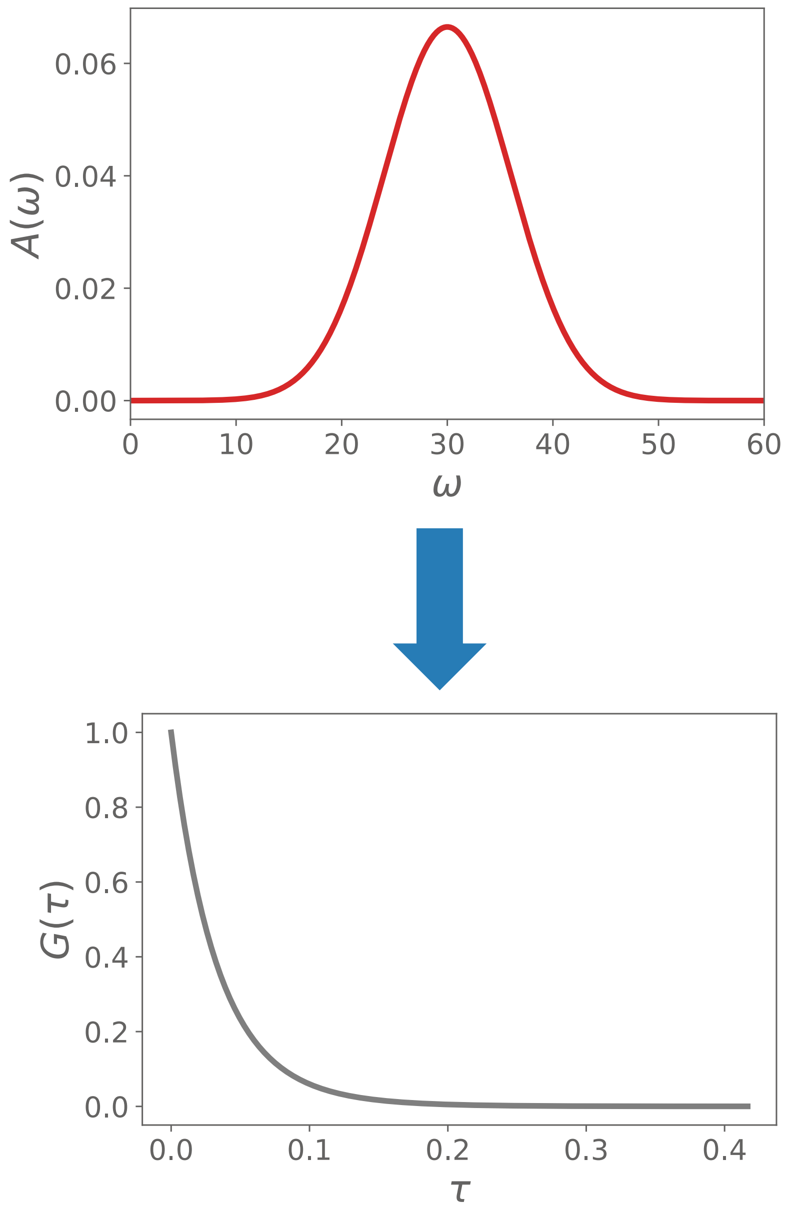
$$G(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$



The problem

Green function:

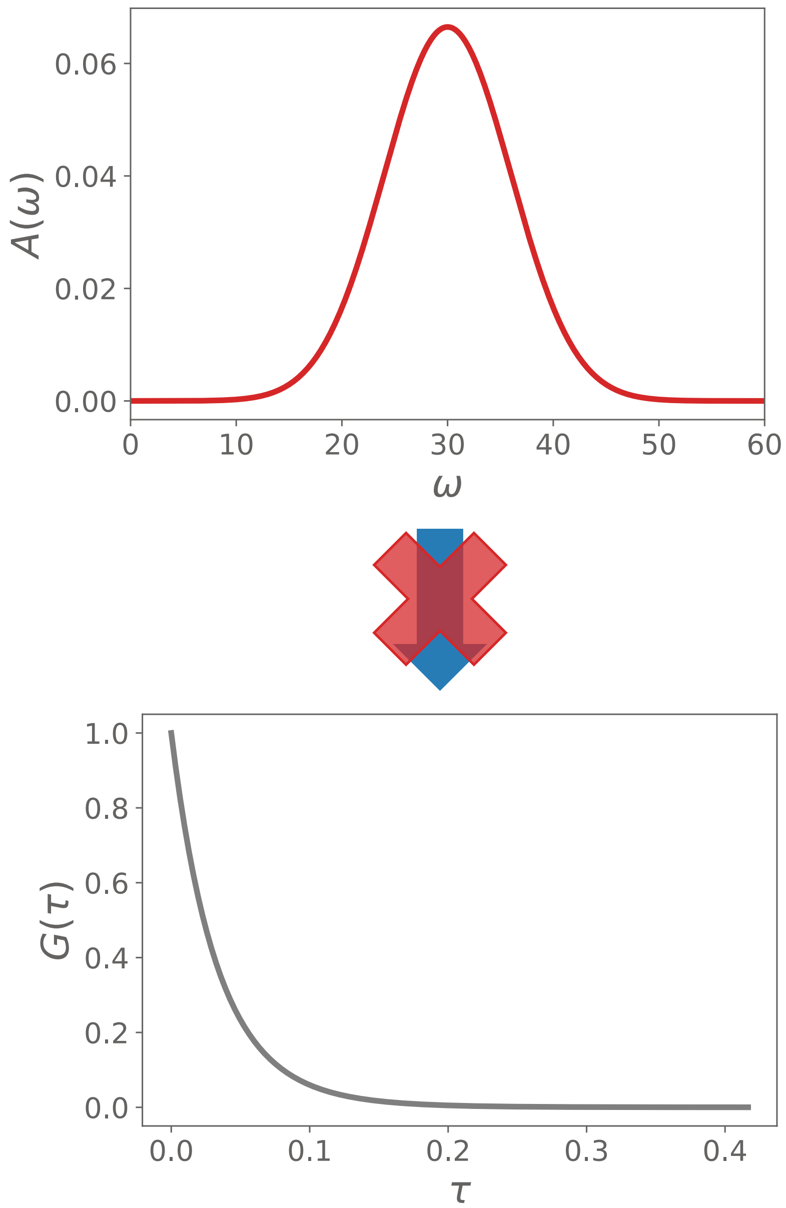
$$G(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$



The problem

Green function:

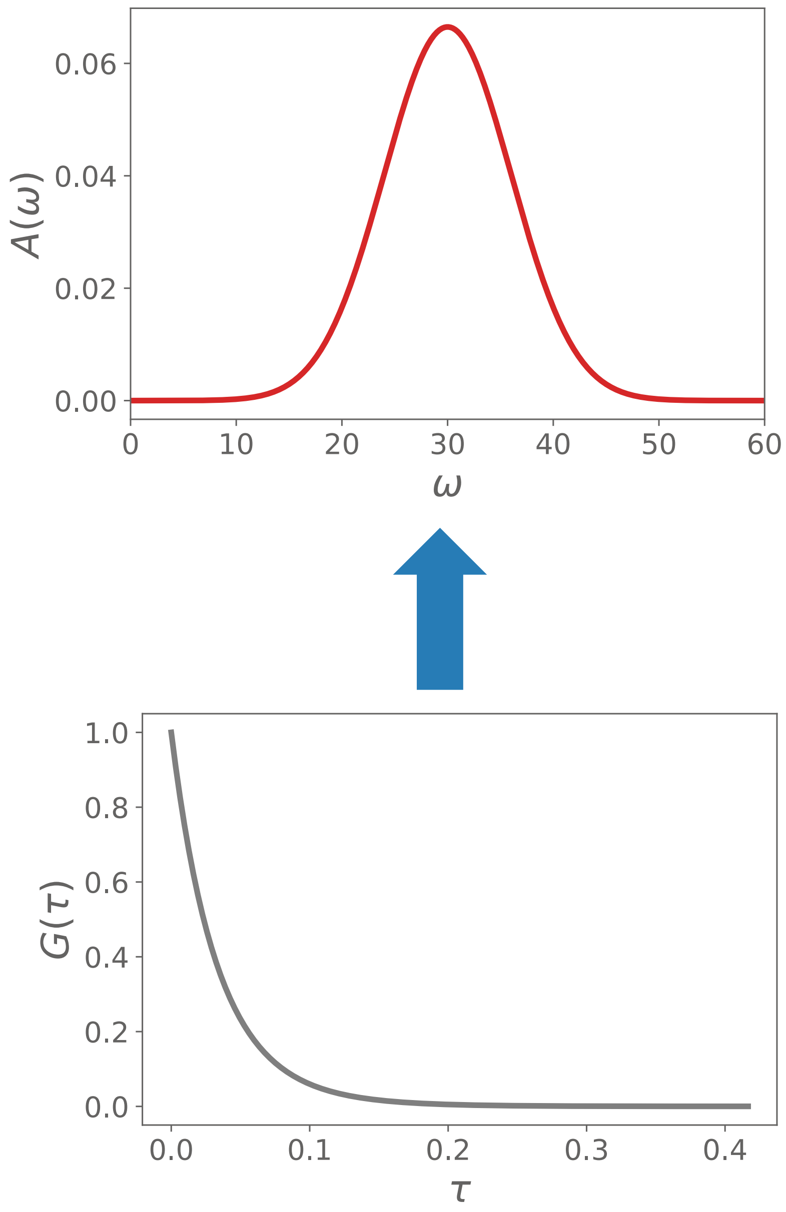
$$G(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$



