Stochastic Analytical Continuation
— Principle, Algorithm & Application

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@ The University of Hong Kong

Spectral function

- Real-time correlation

$$G(t) = \langle \mathcal{O}^\dagger(t)\mathcal{O}(0)\rangle = \langle \mathrm{e}^{\mathrm{i}Ht}\mathcal{O}^\dagger \mathrm{e}^{-\mathrm{i}Ht}\mathcal{O}\rangle \tag{1}$$

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- Fourier transformation ⇒ spectral function

$$\begin{aligned} S(\omega) &= \int \mathrm{d}t \mathrm{e}^{\mathrm{i}\omega t} G(t) \\ &= \frac{1}{\mathcal{Z}}\sum_{mn} \mathrm{e}^{-\beta E_n} \int \mathrm{d}t \langle n|\mathrm{e}^{\mathrm{i}Ht}\mathcal{O}^\dagger \mathrm{e}^{-\mathrm{i}Ht}|m\rangle\langle m|\mathcal{O}|n\rangle \\ &= \frac{1}{\mathcal{Z}}\sum_{mn} \mathrm{e}^{-\beta E_n} \int \mathrm{d}t \mathrm{e}^{\mathrm{i}(\omega - E_m + E_n)t} |\langle m|\mathcal{O}|n\rangle|^2 \\ &= \frac{1}{\mathcal{Z}}\sum_{mn} \mathrm{e}^{-\beta E_n} |\langle m|\mathcal{O}|n\rangle|^2 \delta(\omega - E_m + E_n) \end{aligned} \tag{2}$$

- An excitation state corresponds to a non-zero point in $S(\omega)$ – energy spectrum

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   - Most reliable;
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3. **Quantum Monte Carlo**
   - Formulated in imaginary time;
   - No direct access to real time properties.

$$G(t) = \langle \mathrm{e}^{\mathrm{i}Ht} \mathcal{O}^\dagger \mathrm{e}^{-\mathrm{i}Ht} \mathcal{O} \rangle \tag{3}$$

   - QMC $\rightarrow$ SAC

Ingredients from QMC

- Imaginary time correlation

$$G(\tau = \mathrm{i}t) = \langle \mathcal{O}^\dagger(\tau)\mathcal{O}(0)\rangle = \langle \mathrm{e}^{H\tau}\mathcal{O}^\dagger \mathrm{e}^{-H\tau}\mathcal{O}\rangle \tag{4}$$

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- Connexion to spectral function

$$\begin{aligned} G(t) &= \int \mathrm{d}\omega \mathrm{e}^{-\mathrm{i}\omega t} S(\omega) \quad S(\omega) = \int \mathrm{d}t \mathrm{e}^{\mathrm{i}\omega t} G(t) \\ G(\tau) &= \int \mathrm{d}\omega \mathrm{e}^{-\omega\tau} S(\omega) \end{aligned} \tag{5}$$

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- Inverse Laplacian transformation isn't numerically stable
- 'Analytical continuation' : $G(\tau = it)$ on the imaginary axis $\longrightarrow G(t)$ on the real axis

Parametrization : Convert into fitting problem

- Functional form

$$S(\omega) = A_1\delta(\omega - \omega_q) + A_2 e^{-(\omega-\nu)^2/2\sigma^2} \tag{6}$$

- Easy to control ; biased by the form[1]
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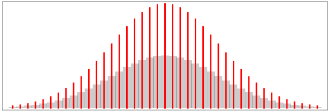
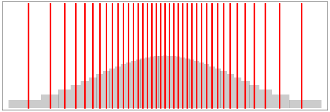


Equal inteval



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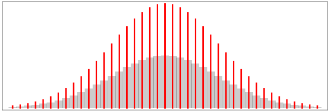

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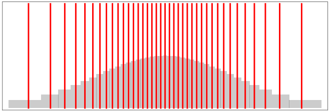

Equal weight

- Constraints
  - Positivity, normalization

Reproduce $G(\tau)$ from fitting

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- Carry out explicitly the integral

$$\tilde{G}(\tau) = \sum_i A_i \frac{1}{\pi} \frac{\mathrm{e}^{-\omega_i \tau} + \mathrm{e}^{-\omega_i (\beta - \tau)}}{1 + \mathrm{e}^{-\omega_i \beta}} \tag{8}$$

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- Write in terms of kernals

$$\tilde{G}(\tau) = \sum_i A_i K(\tau, \omega_i), \quad K(\tau, \omega) = \frac{1}{\pi} \frac{e^{-\omega\tau} + e^{-\omega(\beta-\tau)}}{1 + e^{-\omega\beta}} \tag{9}$$

The kernal for every τ and ω is stored in advance.

