Simulation of Quarkonium Suppression and Stochastic Gradients

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MIT

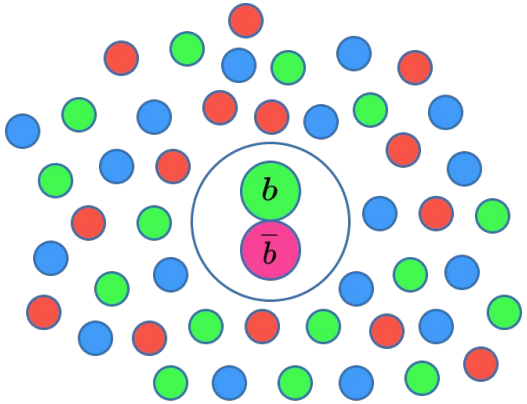
23.01.2025

Quarkonium suppression

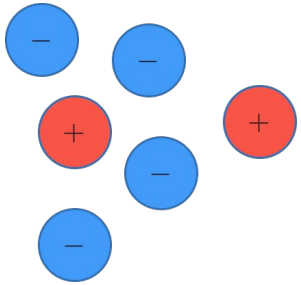
Veres, Gábor I. "Heavy ion physics at CMS and ATLAS: hard probes." *arXiv preprint arXiv:1905.10461* (2019).

Propagation through QGP

$T \approx O(100\mathrm{MeV})$



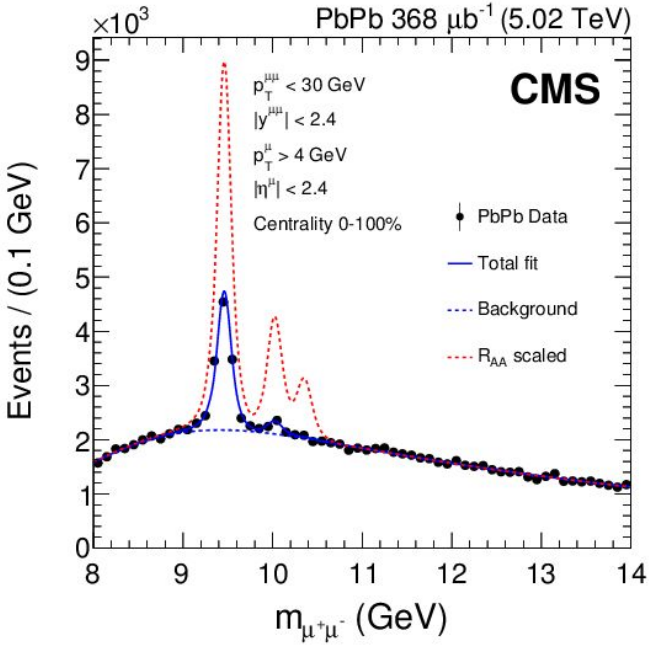
T. Matsui, H. Satz, Phys. Lett. B 178 (1986) 416



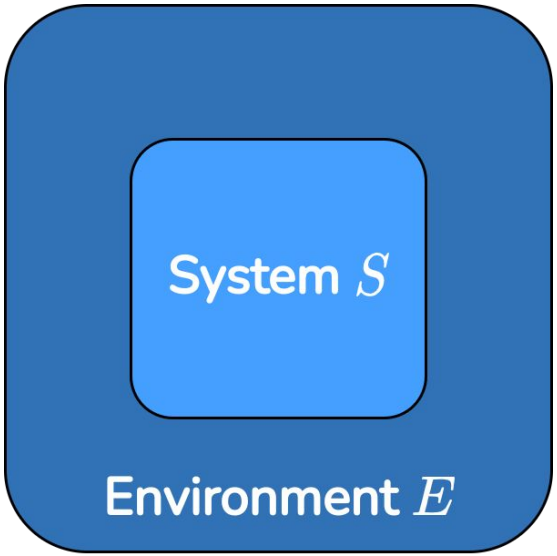
$$V(r) = -\frac{\alpha}{r}$$

$$V(r) = -\frac{\alpha}{r} e^{-m_D r}$$

Debye-screening in medium



Open Quantum Systems



- Quantum system not isolated
- Split into System S and Environment E

$$H = H_S \otimes I_E + I_S \otimes H_E + H_{\text{int}}$$

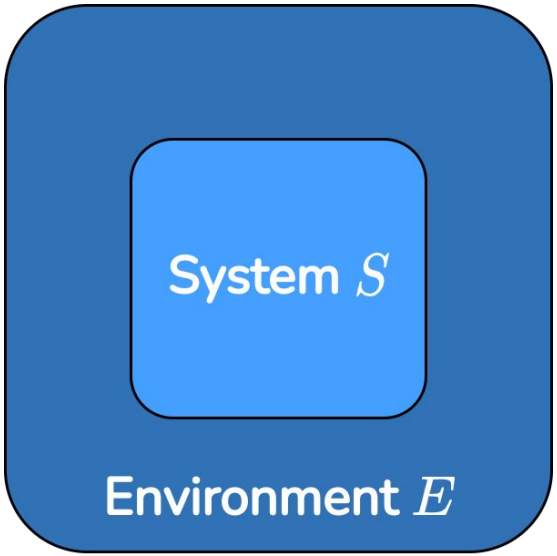
- Time evolution by Von-Neumann Equation

$$\frac{d}{dt}\rho = -i[H, \rho]$$

- Not interested in environmental d.o.f.: **Trace out**!

$$\rho_S = \mathrm{Tr}_E[\rho]$$

Open Quantum Systems

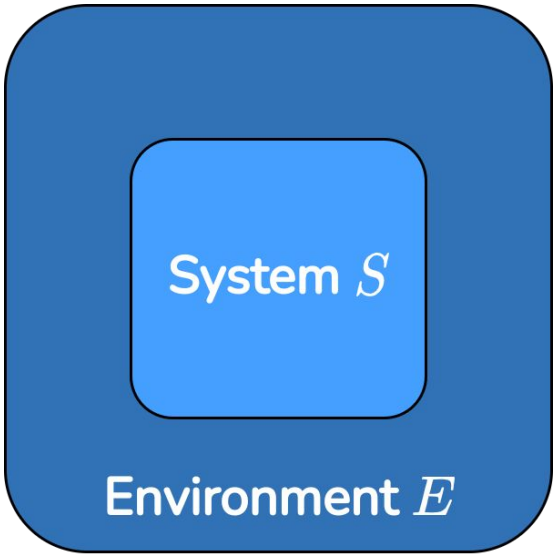


- "Master equation" for the System:

  Lindblad Equation

$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2} \left\{ C_n^\dagger C_n, \rho_S \right\} \right)$$

Open Quantum Systems



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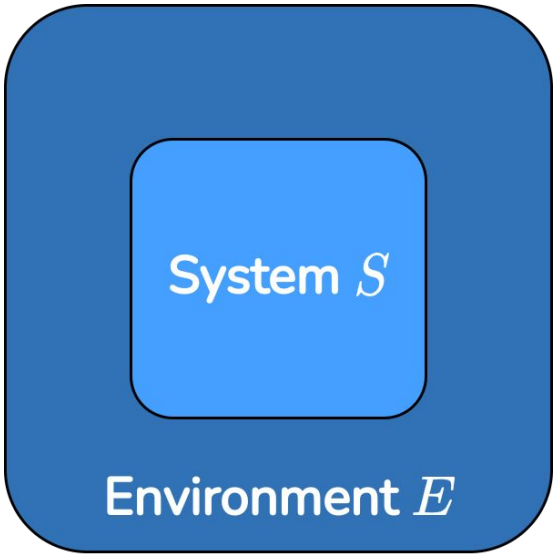
Open Quantum Systems



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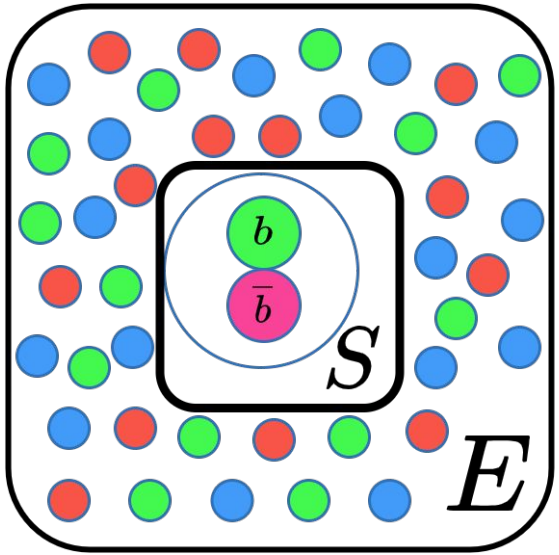
non-unitary

OQS for quarkonium suppression

- Quarkonium: System S
- QGP: Environment E

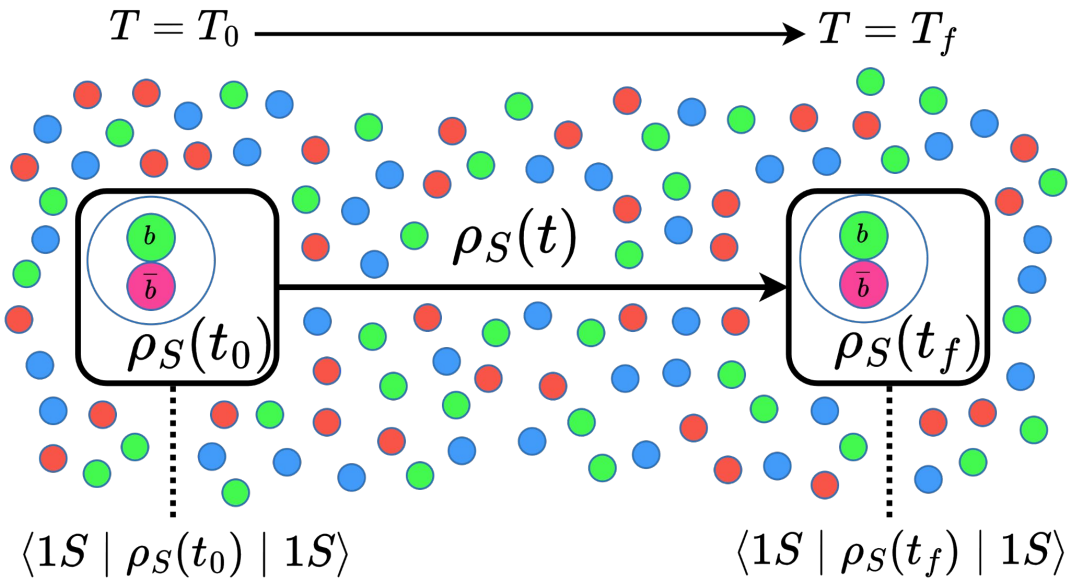


Lindblad equation for quarkonium in medium

$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2} \left\{ C_n^\dagger C_n, \rho_S \right\} \right)$$

OQS for quarkonium suppression

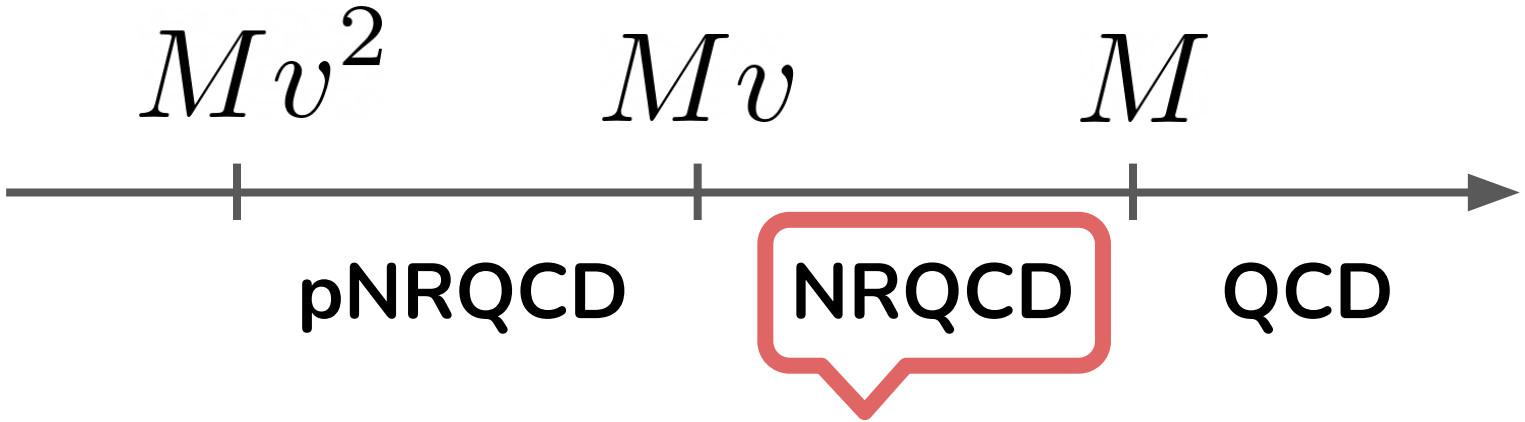
Plan



$$P_{\text{survival}}(1S) = \frac{\langle 1S|\rho(t_f)|1S\rangle}{\langle 1S|\rho(t_0)|1S\rangle}$$

Master equations from EFTs

Yukinao Akamatsu, Prog.Part.Nucl.Phys. 123 (2022), 103932
Xiaojun Yao, Int.J.Mod.Phys.A 36 (2021) 20, 2130010



- Degrees of Freedom: Heavy quarks

Lindblad eq. for *Heavy quarks*:

Akamatsu, Y. (2015). *Physical Review D*, *91*(5), 056002.

Lindblad eq. for *Heavy quarkonium*:

Blaizot, J. P., & Escobedo, M. A. (2018). *Journal of High Energy Physics*, *2018*(6), 1-57.

Blaizot, J. P., & Escobedo, M. A. (2018). *Physical Review D*, *98*(7), 074007.

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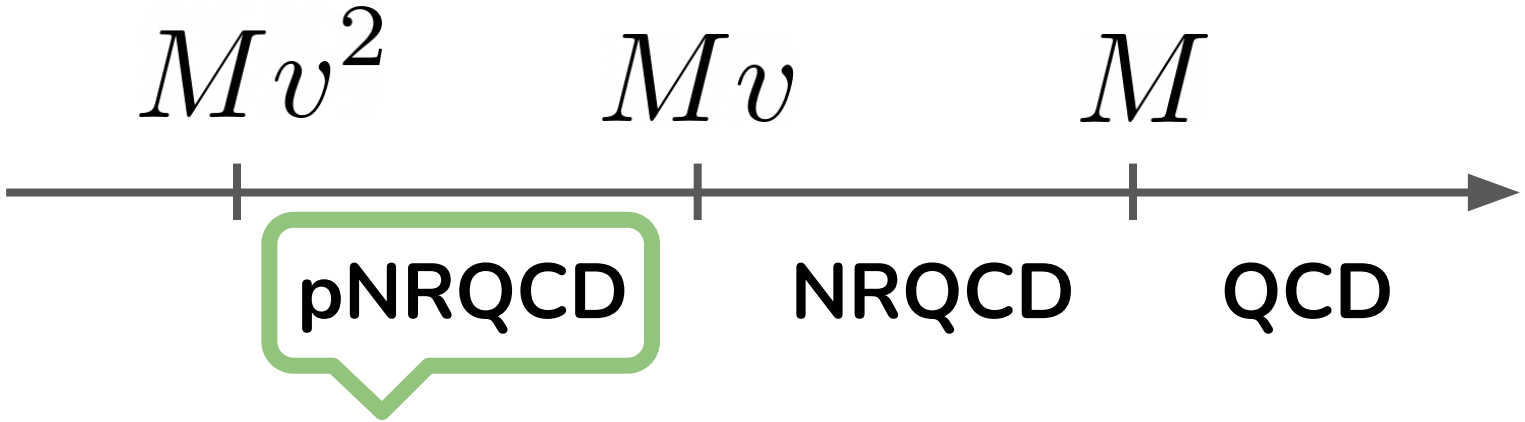

- Degrees of Freedom: Singlet and octet bound states

Lindblad eq. for *Heavy quarkonium*:

Brambilla, N., Escobedo, M. A., Soto, J., & Vairo, A. (2018). *Physical Review D*, *97*(7), 074009.

Brambilla, N., Escobedo, M. A., Soto, J., & Vairo, A. (2017). *Physical Review D*, *96*(3), 034021.

pNRQCD master equation

Brambilla, Escobedo, Soto, Vairo: Phys. Rev. D 97 (2018) 7, 074009

$$\frac{d\rho(t)}{dt} = -i\left[H, \rho(t)\right] + \sum_{nm} h_{nm}\left(L_i^n \rho(t) L_i^{m\dagger} - \frac{1}{2}\left\{L_i^{m\dagger} L_i^n, \rho(t)\right\}\right)$$

$$h = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$L_i^0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} r_i, \quad L_i^1 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{N_c^2-4}{2(N_c^2-1)} A_i^{oo\dagger} \end{pmatrix}$$

$$L_i^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} r_i, \quad L_i^3 = \begin{pmatrix} 0 & \frac{1}{N_c^2-1} A_i^{os\dagger} \\ A_i^{so\dagger} & 0 \end{pmatrix}$$

$$A_i^{uv} \propto \int_0^\infty \mathrm{d}s e^{-ih_u s} r_i e^{ih_v s} \left\langle E_j^a(s) E_j^a(0) \right\rangle$$

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Brambilla, Escobedo, Soto, Vairo: Phys. Rev. D 97 (2018) 7, 074009

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Master equation *not necessarily* of Lindblad type

$$A_i^{uv} \propto \int_0^\infty \mathrm{d}s e^{-ih_u s} r_i e^{ih_v s} \left\langle E_j^a(s) E_j^a(0) \right\rangle$$

pNRQCD master equation

Brambilla, Nora, et al. *Journal of High Energy Physics* 2022.8 (2022): 1-39.

- Simplify using hierarchy of scales $\pi T \gg E$

$$A_i^{uv} \propto \int_0^\infty \mathrm{d}s e^{-ih_u s} r_i e^{ih_v s} \langle E_j^a(s) E_j^a(0) \rangle$$

- Expand exponentials in $E/(\pi T)$
- At **NLO** in $E/(\pi T)$

Transport coefficients

$$A_i^{uv} = \frac{r_i}{2}(\kappa - i\gamma) + \kappa \left(-\frac{ip_i}{2MT} + \frac{\Delta V_{uv}}{4T} r_i \right)$$

$\mathcal{O}(E/T)$

pNRQCD master equation

Brambilla, Nora, et al. *Journal of High Energy Physics* 2022.8 (2022): 1-39.

$$\frac{d\rho(t)}{dt} = -i\left[H, \rho(t)\right] + \sum_{nm} h_{nm}\left(L_i^n \rho(t) L_i^{m\dagger} - \frac{1}{2}\left\{L_i^{m\dagger} L_i^n, \rho(t)\right\}\right)$$

$$h = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \longrightarrow h' = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Negative contributions are of $\mathcal{O}(E^2/T^2)$

neglect!

pNRQCD master equation

Brambilla, Nora, et al. *Journal of High Energy Physics* 2022.8 (2022): 1-39.

$$\frac{d\rho(t)}{dt} = -i\left[H, \rho(t)\right] + \sum_{n=0}^{1}\left(C_i^n \rho(t) C_i^{n\dagger} - \frac{1}{2}\left\{C_i^{n\dagger} C_i^n, \rho(t)\right\}\right)$$

$$H = \begin{pmatrix} h_s + \frac{r^2}{2}\gamma + \frac{\kappa}{4MT}\{r_i, p_i\} & 0 \\ 0 & h_o + \frac{N_c^2-2}{2(N_c^2-1)}\left(\frac{r^2}{2}\gamma + \frac{\kappa}{4MT}\{r_i, p_i\}\right) \end{pmatrix}$$

$$C_i^0 = \sqrt{\frac{\kappa}{N_c^2-1}}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\left(r_i + \frac{ip_i}{2MT} + \frac{\Delta V_{os}}{4T} r_i\right) + \sqrt{\kappa}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\left(r_i + \frac{ip_i}{2MT} + \frac{\Delta V_{so}}{4T} r_i\right),$$

$$C_i^1 = \sqrt{\frac{\kappa(N_c^2-4)}{2(N_c^2-1)}}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\left(r_i + \frac{ip_i}{2MT}\right)$$

Projection on spherical harmonics

$$\frac{d\rho(t)}{dt} = -i\left[H, \rho(t)\right] + \sum_{n=0}^{1}\left(C_{\cancel{i}}^{n}\rho(t)C_{\cancel{i}}^{n\dagger} - \frac{1}{2}\left\{C_{\cancel{i}}^{n\dagger}C_{\cancel{i}}^{n}, \rho(t)\right\}\right)$$

Hilbert space:

$$H_c \otimes H_l \otimes H_r$$

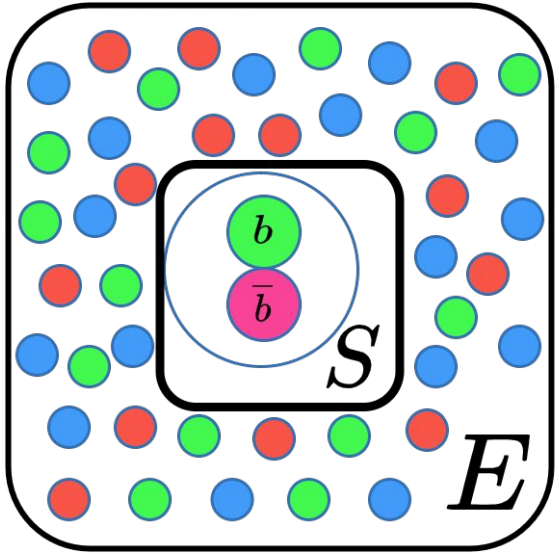
c = s,o

l = 0,1,2,...

Radial wavefunction

$$\rho = \begin{pmatrix} \rho_s^0 & 0 & \dots & 0 & 0 & \dots \\ 0 & \rho_s^1 & \dots & 0 & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \\ 0 & 0 & \dots & \rho_o^0 & 0 & \dots \\ 0 & 0 & \dots & 0 & \rho_o^1 & \dots \\ \vdots & \vdots & & \vdots & \vdots & \ddots \end{pmatrix}$$

pNRQCD master equation



Hilbert space:

$$H_c \otimes H_l \otimes H_r$$

c = s,o

l = 0,1,2,...

Radial wavefunction

- Very large Hilbert space

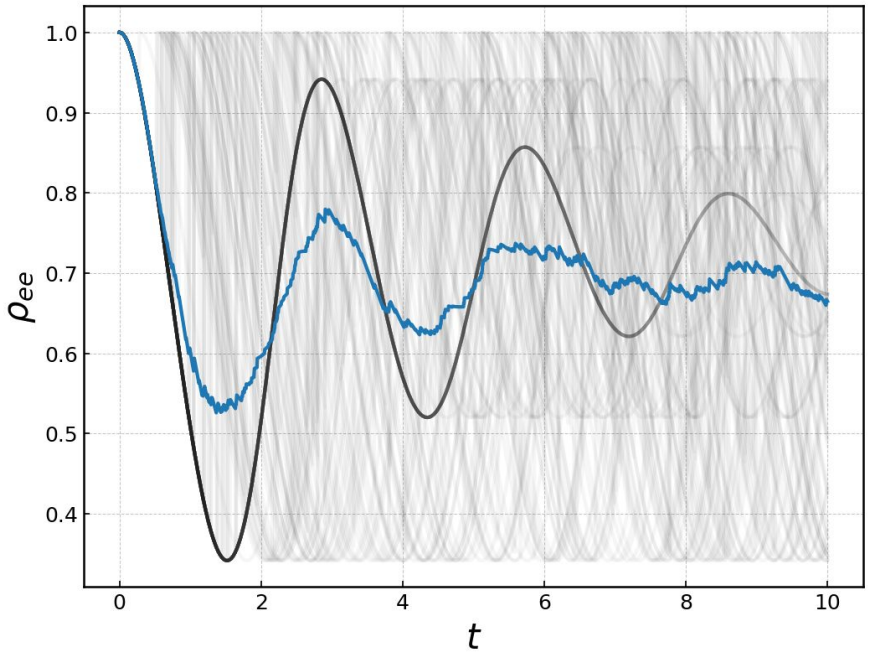
$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2}\left\{C_n^\dagger C_n, \rho_S\right\} \right)$$

E.g. 40000×40000 matrix

Quantum trajectory algorithm

J. Dalibard, Y. Castin, and K. Mølmer, Wave-function approach to dissipative processes in quantum optics, Phys. Rev. Lett. 68 (1992), pp. 580–583.

- Idea:
  1. Evolve individual trajectories $\left|\phi(t)\right\rangle$ **stochastically**
  2. Calculate observables by averaging over trajectories $\overline{\left\langle\phi(t)\middle|A\middle|\phi(t)\right\rangle}$



Quantum Trajectories

e.g.: $U = 1 - iH_{\text{eff}}\delta t$

ψ_0

1. Evolve state $|\psi(t)\rangle$ with $H_{\text{eff}} = H - \frac{i}{2}C^\dagger C$

$$|\psi'(t+\delta t)\rangle = U|\psi(t)\rangle$$

2. Compute norm

$$\langle\psi'(t+\delta t)|\psi'(t+\delta t)\rangle = 1 - \delta p < 1$$

3. Apply jump operator C with probability δp

$$P\left(|\psi(t+\delta t)\rangle = C|\psi(t)\rangle\right) = \delta p$$

$$P\left(|\psi(t+\delta t)\rangle = |\psi'(t+\delta t)\rangle\right) = 1 - \delta p$$

4. Normalize $|\psi(t+\delta t)\rangle$

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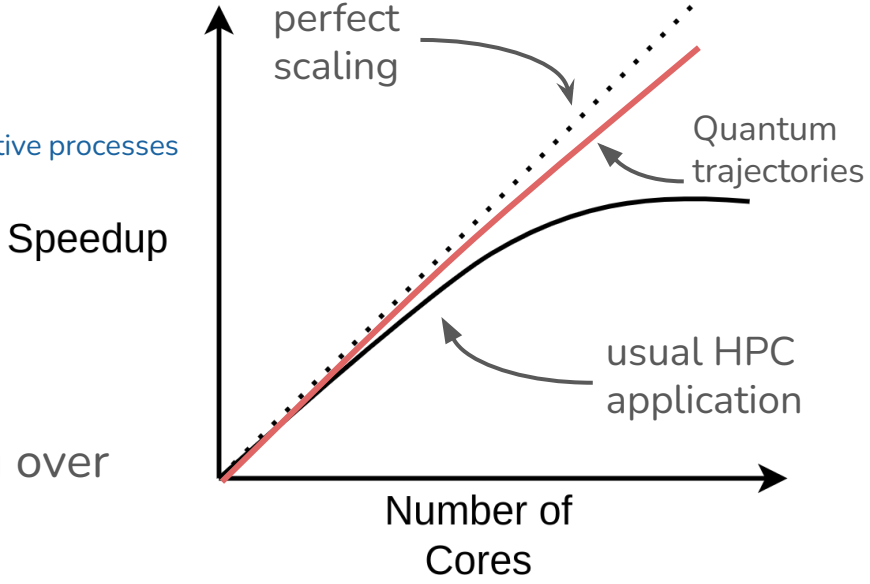
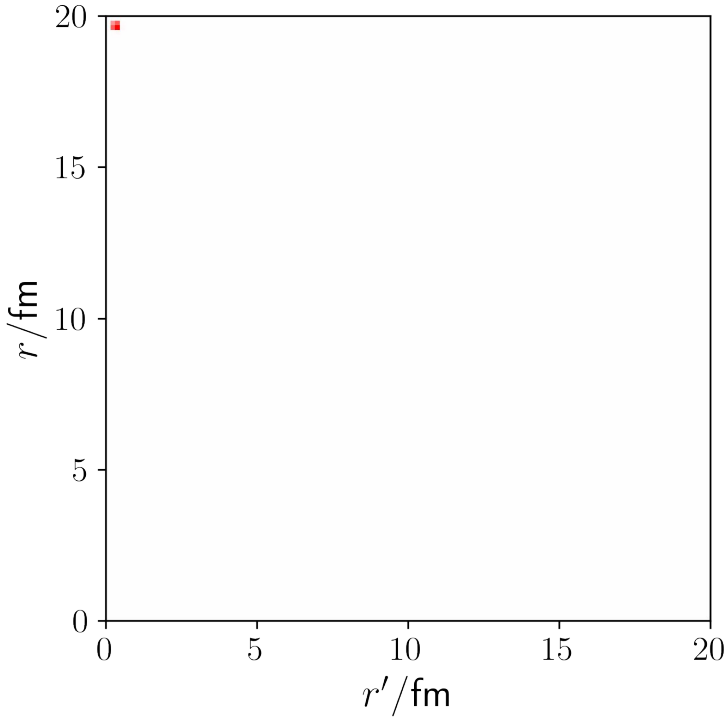


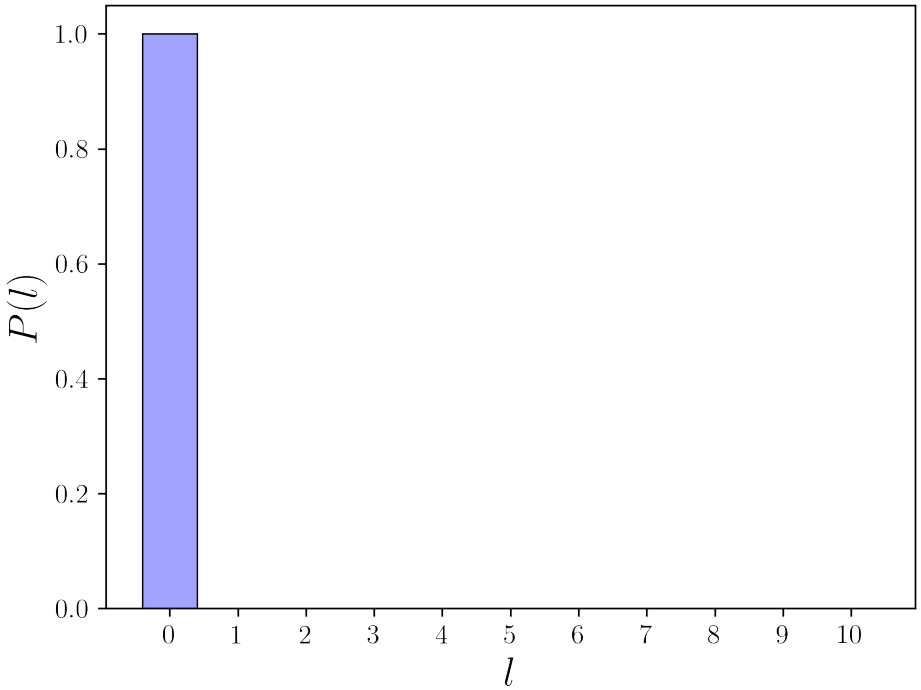
Advantages:

- Evolve vector of size N_H instead N_H^2 density matrix
- Simulation of individual trajectories is **embarrassingly parallel**

singlet
l=0

$t = 0$ $t = 2\,\mathrm{fm}$





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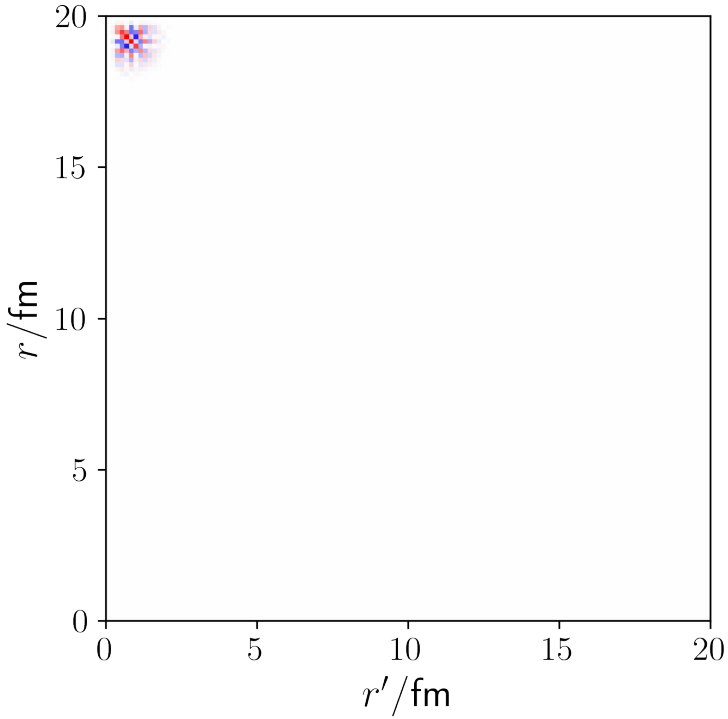

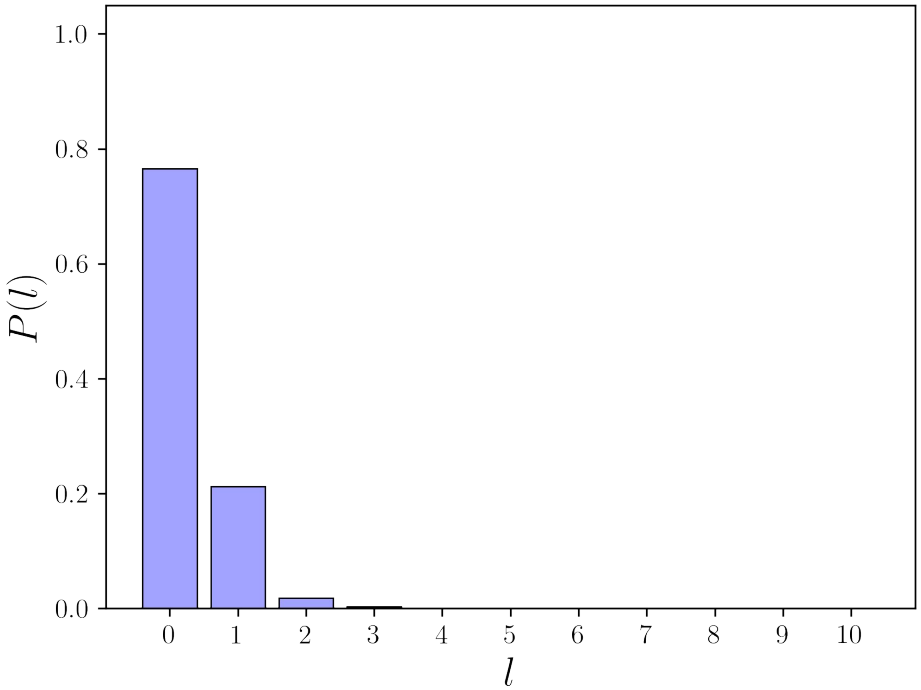

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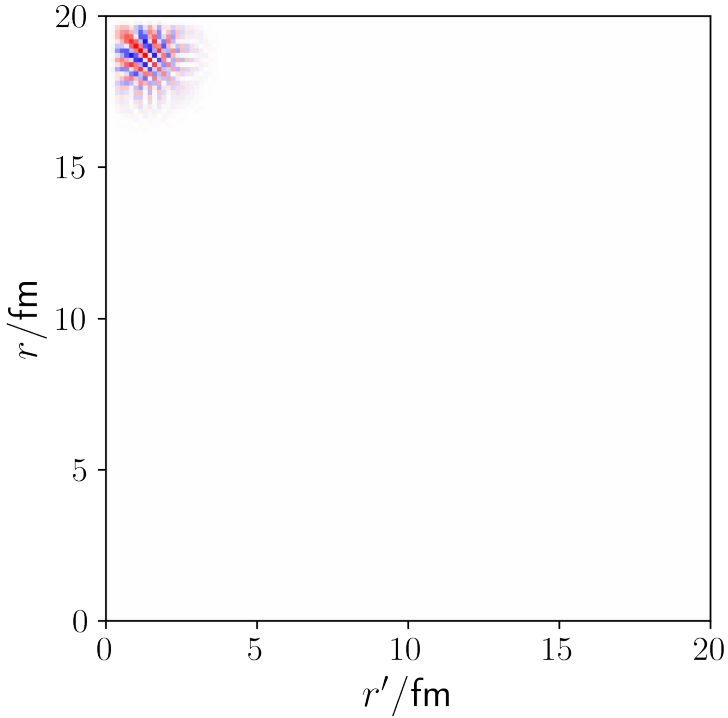