The problem

Green function:

$$G(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$



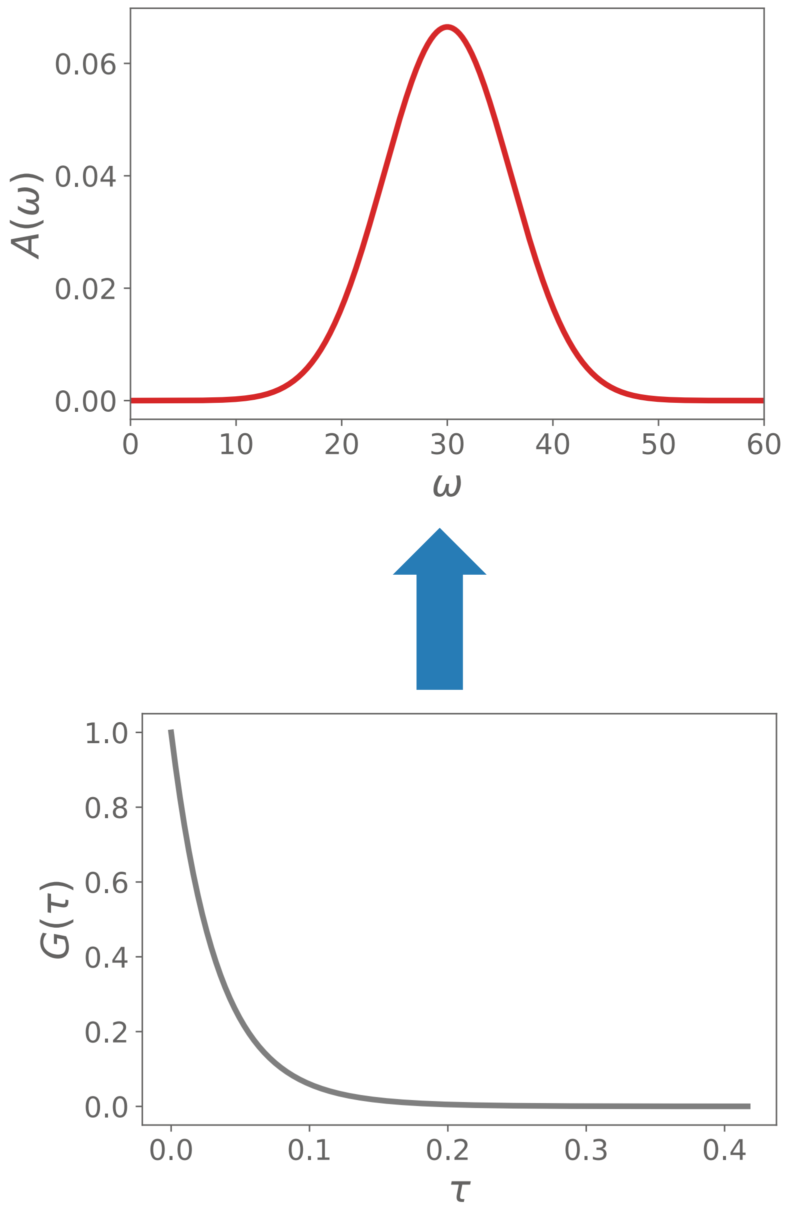
The problem

Green function:

$$G(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

Spectral function:

$$A(\omega) = ?$$



The problem

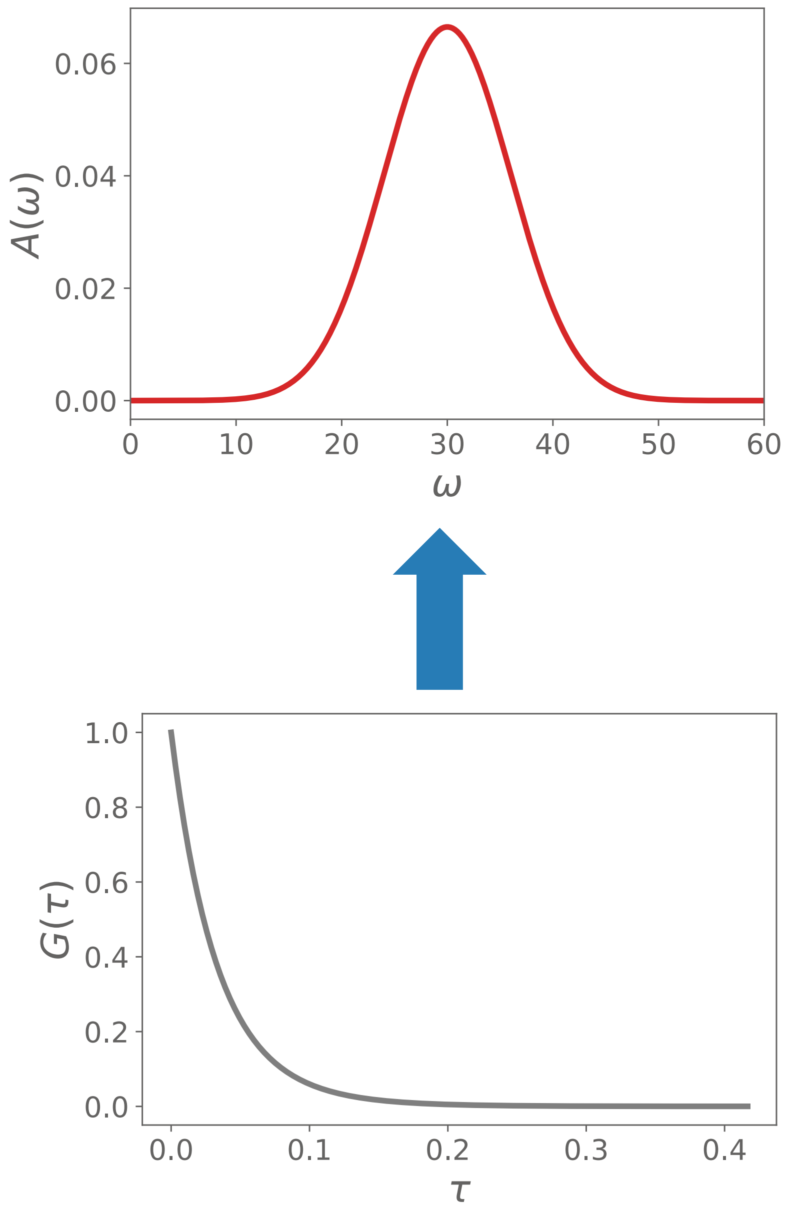
Green function:

$$G(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

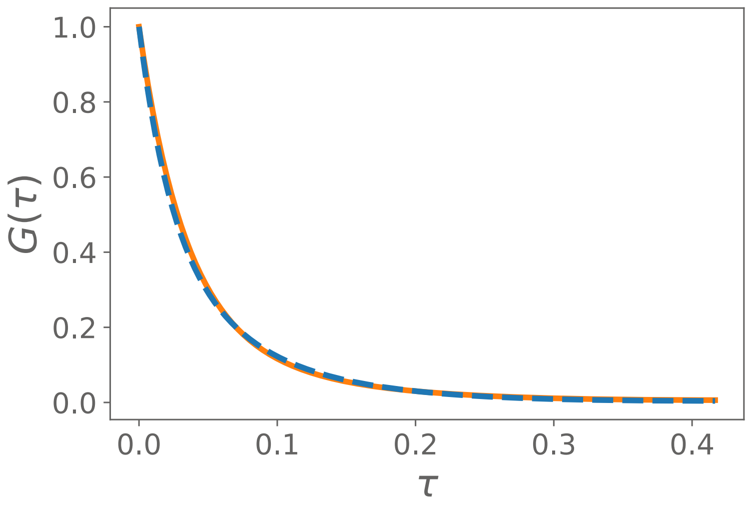
$$G(\tau) = \sum \Delta\omega K(\tau,\omega_i) A(\omega_i)$$

Spectral function:

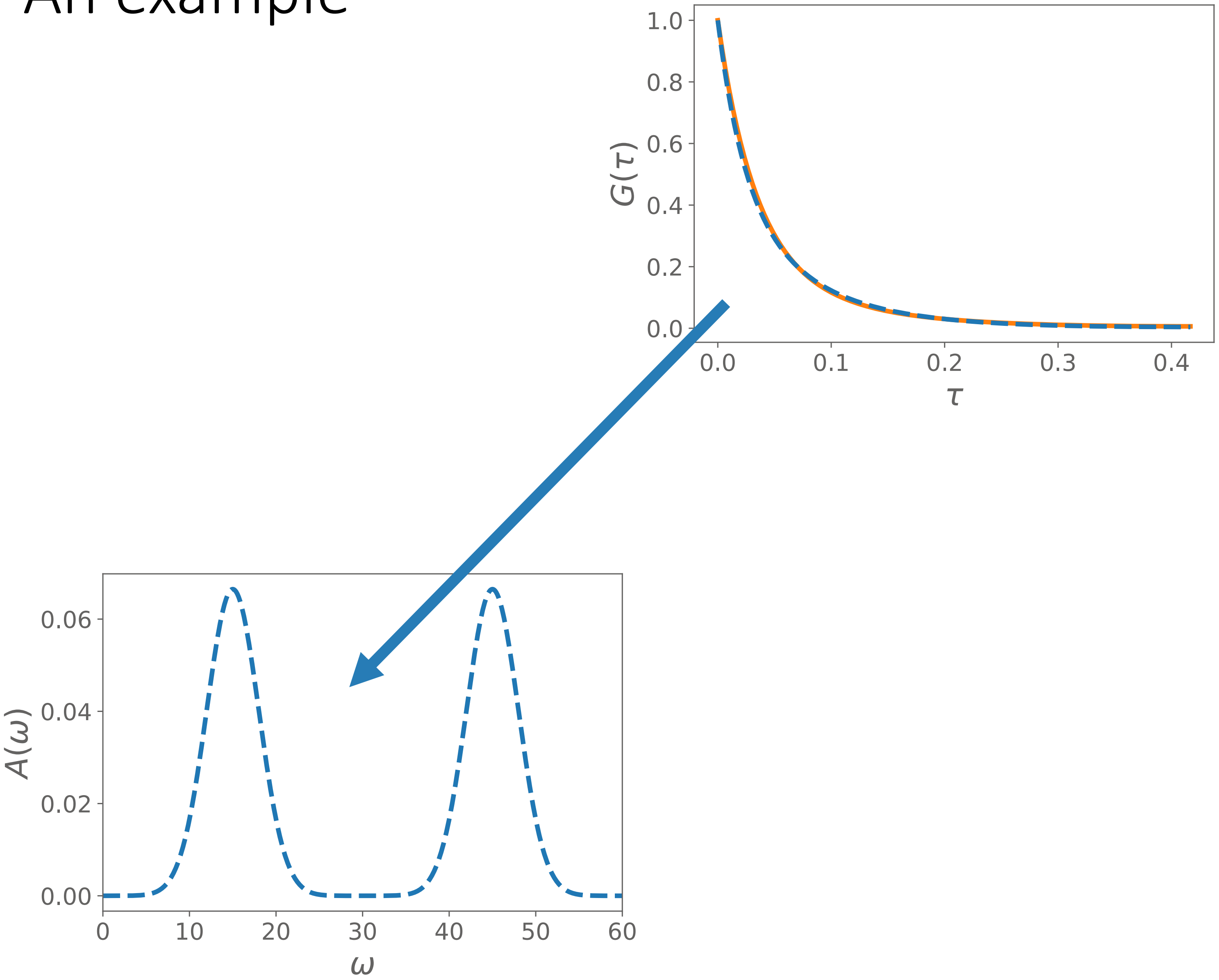
$$A(\omega) = ?$$



An example

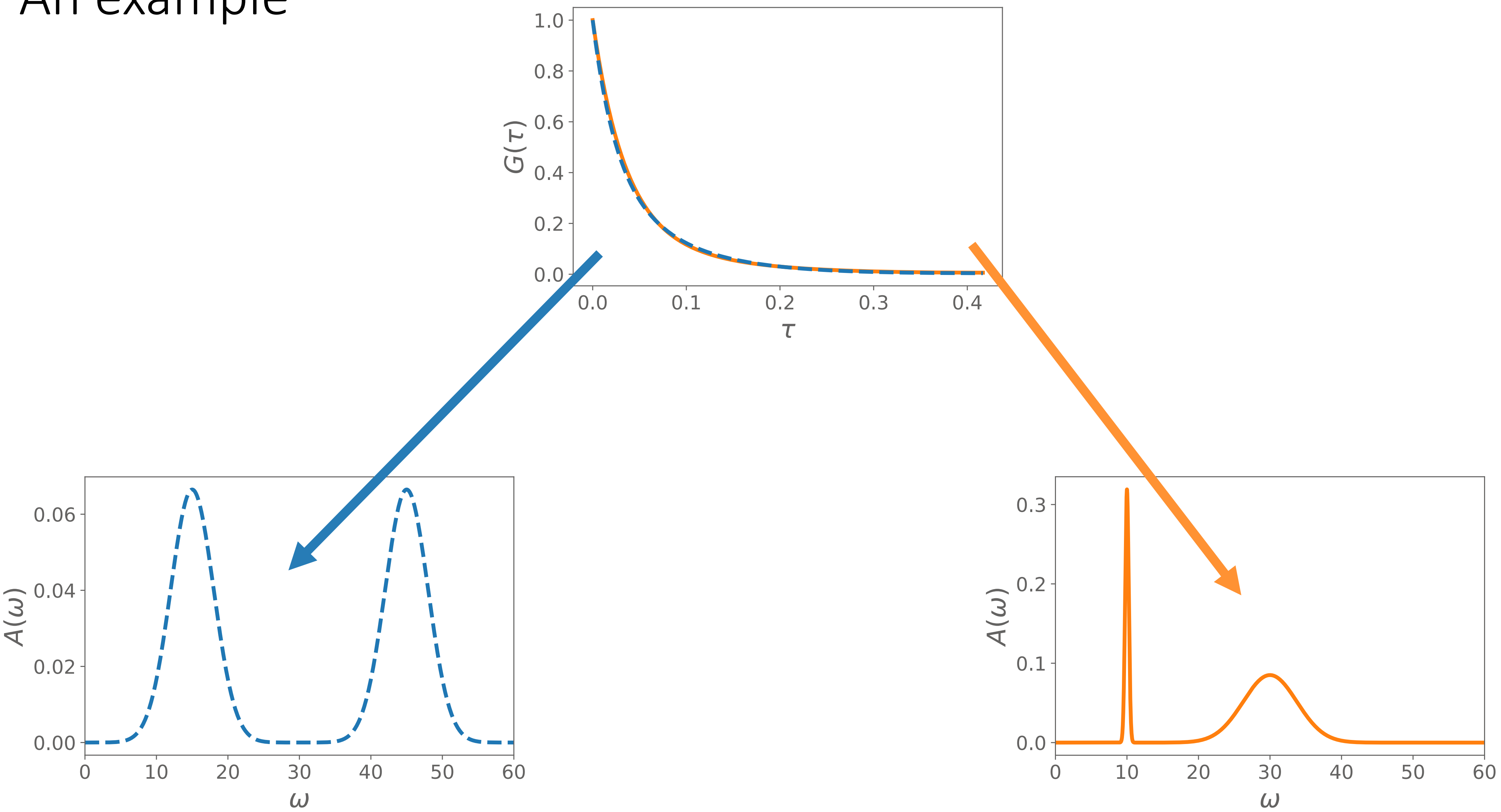


An example



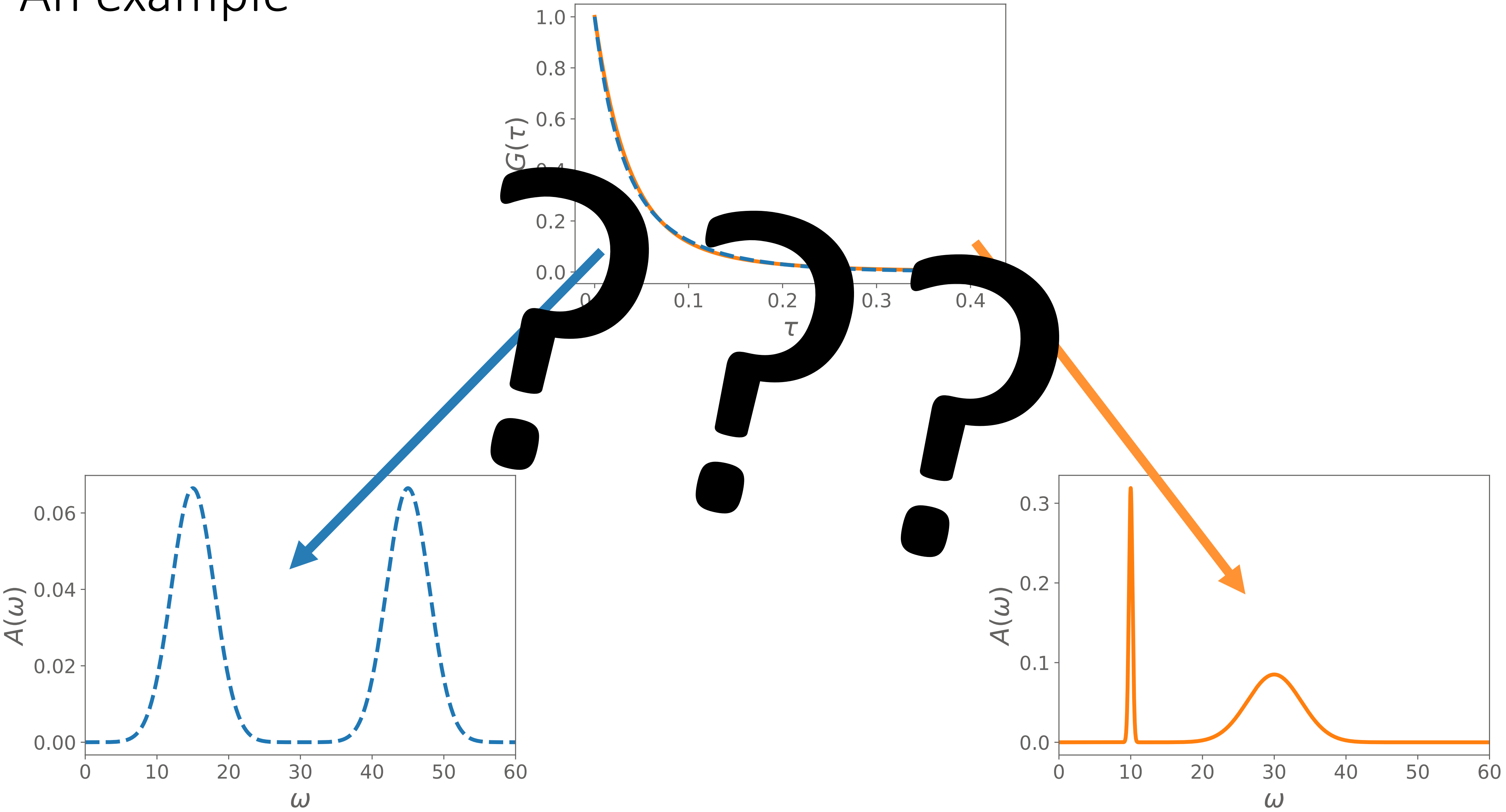
1.0
0.8
0.6
0.4
0.2
0.0
$G(\tau)$
0.0
0.1
0.2
0.3
0.4
τ
0.06
0.04
0.02
0.00
$A(\omega)$
0
10
20
30
40
50
60
ω

An example



1.0
0.8
0.6
0.4
0.2
0.0
$G(\tau)$
0.0
0.1
0.2
0.3
0.4
τ
0.06
0.04
0.02
0.00
$A(\omega)$
0
10
20
30
40
50
60
ω
0.3
0.2
0.1
0.0
$A(\omega)$
0
10
20
30
40
50
60
ω

An example



1.0
0.8
0.6
0.2
0.0
$G(\tau)$
0.1
0.2
0.3
0.4
τ
0.06
0.04
0.02
0.00
$A(\omega)$
0
10
20
30
40
50
60
ω
0.3
0.2
0.1
0.0
$A(\omega)$
0
10
20
30
40
50
60
ω

MaxEnt

Bayes' rule:

$$P(A|G) = \frac{P(G|A)P(A)}{P(G)}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Bayes' rule:

$$P(A|G) = \frac{P(G|A)P(A)}{P(G)}$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Bayes' rule:

$$P(A|G) = \frac{P(G|A)P(A)}{P(G)}$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

Prior probability:

$$P(A) \propto e^{\alpha S}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega)A(\omega)$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega)A(\omega)$$

$$\chi^2 = \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Prior probability:

$$P(A) \propto e^{\alpha S}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Prior probability:

$$P(A) \propto e^{\alpha S}$$

$$S = -\int \frac{d\omega}{2\pi} A(\omega) \ln \frac{A(\omega)}{D(\omega)}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

MaxEnt

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Prior probability:

$$P(A) \propto e^{\alpha S}$$

$$S = -\int \frac{d\omega}{2\pi} A(\omega) \ln \frac{A(\omega)}{D(\omega)}$$

$$P(G|A)P(A) \propto e^{\alpha S - \frac{\chi^2}{2}}$$

D. Bergeron and A.-M. S. Tremblay DOI: 10.1103/PhysRevE.94.023303
M. Jarrell and J. Gubernatis DOI: 10.1016/0370-1573(95)00074-7

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega)A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Algorithm:

$$A_i \rightarrow \chi_i^2$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$

$$\chi^2 = \frac{1}{N} \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau, \omega) A(\omega)$$

$$\chi^2 = \frac{1}{N} \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \rightarrow \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \frac{1}{N} \sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \rightarrow \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i \rightarrow \chi^2_{i+\frac{1}{2}}$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \rightarrow \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i \rightarrow \chi^2_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} \leq \chi_i^2$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \to \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i \to \chi^2_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} \leq \chi_i^2 \to A_{i+1} = A_{i+\frac{1}{2}}$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega)A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \rightarrow \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i \rightarrow \chi^2_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} \leq \chi_i^2 \rightarrow A_{i+1} = A_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} > \chi_i^2$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \to \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i \to \chi^2_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} \le \chi_i^2 \to A_{i+1} = A_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} > \chi_i^2 \to A_{i+1} = A_i$$

Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

Fast and Efficient Stochastic Optimization Method (FESOM)