Fitting goodness – χ^2

- Compare the measured value $\bar{G}(\tau_i) = \sum_b G^b(\tau_i)/N_b$ and fit value $\tilde{G}(\tau_i)$

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- Correlated variables

$$\chi^2 = \sum_{ij}(C^{-1})_{ij}(\bar{G}(\tau_i) - \tilde{G}(\tau_i))(\bar{G}(\tau_j) - \tilde{G}(\tau_j)) \tag{11}$$

$$C_{ij} = \frac{1}{N_b(N_b-1)}\sum_b(G^b(\tau_i) - \bar{G}(\tau_i))(G^b(\tau_j) - \bar{G}(\tau_j)) \tag{12}$$

Rotation to eigenbasis

$$C_{ij} \sim \langle (G_i - \bar{G}_i)(G_j - \bar{G}_j) \rangle \tag{13}$$

In practice, we diagonalize the Green's functions at first

$$\begin{aligned} \epsilon_\alpha \delta_{\alpha\beta} &= \mathbf{TCT}^\dagger \\ G'_\alpha &= \sum_i T_{\alpha i} G(\tau_i) \\ \chi^2 &= \sum_\alpha \frac{1}{\epsilon_\alpha} (\tilde{G}'_\alpha - \bar{G}'_\alpha)^2 \end{aligned} \tag{14}$$

$$\begin{aligned} \tilde{G}'_\alpha &= \sum_i A_i K'_\alpha(\omega_i) \\ K'_\alpha(\omega) &= \sum_j T_{\alpha j} K(\tau_j, \omega) \end{aligned} \tag{15}$$

Direct fitting

- Test on methods
  - Synthesize $S(\omega)$
  - Transform into $G(\tau)$
  - Add Gaussian noise
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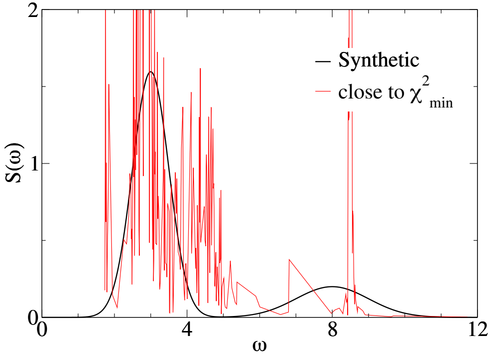
- Annealing process to minimize χ^2
- Overfitting – Fitting to the error bar



Hui Shao's slide on BSSQM at UCAS, 2019

Maximum entropy method

- Bayes' theorem

$$\mathbb{P}(S(\omega)|G(\tau))\mathbb{P}(G(\tau)) = \mathbb{P}(G(\tau)|S(\omega))\mathbb{P}(S(\omega)) \qquad (16)$$

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- MEM assumption : particular choice of $\mathbb{P}(S(\omega))$

$$\mathbb{P}(S(\omega)) \sim \exp(\alpha\mathcal{S}) \tag{18}$$

- Information theory entropy

$$\mathcal{S} = -\int \mathrm{d}\omega S(\omega) \log \frac{S(\omega)}{D(\omega)} \tag{19}$$

- $D(\omega)$ 'default model' : smoothest function consistent with prior knowledge

Silver, Sivia & Gubernatis, Phys. Rev. B 41, 2380 (1990)

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- At the same time evaluate the goodness of fitting and compare with a given spectral
- $\mathcal{S}$ has a smoothing effect.
- Different variants of the method use different criteria to determine α

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Not impose the entropy explicitly as a prior
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$$W \sim \exp\left(-\frac{\chi^2}{2\Theta}\right) \tag{21}$$

Θ is an analogy to thermodynamic temperature

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- Setting the weight of each

$$W \sim \exp\left(-\frac{\chi^2}{2\Theta}\right) \quad (21)$$

Θ is an analogy to thermodynamic temperature

- Monte Carlo sampling of ω_i and A_i of δ-functions

$$S(\omega) = \sum_i A_i \delta(\omega - \omega_i) \quad (22)$$

- MaxEnt method can be regarded as a mean field of SAC.