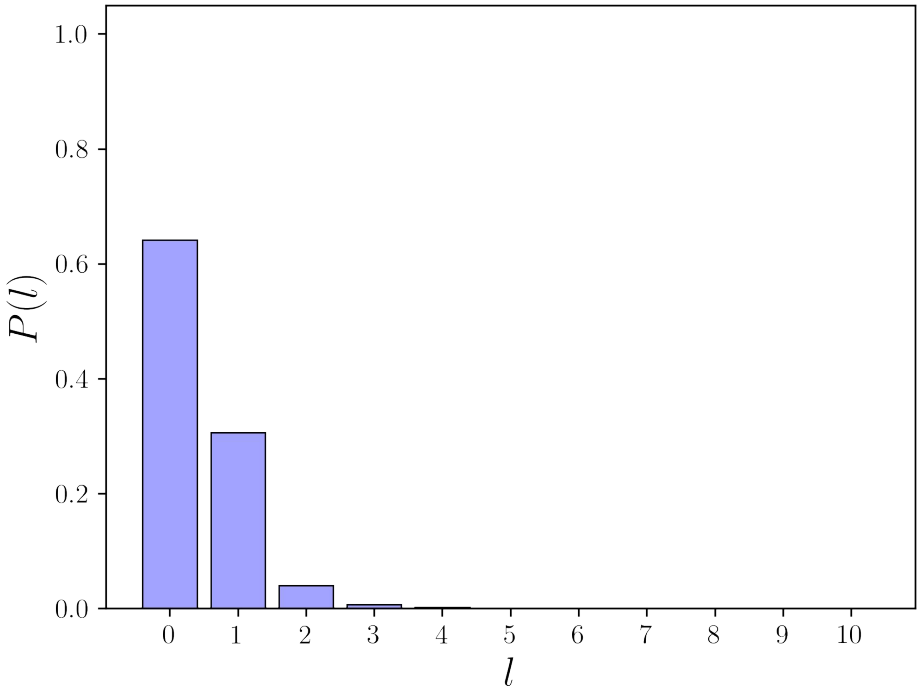

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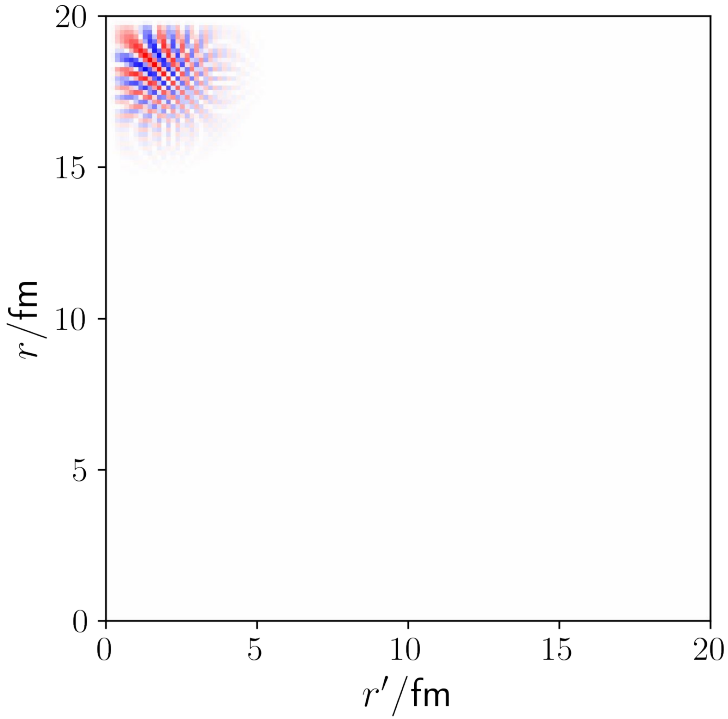

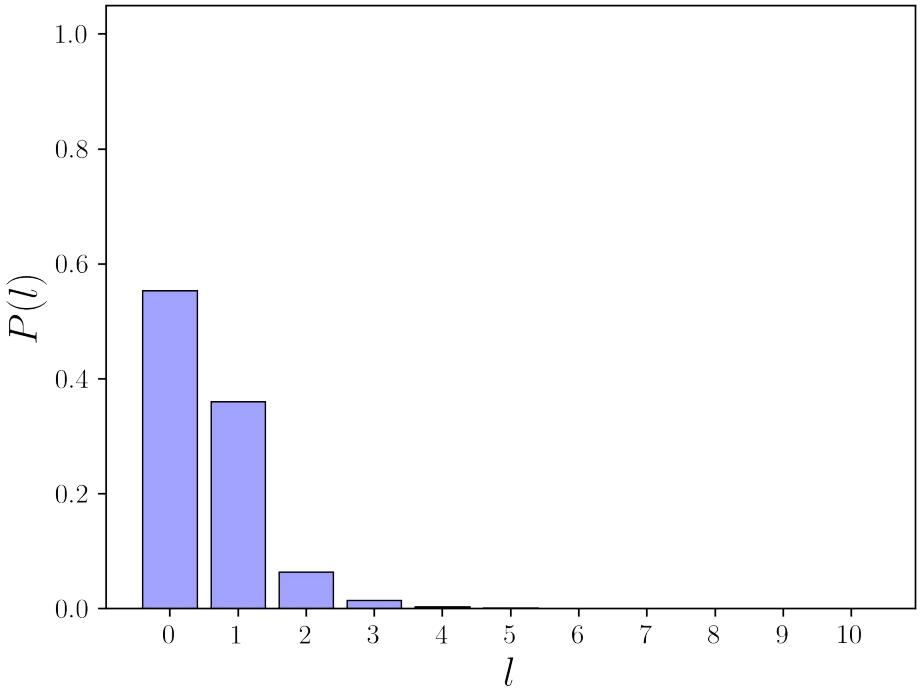

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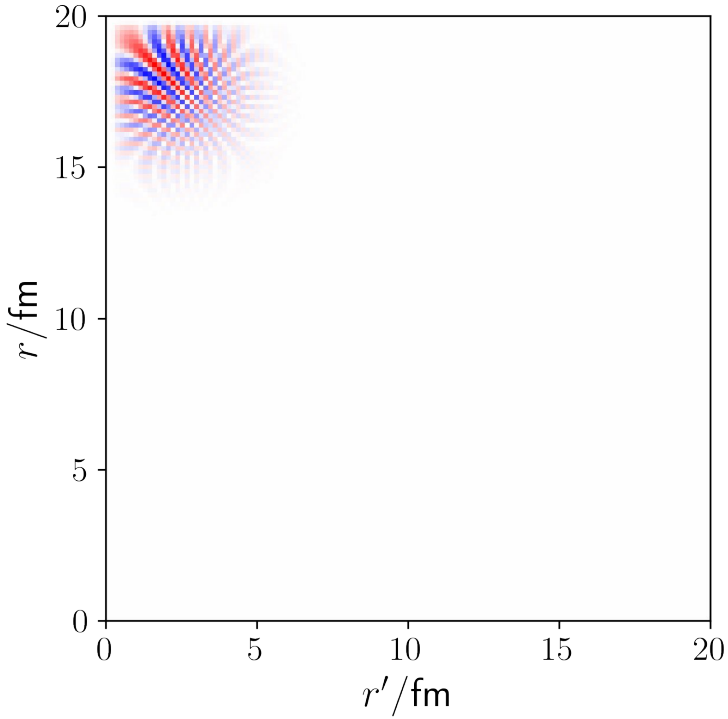

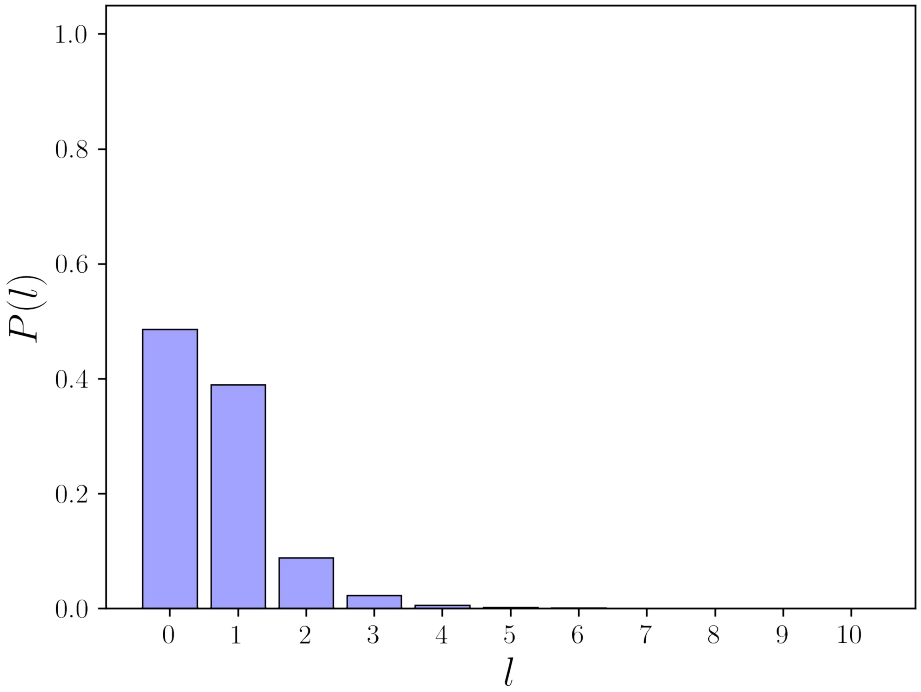

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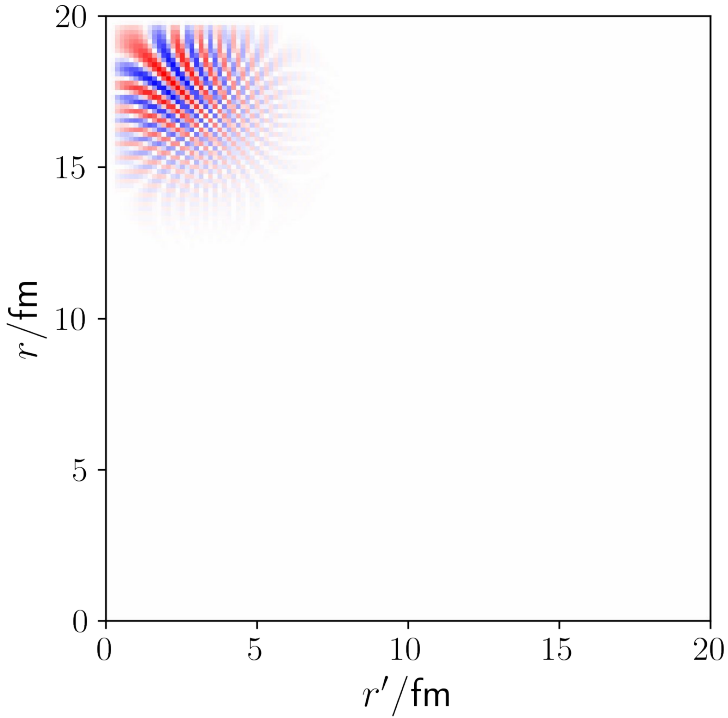

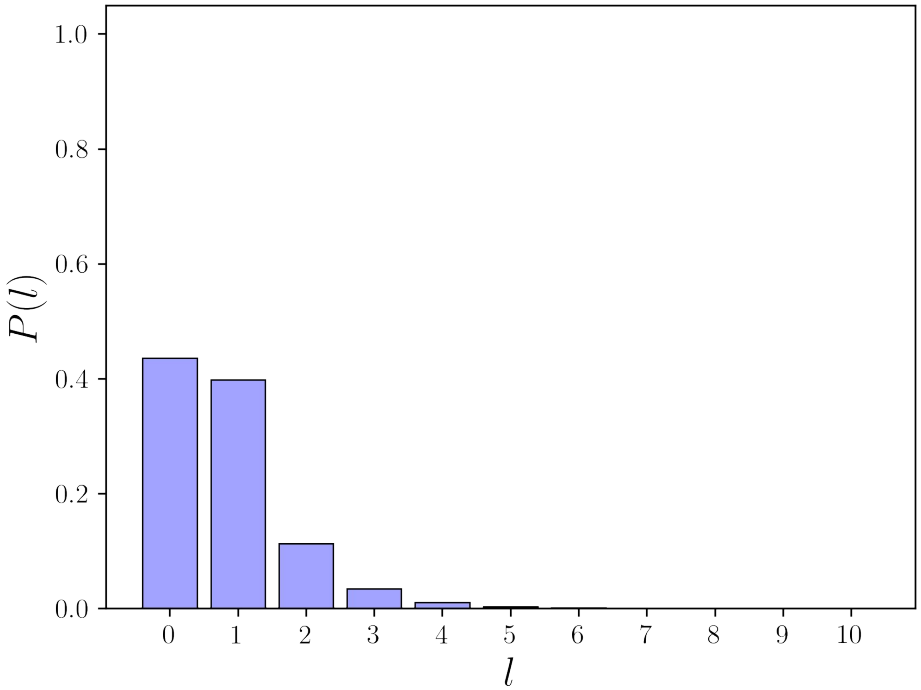

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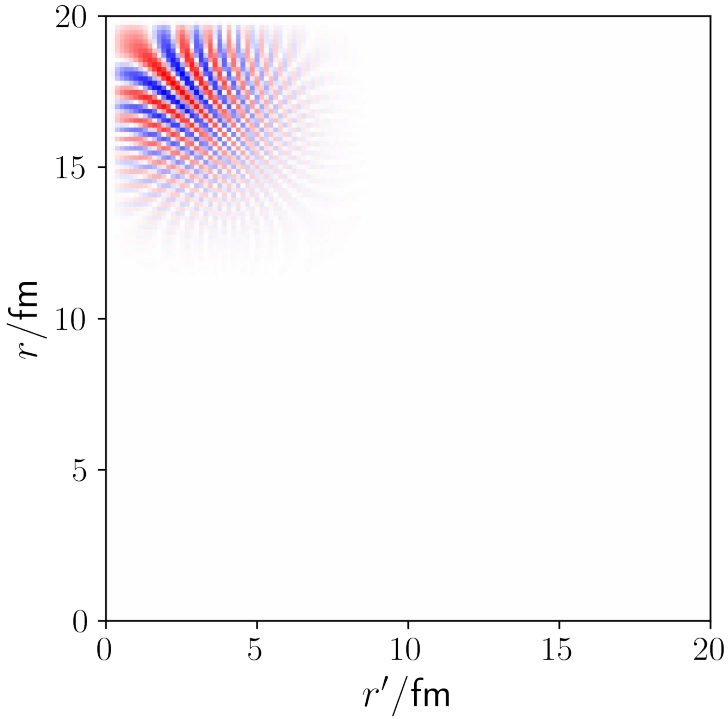

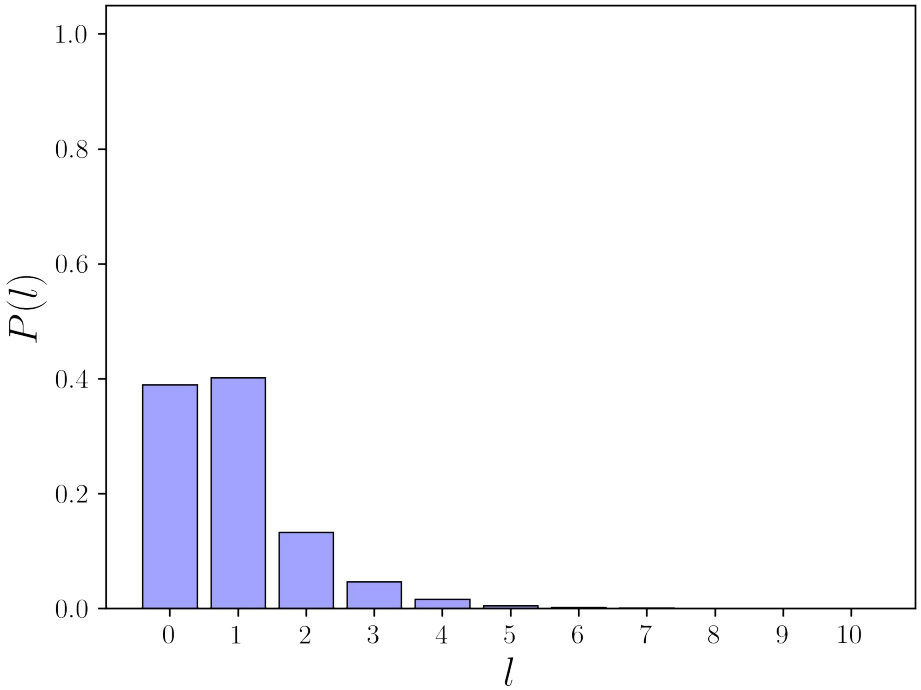

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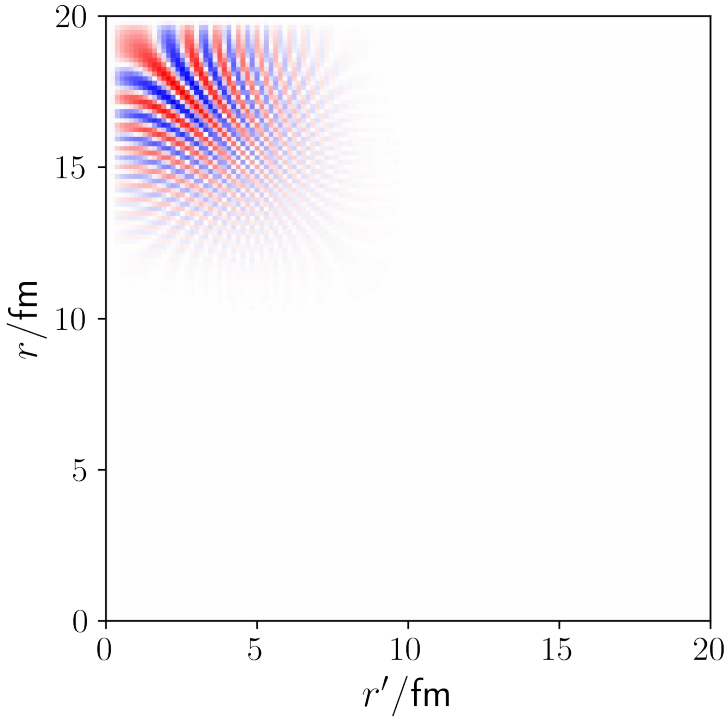
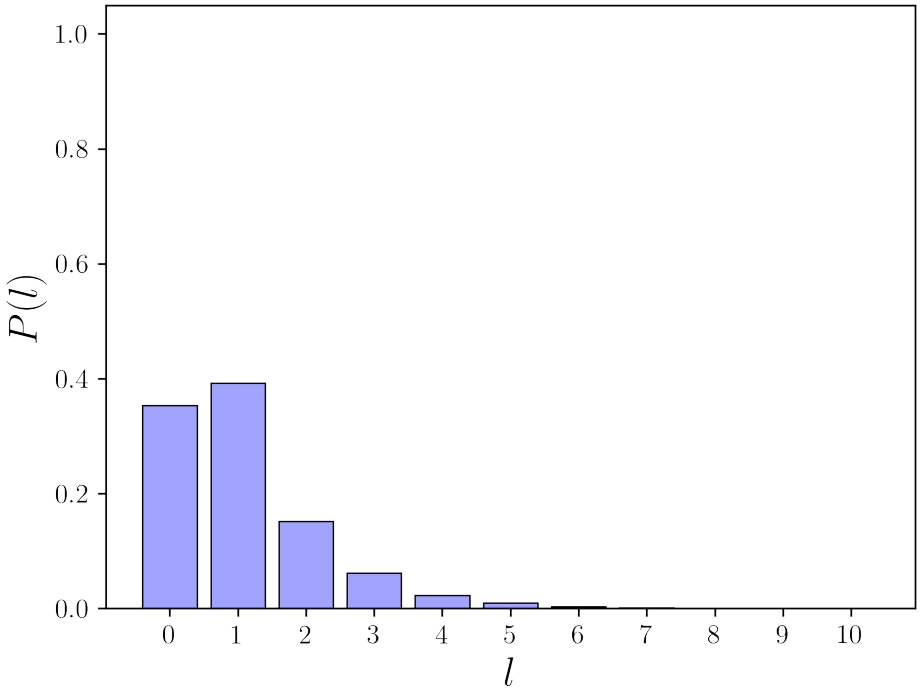
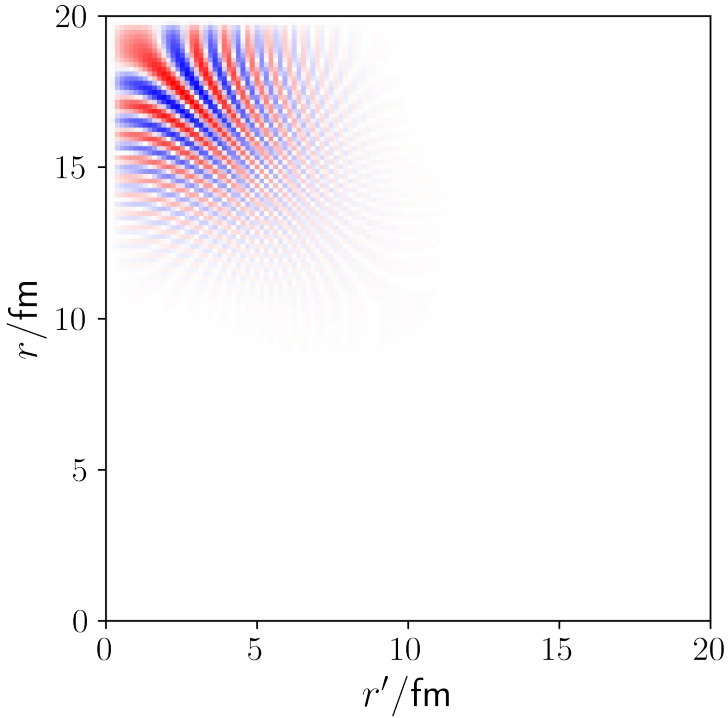
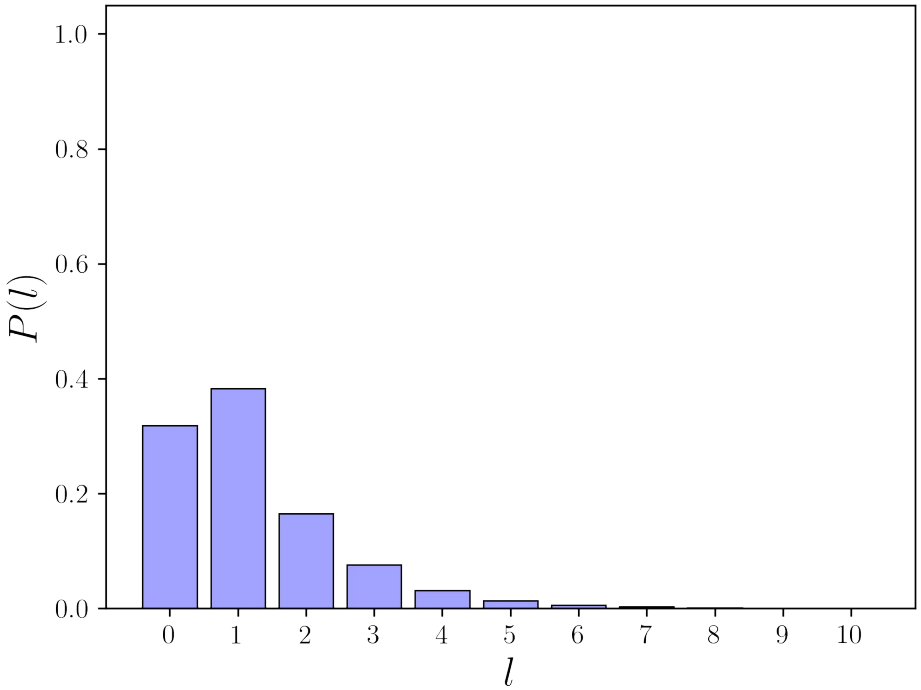




$t = 0$ $t = 2\,\mathrm{fm}$





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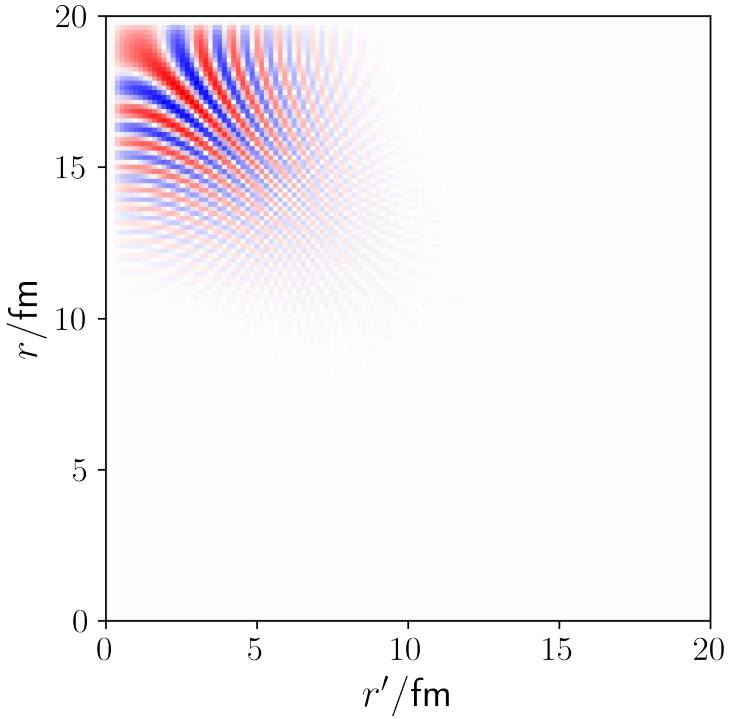

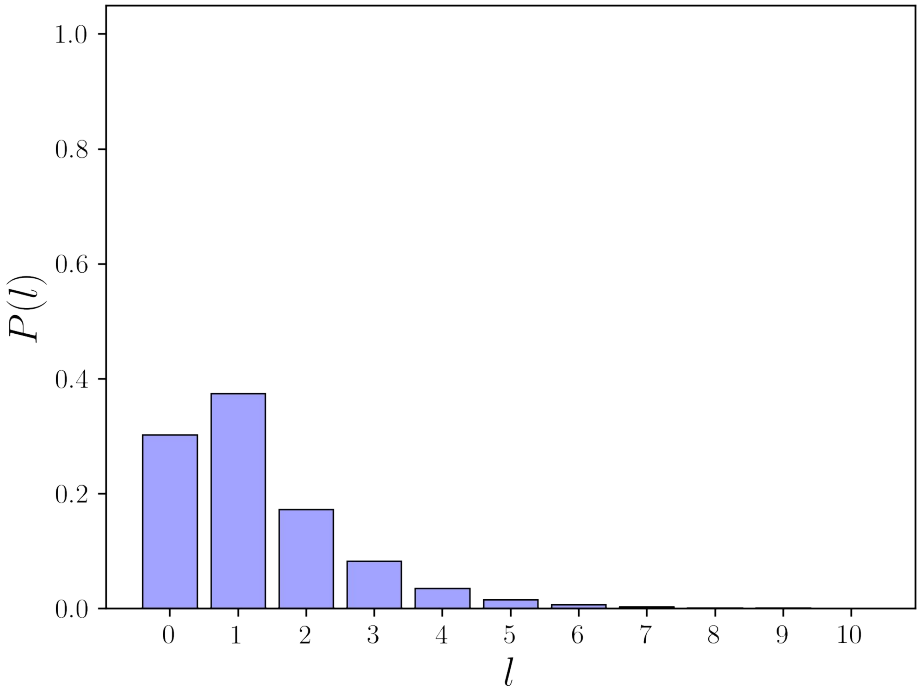

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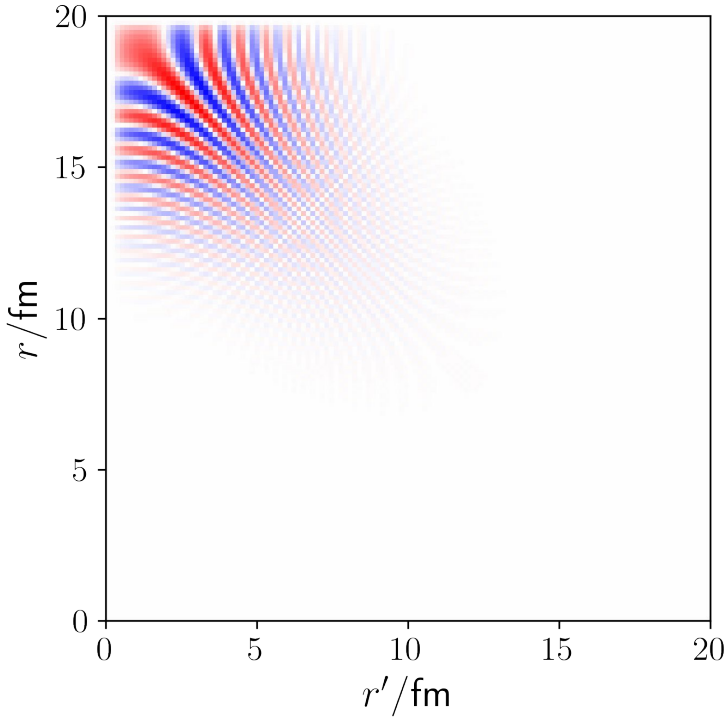

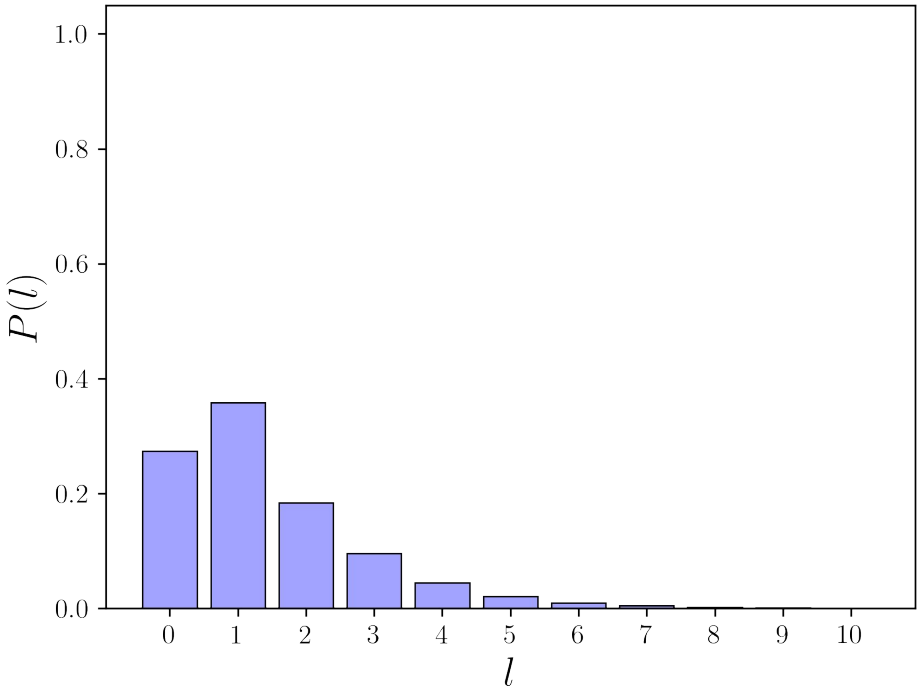

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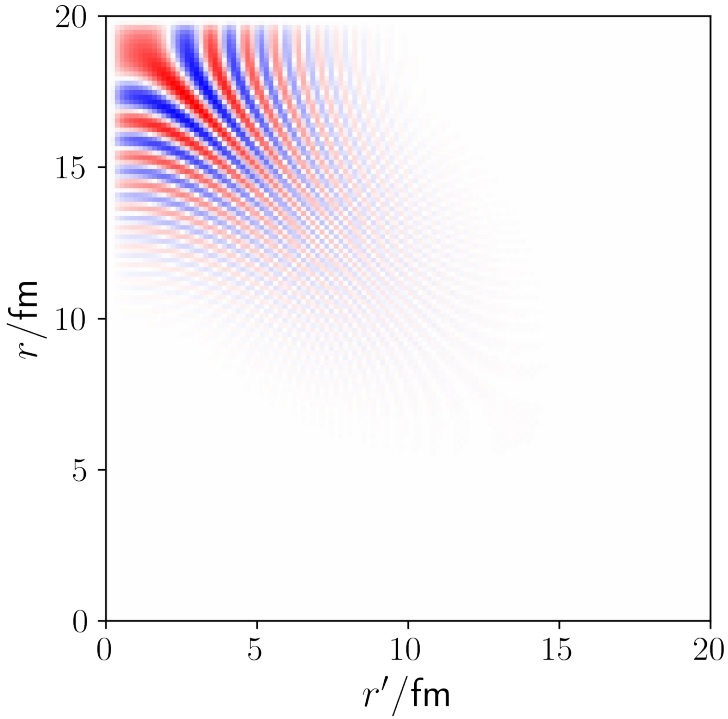

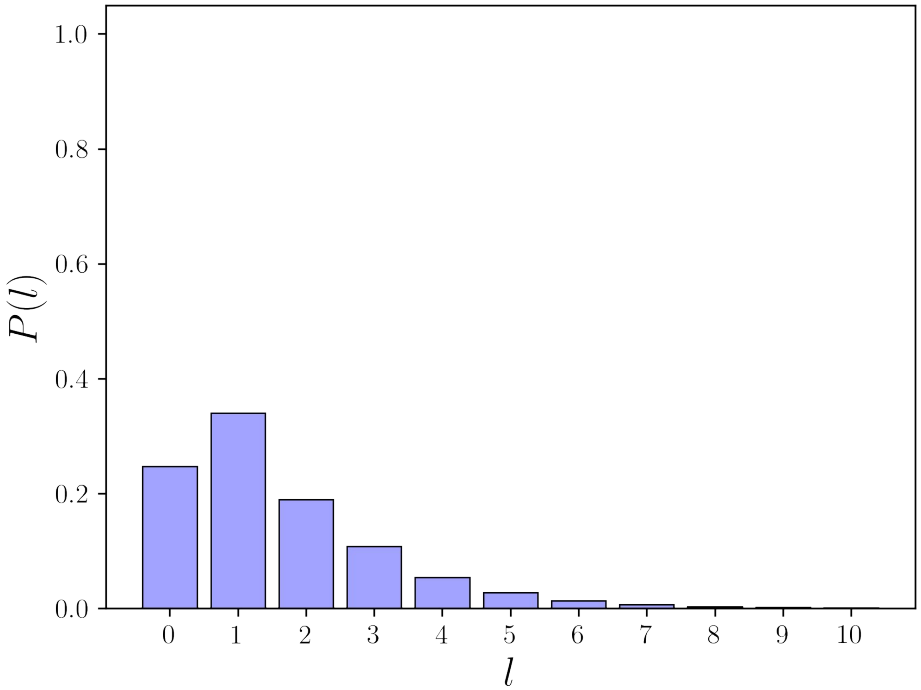

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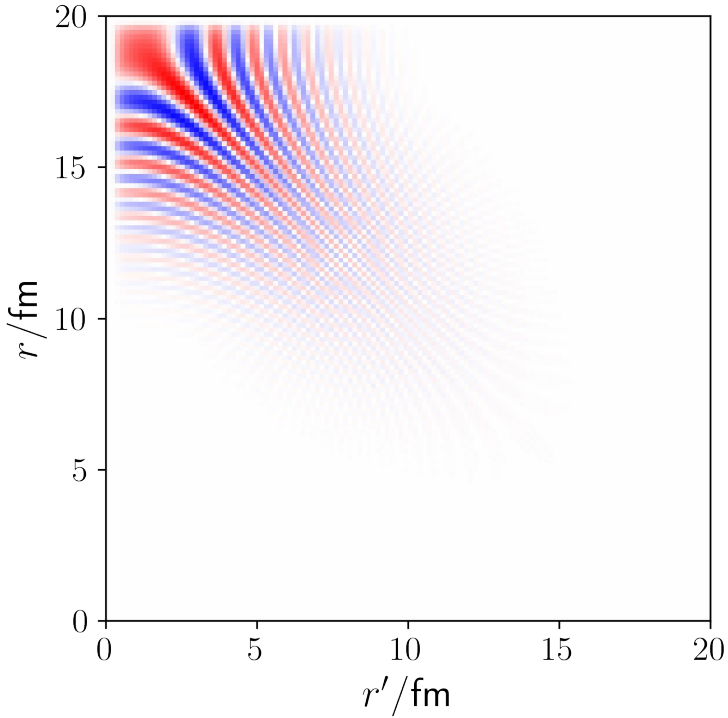