Minimal knowledge of prior probability:

$$P(A|G) = P(G|A)$$

Likelihood:

$$P(G|A) \propto e^{-\frac{\chi^2}{2}}$$

$$\tilde{G}(\tau) = \int d\omega K(\tau,\omega) A(\omega)$$

$$\chi^2 = \frac{1}{N}\sum_i \frac{\left(\tilde{G}_i - G_i\right)^2}{\sigma^2}$$

Algorithm:

$$A_i \rightarrow \chi_i^2$$

$$A_{i+\frac{1}{2}} = A_i + \lambda_i \rightarrow \chi^2_{i+\frac{1}{2}}$$

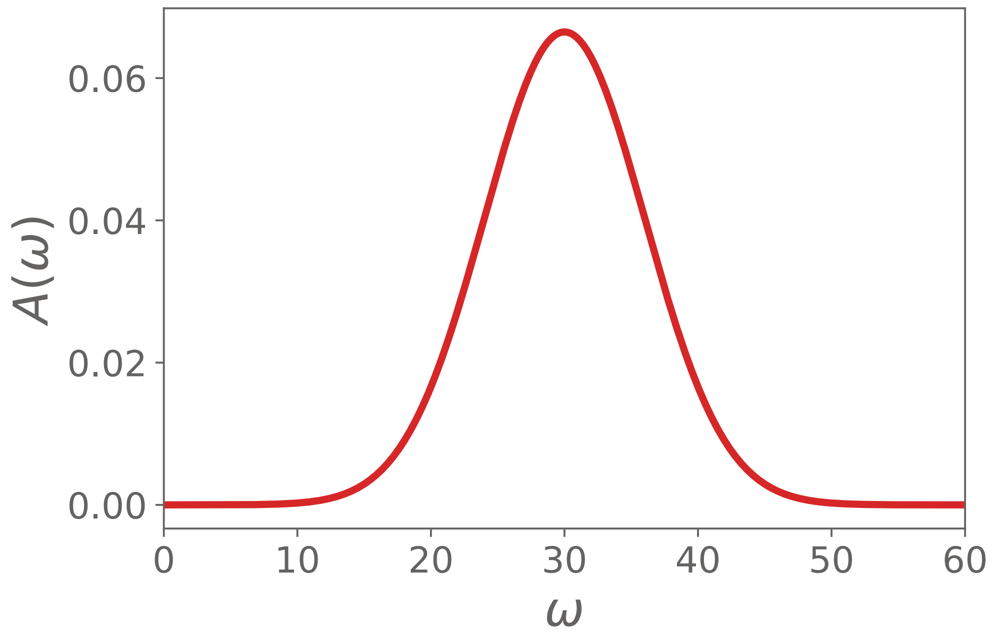
$$\chi^2_{i+\frac{1}{2}} \leq \chi_i^2 \rightarrow A_{i+1} = A_{i+\frac{1}{2}}$$

$$\chi^2_{i+\frac{1}{2}} > \chi_i^2 \rightarrow A_{i+1} = A_i$$

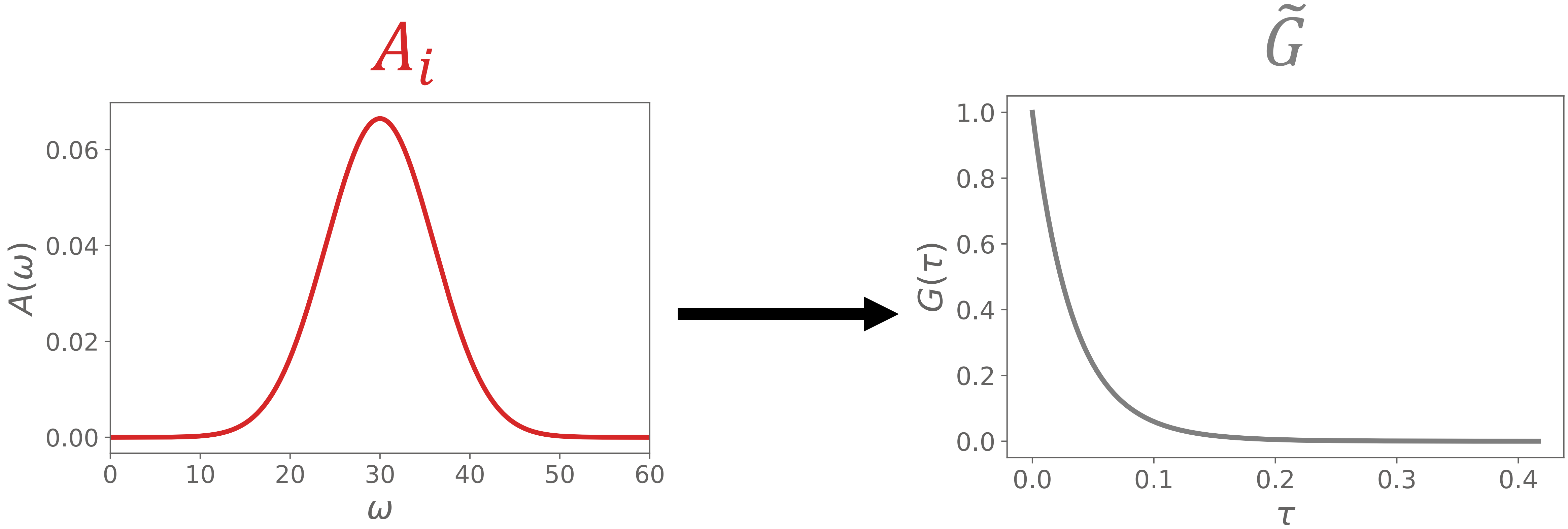
Bao *et al.* DOI: 10.1103/PhysRevB.94.125149