Shao, Qin, Capponi et al., Phys. Rev. Lett. 7, 041072 (2017)

Determining Θ

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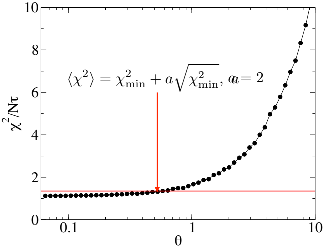
- Statistically motivated method: raise the χ^2 by a standard deviation with respect to the minimum

$$\chi^2(\theta) = \chi^2_{\min} + a\sigma_{\chi^2} \qquad (23)$$

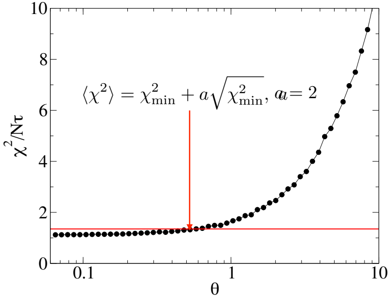
$$\chi^2_{\min} \sim N_\tau, \quad \sigma_{\chi^2} \sim \sqrt{2N_\tau} \quad (24)$$

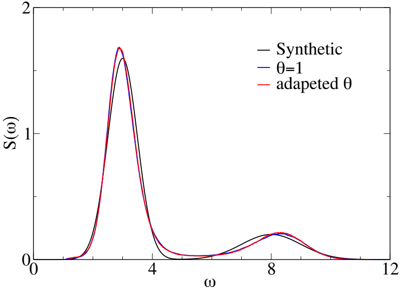


  - *Sandvik, Phys. Rev. E 94, 063308 (2016)*

Determining Θ

- Use simulated annealing to find the lowest χ^2
- Raise Θ to meet the criteria

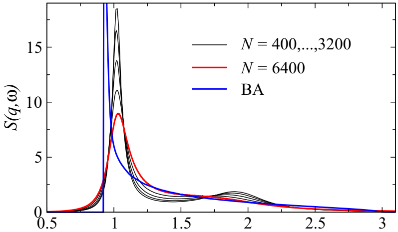


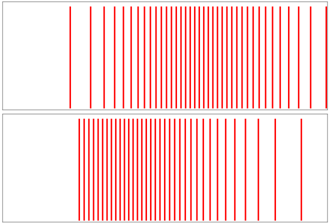


Shao, Qin, Capponi et al., Phys. Rev. Lett. 7, 041072 (2017)

Sharp peaks

- Sharp peak feature – Spinon mode in spin-1/2 Heisenberg





- Unrestricted result: peak suppressed and moved

Sandvik, Phys. Rev. E 94, 063308 (2016)

- Restriction 1: Cut-off frequency

Sharp peaks

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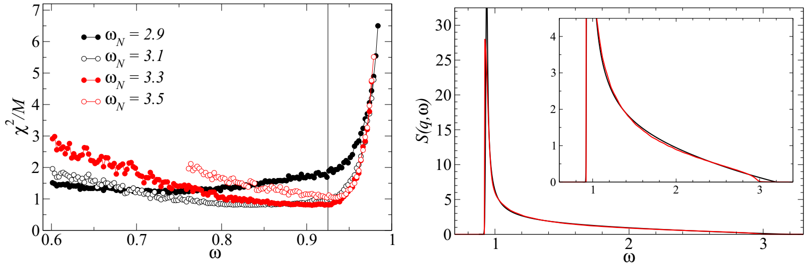
- Determine ω_{inf} by minimizing χ^2