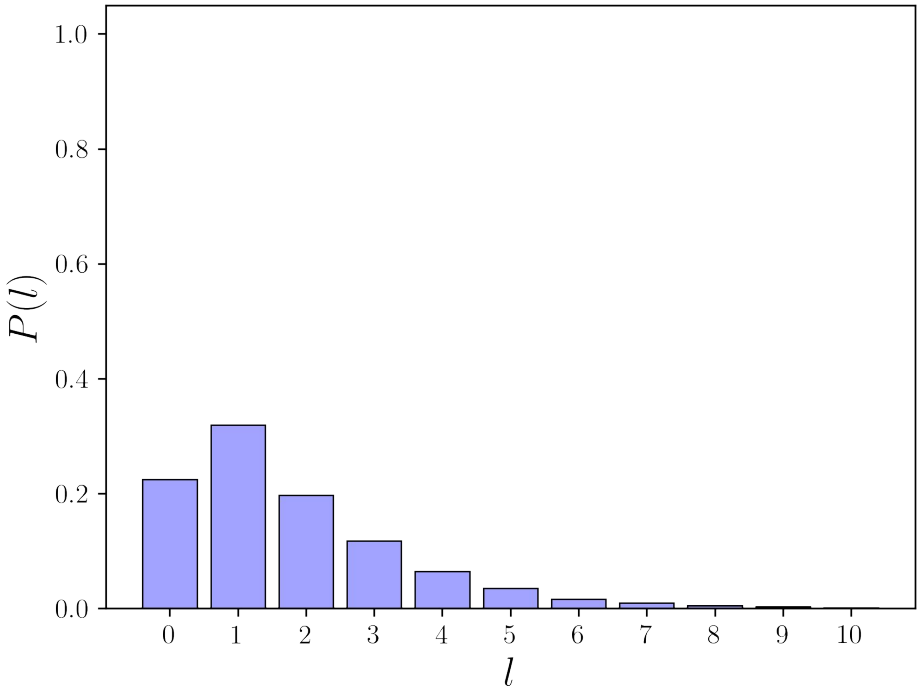

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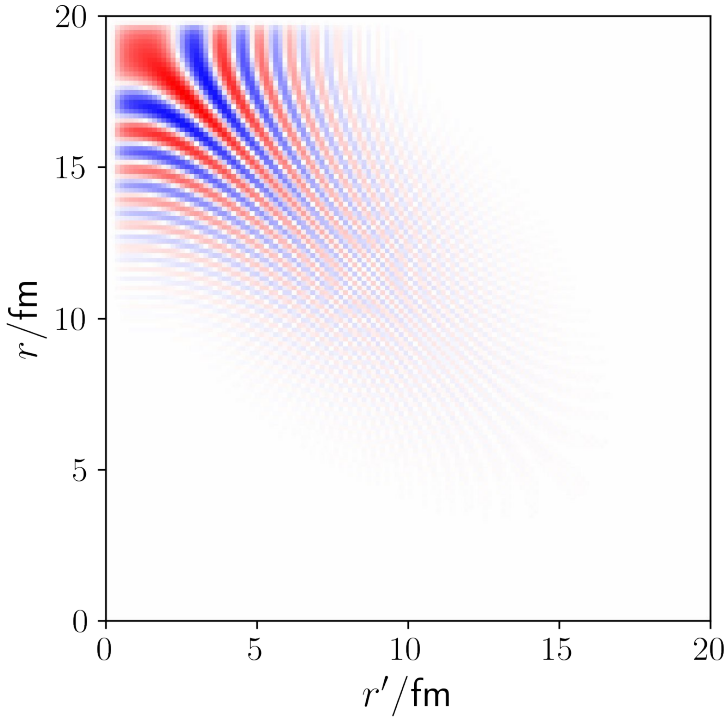

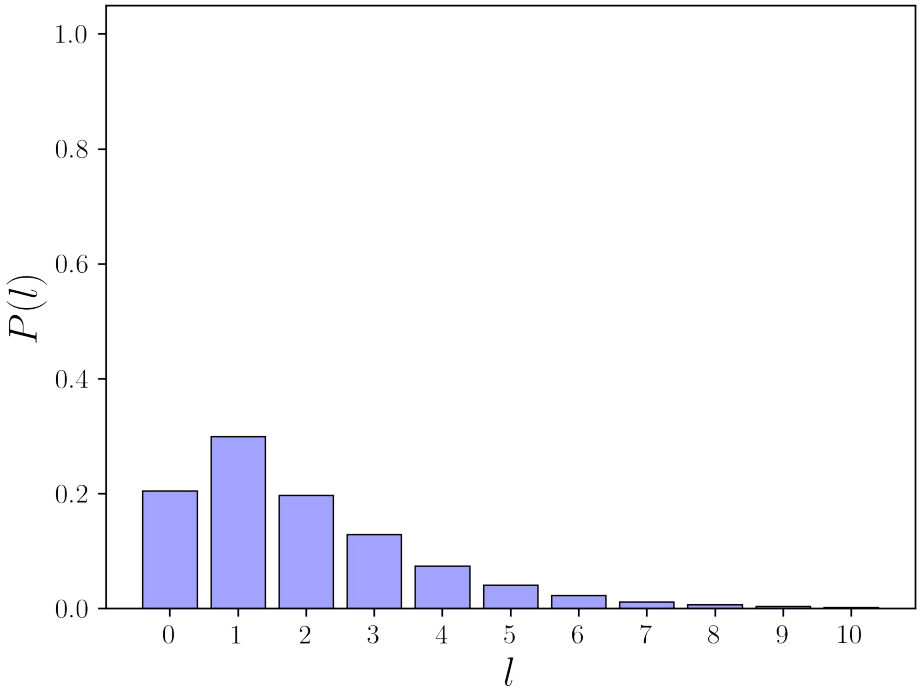

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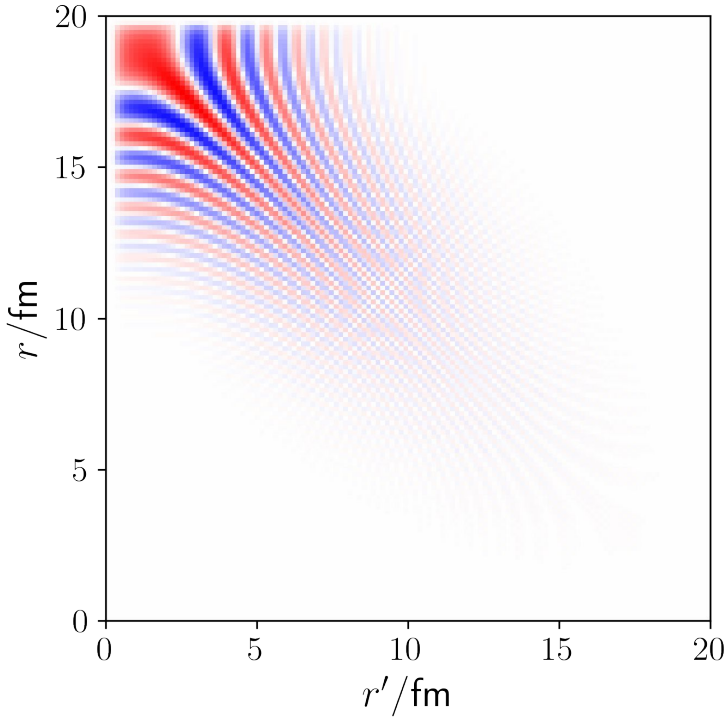

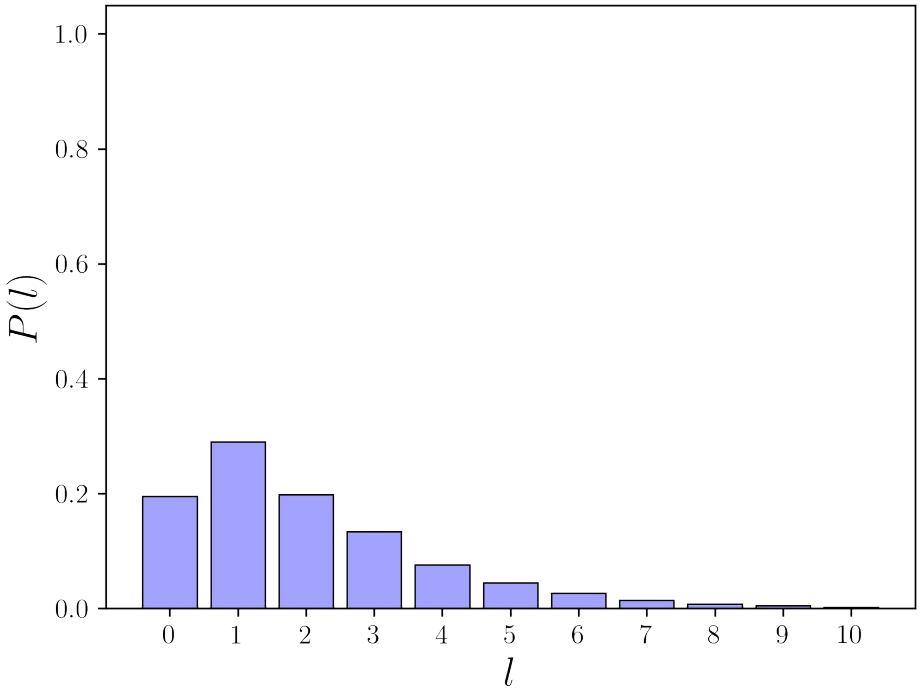

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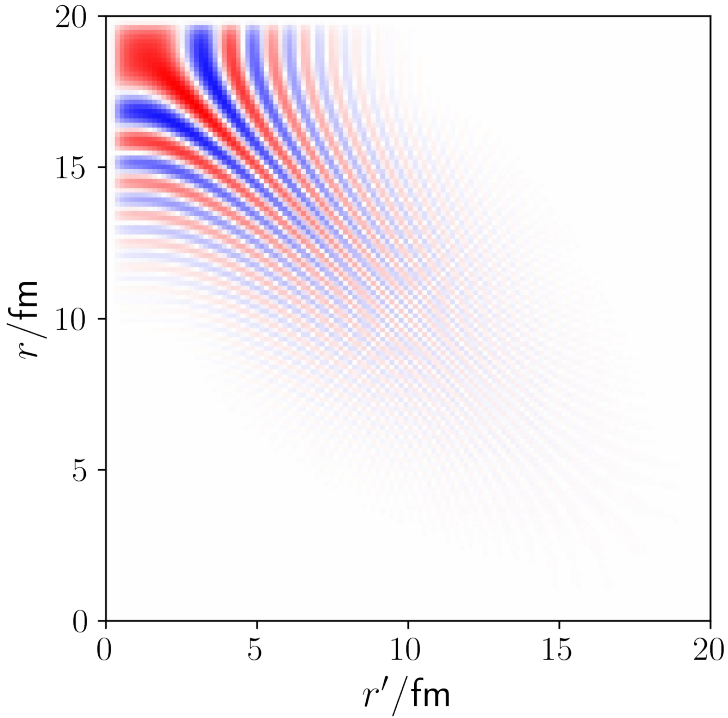

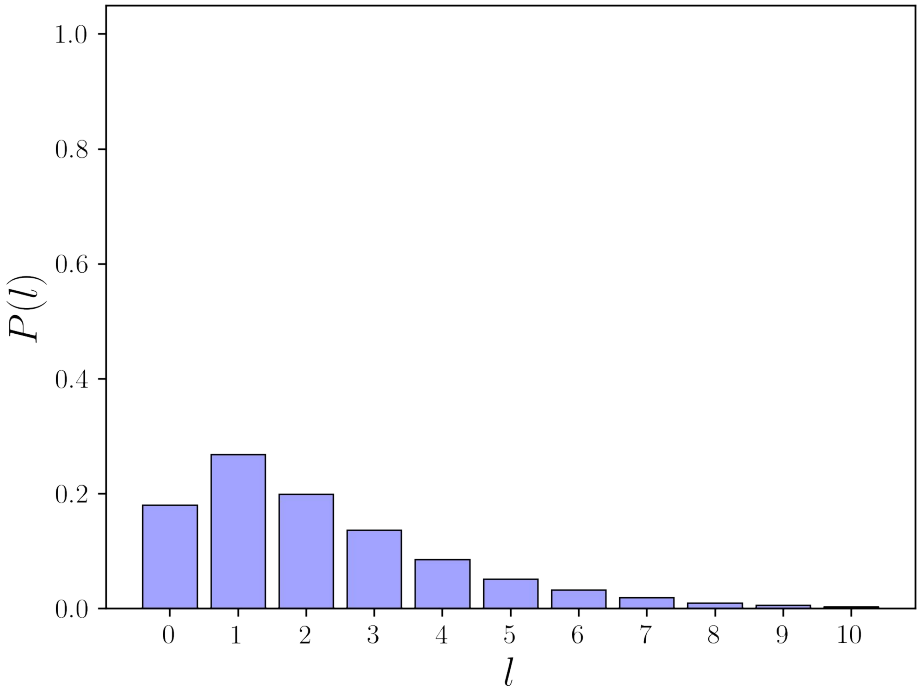

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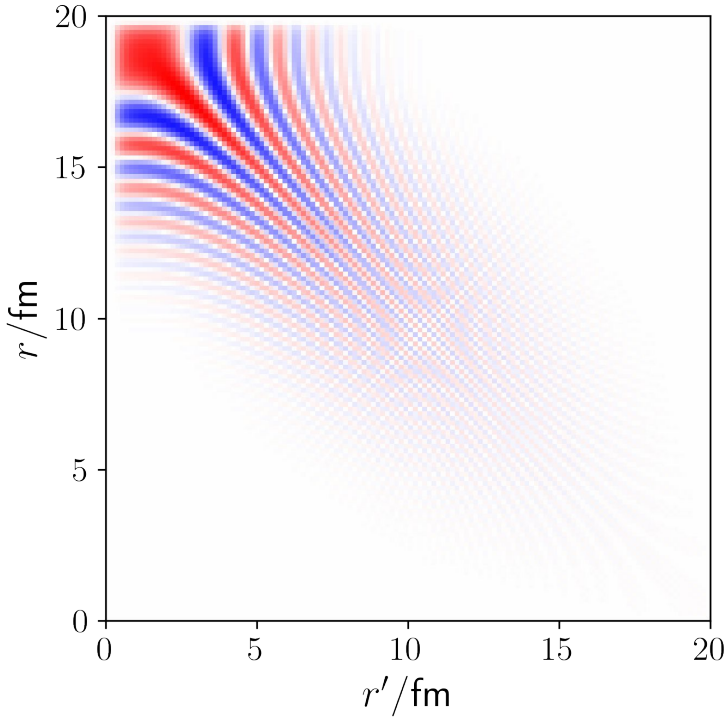

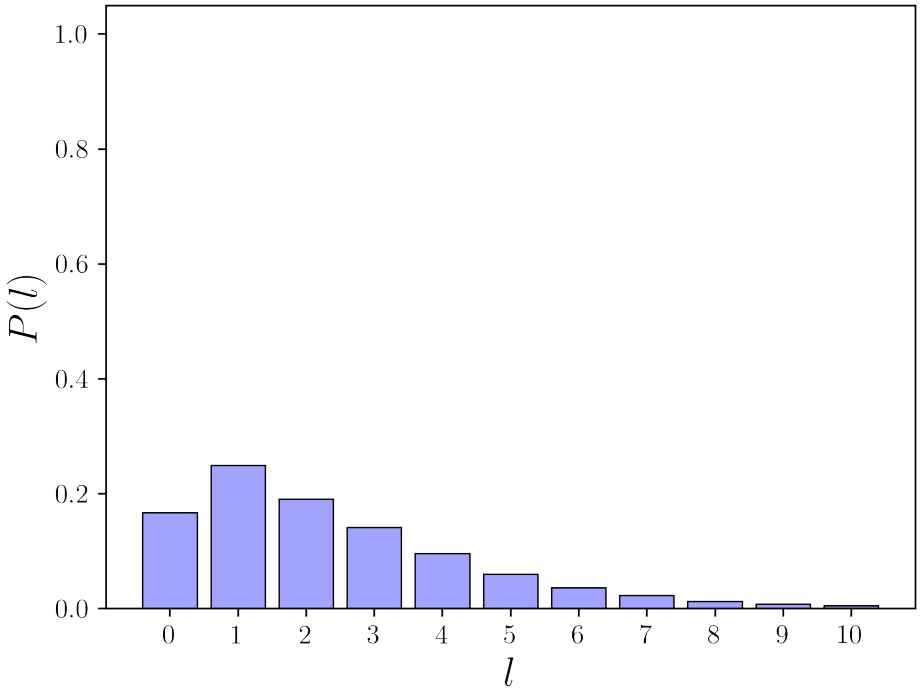

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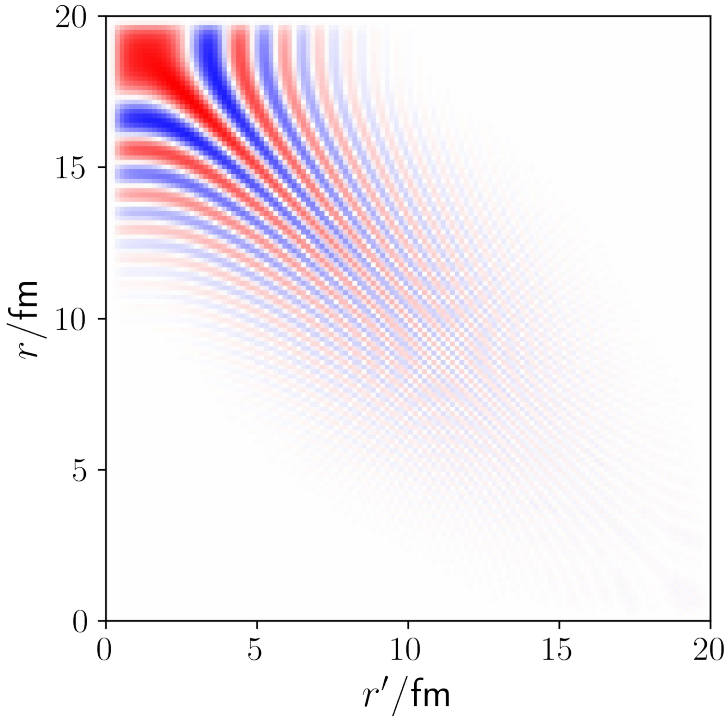

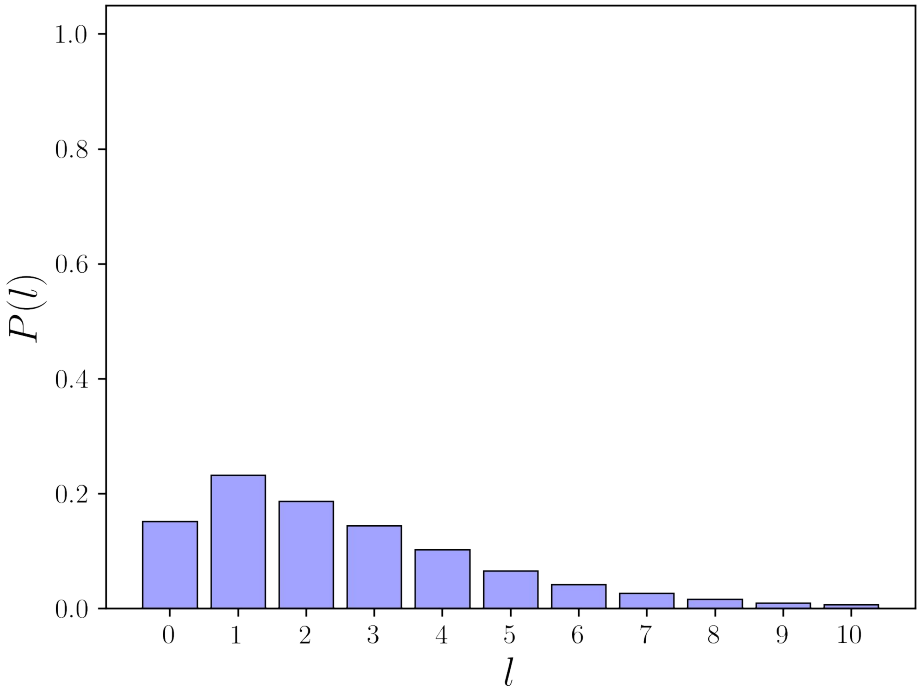

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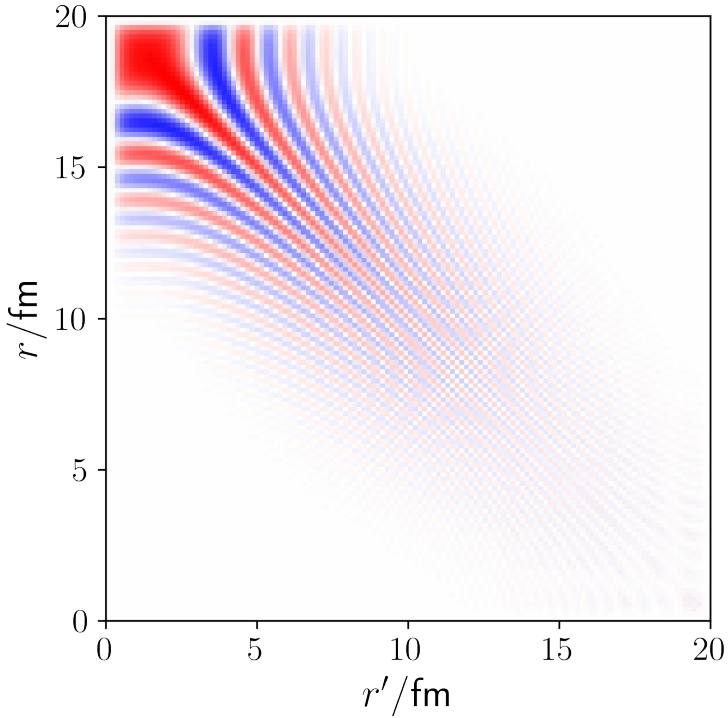

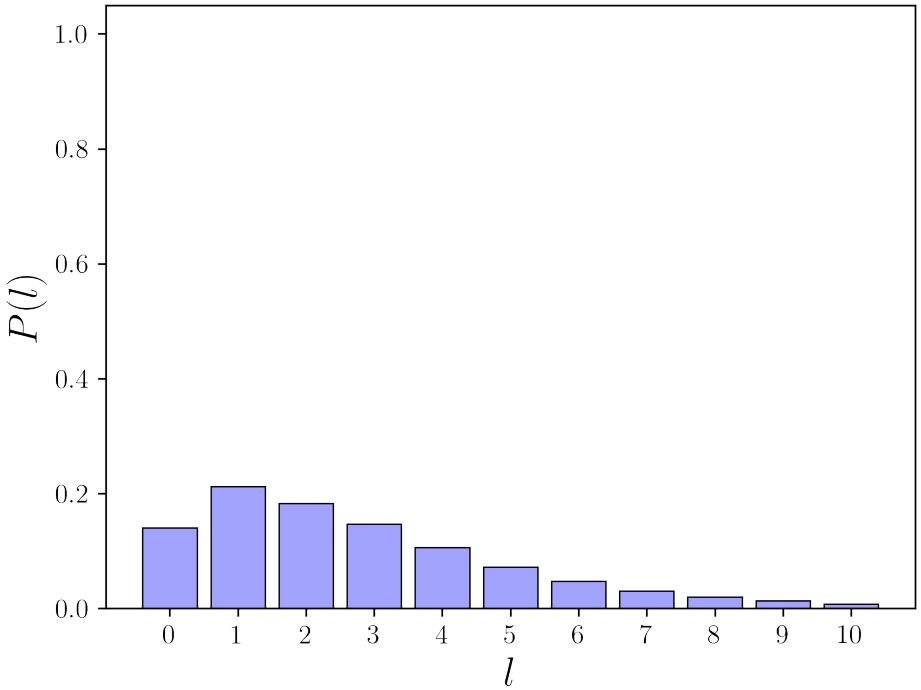

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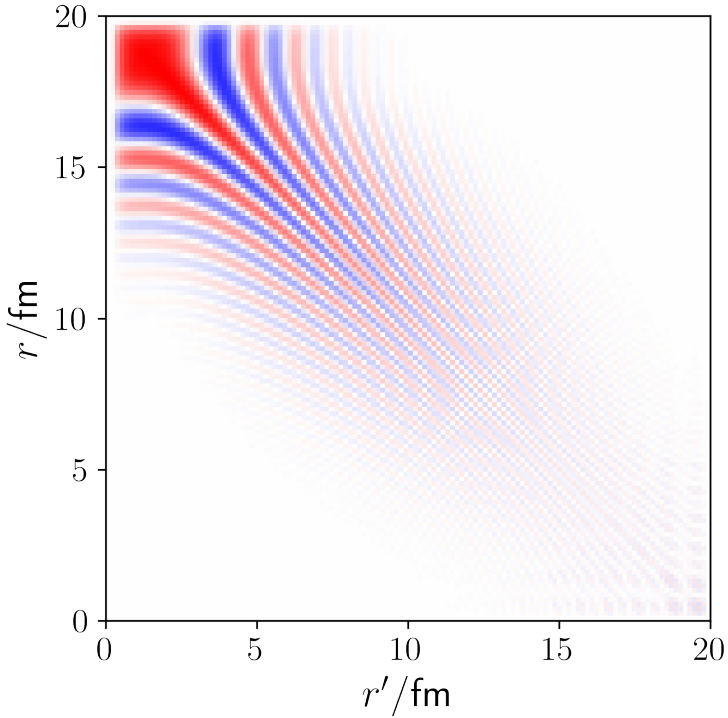

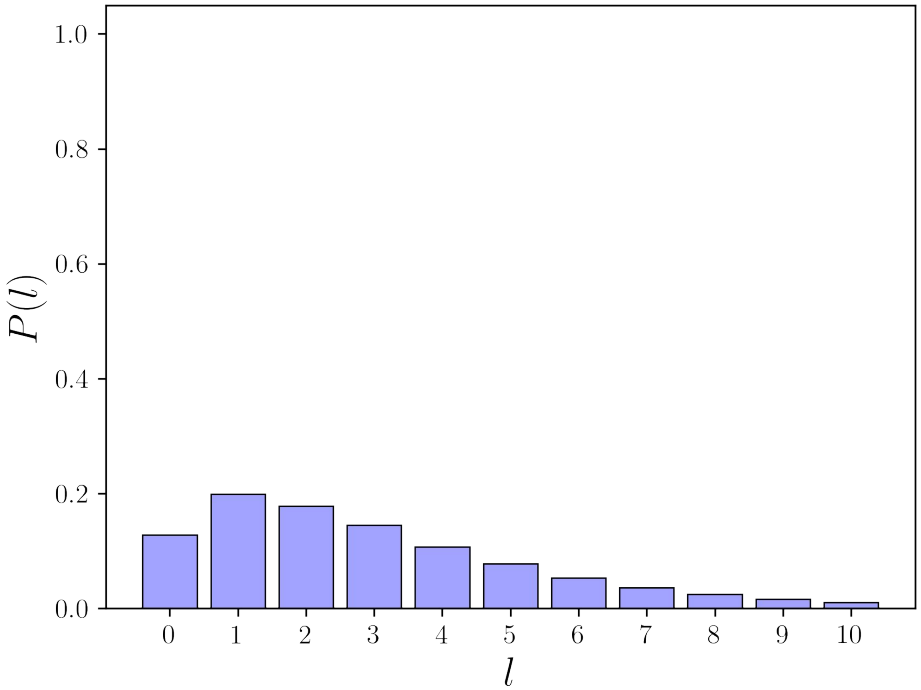

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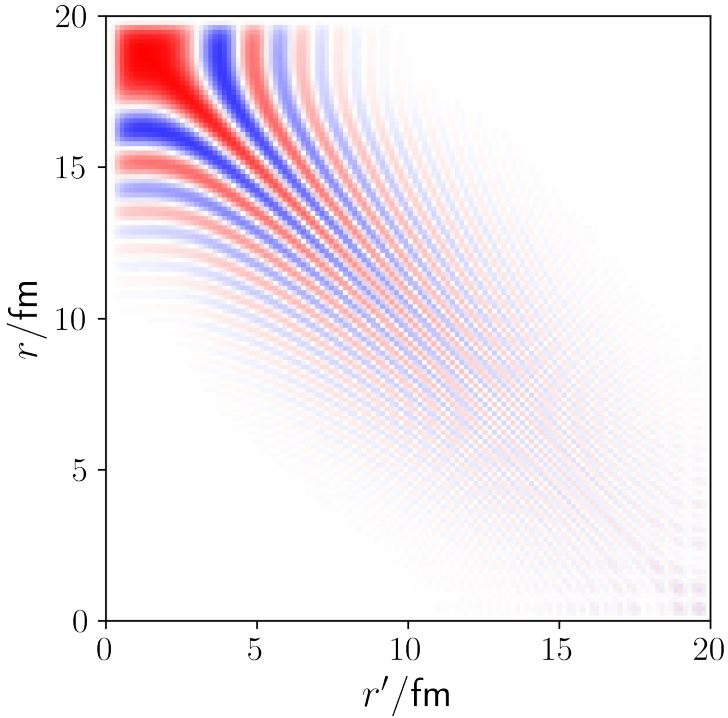

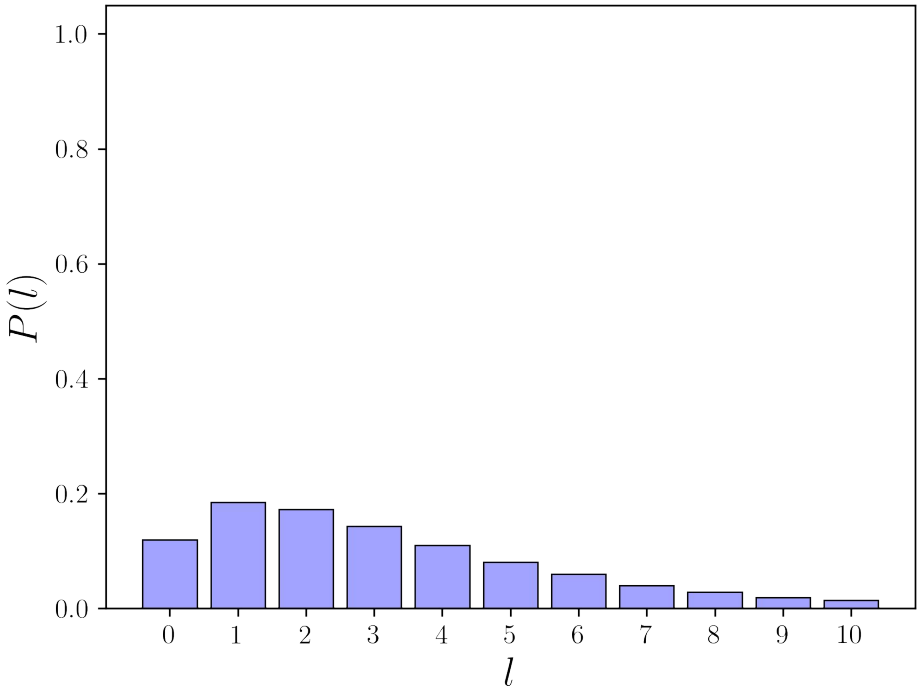

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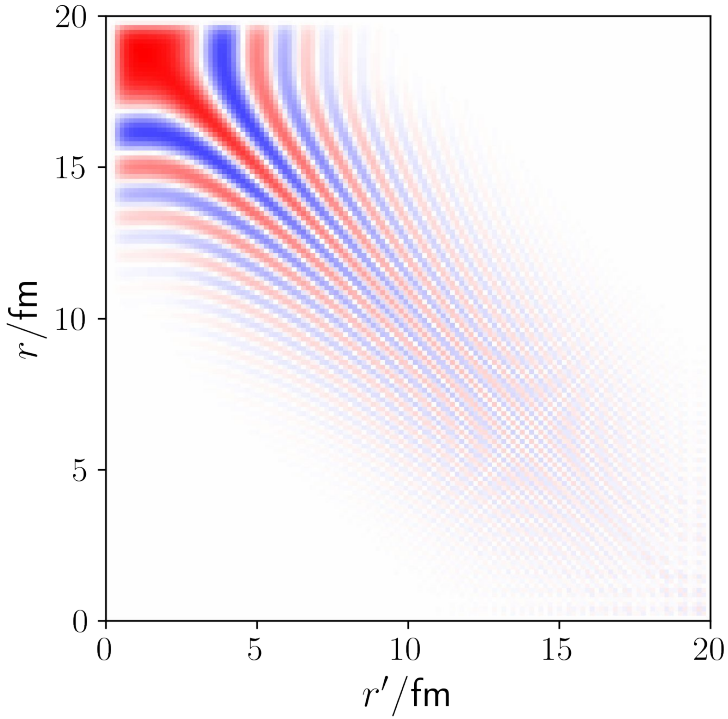

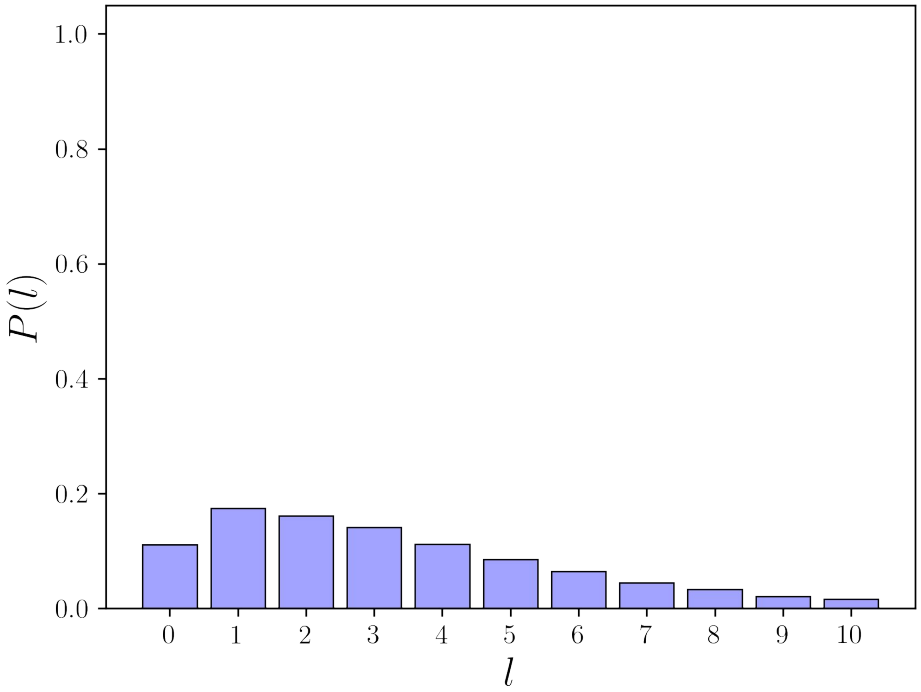

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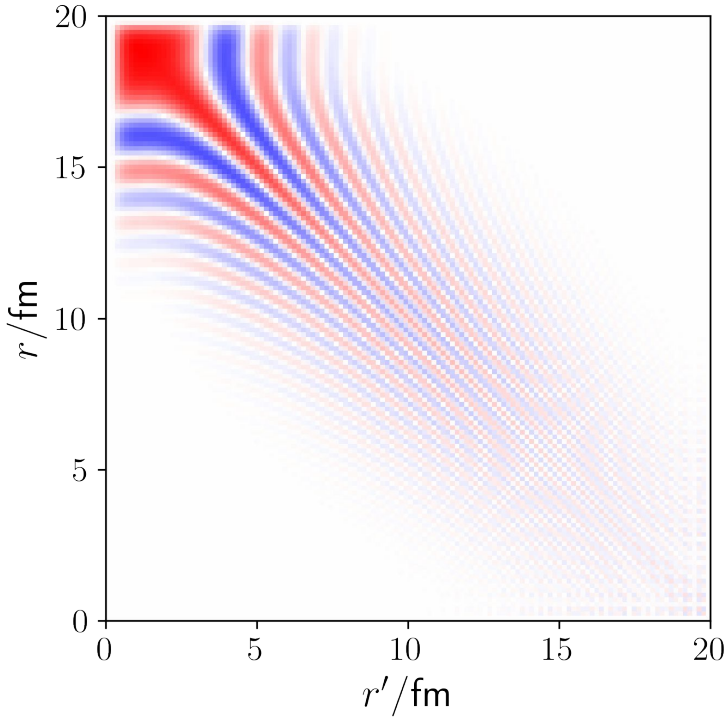

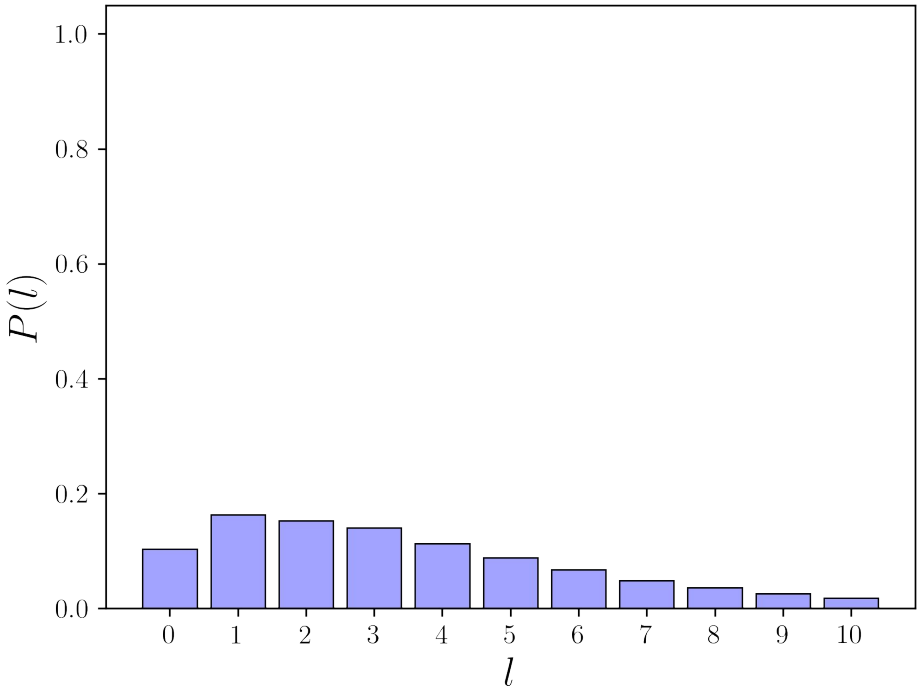

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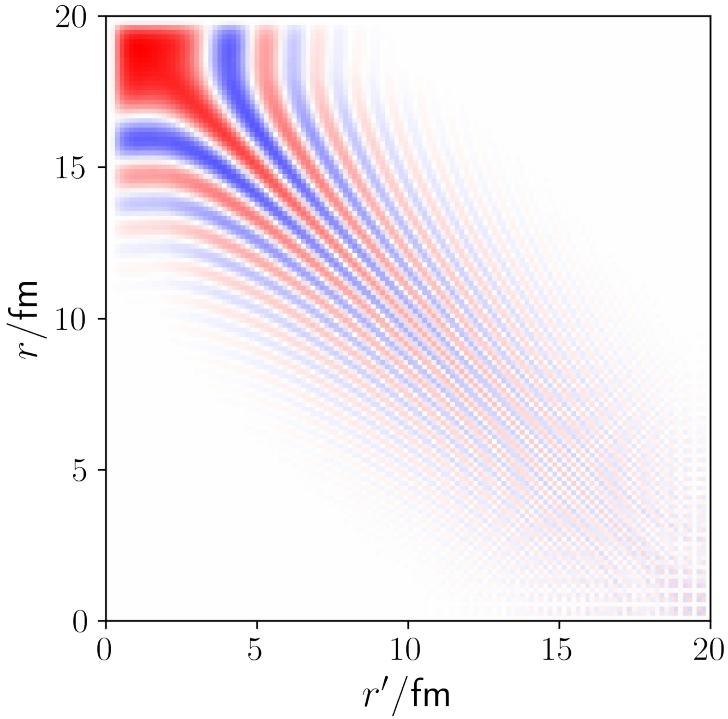