FESOM example

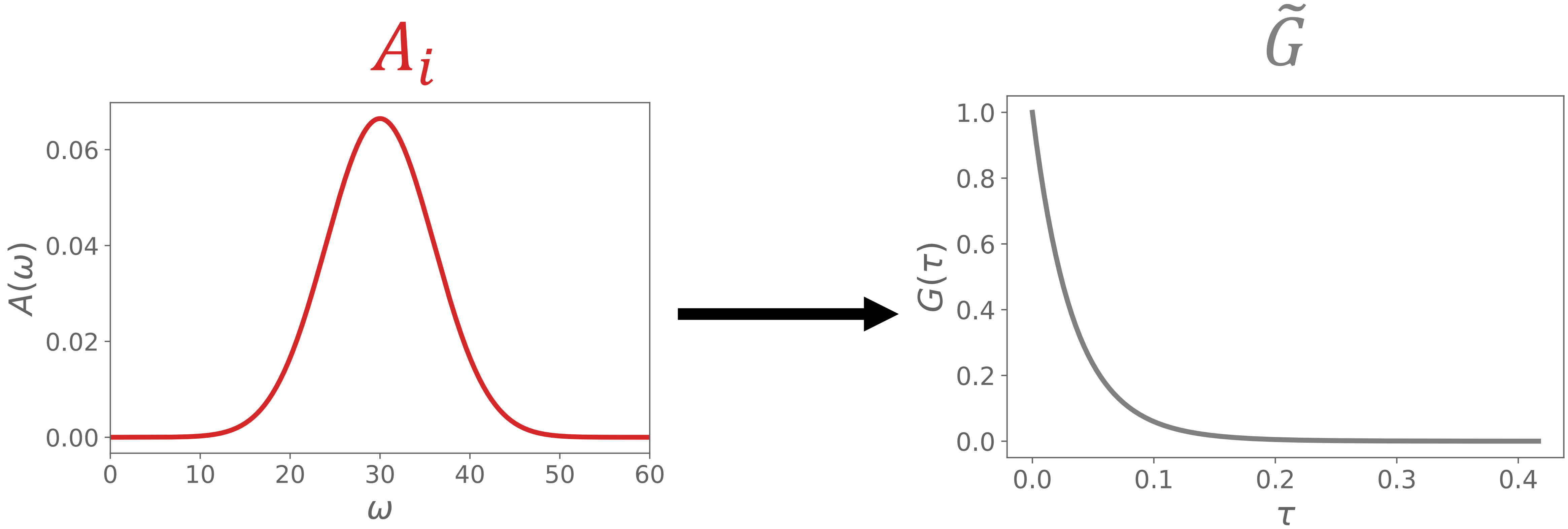
A_i



FESOM example

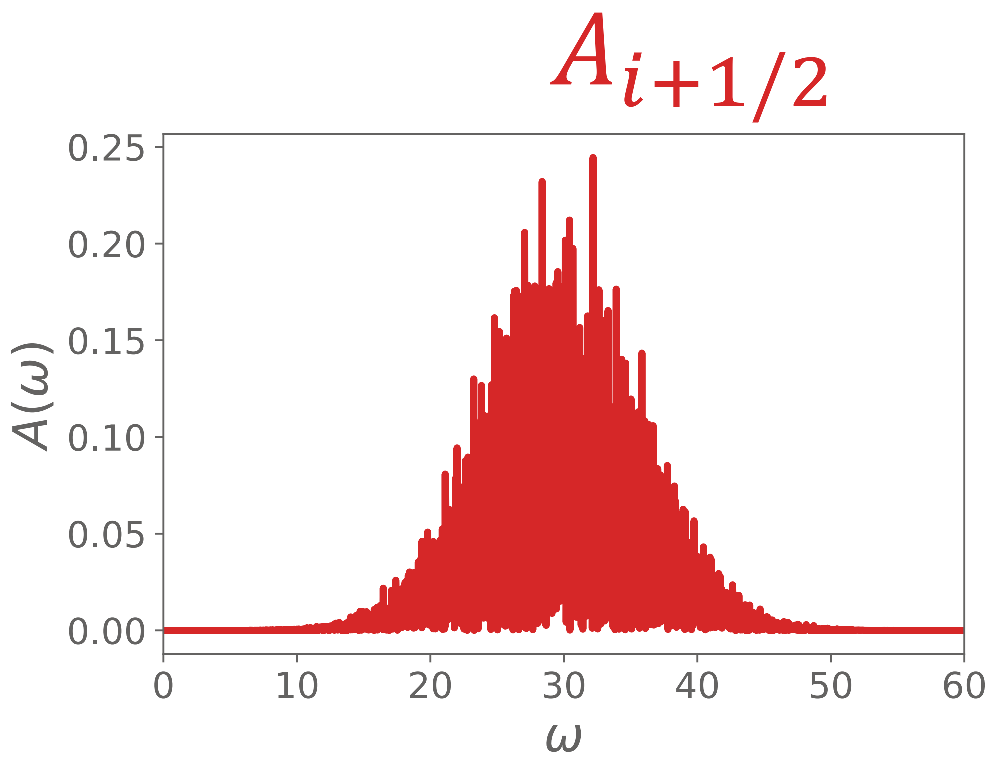


FESOM example

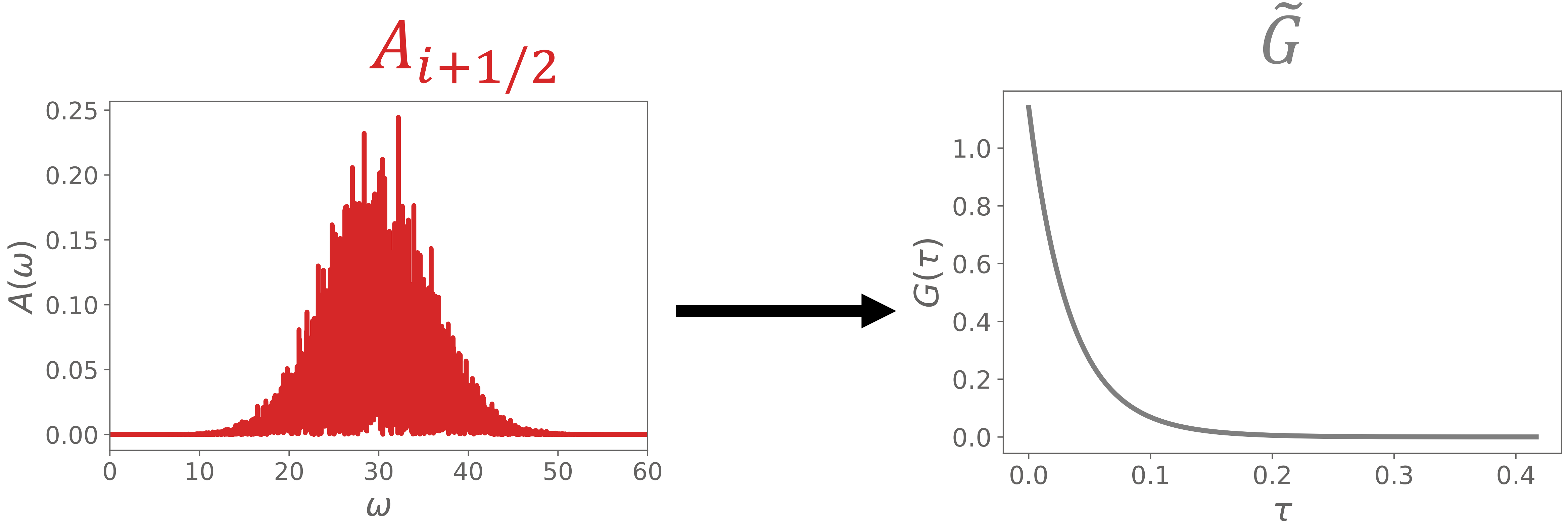


$$\chi_i^2 = 5.53$$

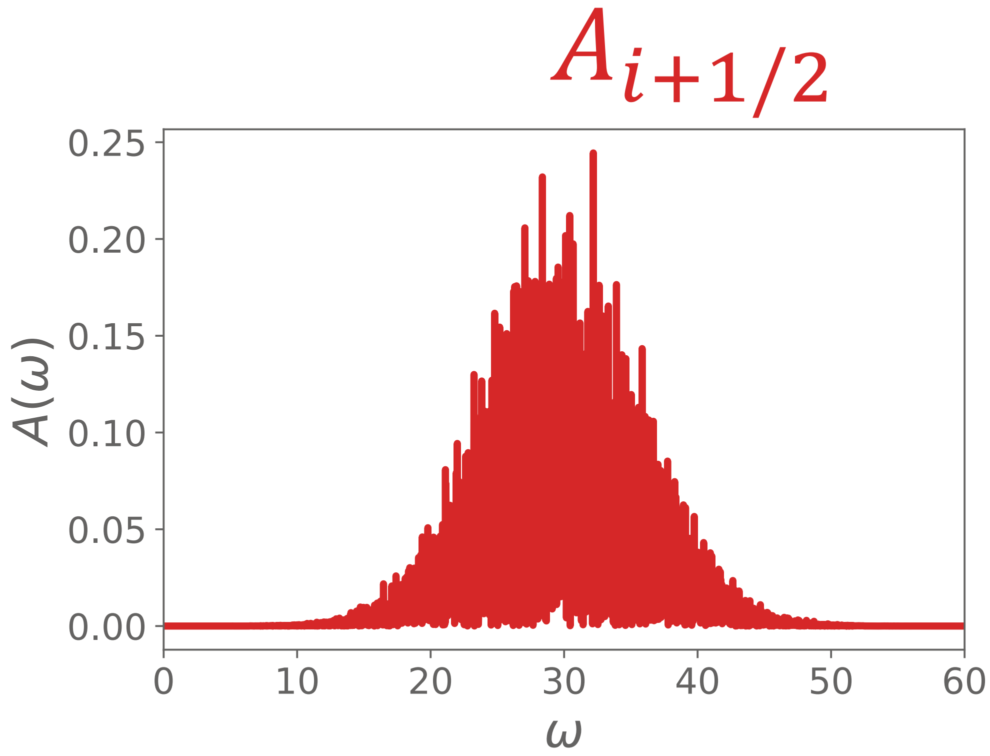
FESOM example

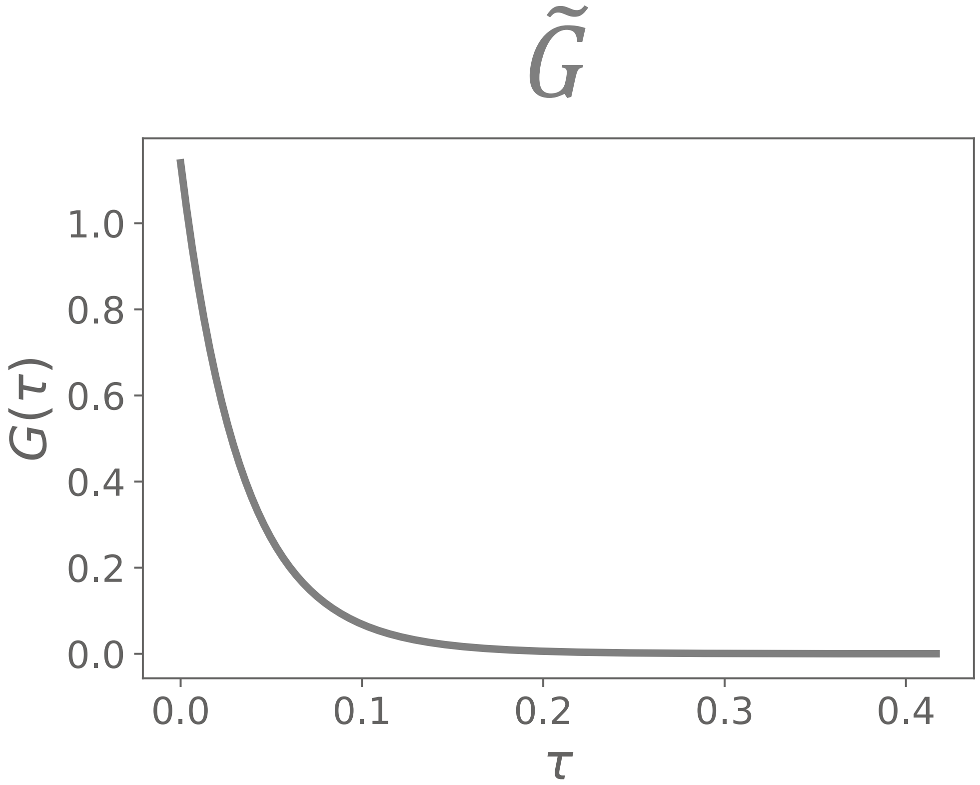


FESOM example



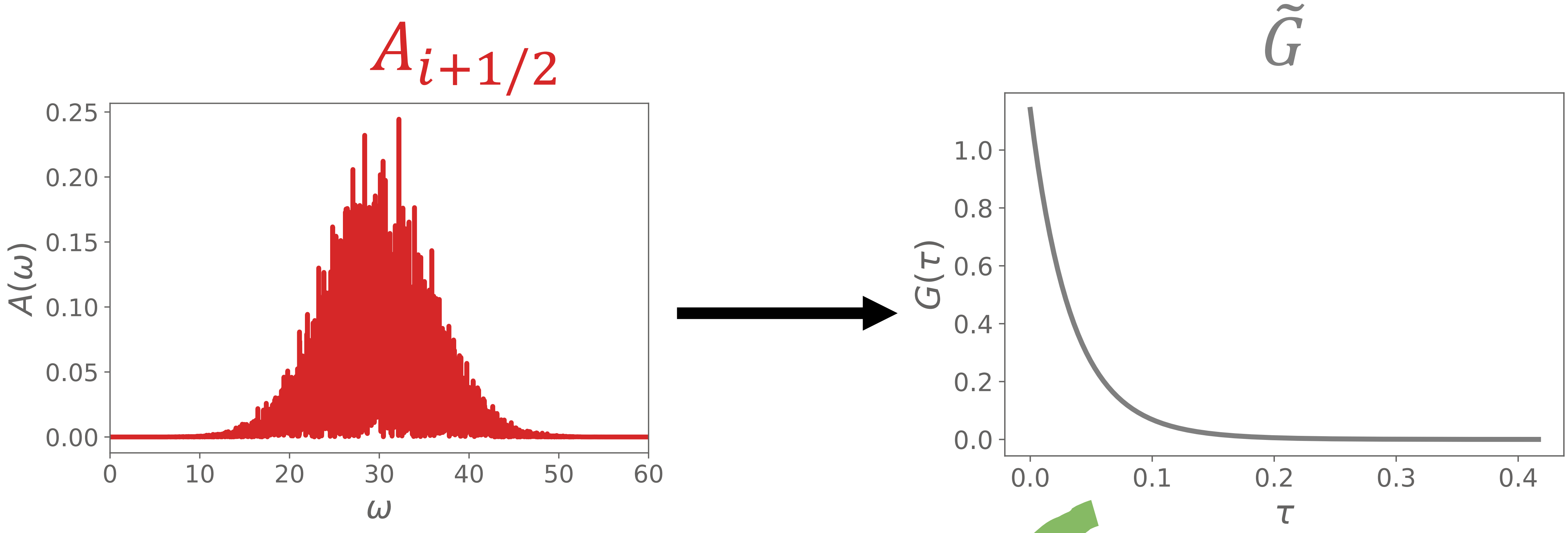
FESOM example





$$\chi^2_{i+1/2} = 5.25$$

FESOM example



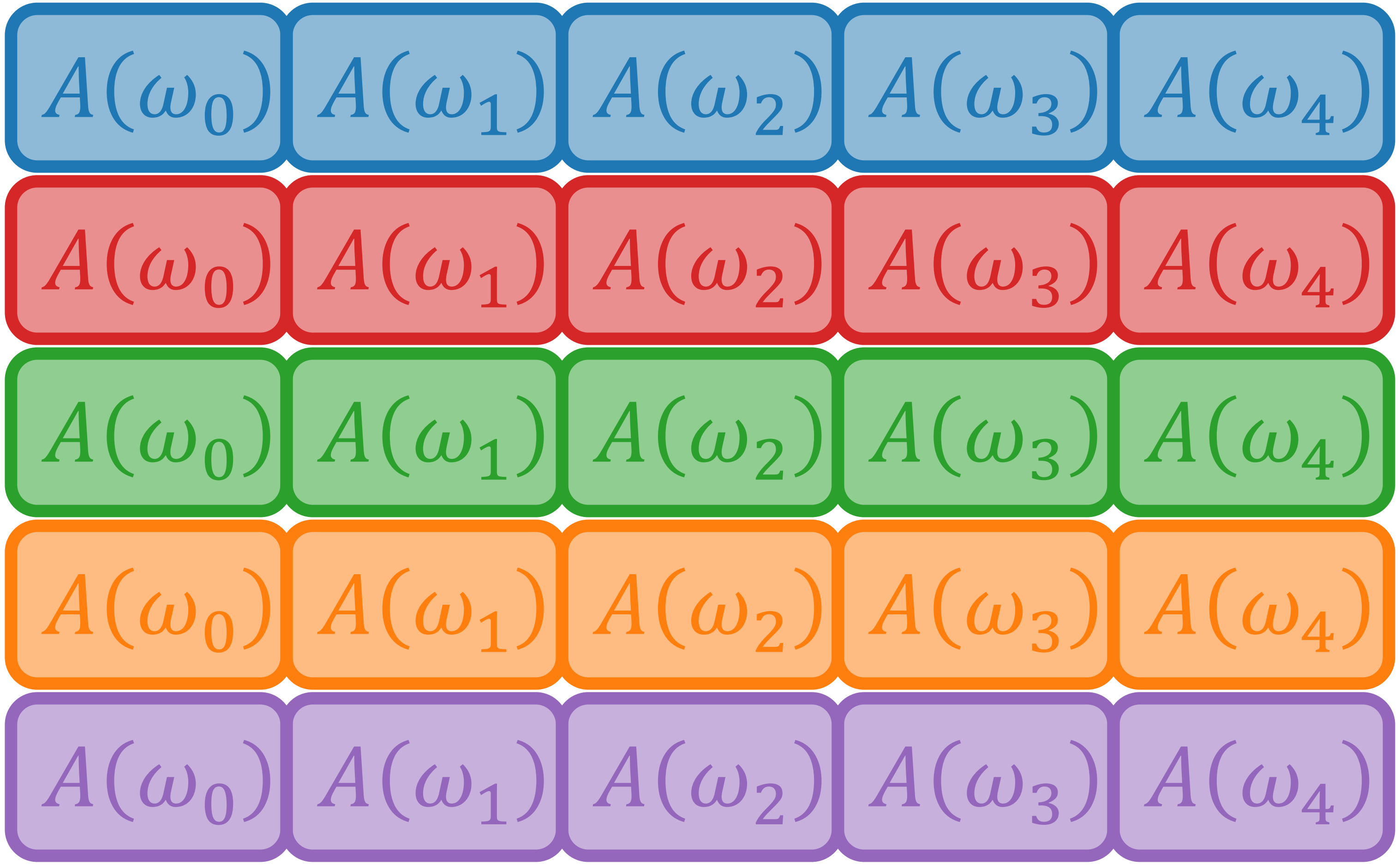
$$\chi^2_{i+1/2} = 5.25$$