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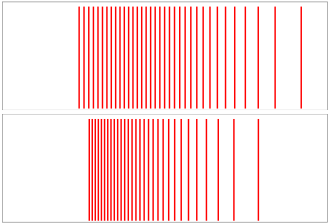
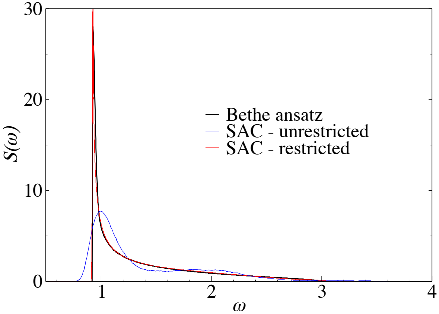
Sharp peaks

- Restriction 2: Monotonically increasing distances ⇔ monotonically decreasing $S(\omega)$

$$S(\omega) \approx A/\delta\omega \tag{25}$$





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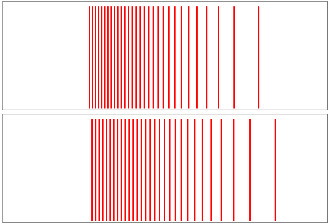
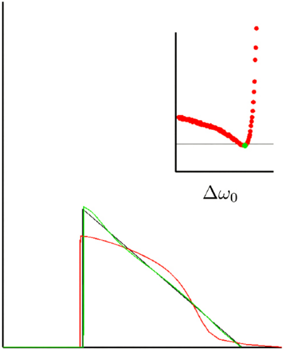
- Restriction 3: Fix the initial inteval $\delta\omega|_{\omega_{\text{inf}}}$

$$S(\omega) \approx A/\delta\omega \tag{26}$$





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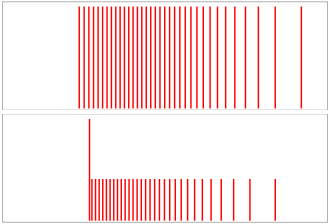
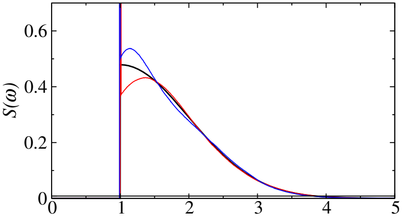
Delta peak

- Magnon mode : A discrete peak followed by a continue spectrum
- Restriction : Add a predominate δ peak at the inferior limit





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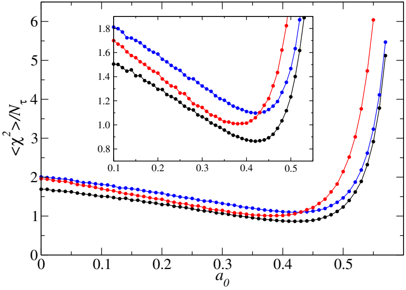
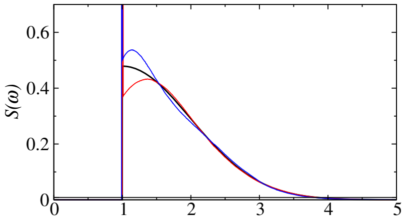
Delta peak

- Restriction : Add a predominate δ peak at the inferior limit
- Determine the height of the predominant peak by minimizing χ^2





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Dynamic spin structure factor

$$S(\omega) = \int \mathrm{d}t \mathrm{e}^{\mathrm{i}\omega t} G(t), \quad G(t) = \langle \mathcal{O}^{\dagger}(t) \mathcal{O}(0) \rangle \tag{27}$$

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Choose

$$\mathcal{O} \to S^\alpha(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_i S_i^\alpha \mathrm{e}^{-\mathbf{i}\mathbf{q}\cdot\mathbf{r}_i} \tag{28}$$

$$G(\tau) = \frac{1}{N} \sum_{ij} \langle S_i^\alpha(\tau) S_j^\alpha(0)\rangle \cos \mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j) \tag{29}$$