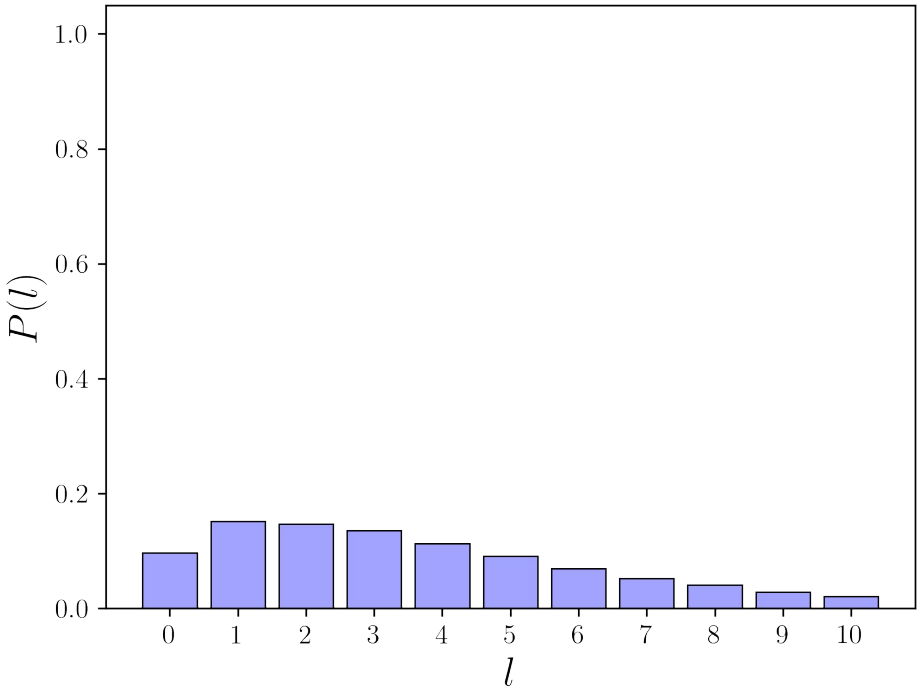

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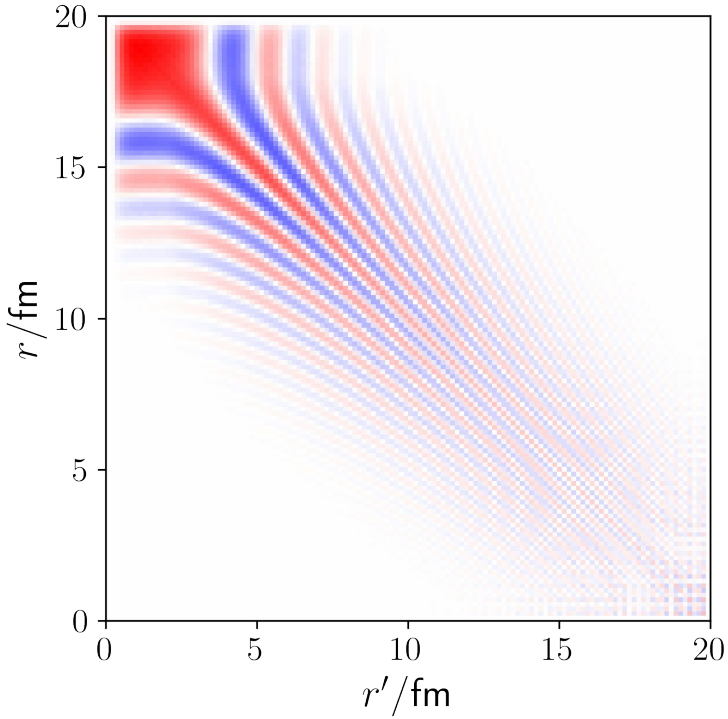

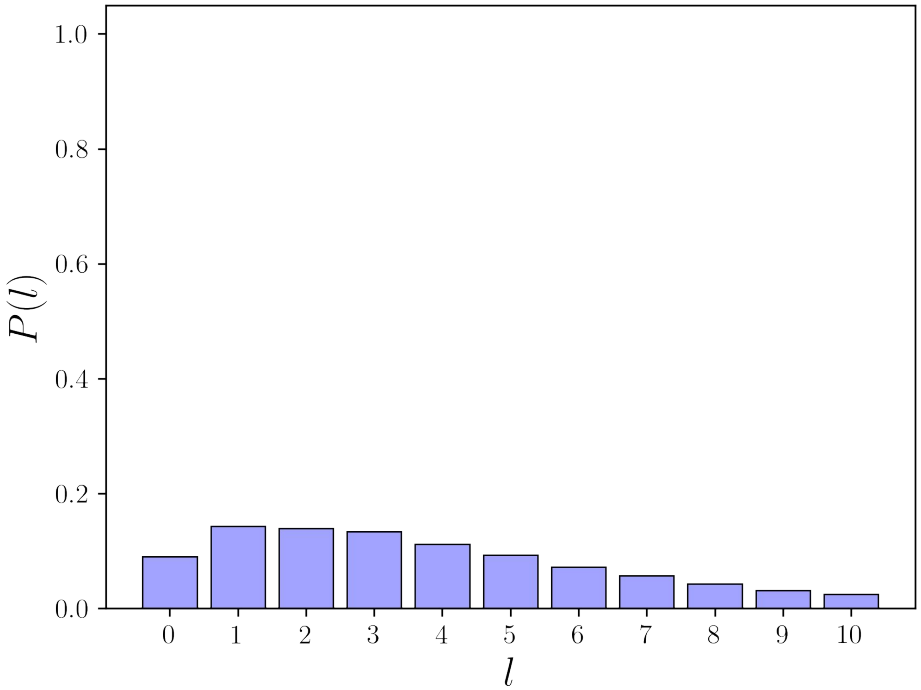

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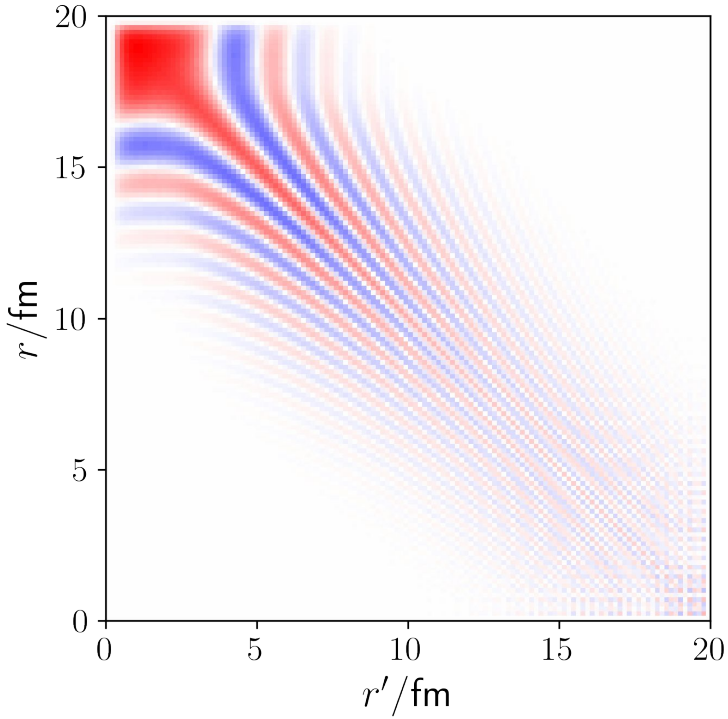

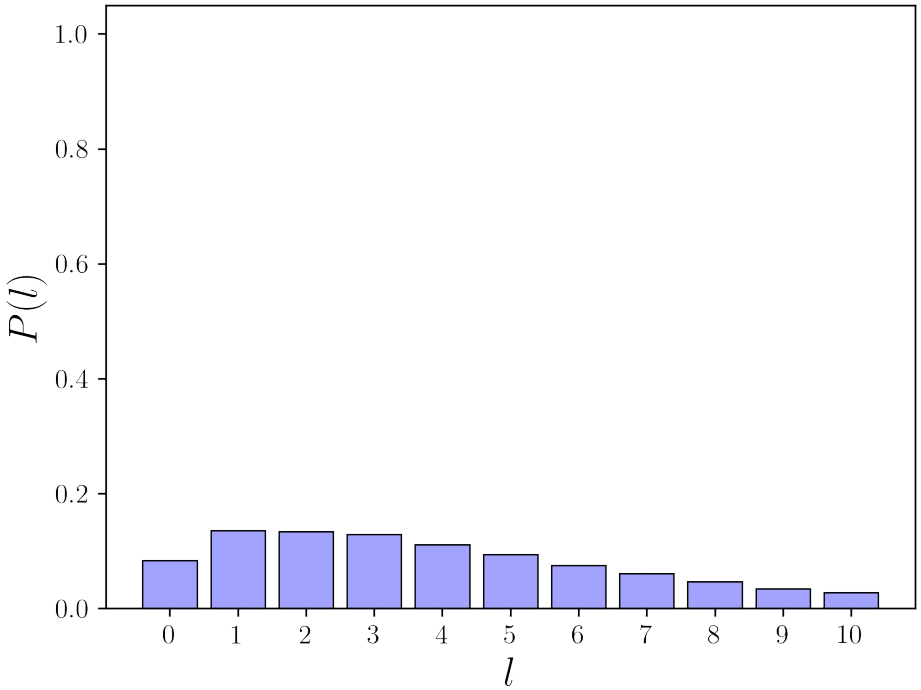

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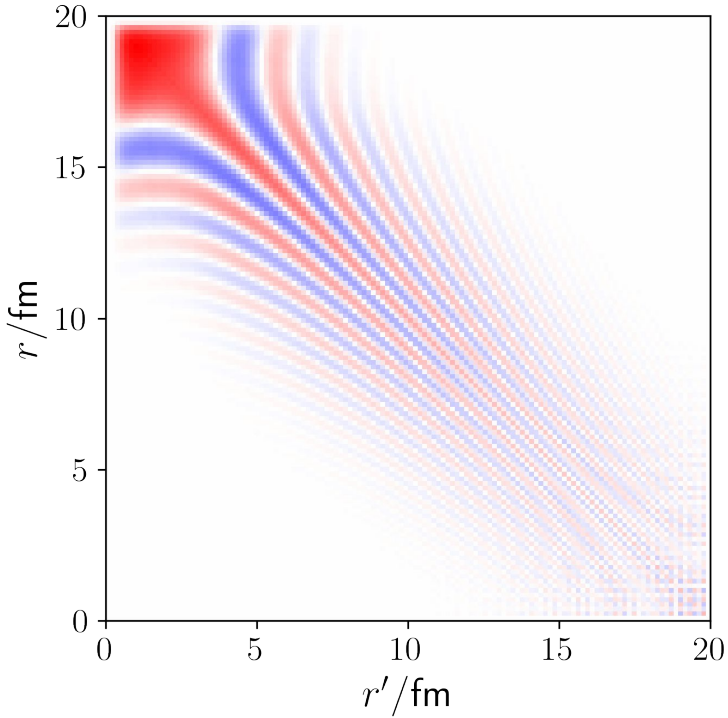

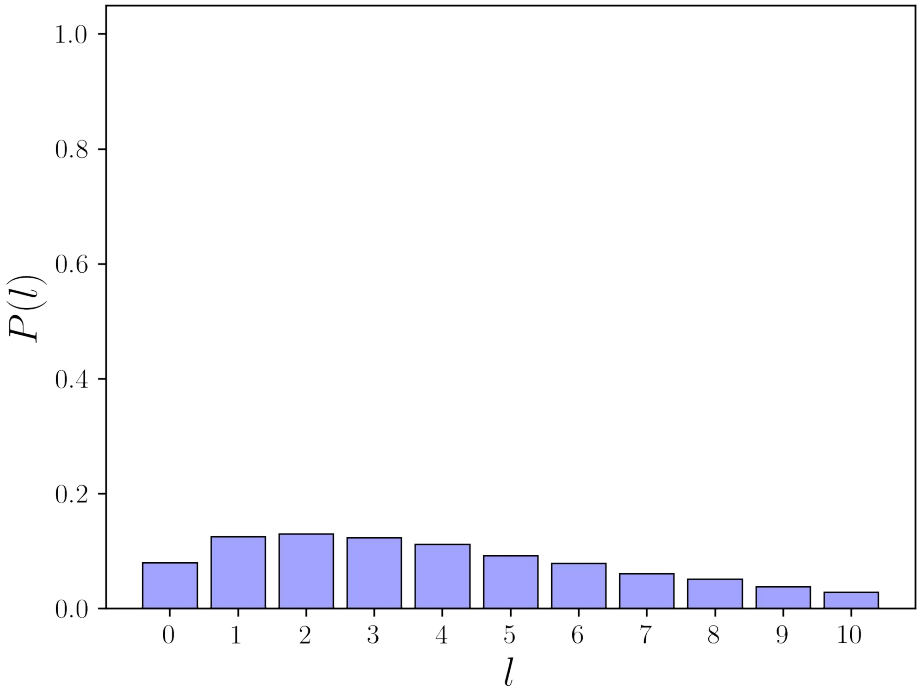

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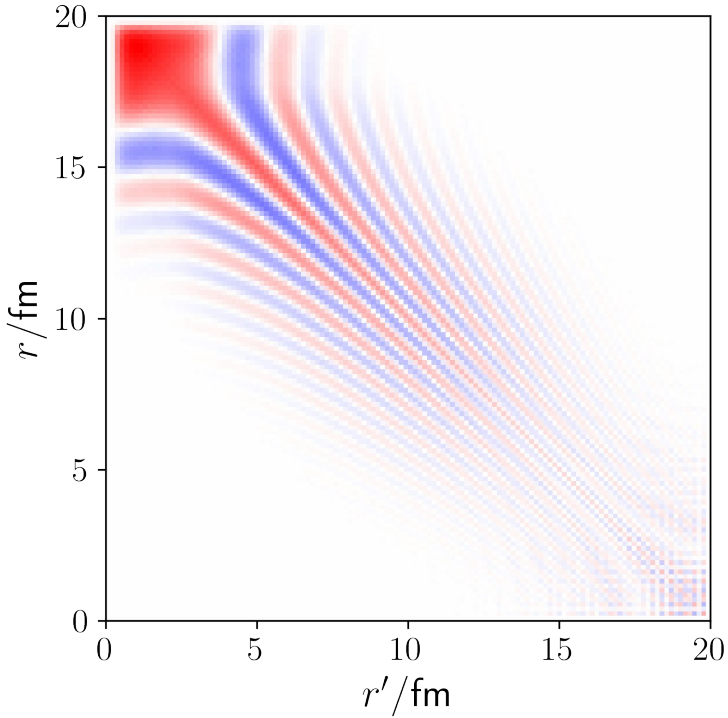

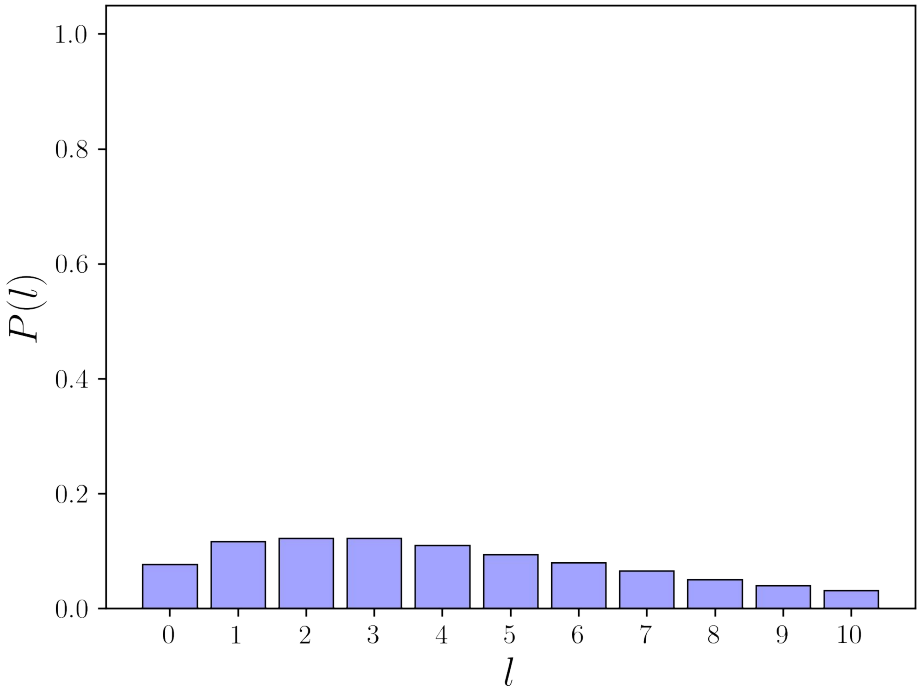

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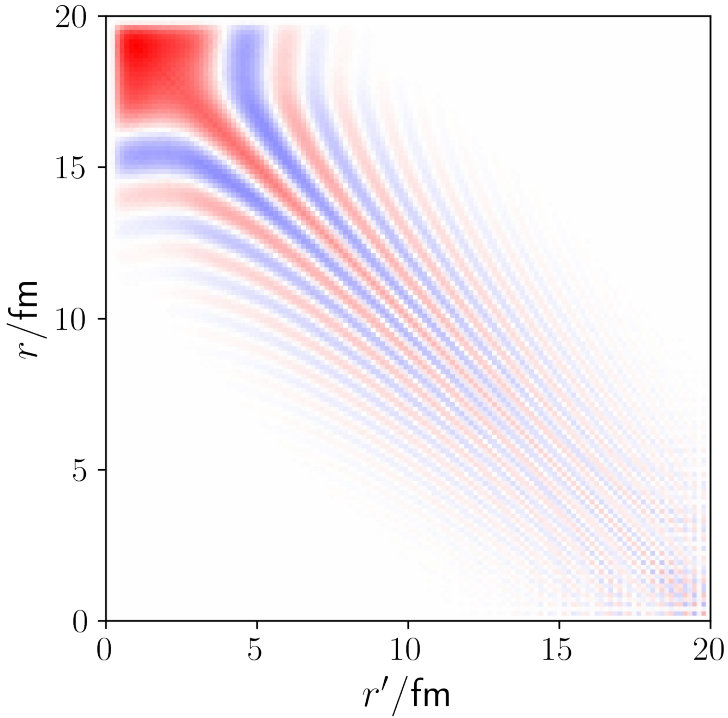

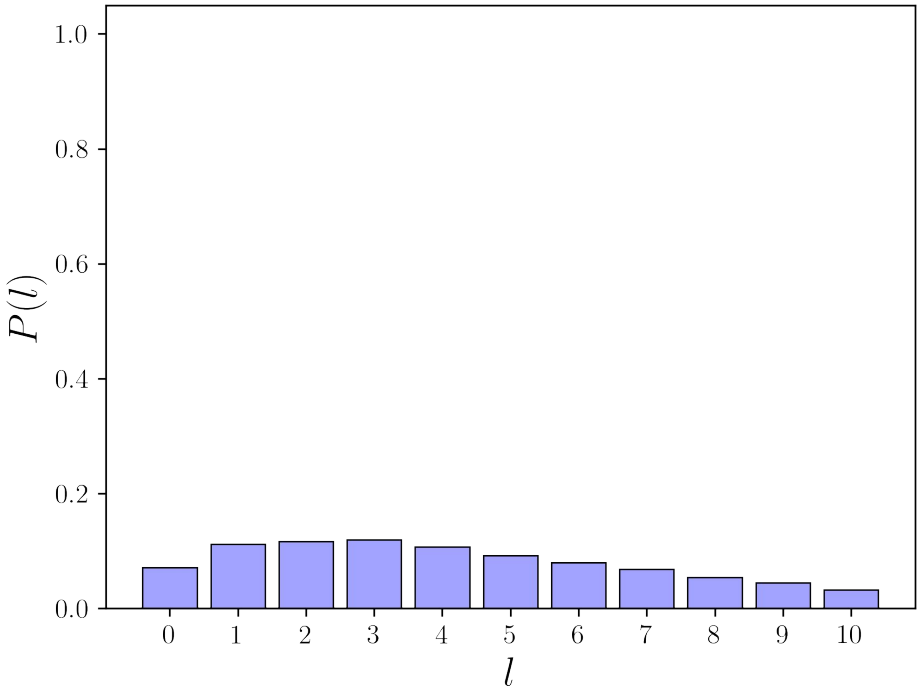

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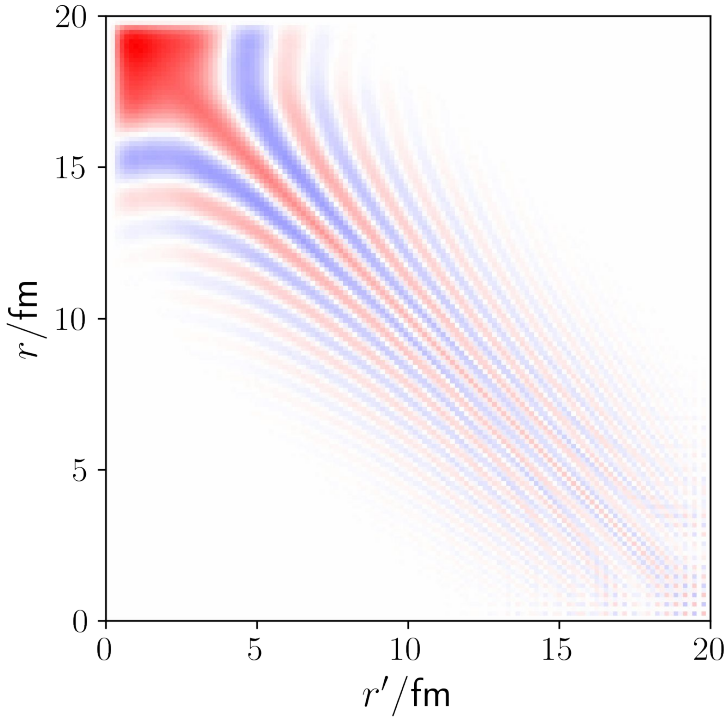

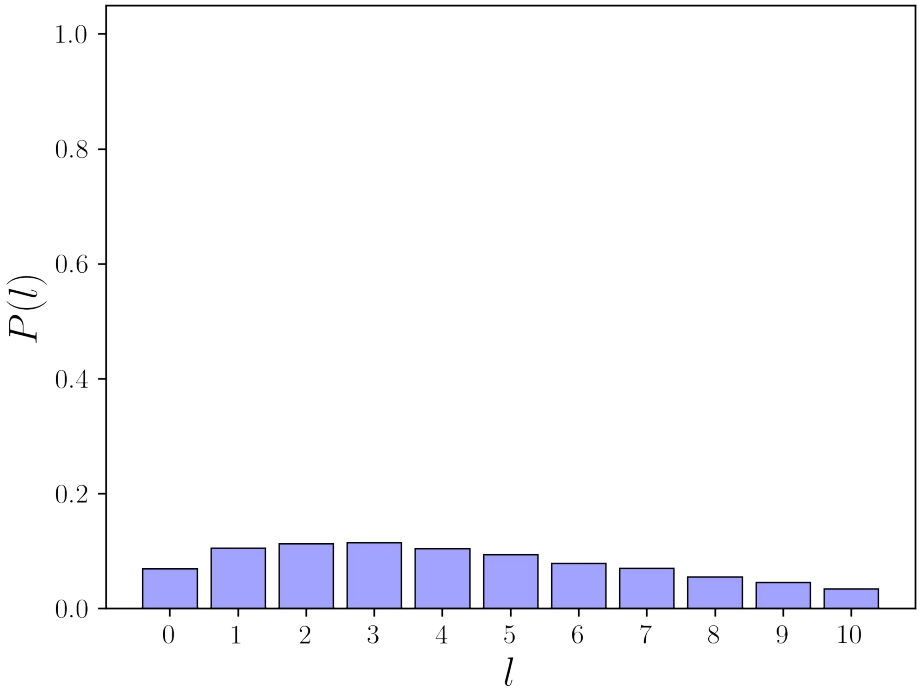

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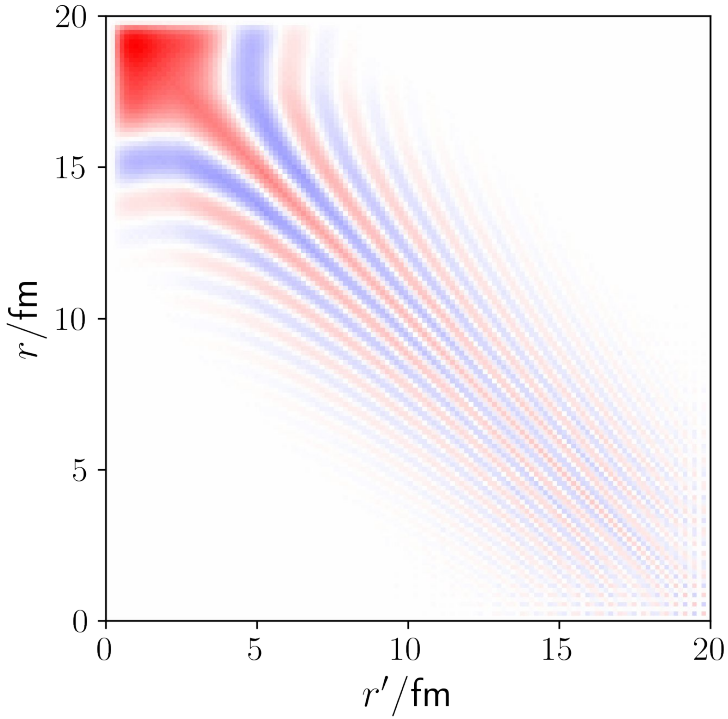

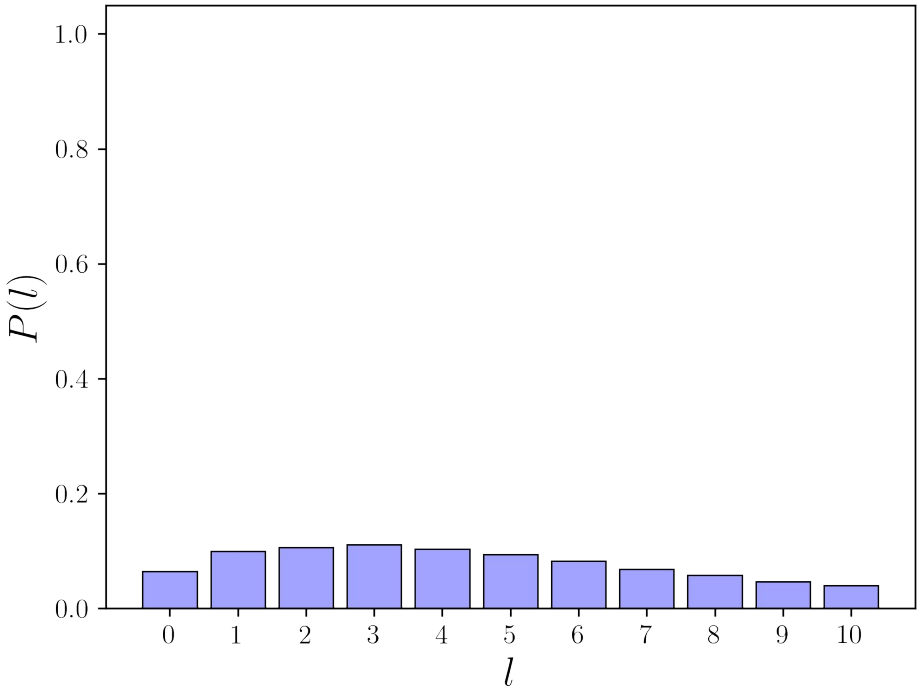

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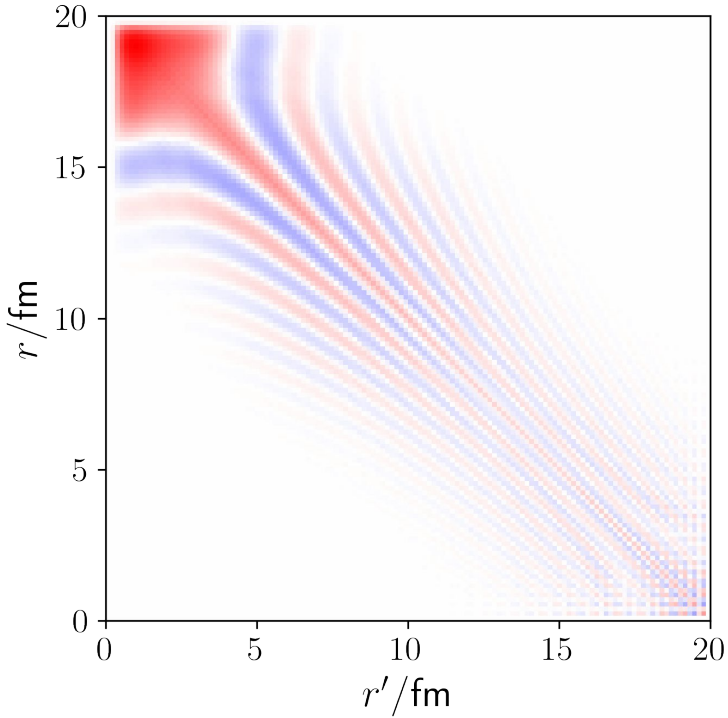

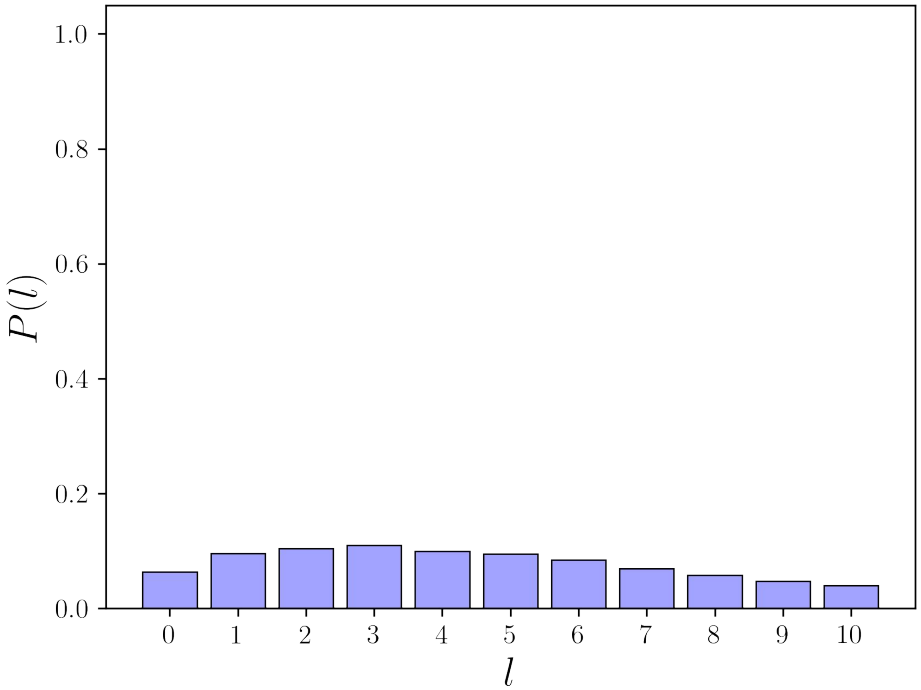

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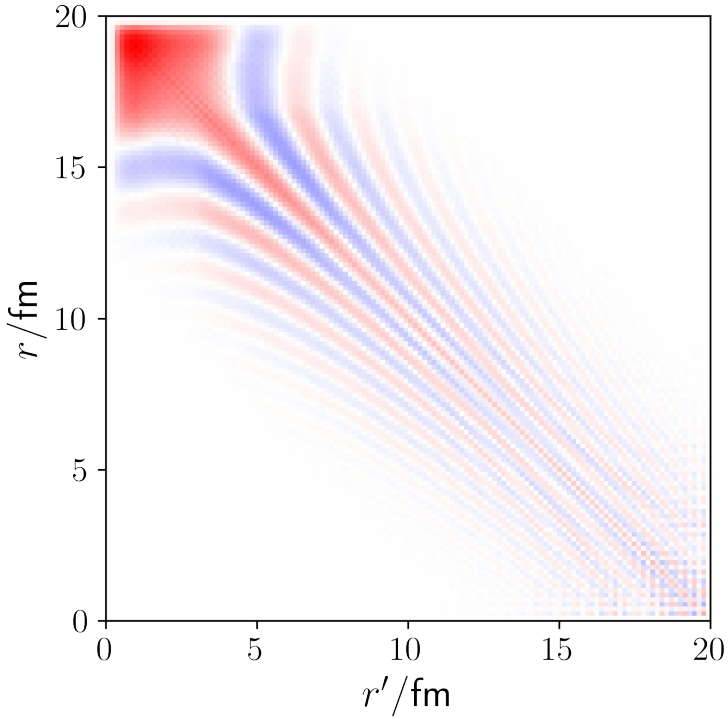

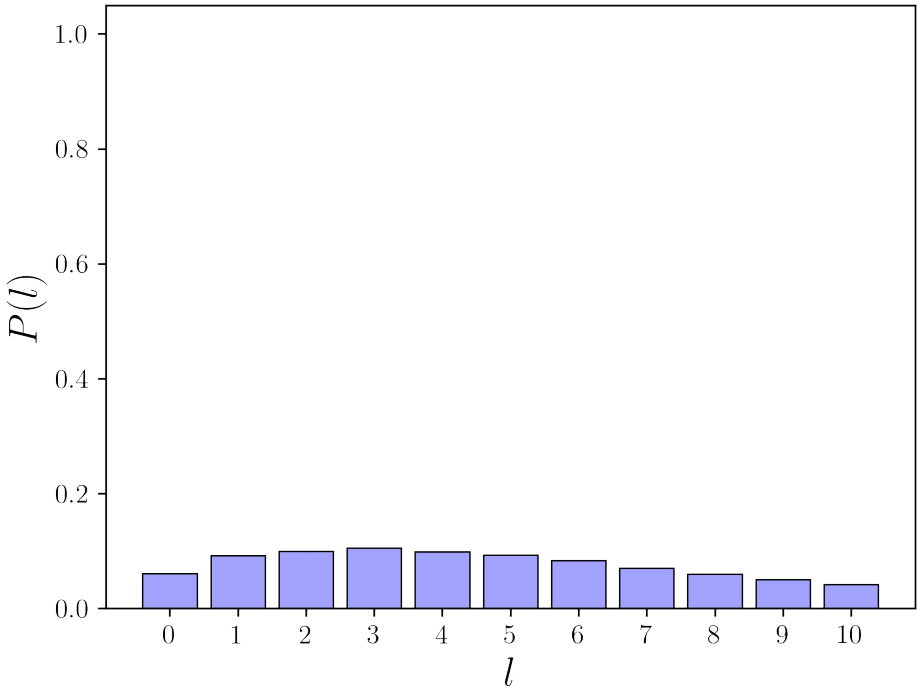

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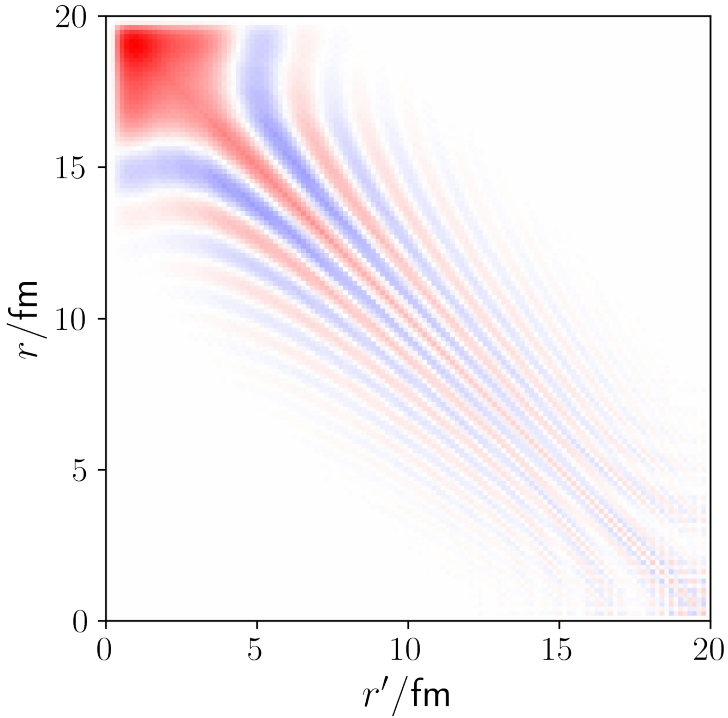