Differential Evolution for Analytic Continuation (DEAC)

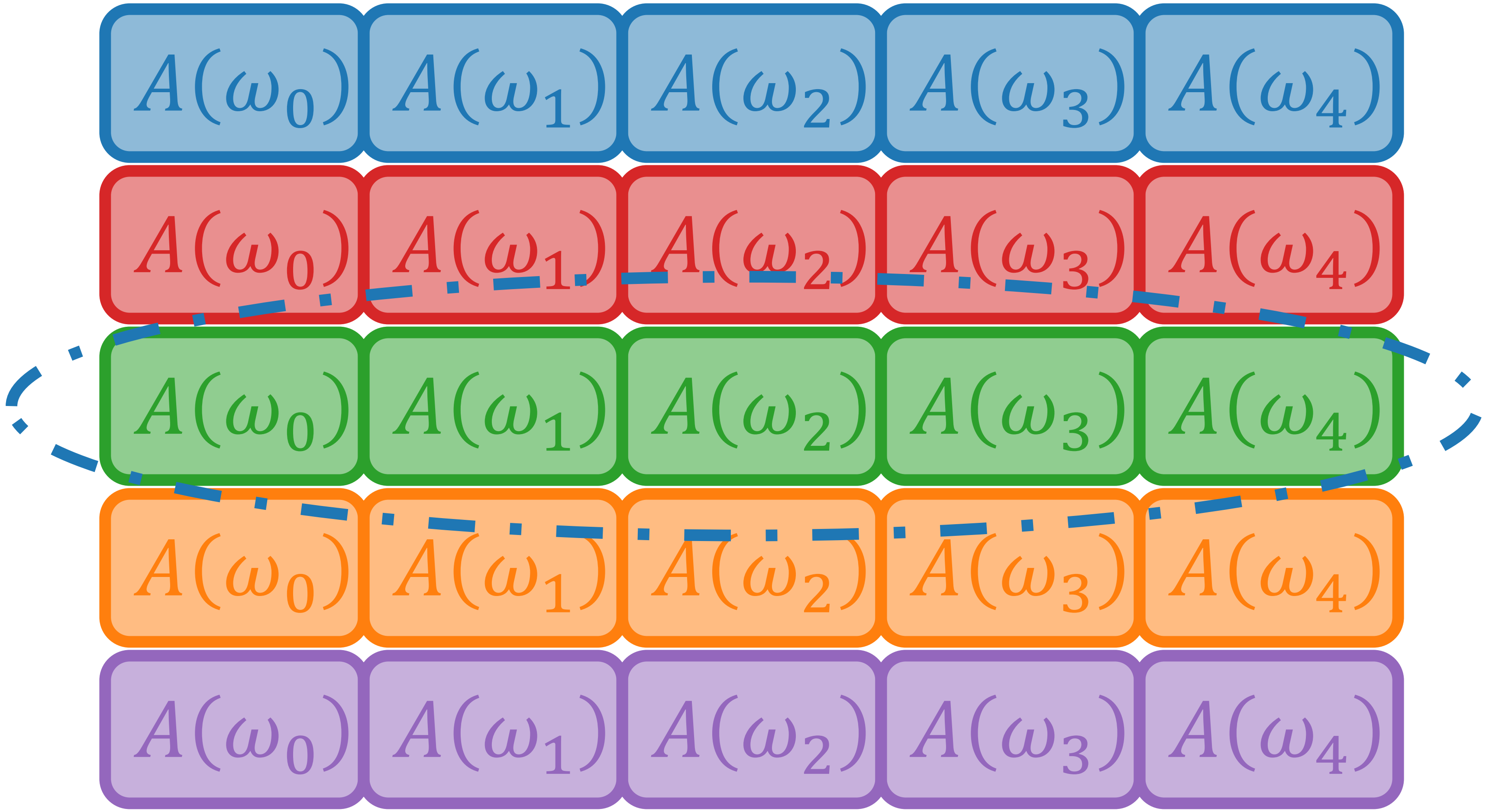
- Inspired by GIFT
- Evolutionary algorithm
  - Population of individuals
  - Genome $\longrightarrow$ $A(\omega_i)$
  - Mutations $\longrightarrow$ vector differences
  - Fitness $\longrightarrow$ $f\left(A;\chi^2,\langle\omega^k\rangle\right)$
  - Rejection $\longrightarrow$ keep most fit

Vitali *et al.* DOI: 10.1103/PhysRevB.82.174510
Storn and Price DOI: 10.1023/A:1008202821328