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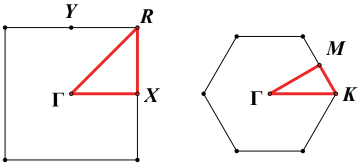
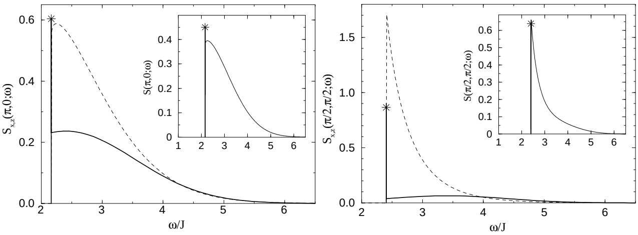


Antiferromagnetic Heisenberg model

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{30}$$



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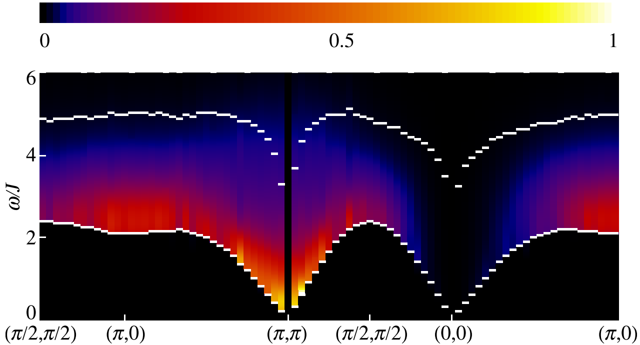
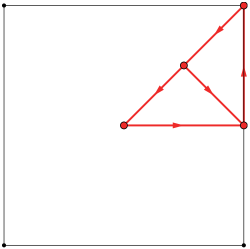
SAC spectrum





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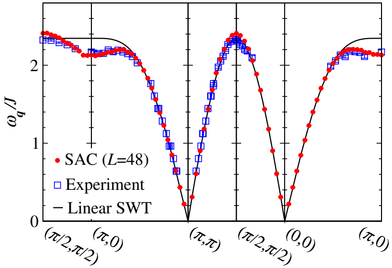
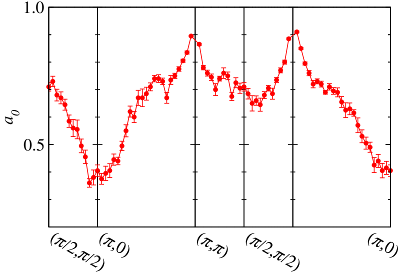
Predominant feature





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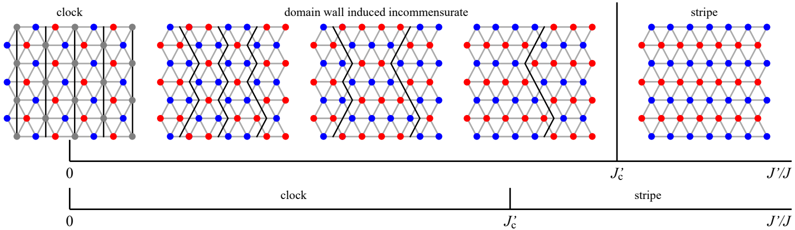
Frustrated Ising Model

$$H = J \sum_{\langle ij \rangle} S_i^z S_j^z + J' \sum_{\langle\langle ij \rangle\rangle} S_i^z S_j^z - h \sum_i S_i^x \tag{31}$$