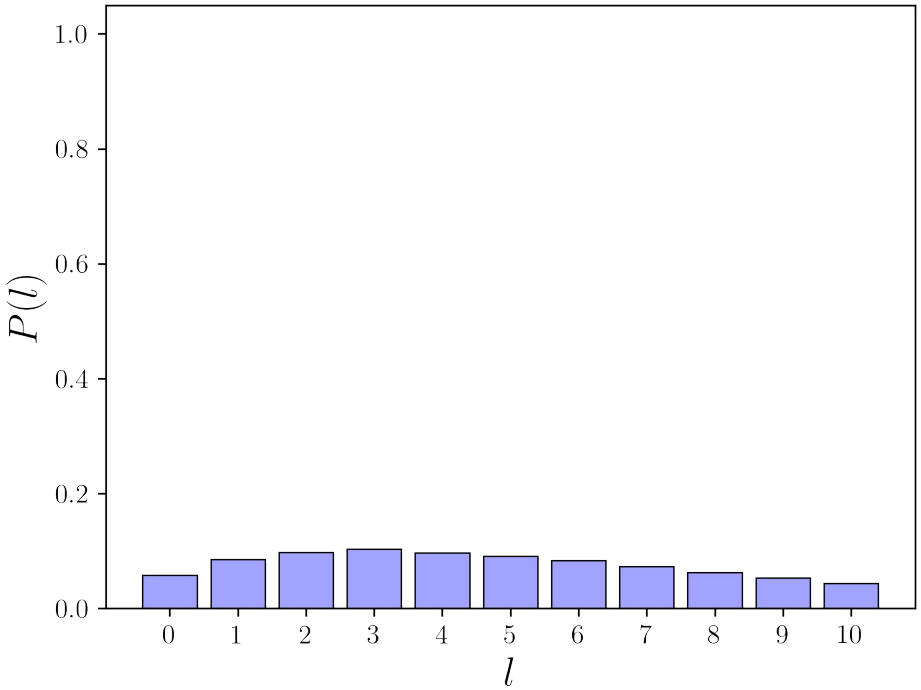

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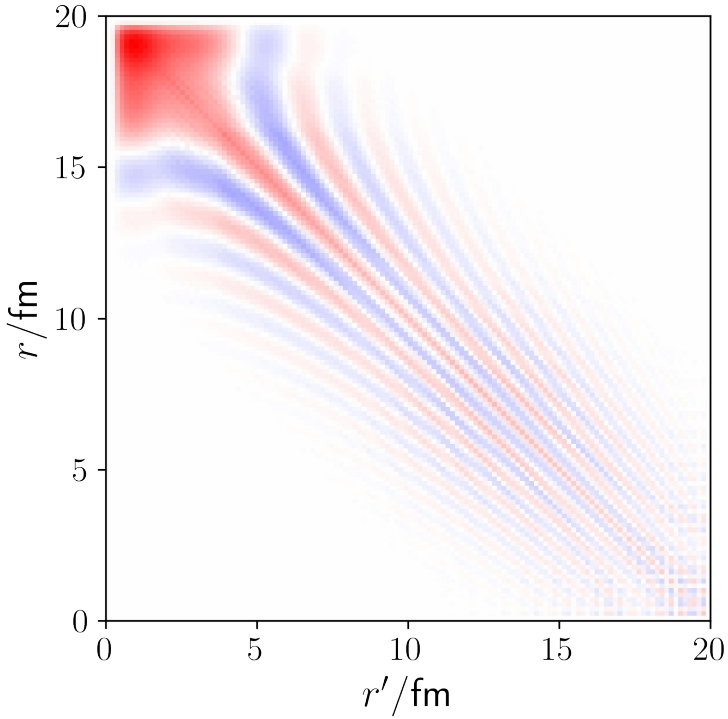

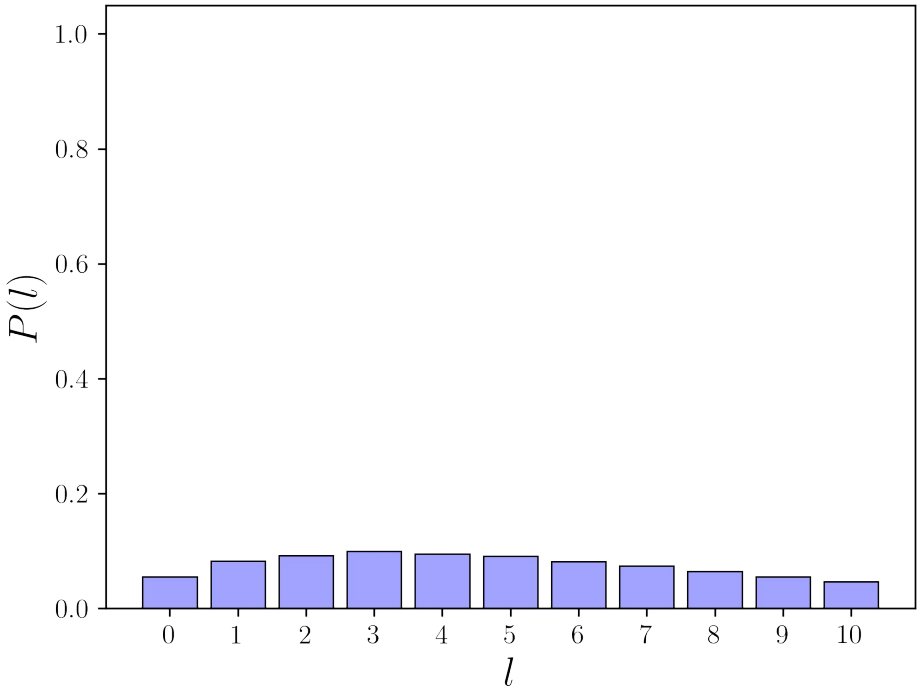

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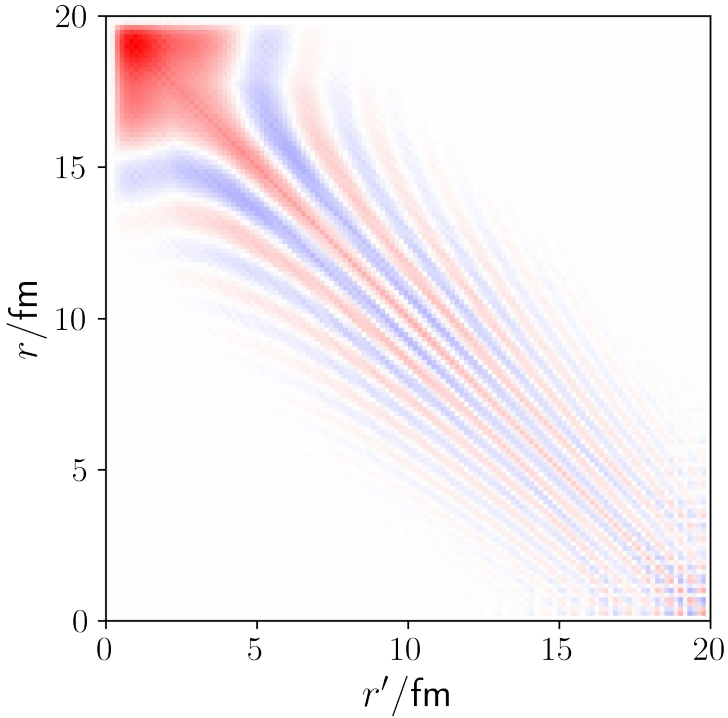

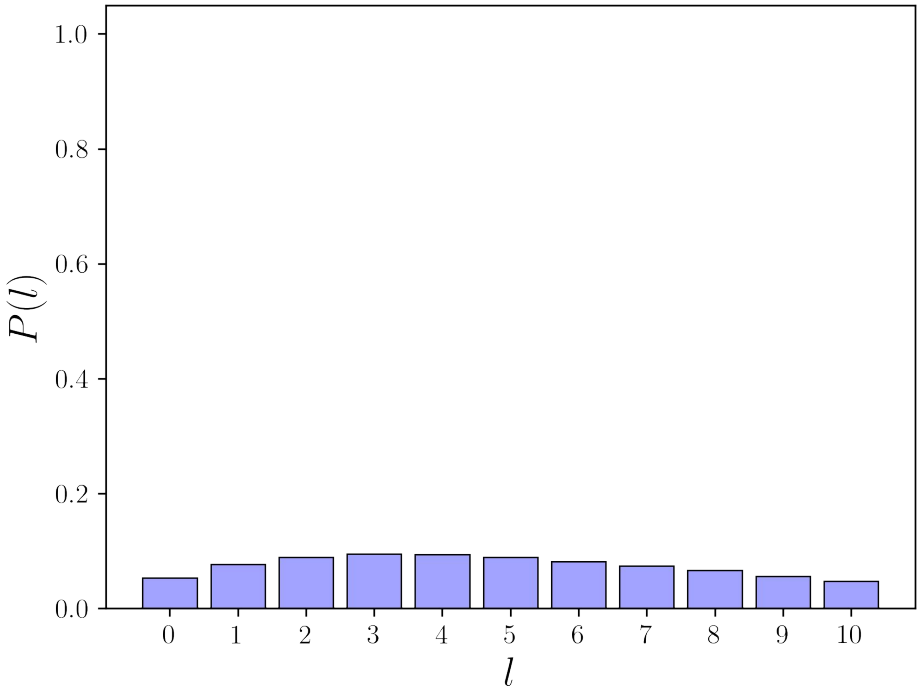

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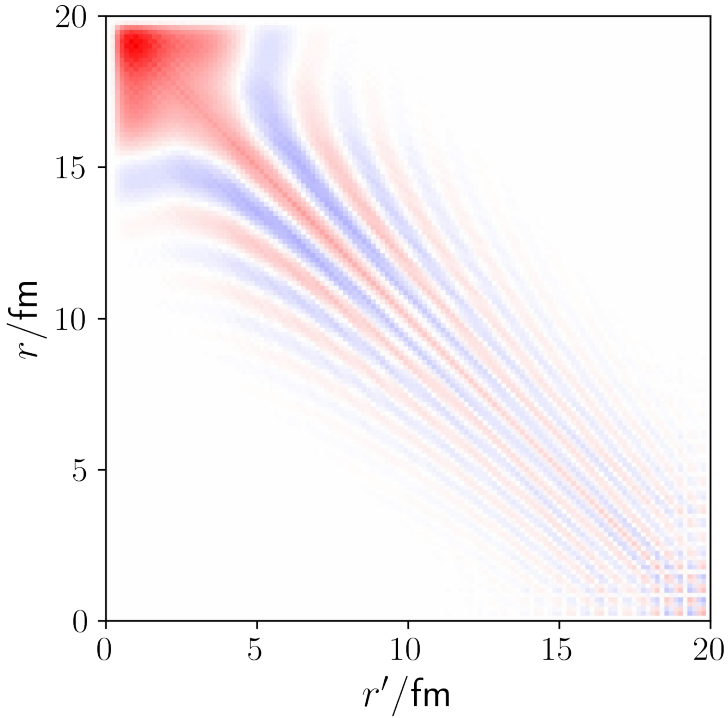

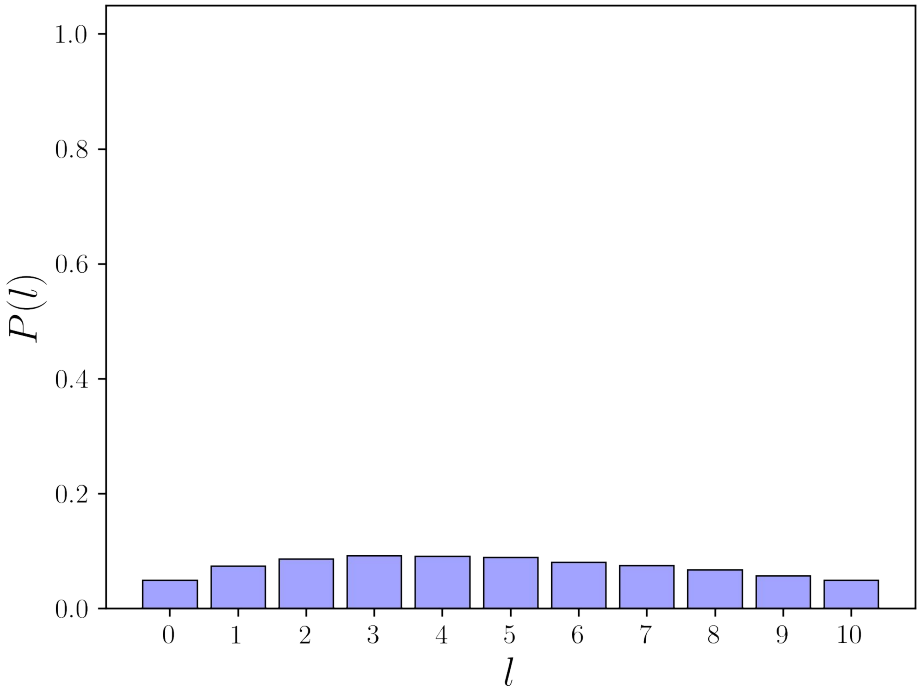

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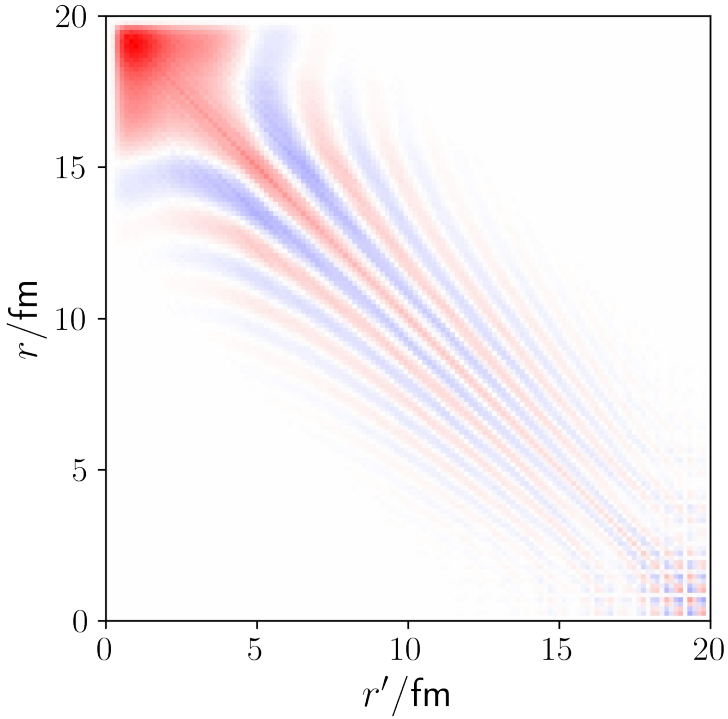

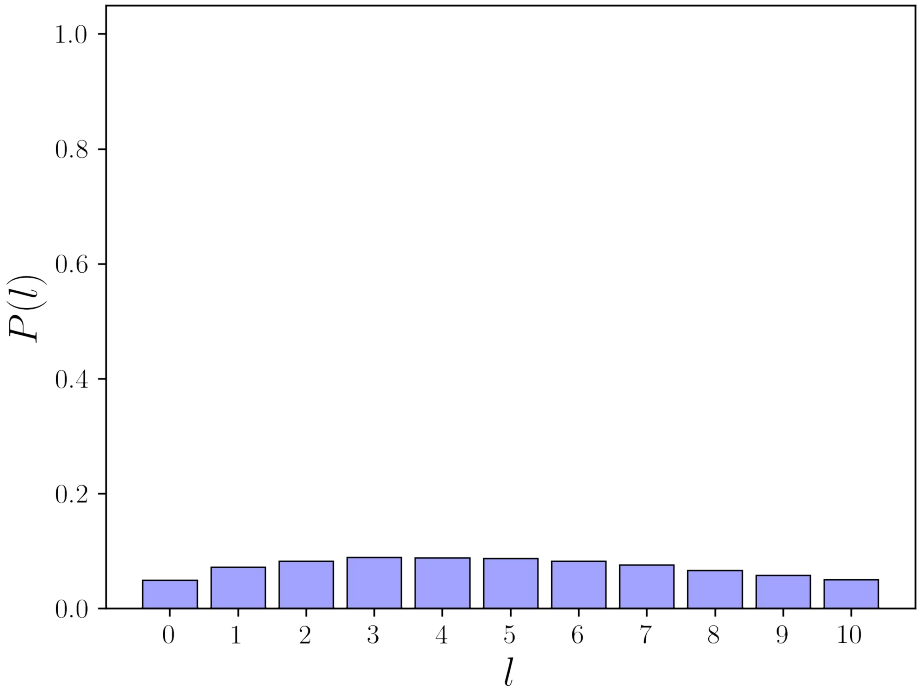

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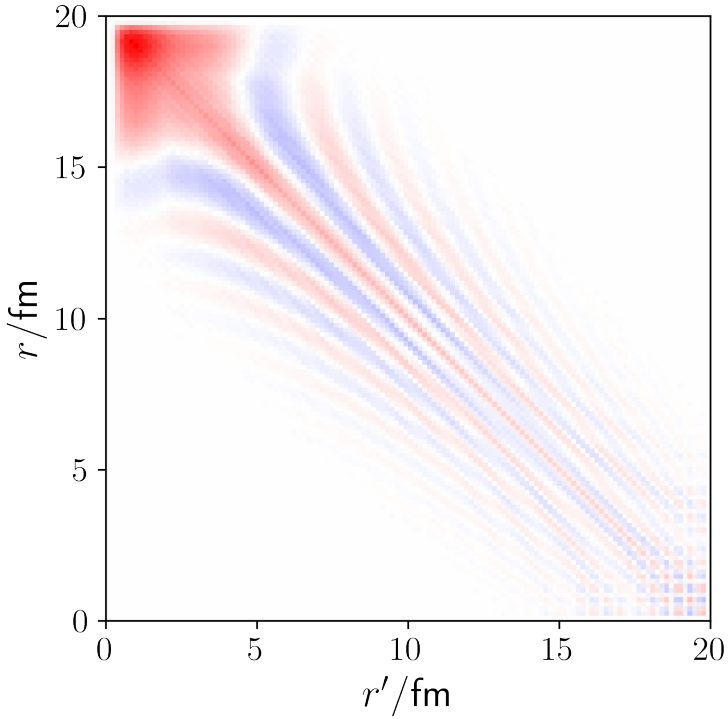

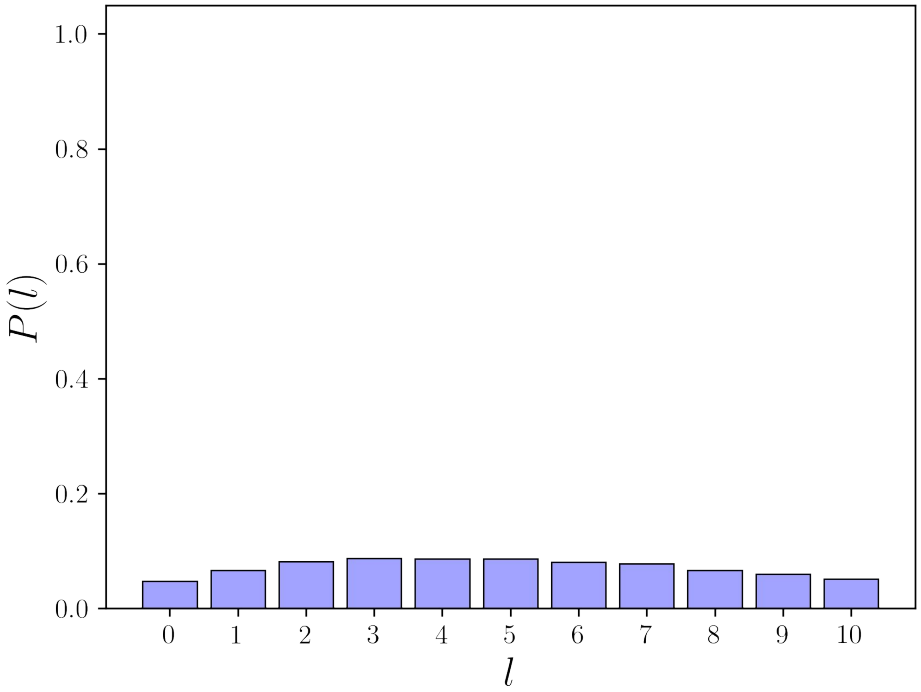

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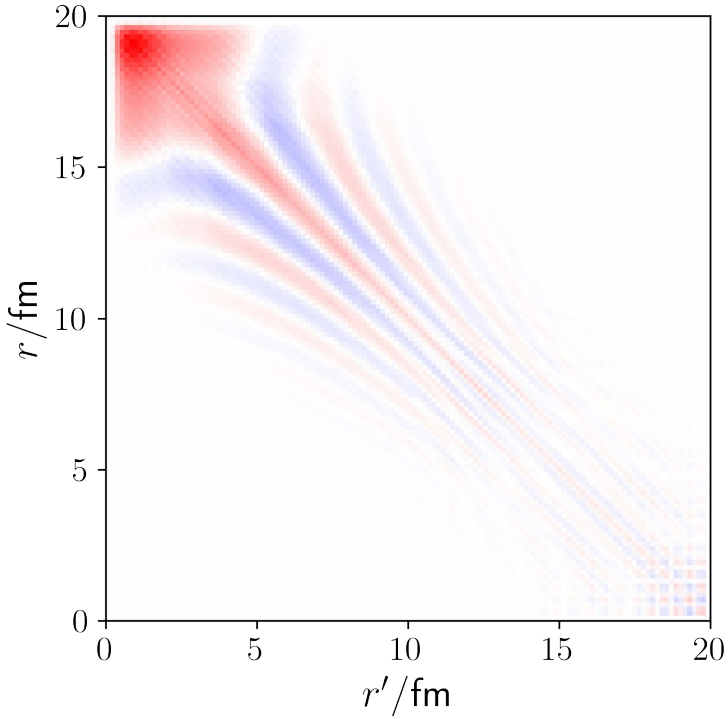

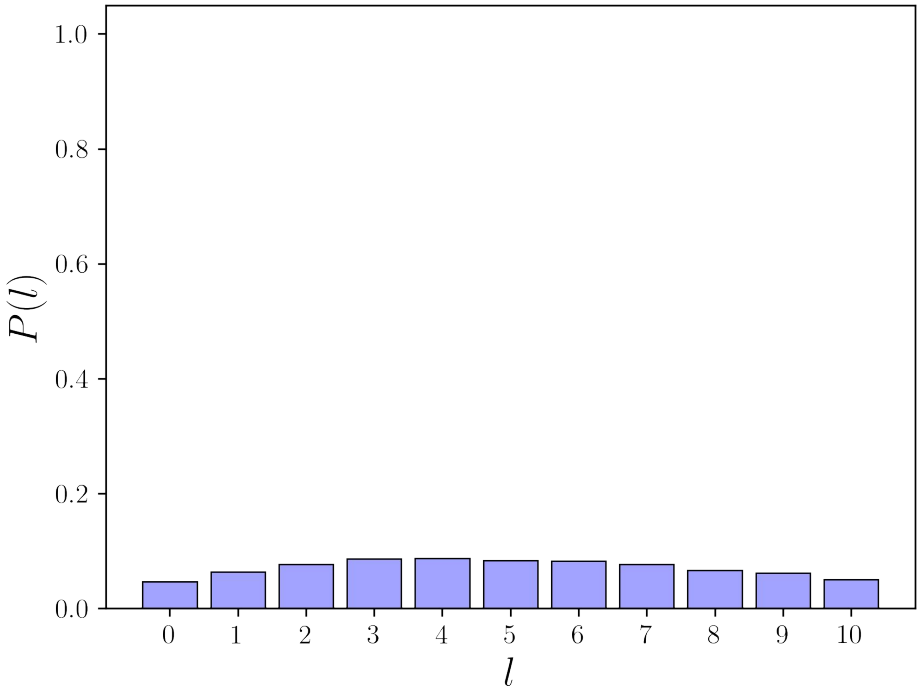

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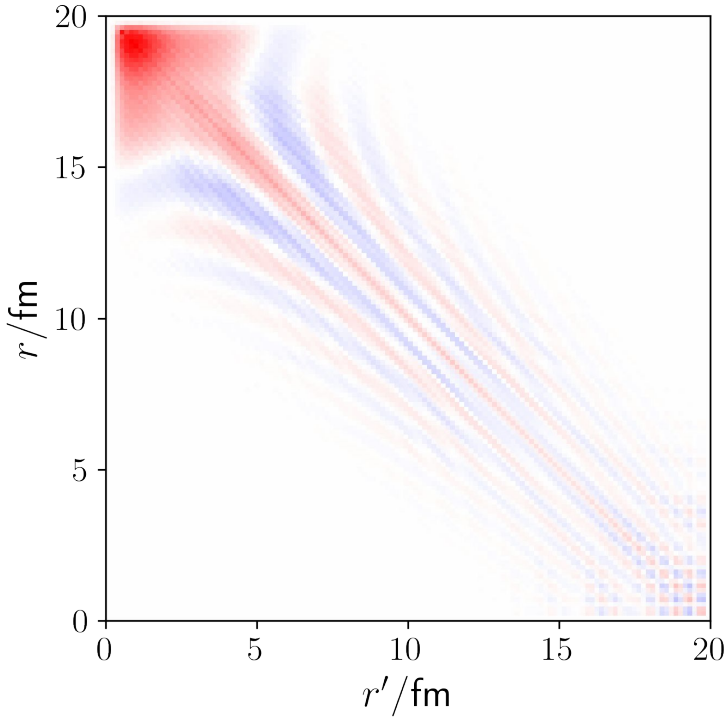

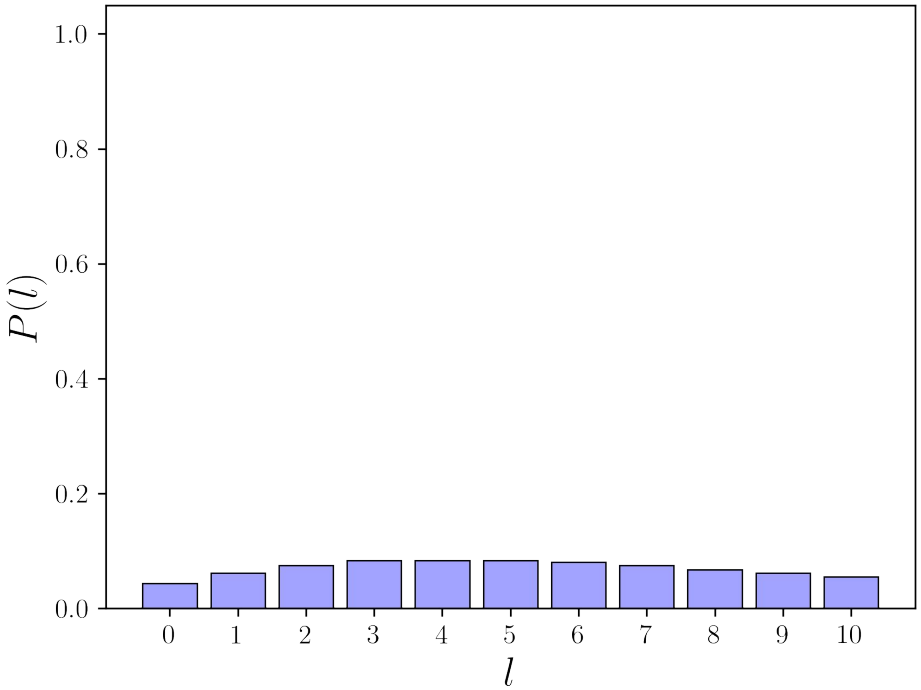

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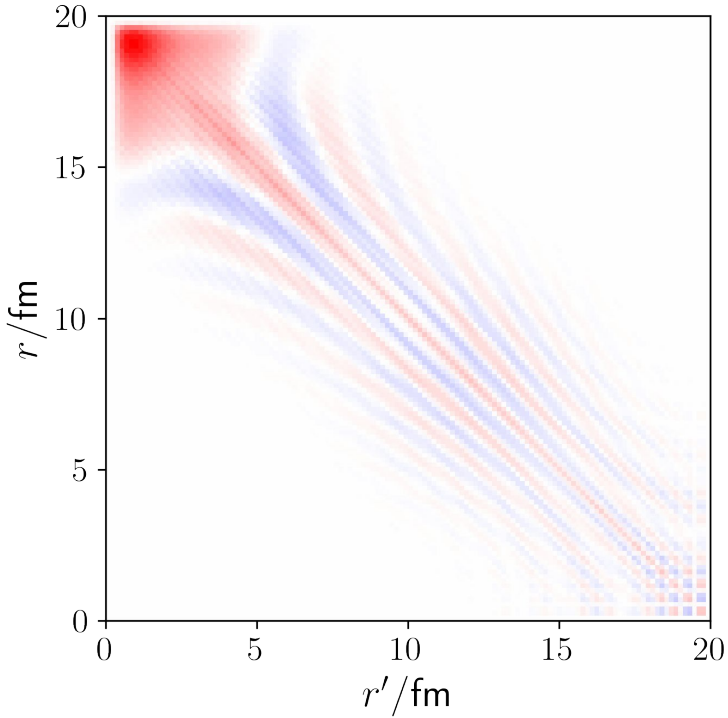

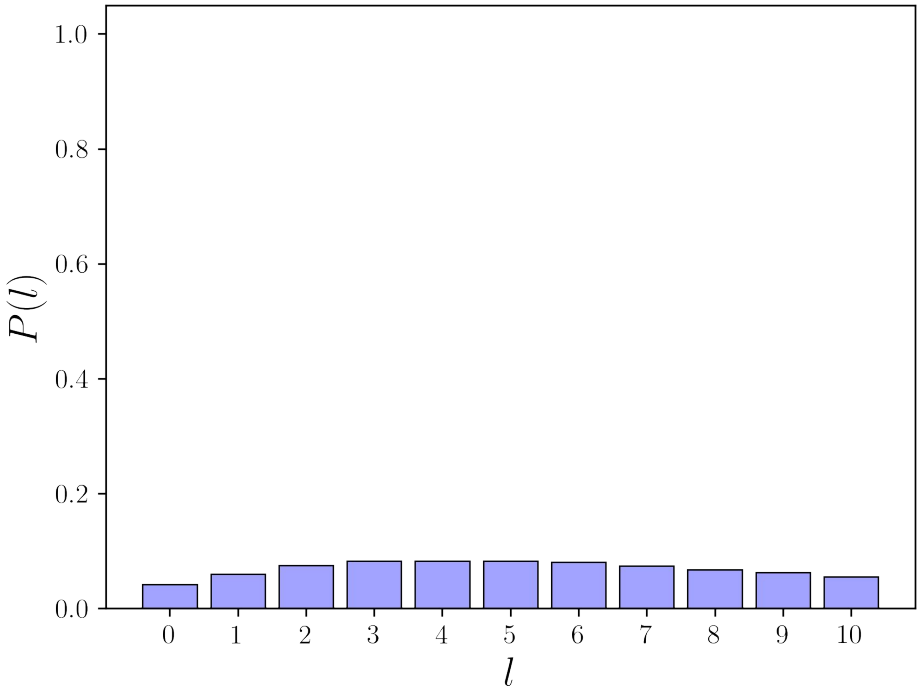

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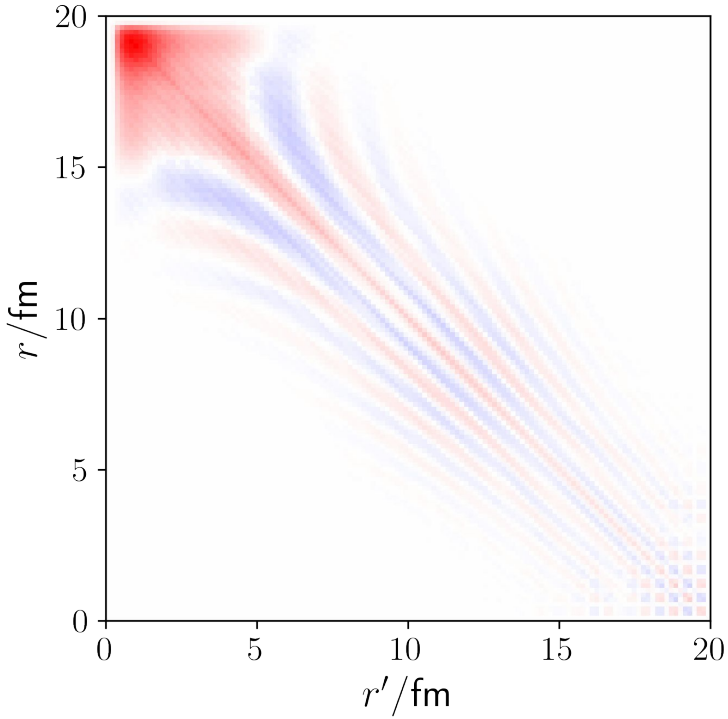

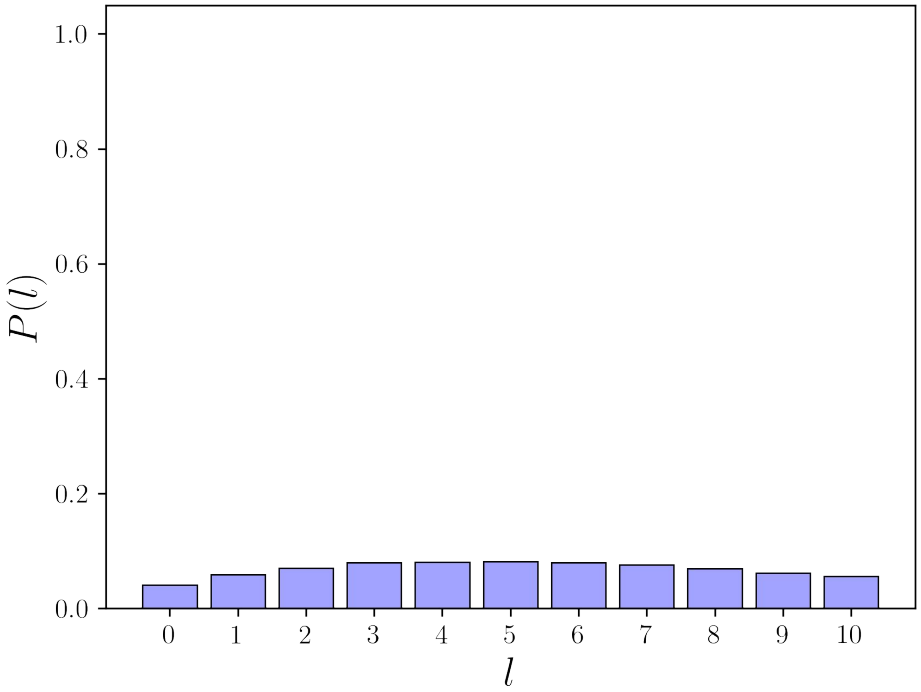

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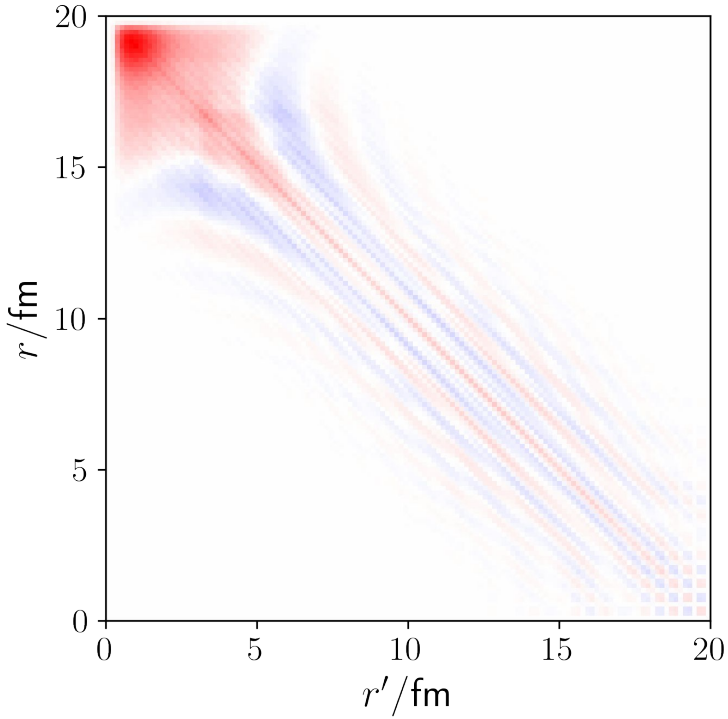