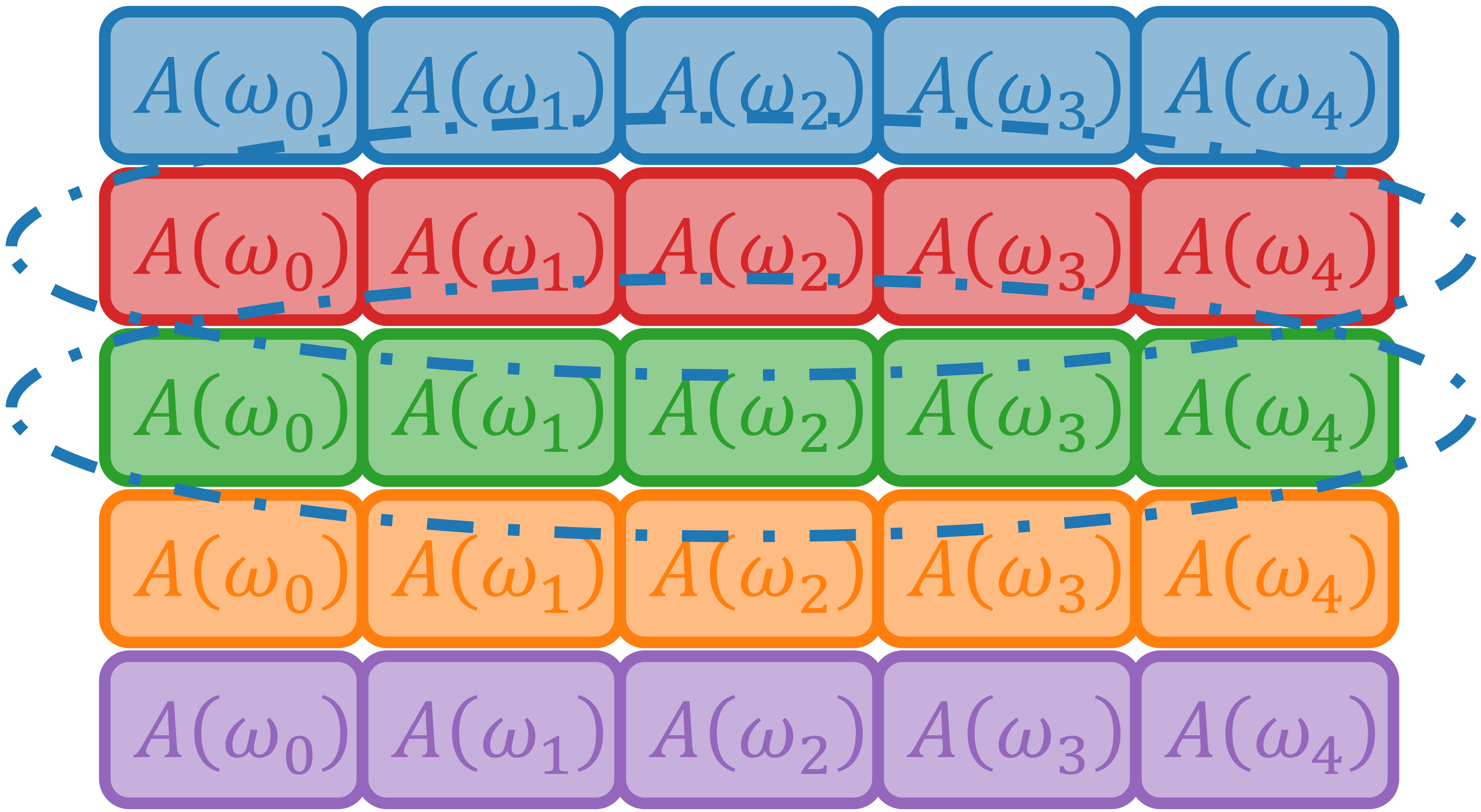
DEAC Population



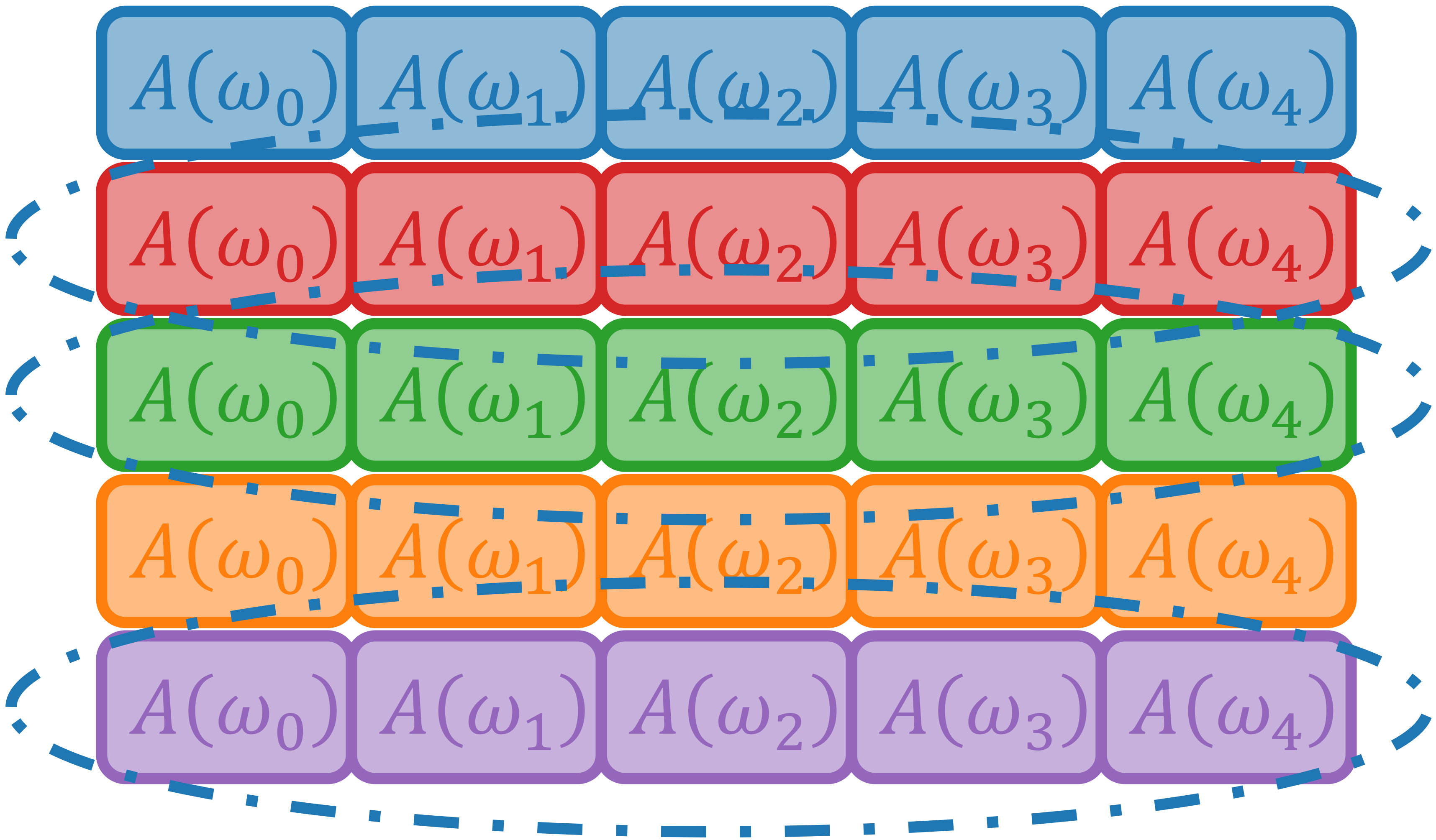
DEAC Mutation



DEAC Mutation



DEAC Mutation



DEAC Mutation

$\tilde{A}(\omega_i)$

DEAC Mutation

$$U(0,1) < C$$

$$\tilde{A}(\omega_i)$$

DEAC Mutation

$$U(0,1) < C$$

$$\tilde{A}(\omega_i) = A(\omega_i) + F \times \left(A(\omega_i) - A(\omega_i) \right)$$

DEAC Mutation

$$U(0,1) < C$$

$$\tilde{A}(\omega_i) = A(\omega_i) + F \times \left(A(\omega_i) - A(\omega_i) \right)$$

$$U(0,1) \geq C$$

$$\tilde{A}(\omega_i) = A(\omega_i)$$

DEAC Mutation

$U(0,1) < C$

$$\tilde{A}(\omega_i) = A(\omega_i) + F \times \left(A(\omega_i) - A(\omega_i) \right)$$

$U(0,1) \geq C$

$$\tilde{A}(\omega_i) = A(\omega_i)$$

$$f(\tilde{A}) < f(A)$$

DEAC Mutation

$U(0,1) < C$

$$\tilde{A}(\omega_i) = A(\omega_i) + F \times \left(A(\omega_i) - A(\omega_i) \right)$$

$U(0,1) \geq C$

$$\tilde{A}(\omega_i) = A(\omega_i)$$

$$f(\tilde{A}) < f(A)$$

DEAC Mutation

$U(0,1) < C$

$\tilde{A}(\omega_i) = A(\omega_i) + F \times \left(A(\omega_i) - A(\omega_i) \right)$

$U(0,1) \geq C$

$\tilde{A}(\omega_i) = A(\omega_i)$

$f(\tilde{A}) < f(A)$

DEAC Mutation

$$U(0,1) < C$$

$$\tilde{A}(\omega_i) = A(\omega_i) + F \times \left(A(\omega_i) - A(\omega_i) \right)$$