Excitation spectrum

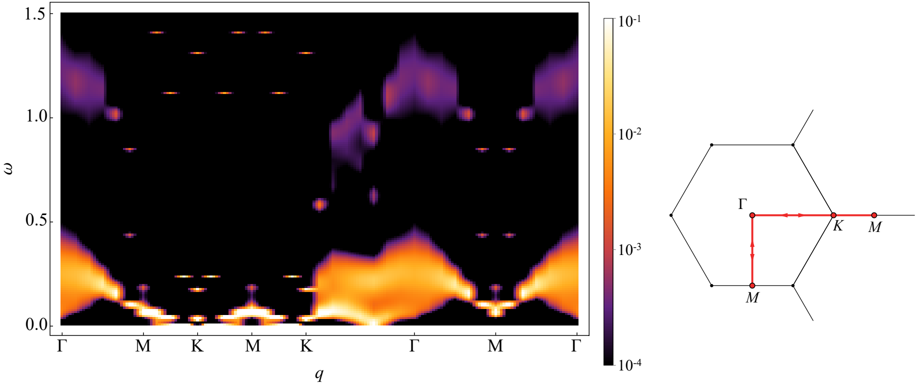


Figure: $J' = 0.04$, $\rho = 1/2$, $h = 0.3$

Low frequency spectrum along high-symmetry lines

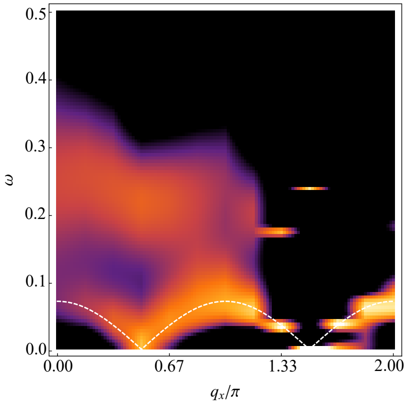


Figure: x-axis, ΓKM Line

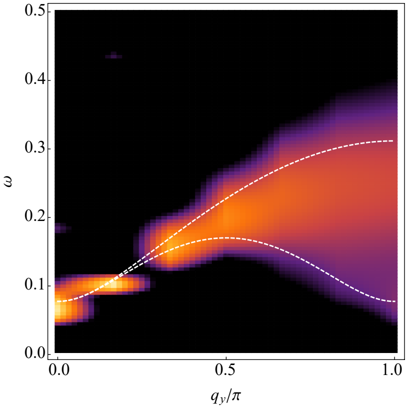


Figure: y-axis, ΓM Line

Code from Hui Shao on BSSQM

http://ddl.escience.cn/f/SPoD

tres.f90

dealdata/tres.f90: To process the data of every bin correlation from QMC into input of SAC.

- Calculate the mean $G(\tau_i)$; calculate and diagonalize covariance matrix.
- Input *tgrid.dat*: imaginary time grid τ_i
- Input *cor.dat*: $G^b(\tau_i)$, $N_b \times N_\tau$ data from QMC measurement
- Input *tres.dat*: parameters of processing
  - *nq* Number of q-points (set 1)
  - *beta* Inverse temperature of QMC
  - *qq* Assign which q to use (set 0)
  - *nb* Number of bins (set 0 =All)
  - *rb* Rebinning factor
  - *sk* Skipping some of the bins
  - *nbt* Number of bootstrap samples

tres.f90

dealdata/tres.f90: To process the data of every bin correlation from QMC into input of SAC.

- Output *sq.dat*: the average of $G(0)$ and errorbar
- Output *tq.dat*: the averages of $G(\tau_i)$ and errorbars
- **Output *q001.dat***: the eigenvalues and eigenvectors of covariance matrix
  - τ_i, $G(\tau_i)$, $\delta G(\tau_i)$, eigenvalue of C_{ij}
  - Eigenvectors of C_{ij}
- Command: *ifort tres.f90 dsyev.f -o ***.out*

sac.f90

sac/sac.f90: the main SAC programme

- Input *t.in*: renamed from *dealdata/q001.dat*
- Input *samp.in*: parameters of SAC.
  - *nw*: number of δ's in parametrization;
  - *th*: the initial temperature
  - *da*: the minimum inteval in histogram
  - *dw*: the minimum inteval in gridding
  - *w1,w2*: the lower/upper bound of the
  - *istps,mspts*: the MCS's used in initialization and measurement

sac.f90

sac/sac.f90: the main SAC programme

- Output *sw.dat*: accumulated spectral function
- Output *log.log*: the log file while the programme is running
  - index, index, Θ, χ^2_{min}, $\langle\chi^2\rangle$, two kinds of update success rates and window widths