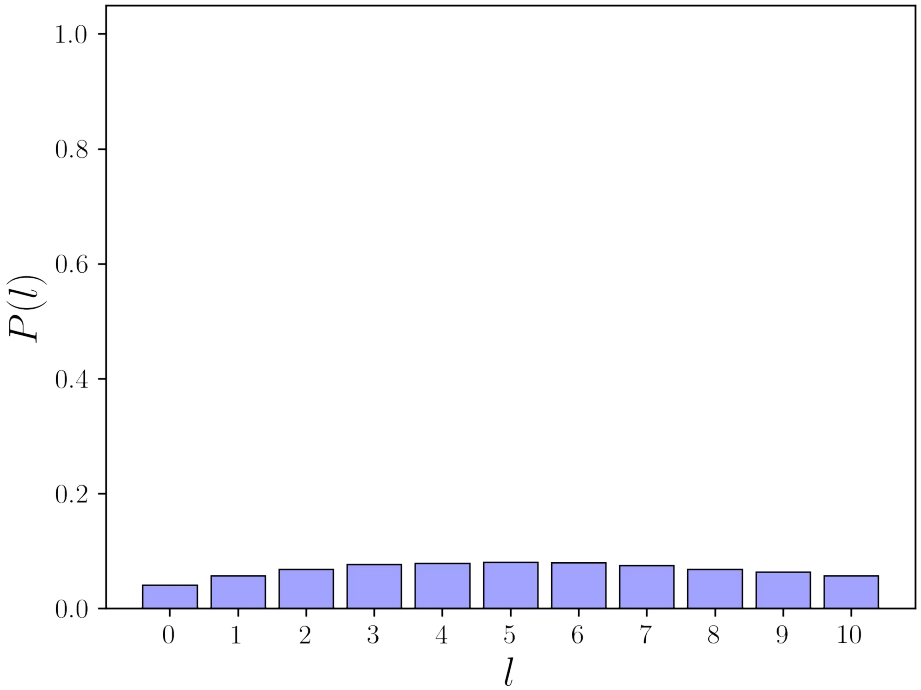

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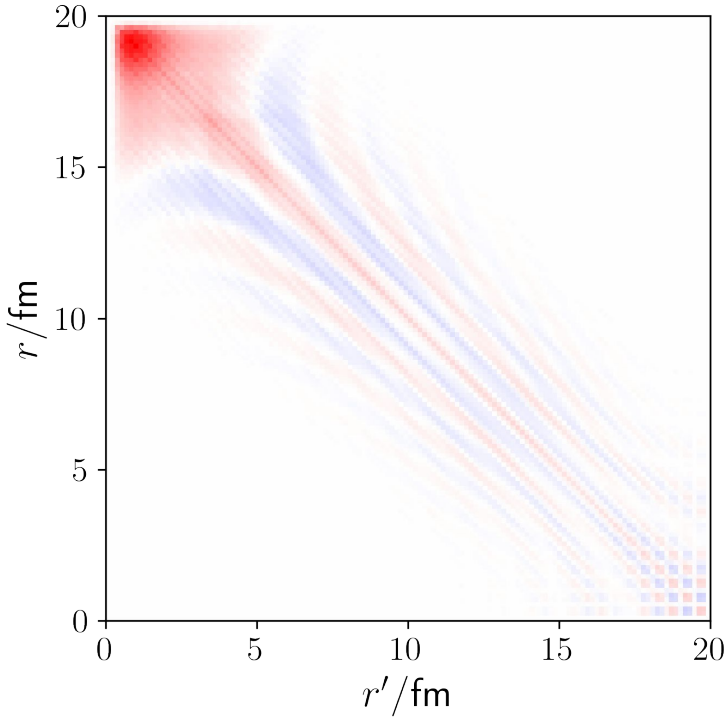

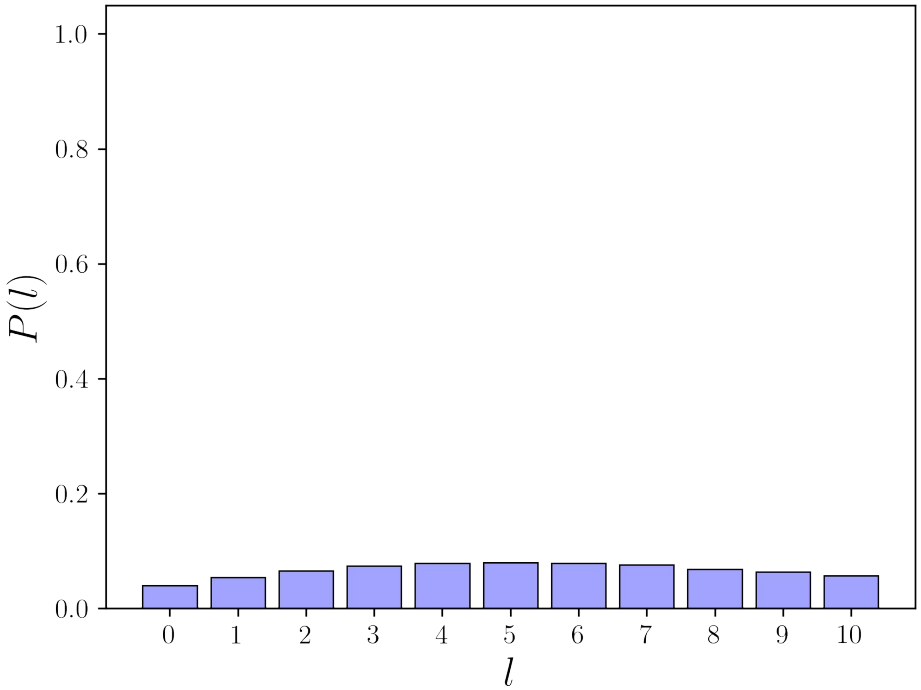

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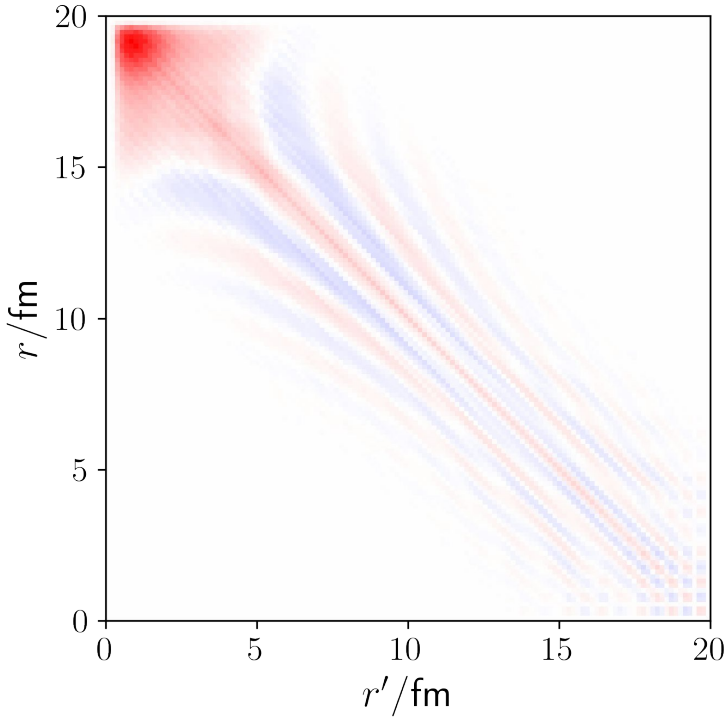

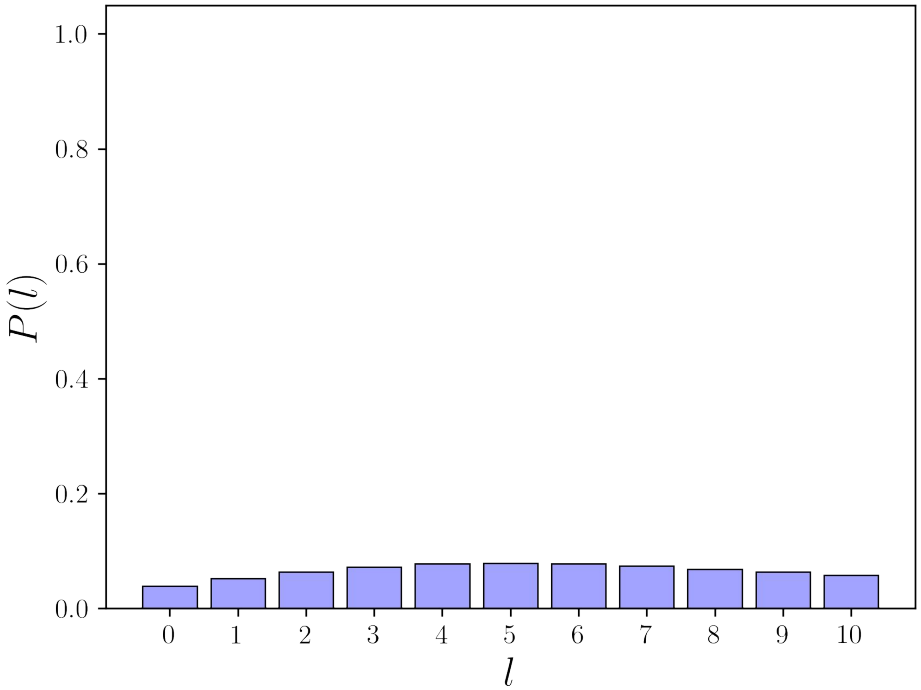

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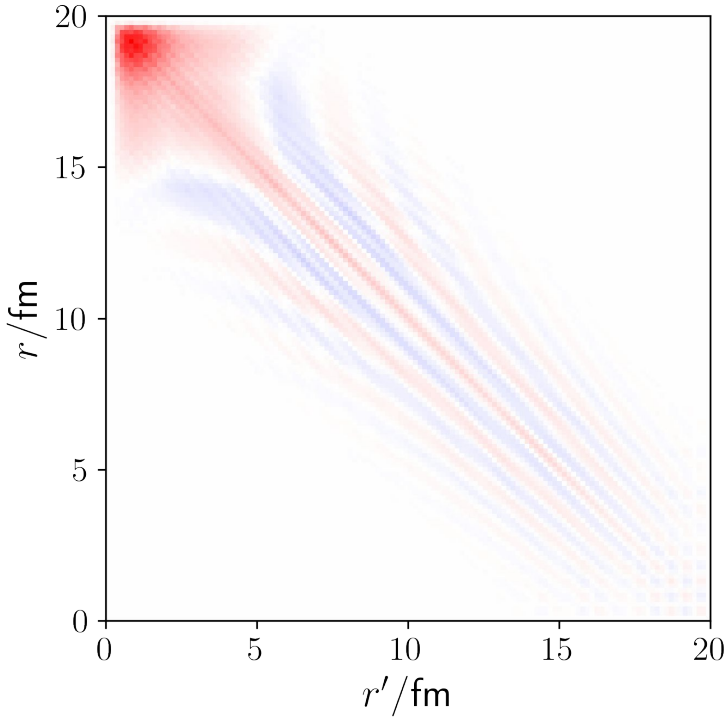

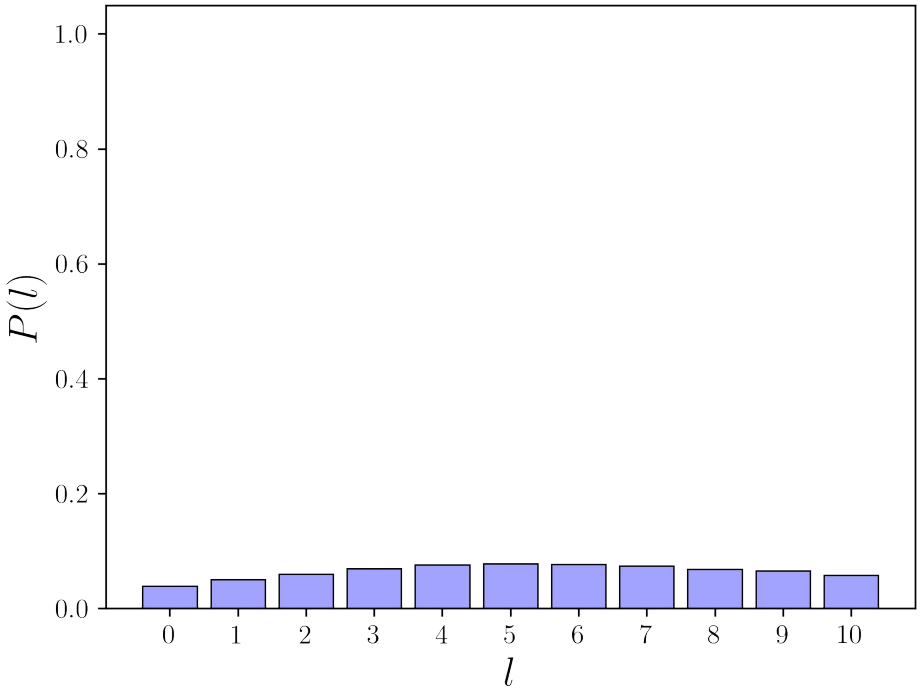

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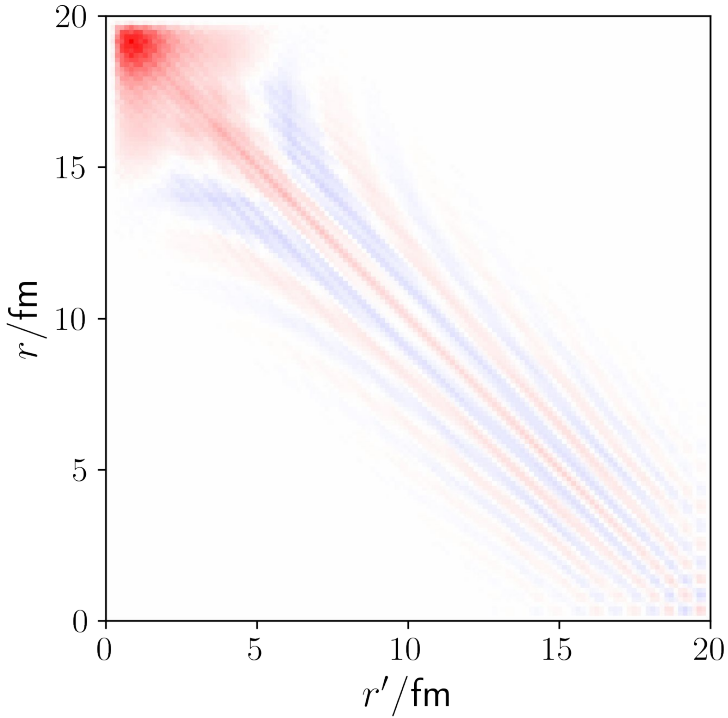

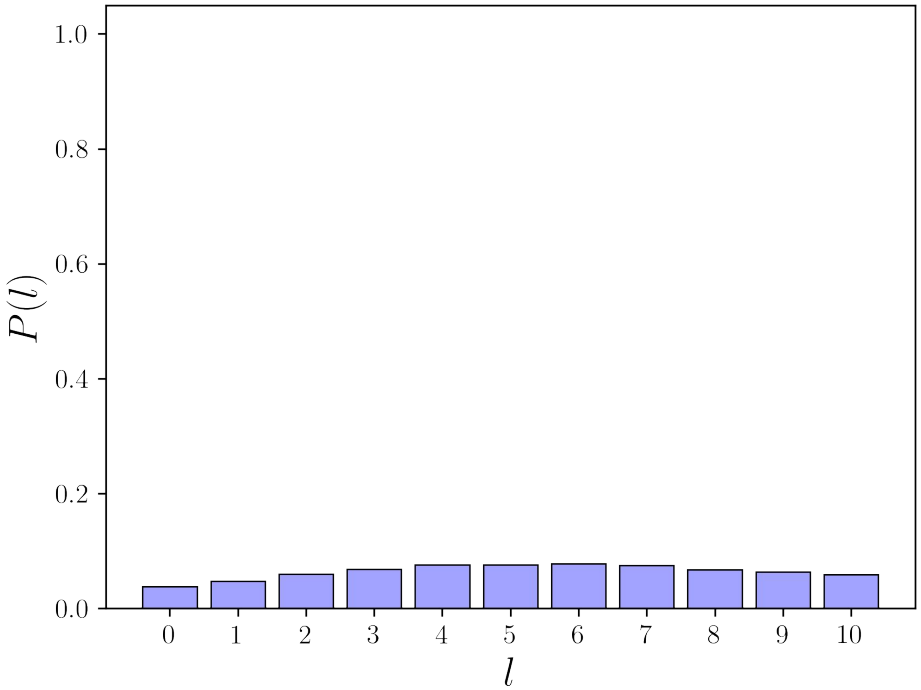

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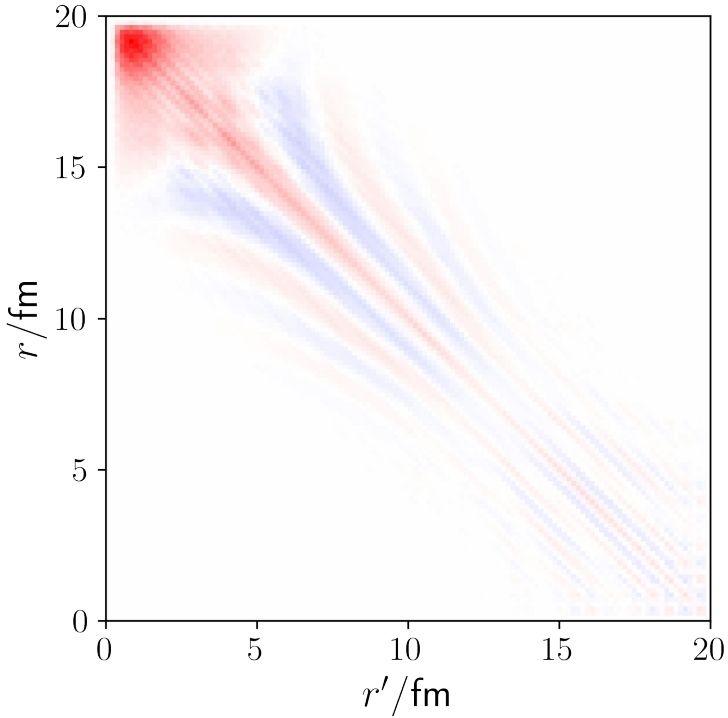

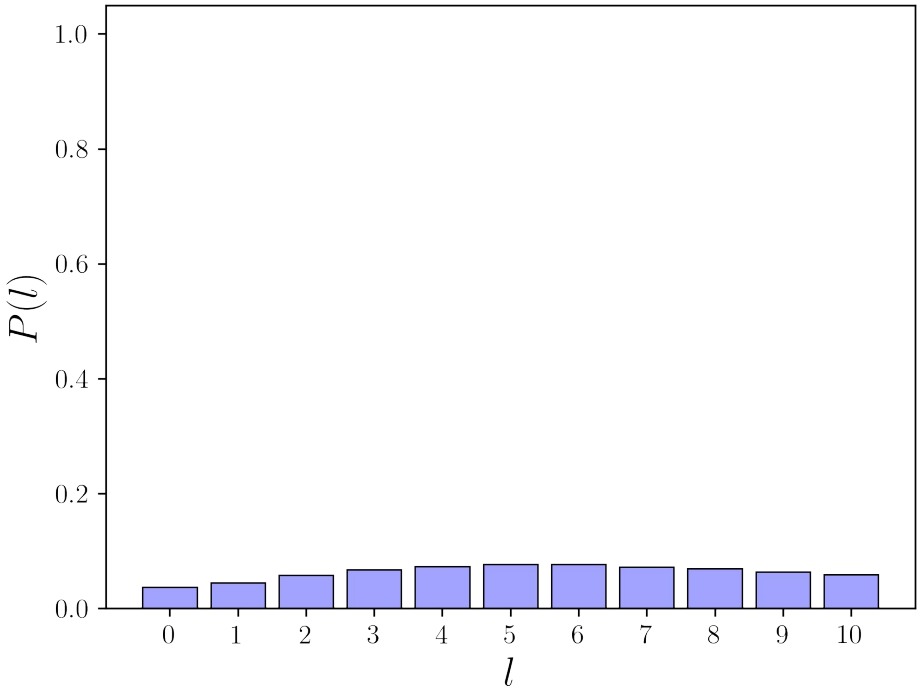

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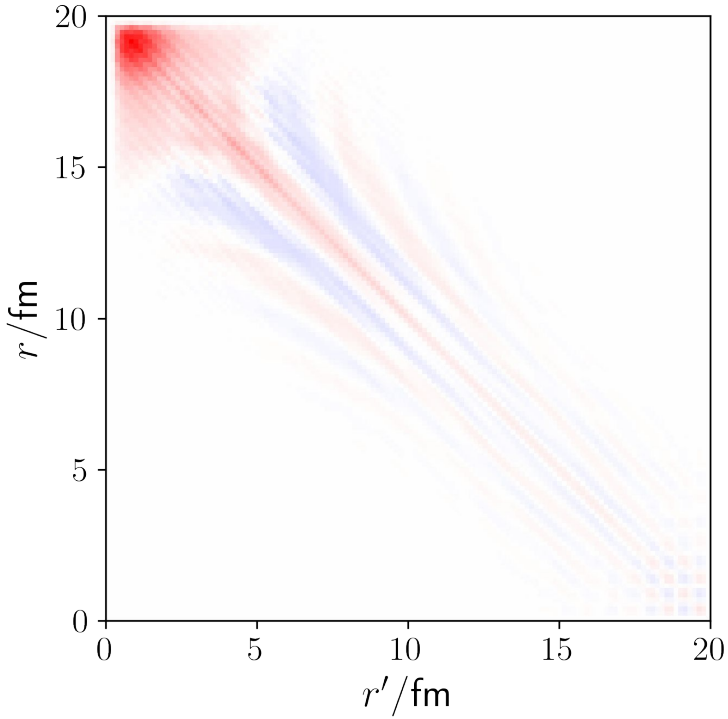

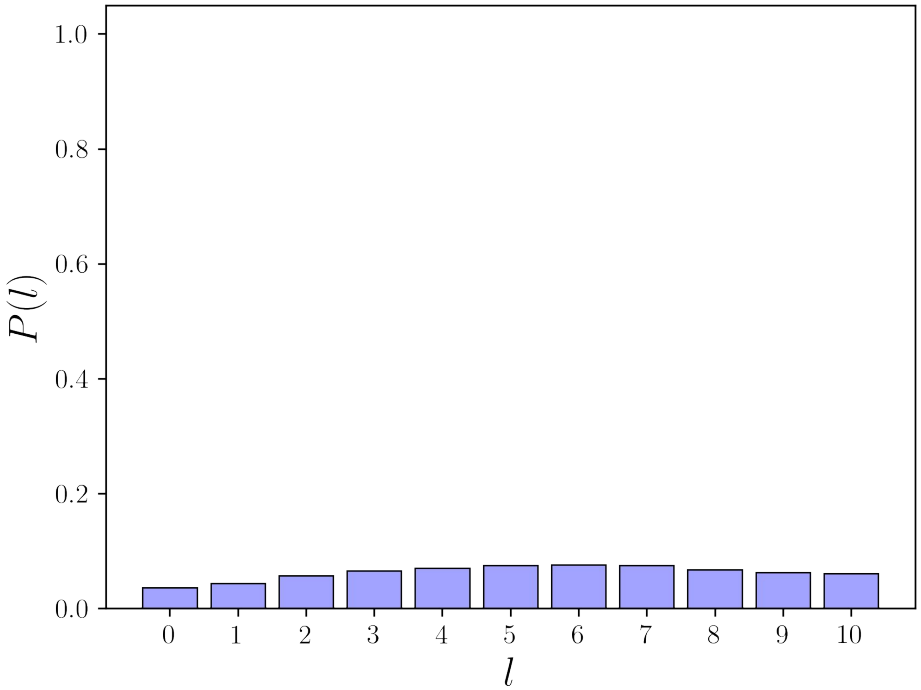

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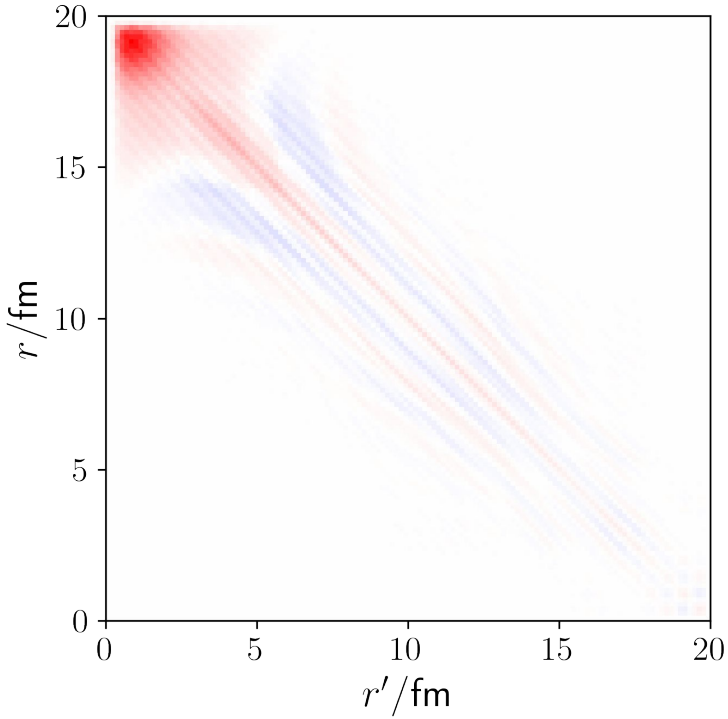

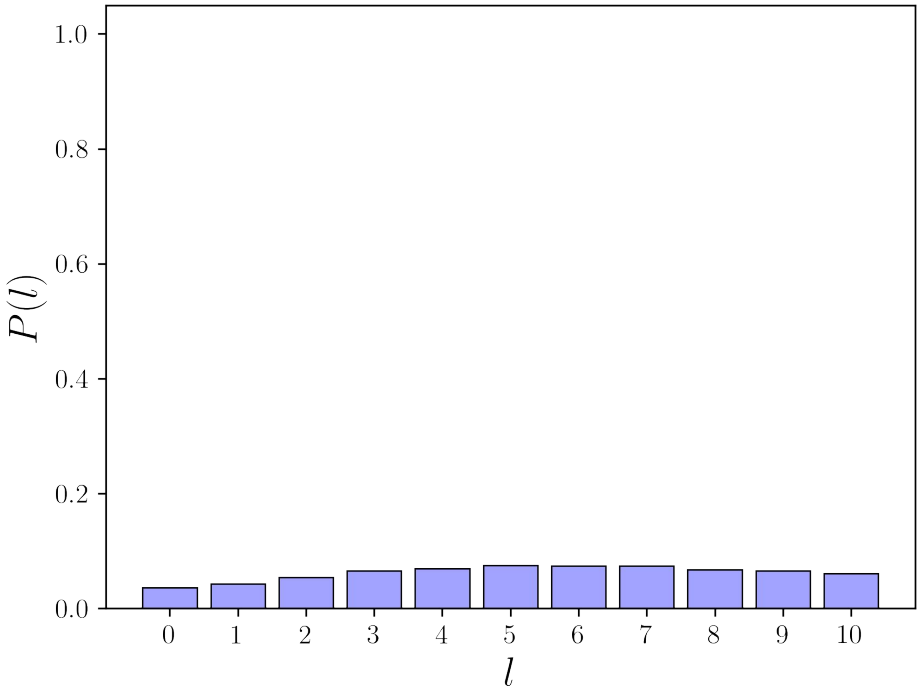

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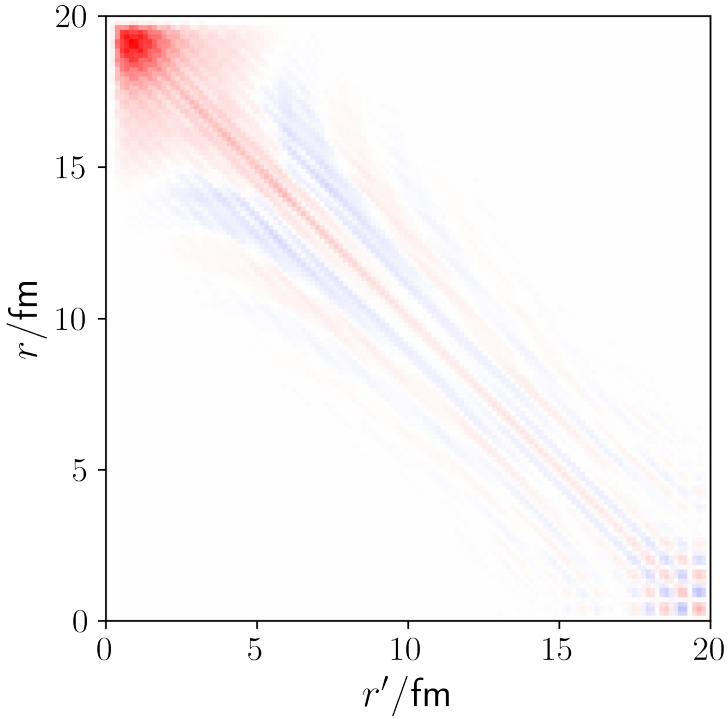

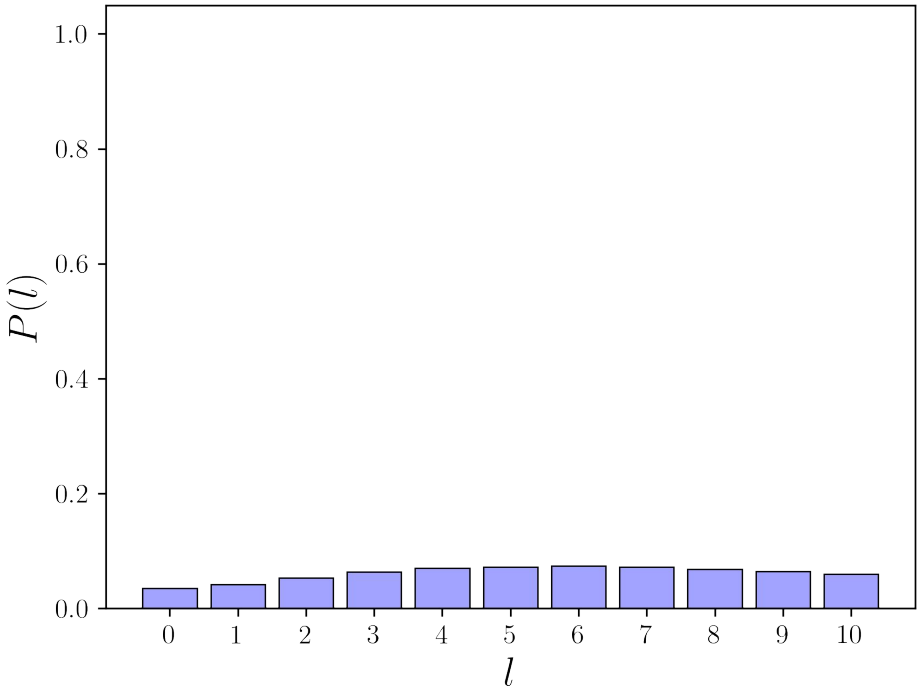

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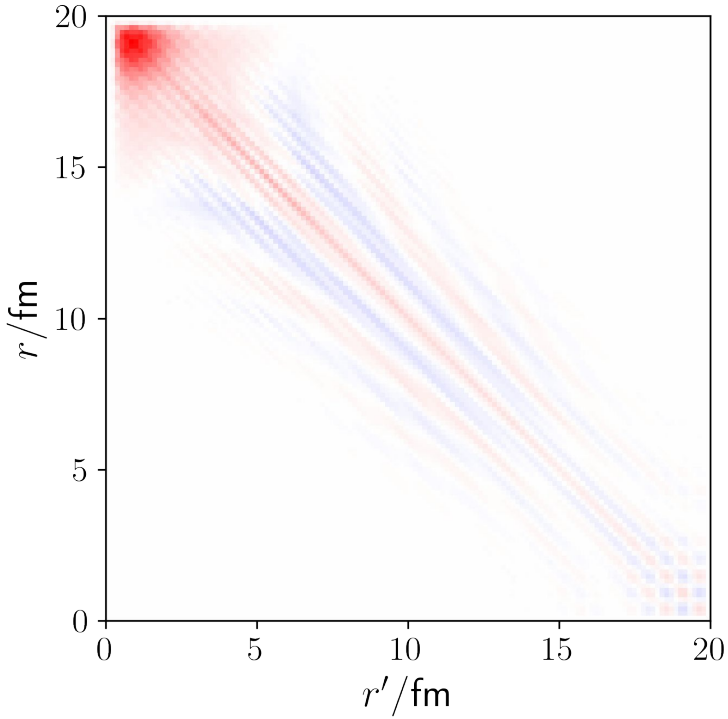

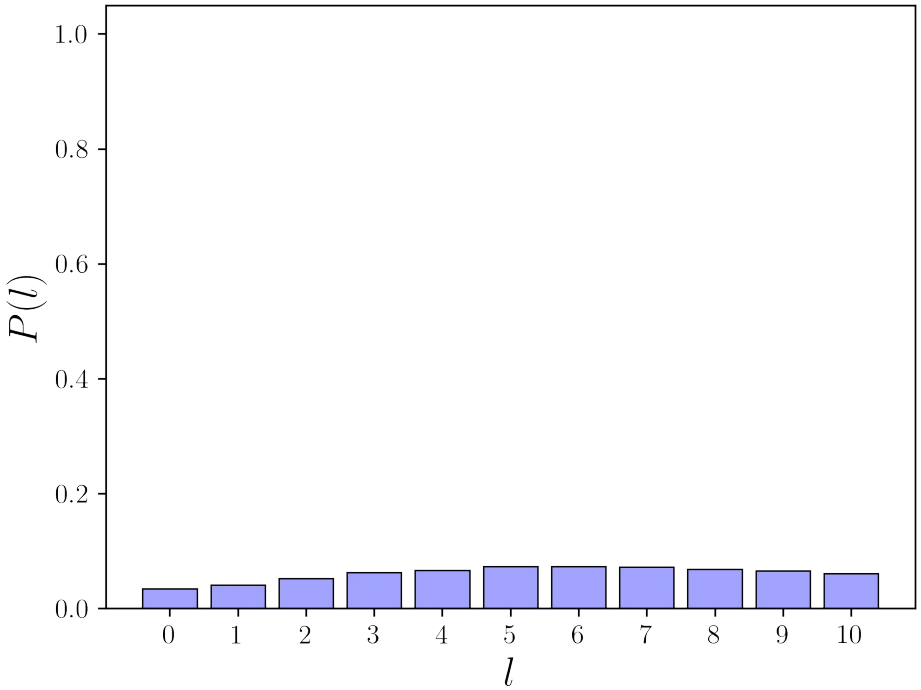

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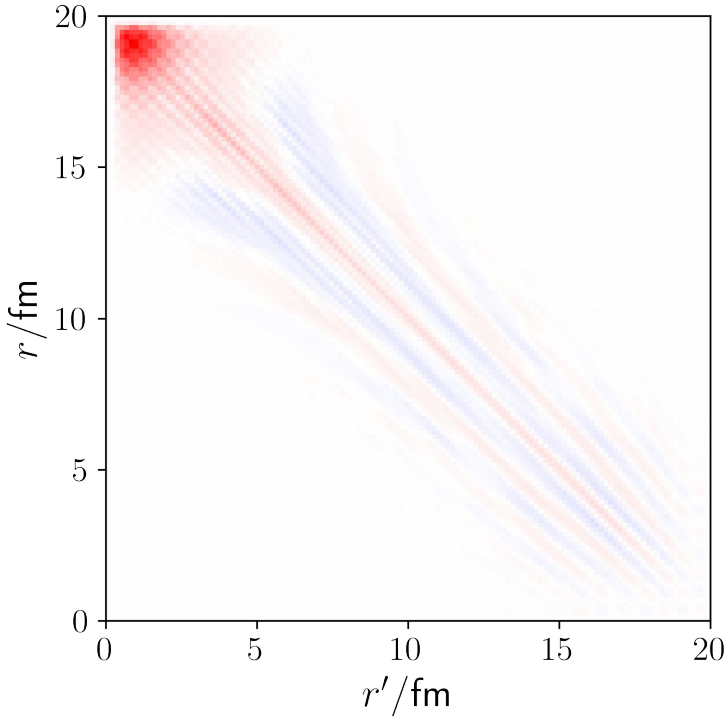