$$U(0,1) \geq C$$

$$\tilde{A}(\omega_i) = A(\omega_i)$$

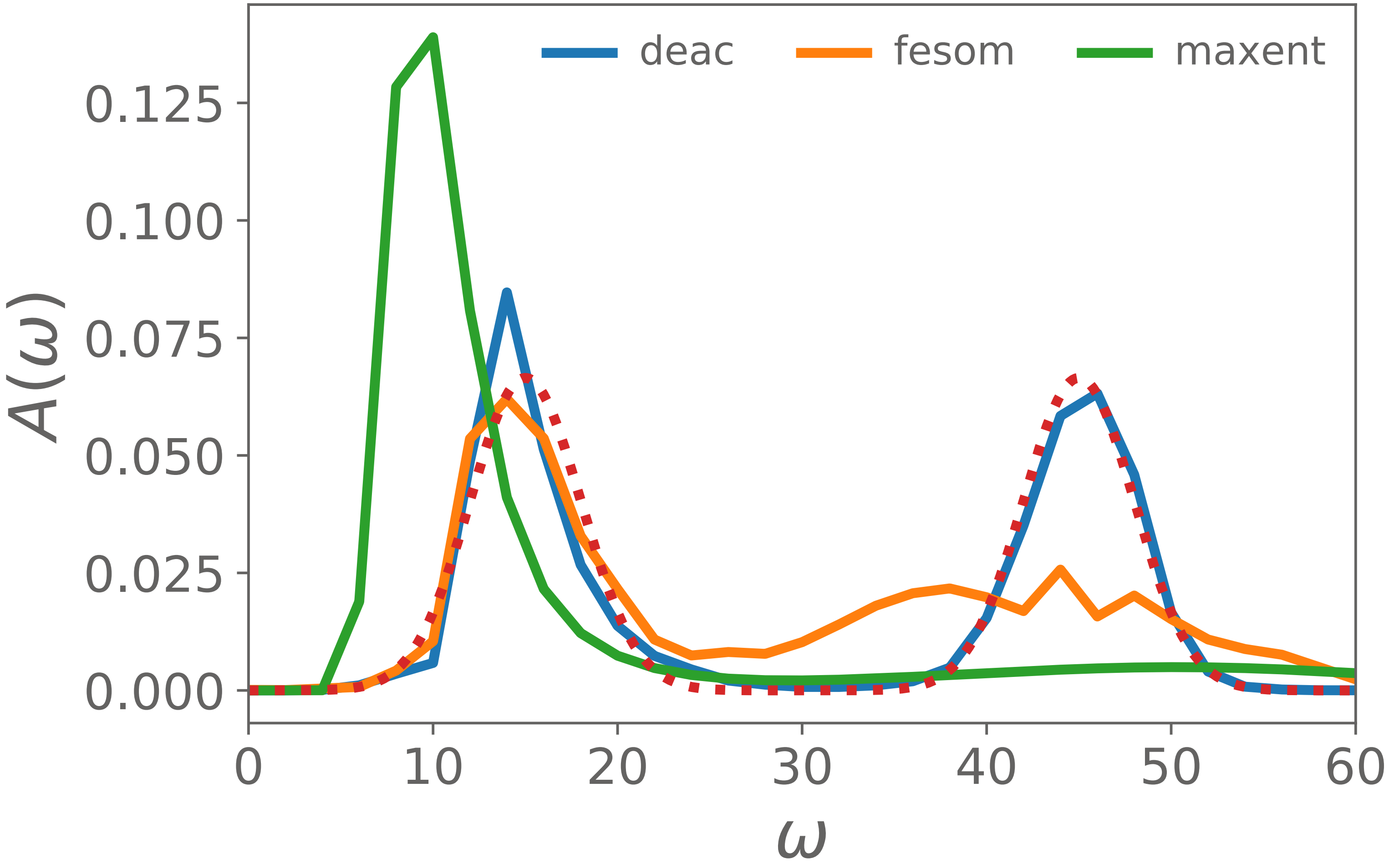
$$f(\tilde{A}) < f(A)$$

DEAC Population

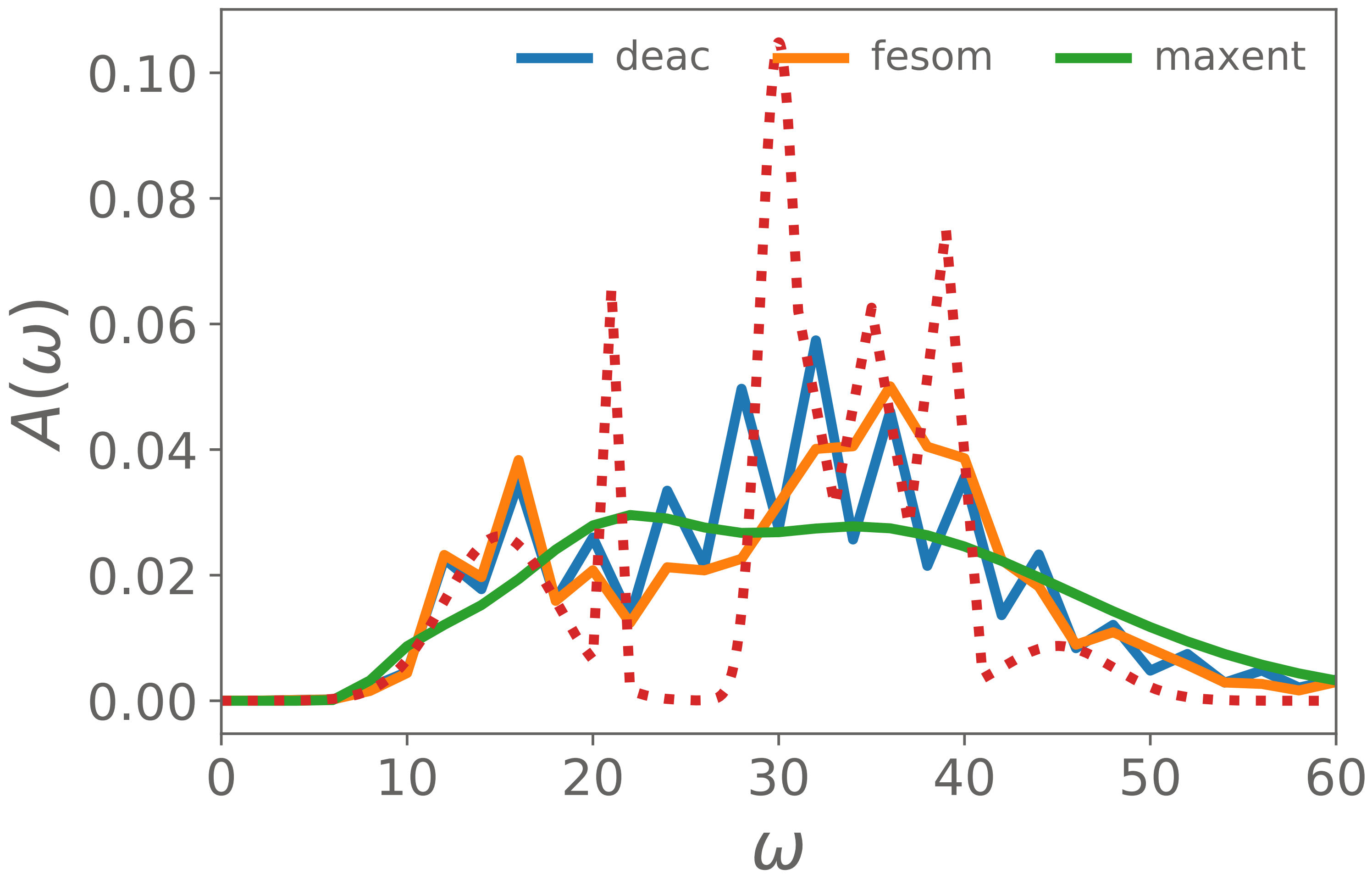
$A(\omega_0)$	$A(\omega_1)$	$A(\omega_2)$	$A(\omega_3)$	$A(\omega_4)$	F	C
$A(\omega_0)$	$A(\omega_1)$	$A(\omega_2)$	$A(\omega_3)$	$A(\omega_4)$	F	C
$A(\omega_0)$	$A(\omega_1)$	$A(\omega_2)$	$A(\omega_3)$	$A(\omega_4)$	F	C
$A(\omega_0)$	$A(\omega_1)$	$A(\omega_2)$	$A(\omega_3)$	$A(\omega_4)$	F	C
$A(\omega_0)$	$A(\omega_1)$	$A(\omega_2)$	$A(\omega_3)$	$A(\omega_4)$	F	C

Qin and Suganthan DOI: 10.1109/CEC.2005.1554904

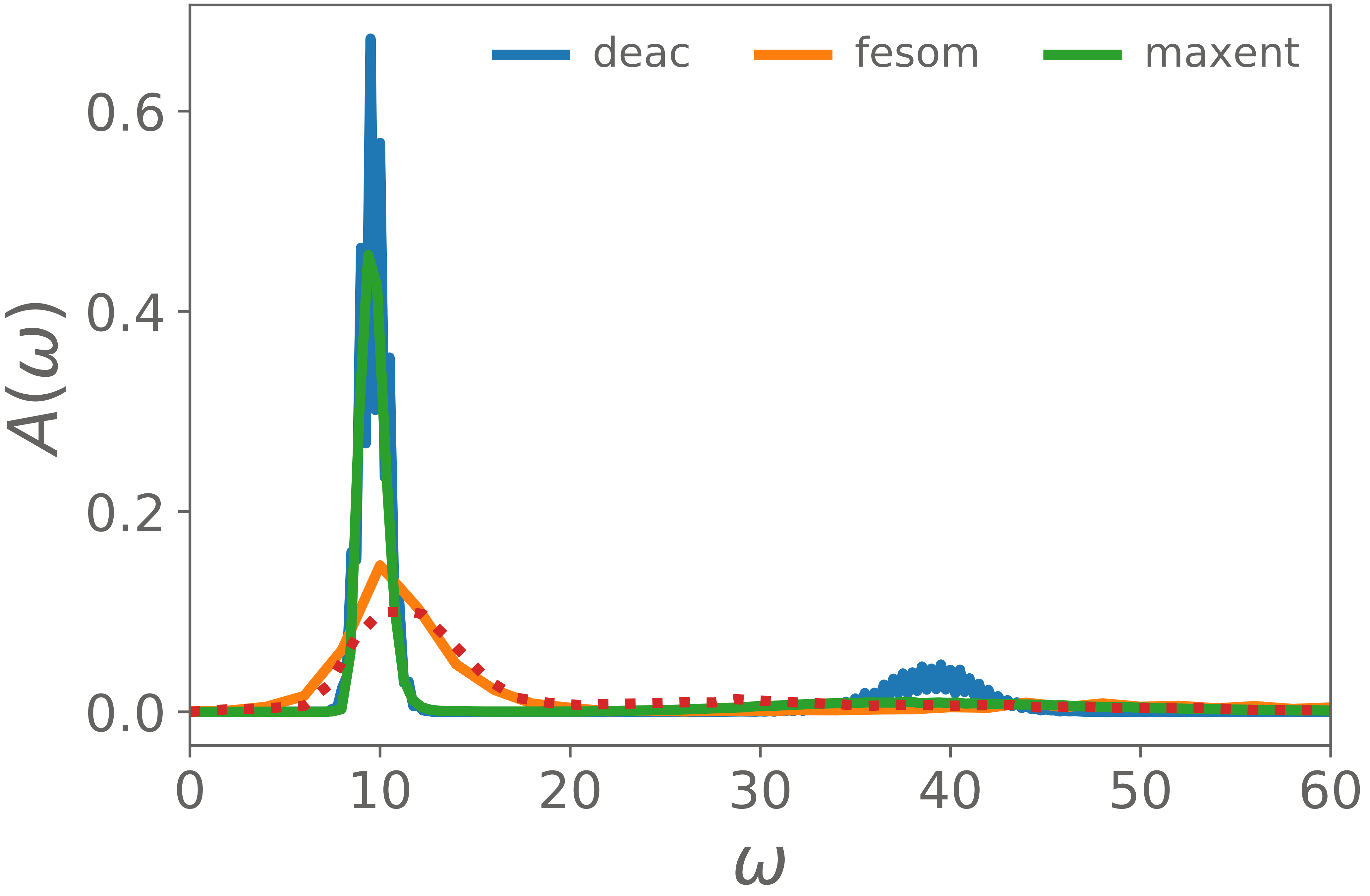
How do the three methods compare?



Method	χ^2
MEM	3.5×10^{-4}
FESOM	5.2×10^{-5}
DEAC	8.6×10^{-6}



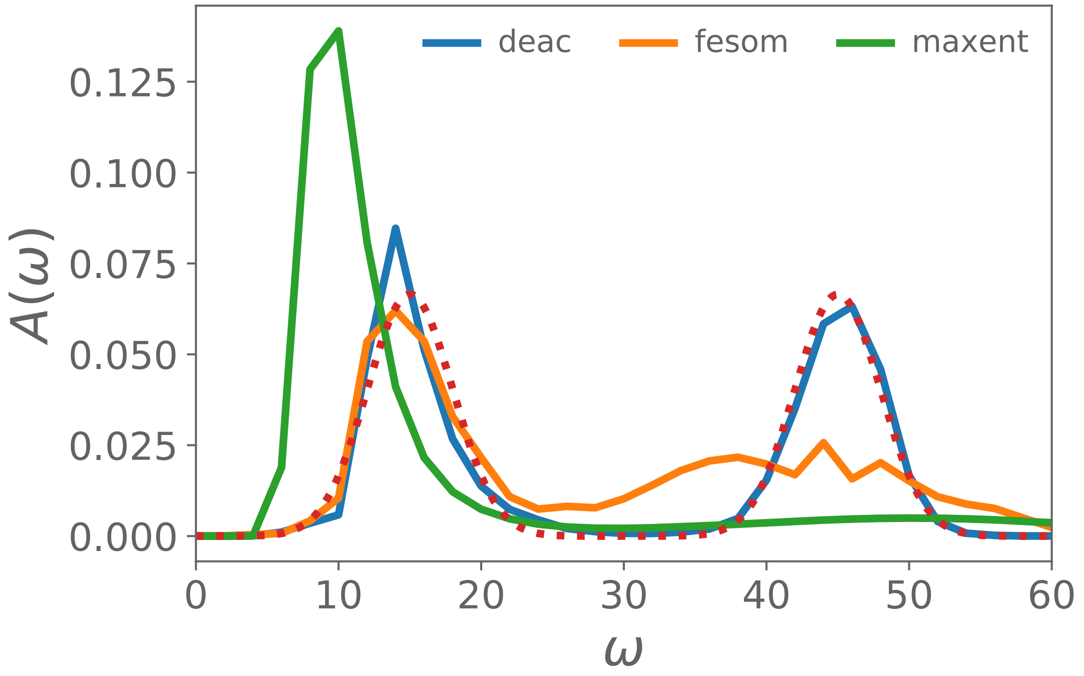
Method	χ^2
MEM	9.3×10^{-5}
FESOM	6.0×10^{-5}
DEAC	8.9×10^{-5}



deac
fesom
maxent
0.6
0.4
0.2
0.0
A(ω)
0
10
20
30
40
50
60
ω

Future Work

- Use DEAC on new qmc data
- Port code to gpu



GitHub

DelMaestroGroup

nscottnichols

The University of Vermont