Code Structure

- Read input & initializations
  - Initialize *ran* 503–549
  - Read τ_i, $G(\tau_i)$ & C_{ij} 437–471
  - Initialize spectrum 397–416
  - Initialize kernal 418–434
- Decide temperature & equiliberate
  - Annealing process to determine Θ 99–154 (if $\Theta_{\text{init}} > 1$)
  - Equiliberate again
- Sample & measure
  - Collect spectrum while sampling
  - Write spectrum 244–263

Initializations

Read parameters 70–74
Initialize random number 503–549
Clear files *initfiles* 474–484
Read data *readsqt* 437–471

- Transform $G(\tau_i)$ into the eigenbasis of covaraince matrix.
- Calculate the average frequency

Initializations

Initialize spectrum *initspec* 397–416

- Convert all the frequencies into the unit of grid inteval *dw*
- Set the amplitudes of the δ's to be the same.
- Set the initial positions to be the same at the average frequency (if not too low)
- Set the intial window width *dd* to be 1/10 of the average frequency

Initialize kernal *inikern* 418–435

$$\tilde{G}(\tau) = \sum_i A_i K(\tau, \omega_i), \quad K(\tau, \omega_i) = \frac{1}{\pi} \frac{e^{-\omega\tau} + e^{-\omega(\beta-\tau)}}{1 + e^{-\omega\beta}} \tag{32}$$

$$G'^{F}_{\alpha} = \sum_j U_{\alpha j} \tilde{G}(\tau_j) = \sum A_i K_\alpha(\omega_i), \quad K_\alpha = \sum_j U_{\alpha j} K(\tau_j, \omega_i) \tag{33}$$

Updating process

Updating single δ *dmove1(dd,ar)* 299–336

- Update nw times, each time take a random single peak
- Find a random $\delta\omega$ within the window, $\omega \leftarrow \omega + \delta\omega$
- Check the updated value is allowed
- Calculate the updated $\tilde{G}_\alpha$'s and χ^2's *chi2* 385–395
- Accept the update according to probability $p = \max(1, \mathrm{e}^{-(\chi^2 - \chi'^2)/2\Theta})$
- Calculate the success rate

Updating δ pairs *dmove2(dd,ar)* 338–383

- Update $nw/2$ times, each time take two random peaks
- Find a random $\delta\omega$ within the window, $\omega_1 \leftarrow \omega_1 + \delta\omega, \omega_2 \leftarrow \omega_2 - \delta\omega$

Sampling and equiliberate process

Sampling *sample(stps,sp,del)* 183–205

- *stps* MCS's, each step two kinds of update is carried out once.
- Each ten steps the Green's functions are re-calculated to avoid accumulation of errors. *calcxt* 280–297
- Current spectrum is calculated if needed *collectspec* 225–241
- Average χ^2 is measured

Equiliberate *equiliberate(ia,stp,nbin,del)* 156–180

- *nbin* bins, each bin sample *stp* MCS's.
- Adjust window width so that the success rates ~ 0.5.
- Measure the mean and deviation of χ^2 *expvalues* 207–223

Determine Θ

If $\Theta_{\text{init}} > 1$, *fixtheta* 101–154

- Annealing process
  - Each time decrease the temperature by 1/10, until $\langle\chi^2\rangle$ is close to its minimum value
  - Equiliberate
  - Save the Θ, $\langle\chi^2\rangle$, window widths and current spectrum of all the $\theta's$
- Choose the set of data whose $\langle\chi^2\rangle = \chi^2_{\text{min}} + 2\sqrt{\chi^2_{\text{min}}}$, read the saved window widths and spectrum

Conclusion

1. SAC is a numerical method to carry out anti-Laplacian transformation to obtain $S(\omega)$ out of $G(\tau)$, which is a numerically unstable problem.
2. We parametrize $S(\omega)$ into a series of δ function and perform a fitting process and evaluate the goodness of the fitting by a parameter χ^2.
3. To avoid overfitting we sample over all possible $S(\omega)$'s and average with the weight of each $\exp(-\chi^2/2\Theta)$
4. Features can be added such as a predominant δ peak or a sharp peak.
5. Basic code is given. Its structure and instruction are overviewed.
6. Applications such as spectra of Heisenberg and frustrated Ising magnets are introduced.

Stochastic Analytical Continuation — Principle, Algorithm & Application

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