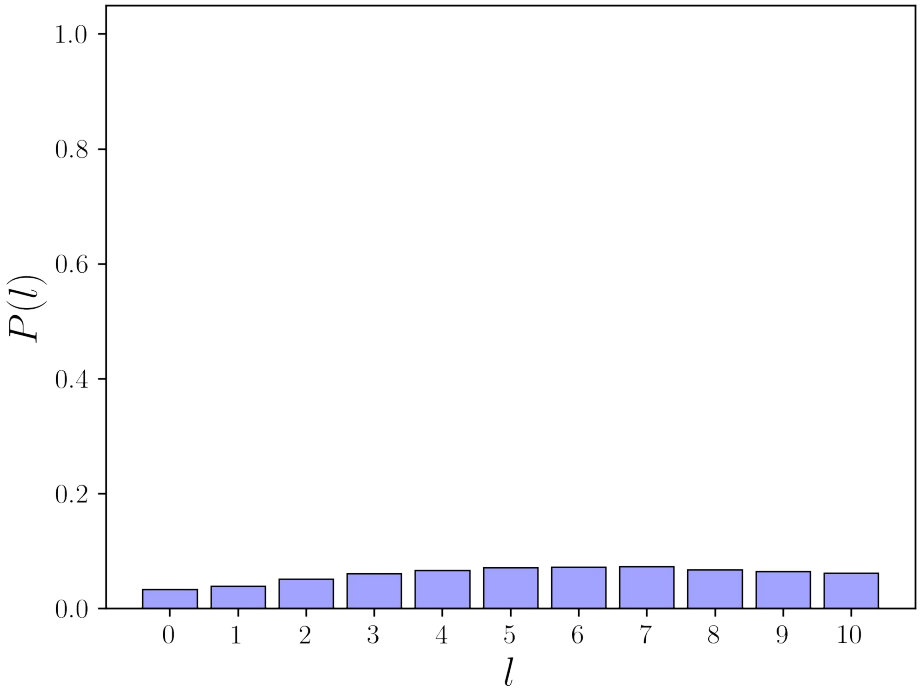

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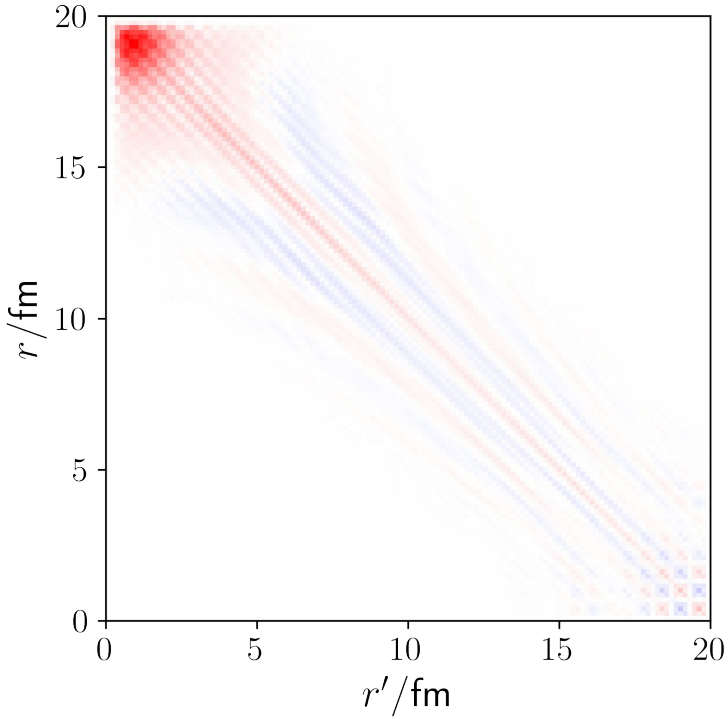

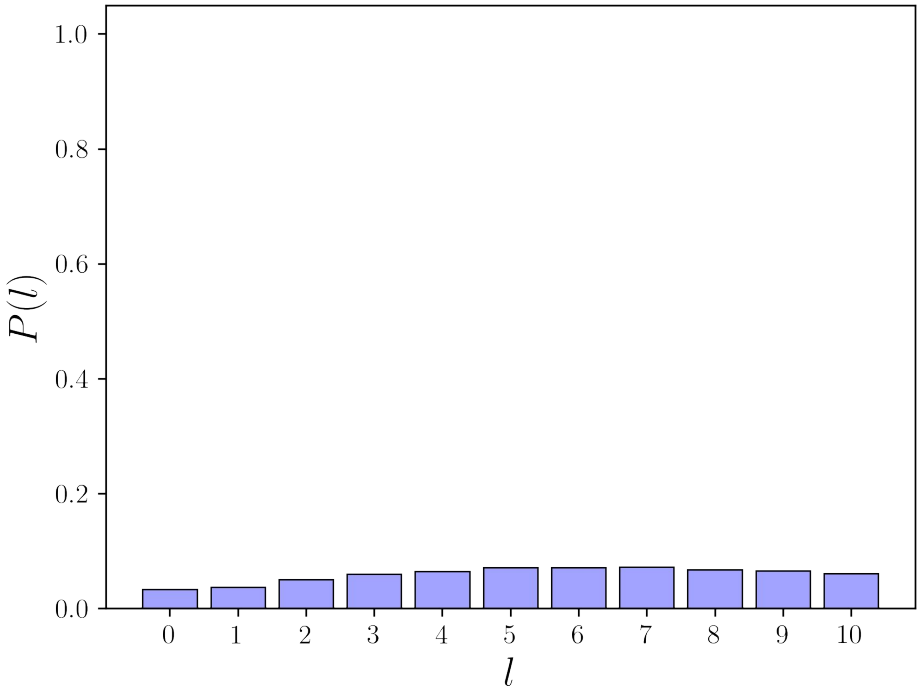

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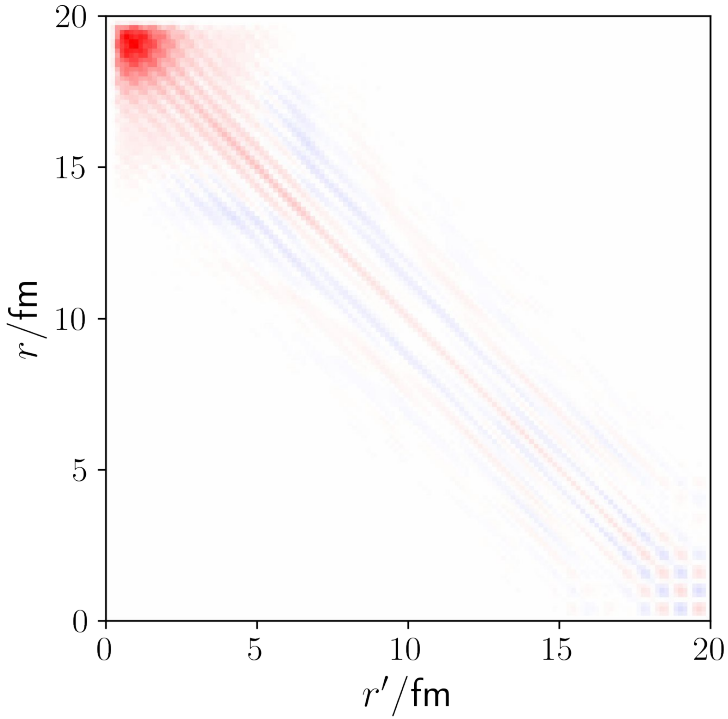

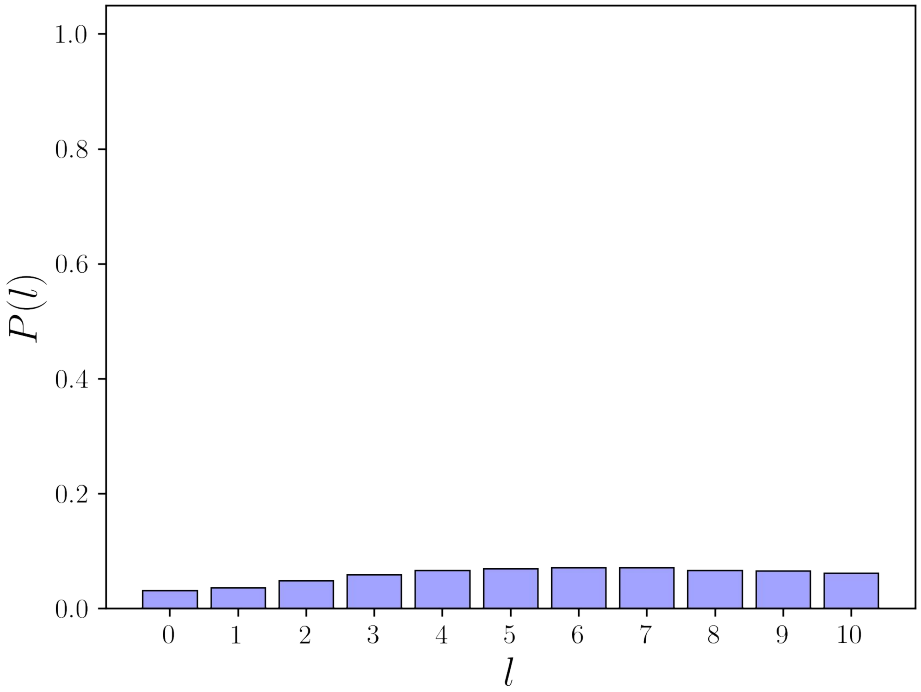

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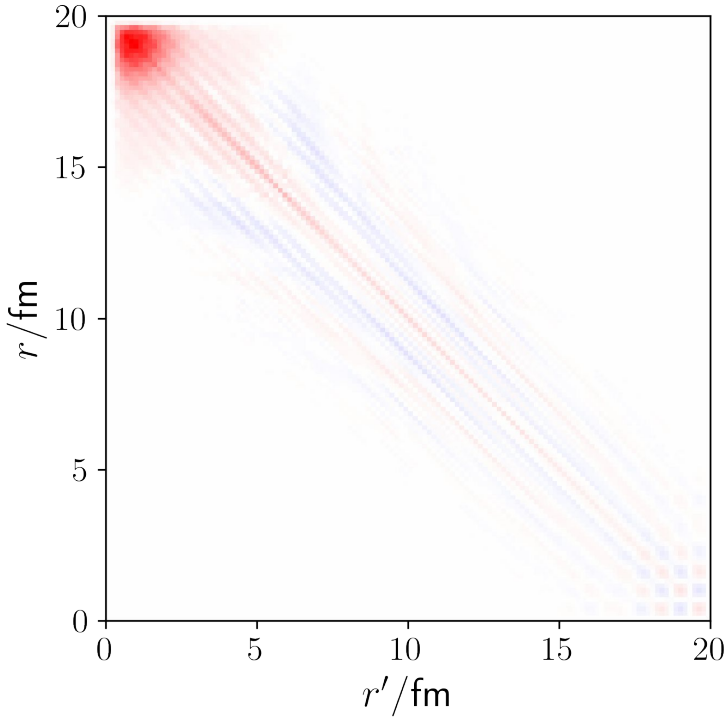

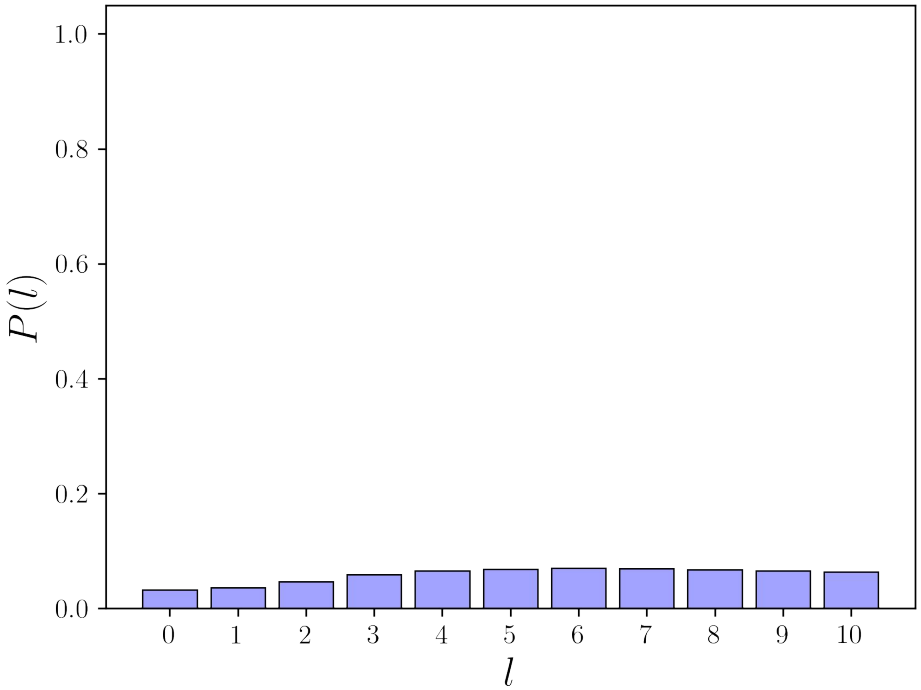

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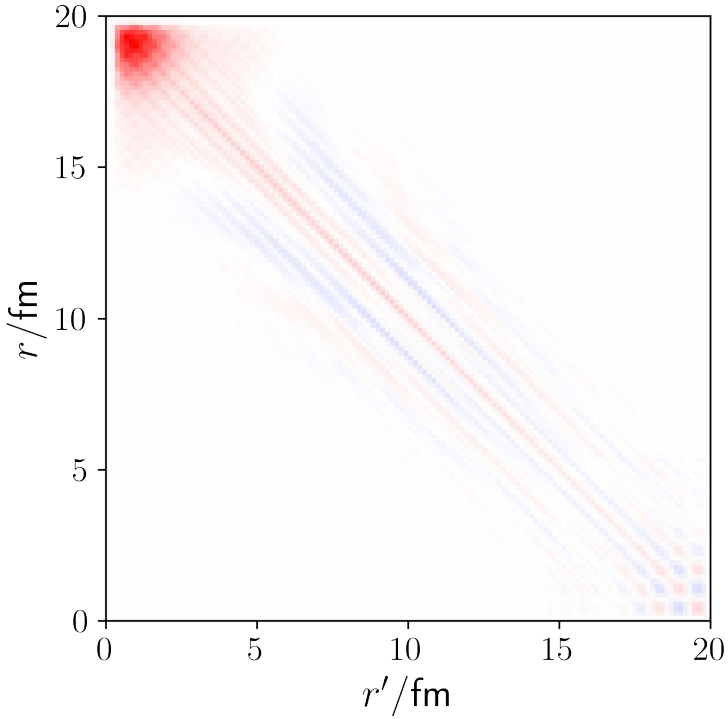

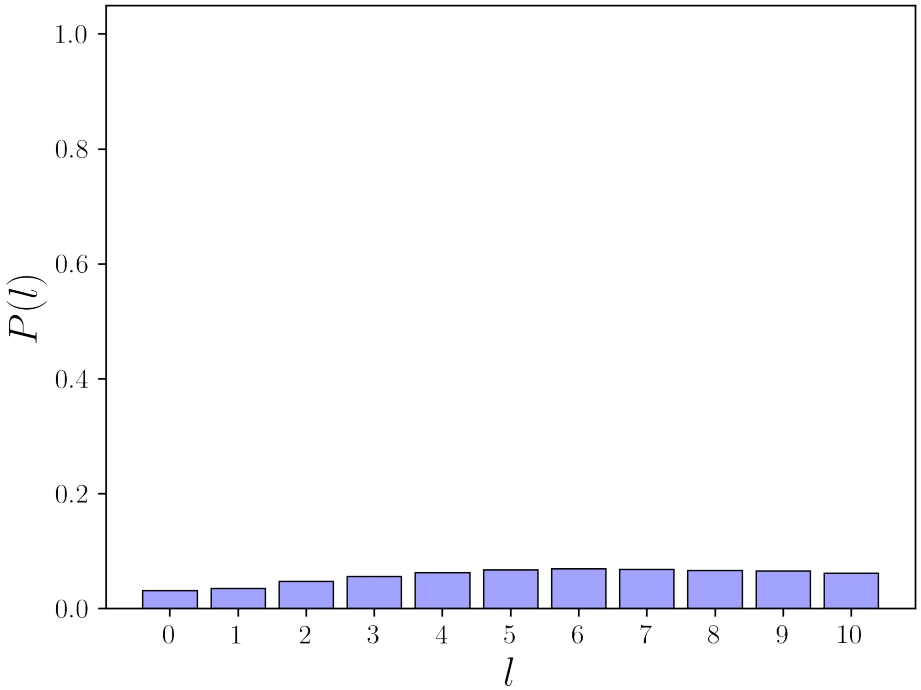

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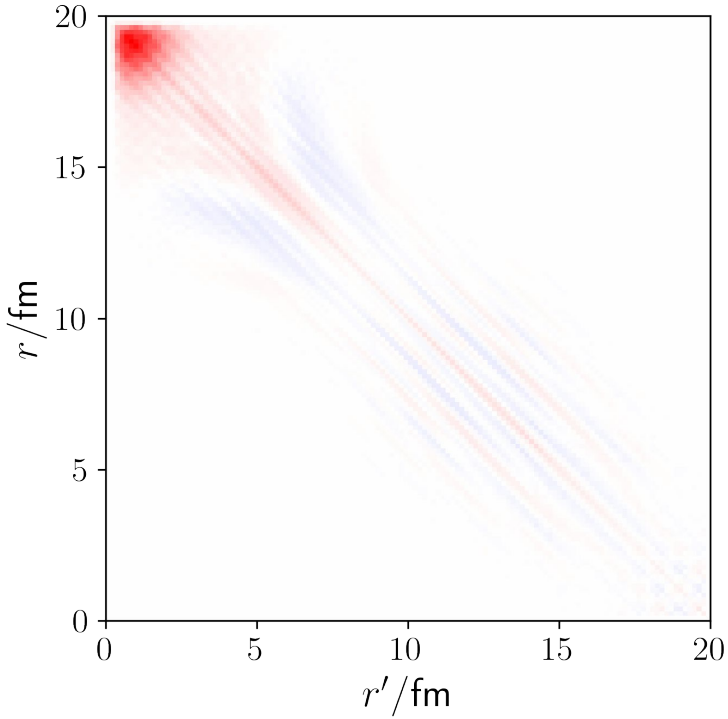

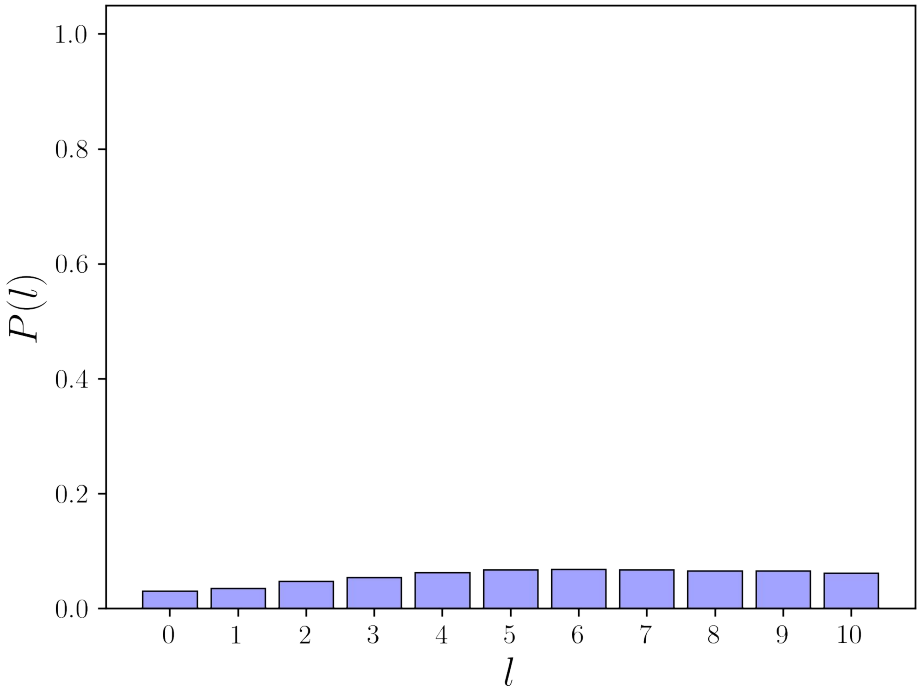

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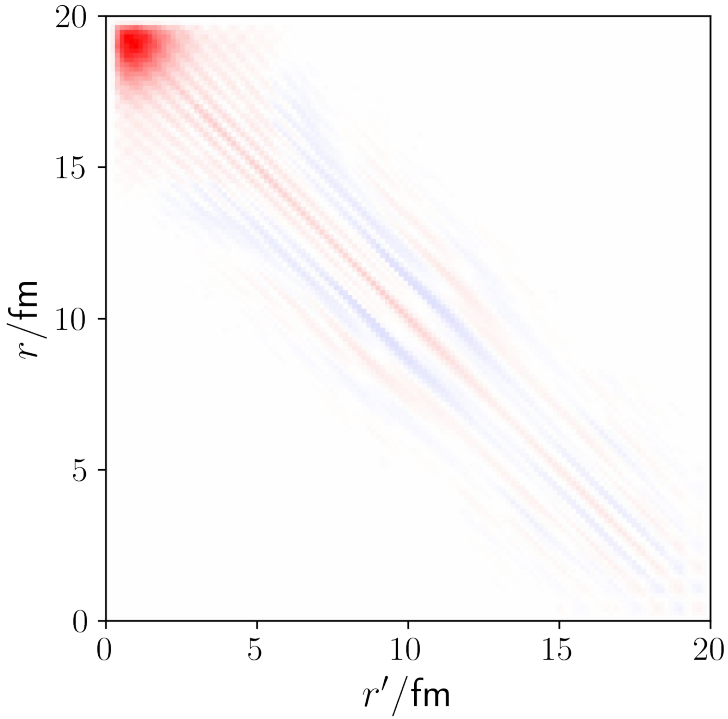

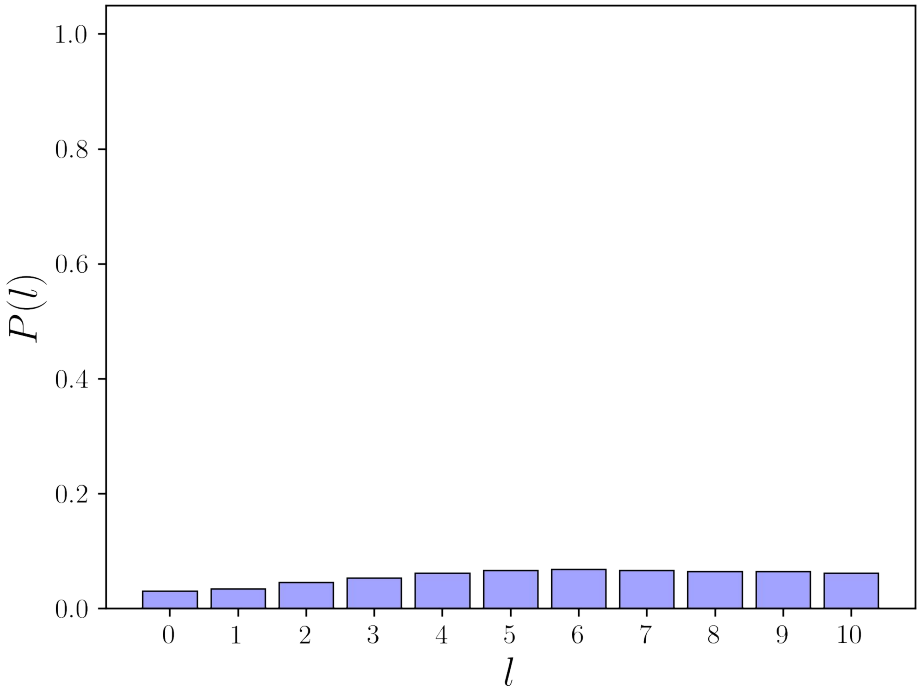

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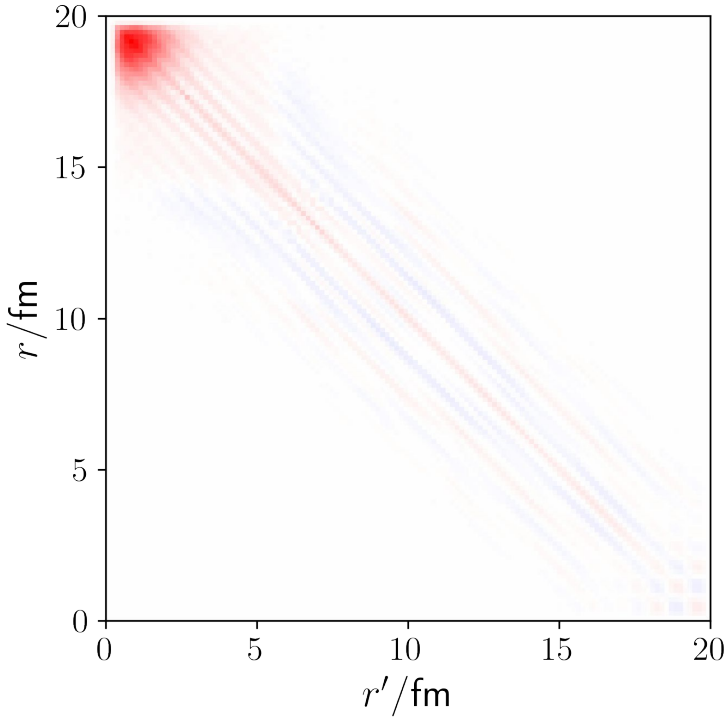

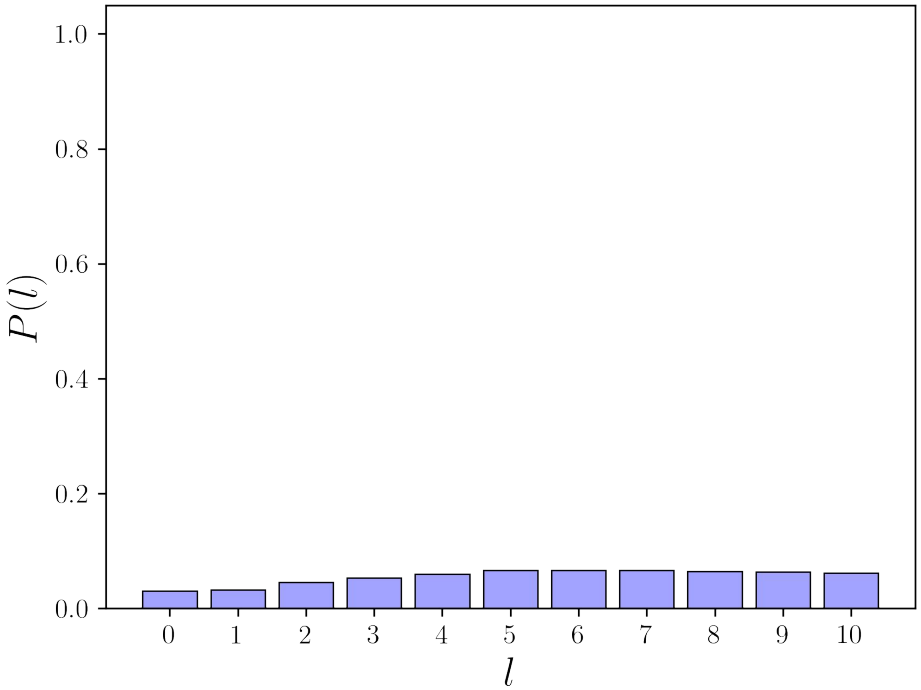

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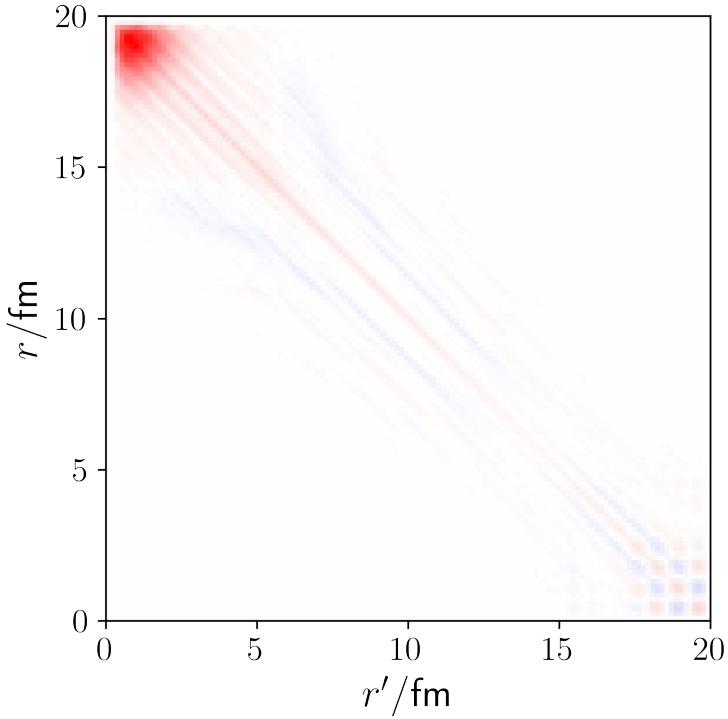
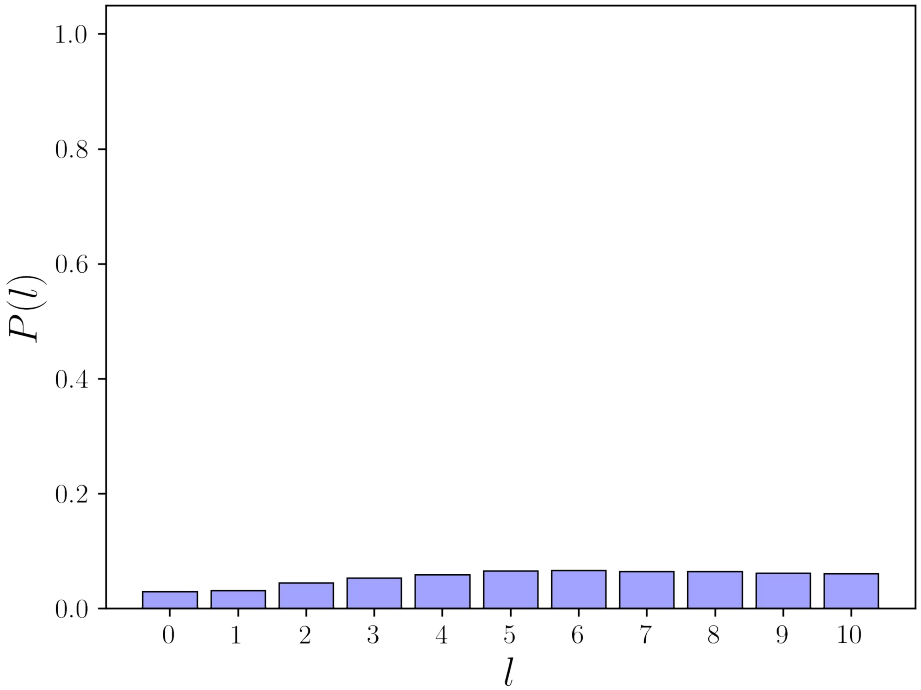
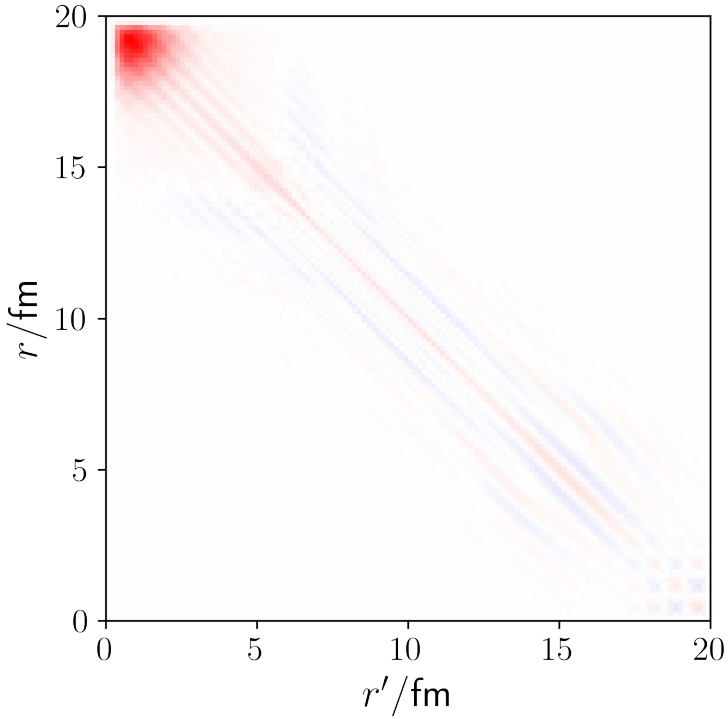
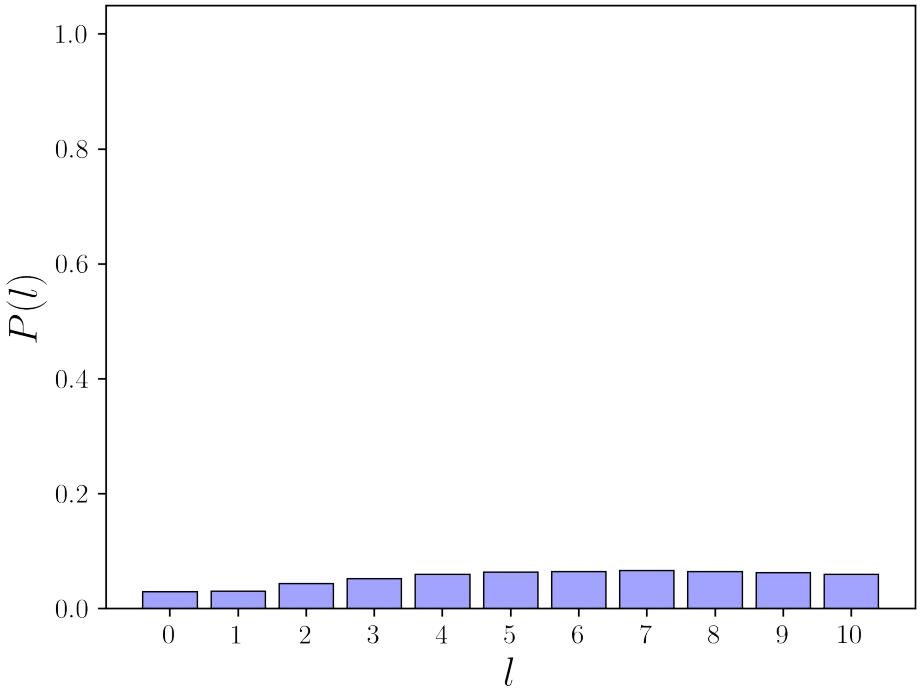


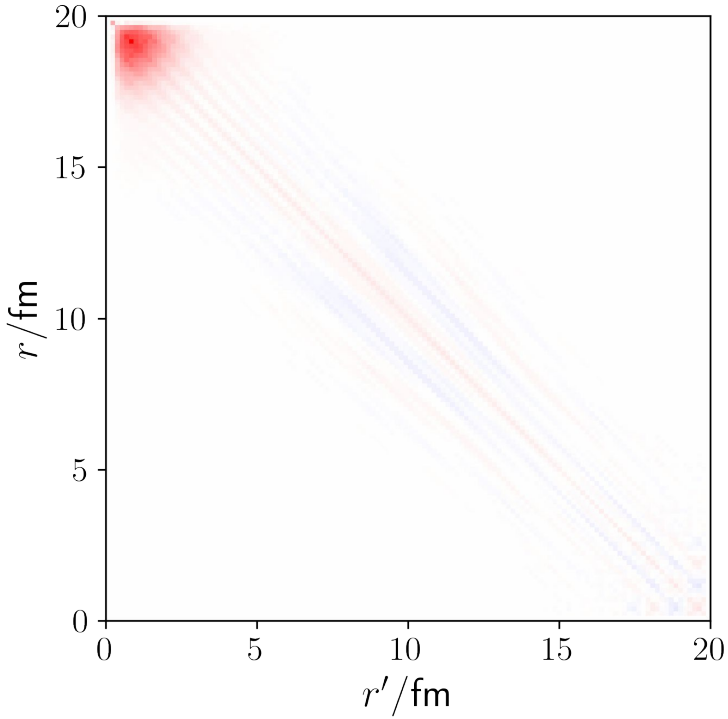


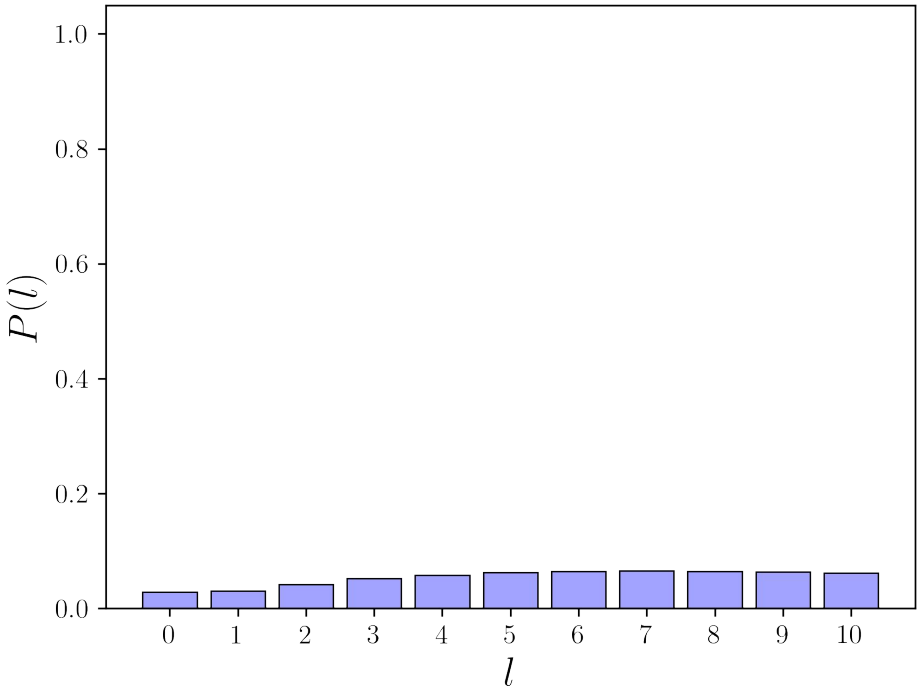
$t = 0$ $t = 2\,\mathrm{fm}$



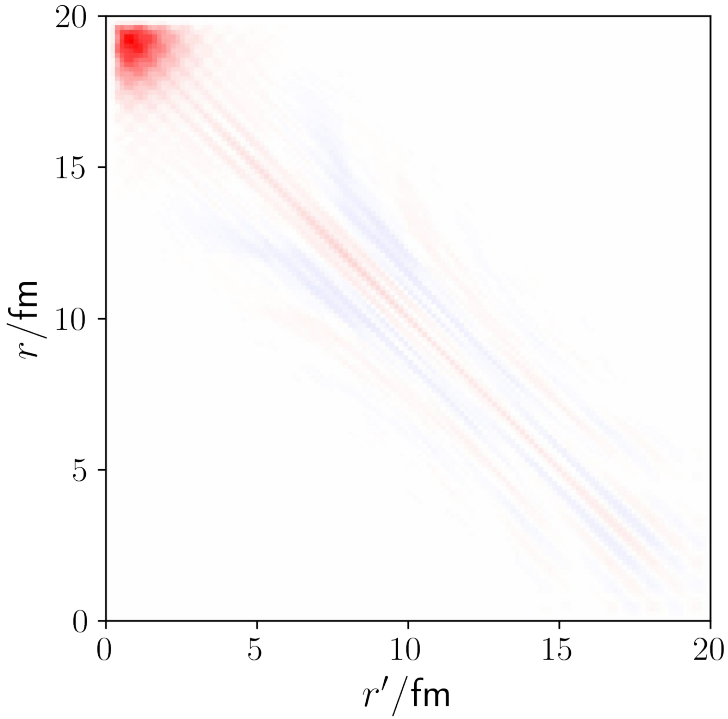


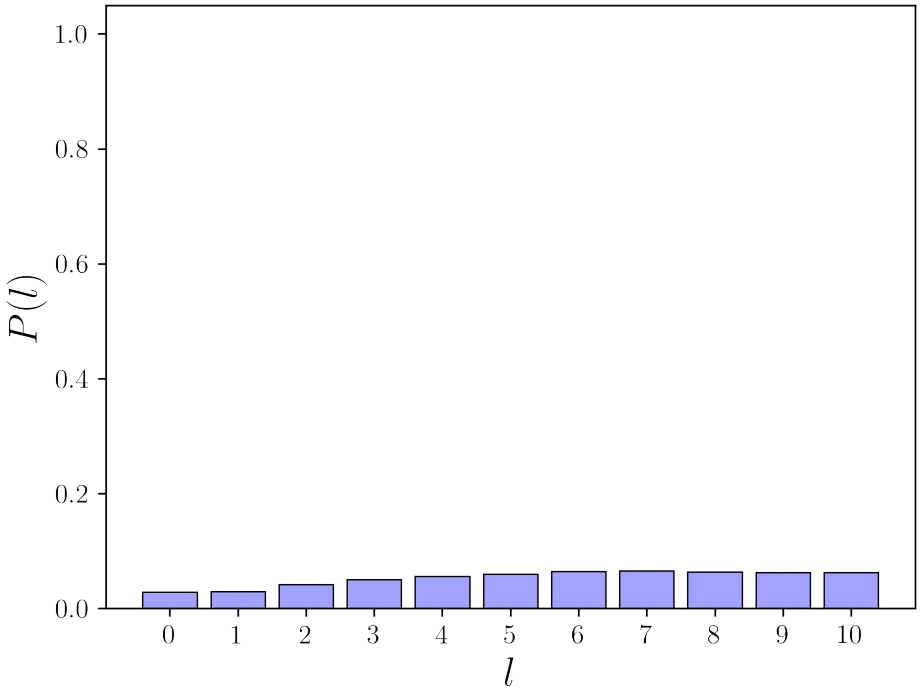
$t = 0$ $t = 2\,\mathrm{fm}$





$t = 0$ $t = 2\,\mathrm{fm}$





Connecting to phenomenology

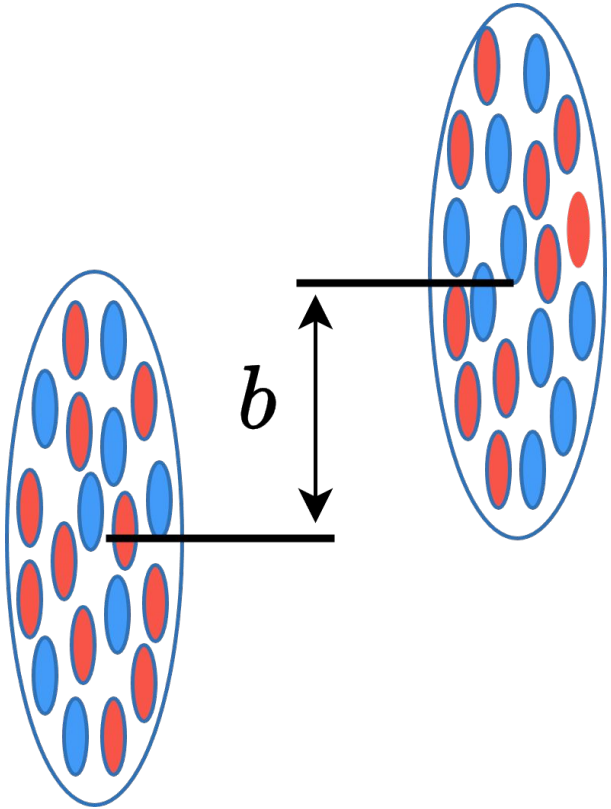
$$R_{AA}^{i}(c) = \frac{\left(F \cdot S(c) \cdot \vec{\sigma}_{\text{direct}}\right)^{i}}{\sigma_{\text{exp}}^{i}}$$

$$S_{ii} = P_{\text{survival}}(i) = \frac{\langle i|\rho(t_f)|i\rangle}{\langle i|\rho(t_0)|i\rangle}$$

Connecting to phenomenology

centrality

$$R^i_{AA}(c) = \frac{(F \cdot S(c) \cdot \vec{\sigma}_{\text{direct}})^i}{\sigma^i_{\text{exp}}}$$



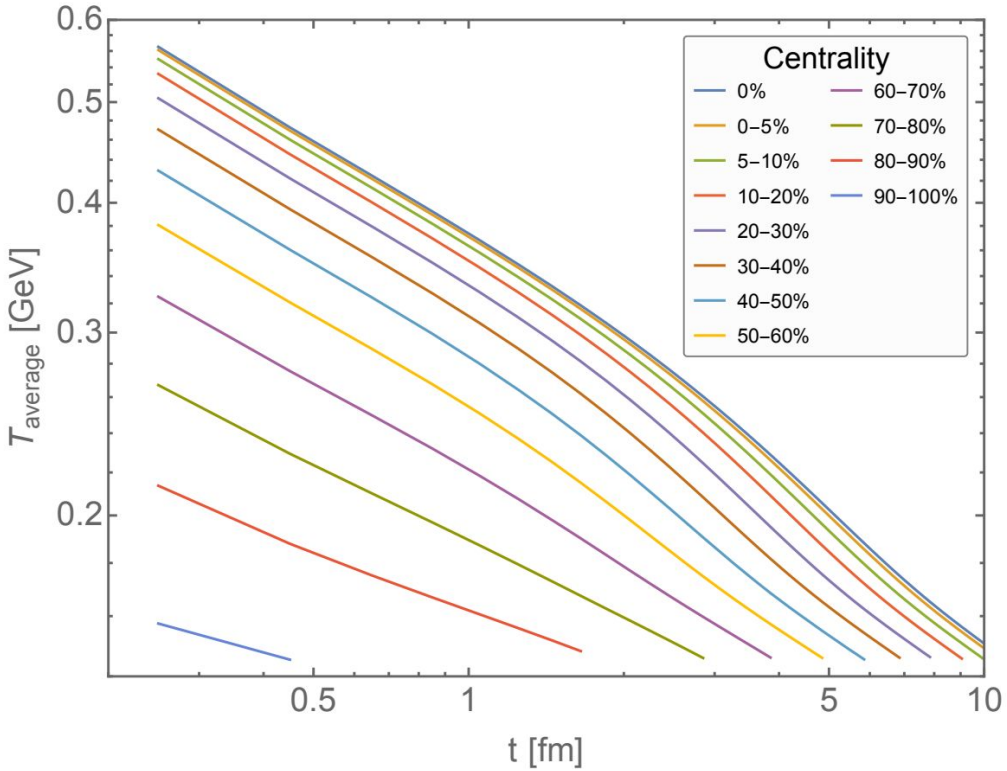
b : Impact parameter

Connecting to phenomenology

Brambilla, Nora, et al. *Journal of High Energy Physics* 2021.5 (2021): 1-47.

centrality

$$R^i_{AA}(c) = \frac{(F \cdot S(c) \cdot \vec{\sigma}_{\text{direct}})^i}{\sigma^i_{\text{exp}}}$$

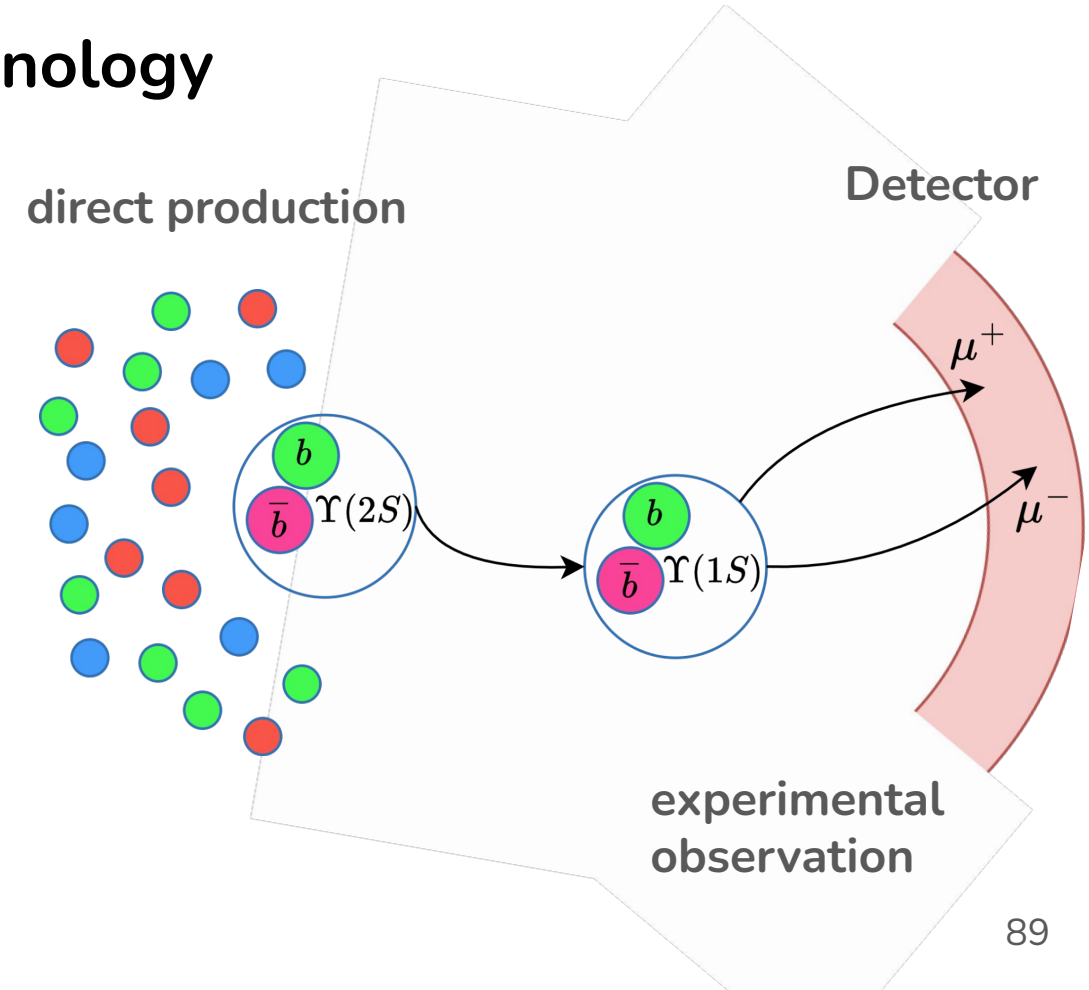


Connecting to phenomenology

Feeddown matrix

$$R^i_{AA}(c) = \frac{\left(F \cdot S(c) \cdot \vec{\sigma}_{\text{direct}}\right)^i}{\sigma^i_{\text{exp}}}$$

$$\vec{\sigma}_{\text{direct}} = F^{-1}\vec{\sigma}_{\text{exp}}$$

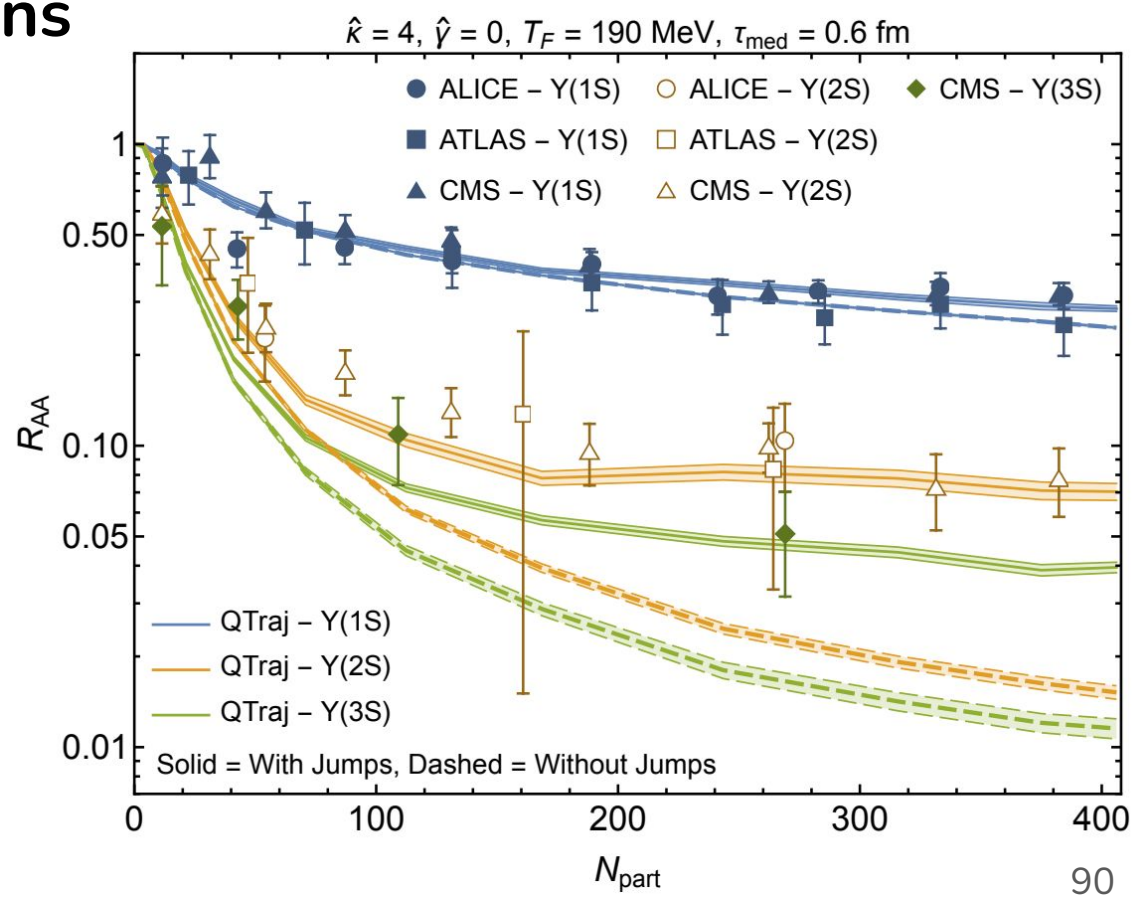


Suppression predictions

Brambilla, Nora, et al. "Regeneration of bottomonia in an open quantum systems approach." *Physical Review D* 108.1 (2023): L011502.

- Transport coefficients:

$$\hat{\kappa} = 4$$
$$\hat{\gamma} = 0$$



Suppression predictions

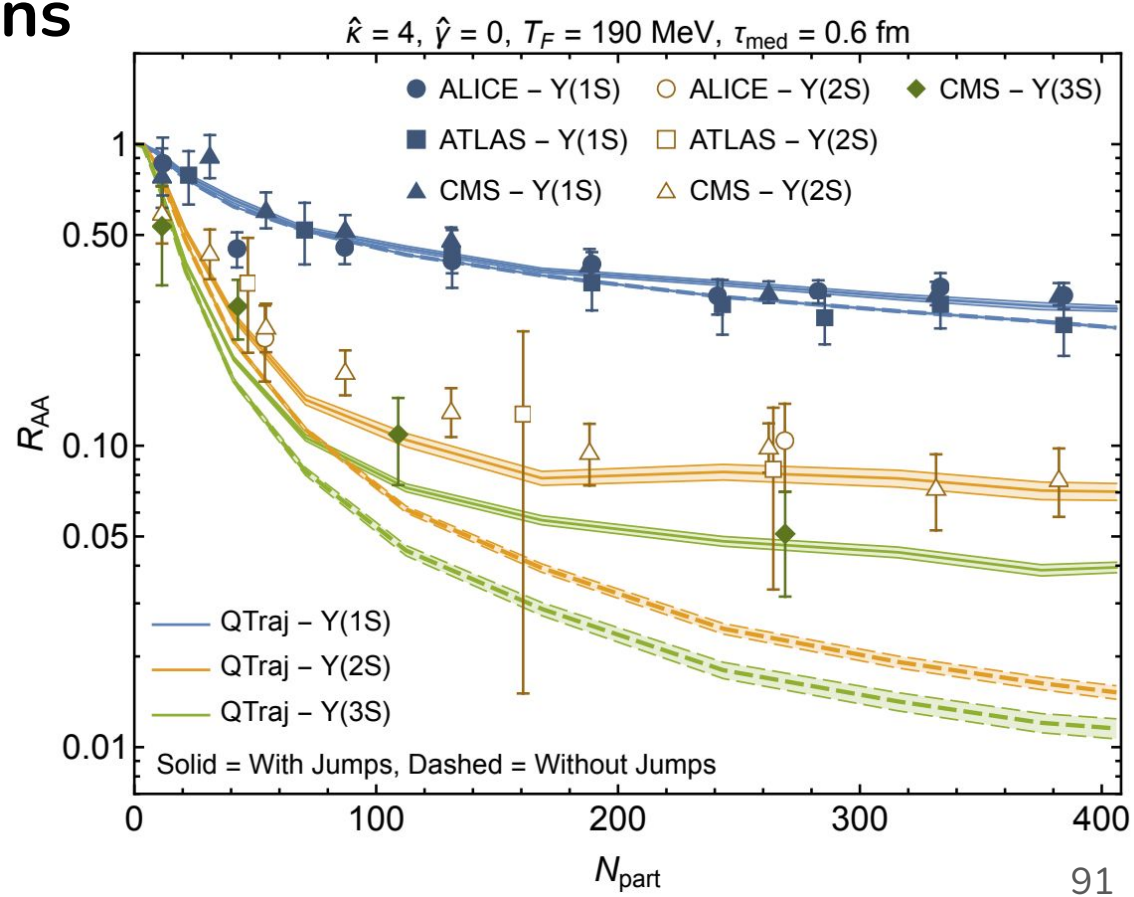
Brambilla, Nora, et al. "Regeneration of bottomonia in an open quantum systems approach." *Physical Review D* 108.1 (2023): L011502.

- Transport coefficients:

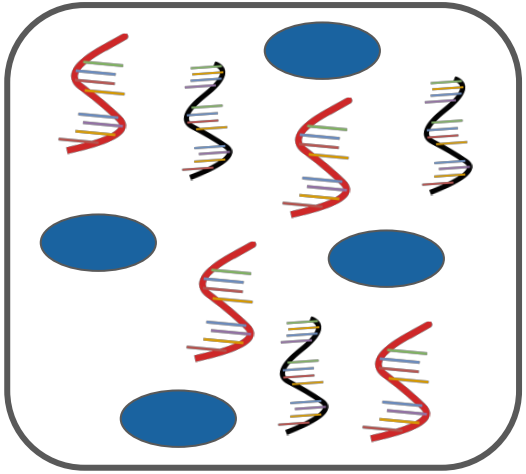
$$\hat{\kappa} = 4$$
$$\hat{\gamma} = 0$$

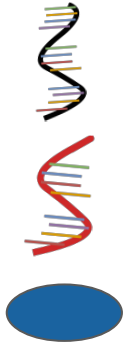
- More transport coefficients:

Possibility to Fit them ?



Stochastic simulation in Biophysics:





Reactions:

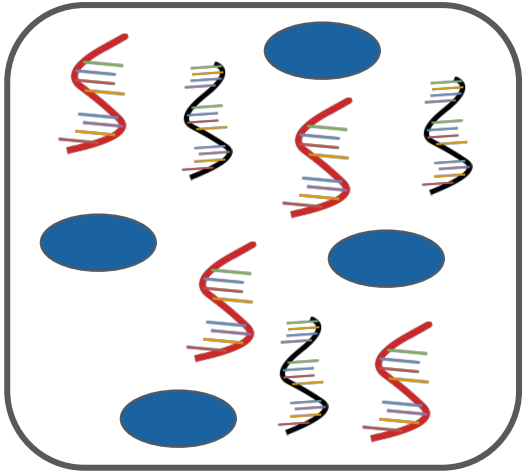
$$A + E \xrightarrow{k_{\mathrm{on},A}} AE$$

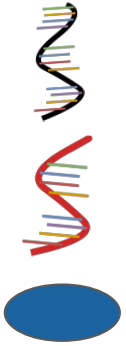
$$AE \xrightarrow{k_{\mathrm{rep},AE}} A + B + E$$

$$B + E \xrightarrow{k_{\mathrm{on},B}} BE$$

$$BE \xrightarrow{k_{\mathrm{rep},BE}} A + B + E$$

Stochastic simulation in Biophysics:





RNA A

RNA B

Enzyme E

Reactions:

$$A + E \xrightarrow{k_{\mathrm{on},A}} AE$$

$$AE \xrightarrow{k_{\mathrm{rep},AE}} A + B + E$$

$$B + E \xrightarrow{k_{\mathrm{on},B}} BE$$

$$BE \xrightarrow{k_{\mathrm{rep},BE}} A + B + E$$

N_i Number of Molecules of type i

Gillespie Algorithm

1. Randomly draw time t ***when*** the next reaction will happen: depends on $\sum_i k_i N_i$
2. Randomly draw which reaction will happen: depends on $k_i N_i$
3. Adjust N_i

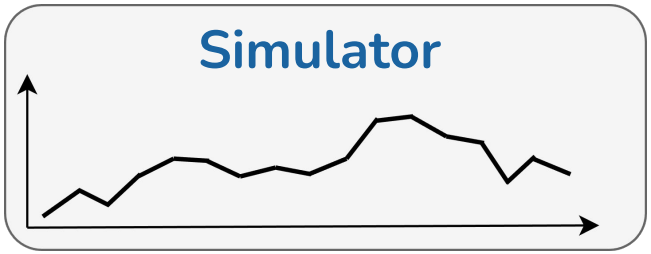
Parameter estimation

Input parameters

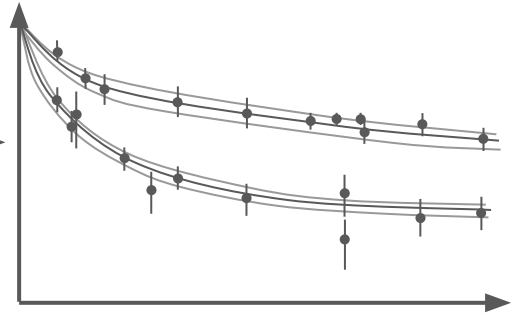
$$\hat{\gamma}$$

$$\hat{\kappa} \quad k_{\mathrm{rep,BE}}$$

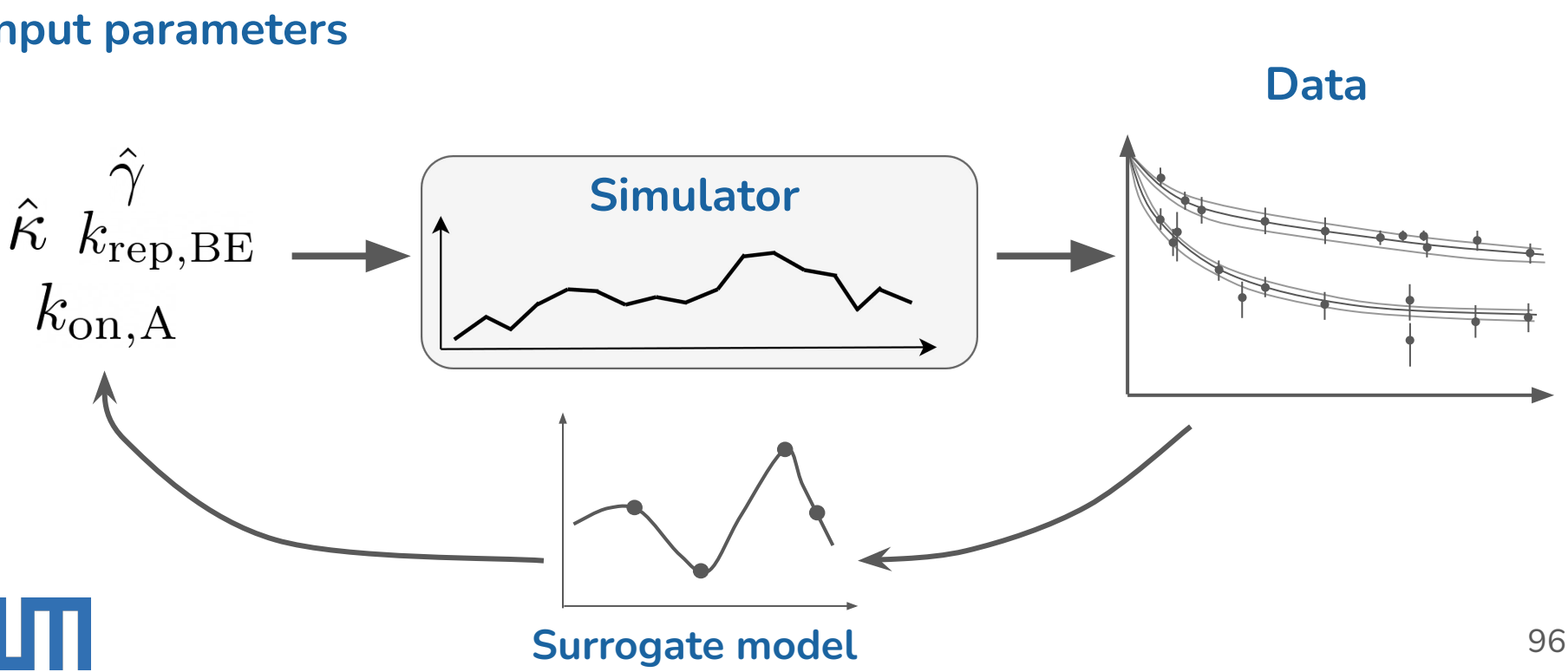
$$k_{\mathrm{on,A}}$$



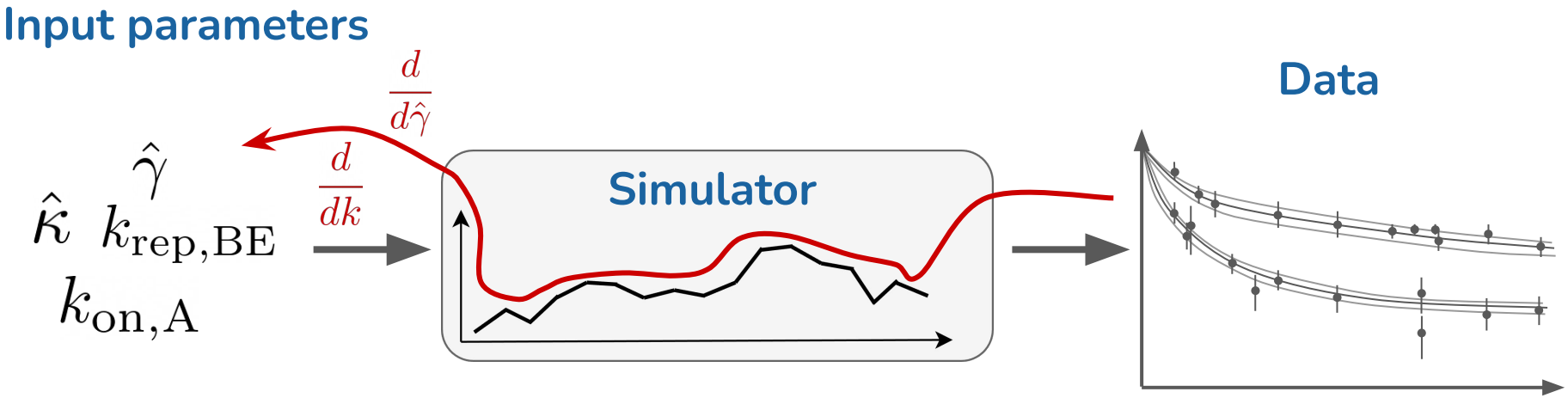
Data



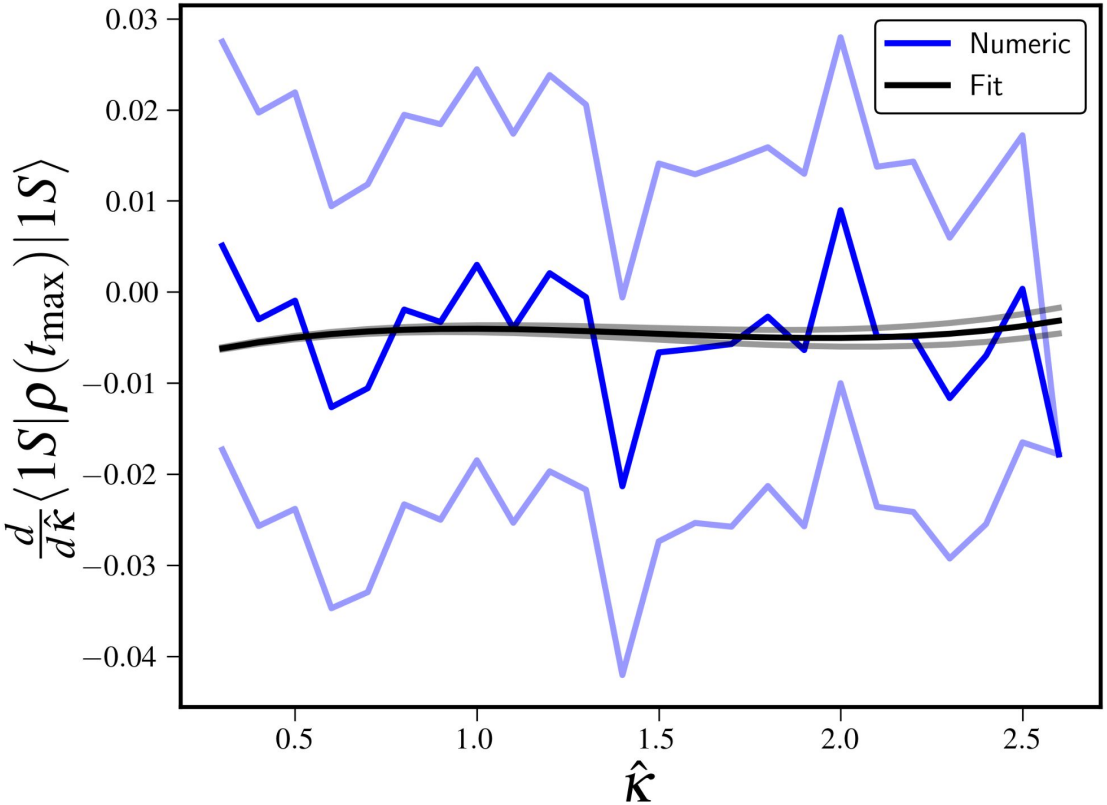
Parameter estimation: Bayesian optimization



Parameter estimation: Gradient descent



Estimate gradient: Variance of naive finite difference



Score function based gradient estimation

- Quantum trajectory contains **discrete probabilities**

$$\frac{d}{d\Theta} E_{x\sim p(x|\Theta)}[f(x,\Theta)]$$

$$= \int dx \frac{d}{d\Theta}\left[p(x|\Theta) f(x,\Theta)\right]$$

$$= \int dx\, p(x|\Theta)\left[\frac{d\log\left(p(x|\Theta)\right)}{d\Theta} f(x,\Theta) + \frac{d}{d\Theta} f(x,\Theta)\right]$$

$$\boxed{= E_{x\sim p(x|\Theta)}\left[\frac{d\log\left(p(x|\Theta)\right)}{d\Theta} f(x,\Theta) + \frac{d}{d\Theta} f(x,\Theta)\right]}$$

Variance reduction

$$E_{x\sim p(x|\Theta)}\left[\frac{d\log(p(x|\Theta)}{d\Theta}f(x,\Theta)-h(x)+\frac{d}{d\Theta}f(x,\Theta)\right]$$

Unbiased if: $E_{x\sim p(x|\Theta)}\left[h(x)\right]=0$

Variance changes: $\mathrm{Var}(g(x)-h(x))=\mathrm{Var}(g)+\mathrm{Var}(h)-2\mathrm{Cov}(g,h)$

Variance reduction

$$E_{x \sim p(x|\Theta)} \left[\frac{d \log(p(x|\Theta))}{d\Theta} \right] = 0$$

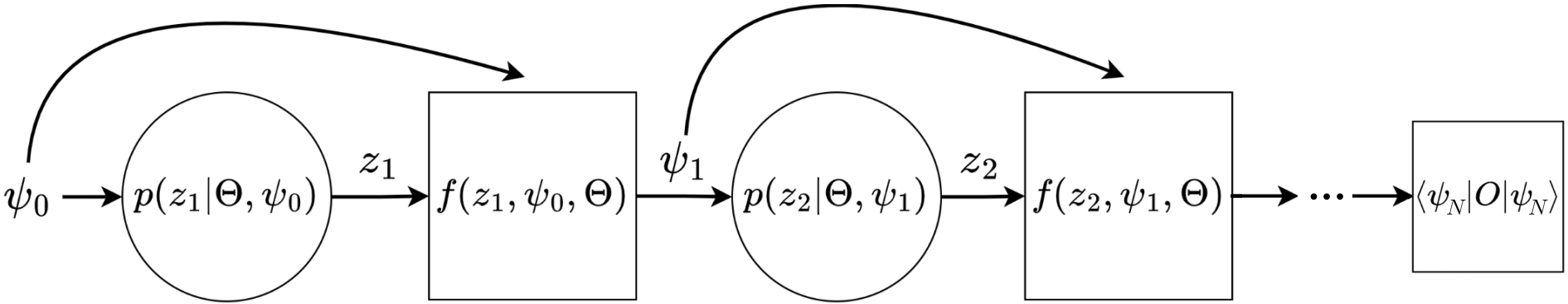
$$E \left[\frac{d \log(p(x|\Theta))}{d\Theta} f(x, \Theta) \right] = E \left[\frac{d \log(p(x|\Theta))}{d\Theta} (f(x, \Theta) - b(\Theta)) \right]$$

Variance reduction by appropriate **baseline**

Common choice

$$b(\Theta) = E[f(x, \Theta)]$$

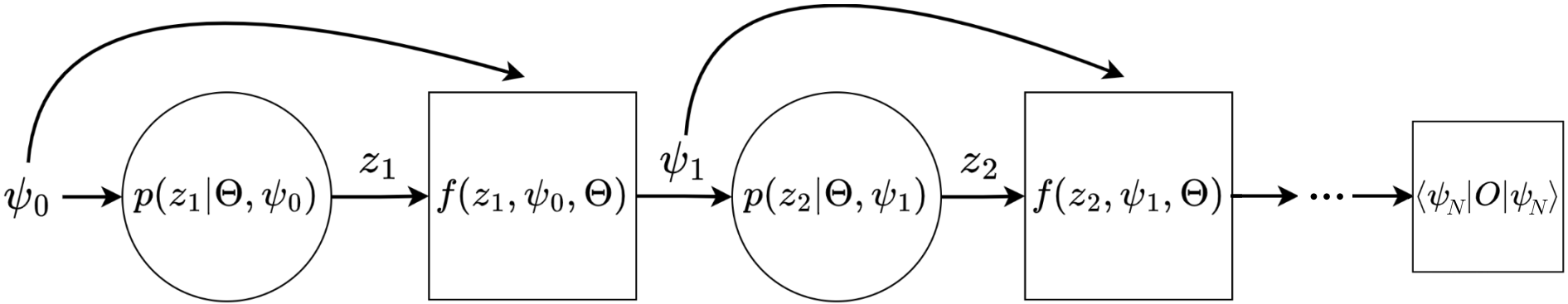
Score based gradient for quantum trajectories



$$p(z|\Theta, \psi_{n-1}) = \begin{cases} 1 - \delta p(\Theta, \psi_{n-1}), & z = 1 \\ \delta p(\Theta, \psi_{n-1}), & z = 0 \end{cases}$$

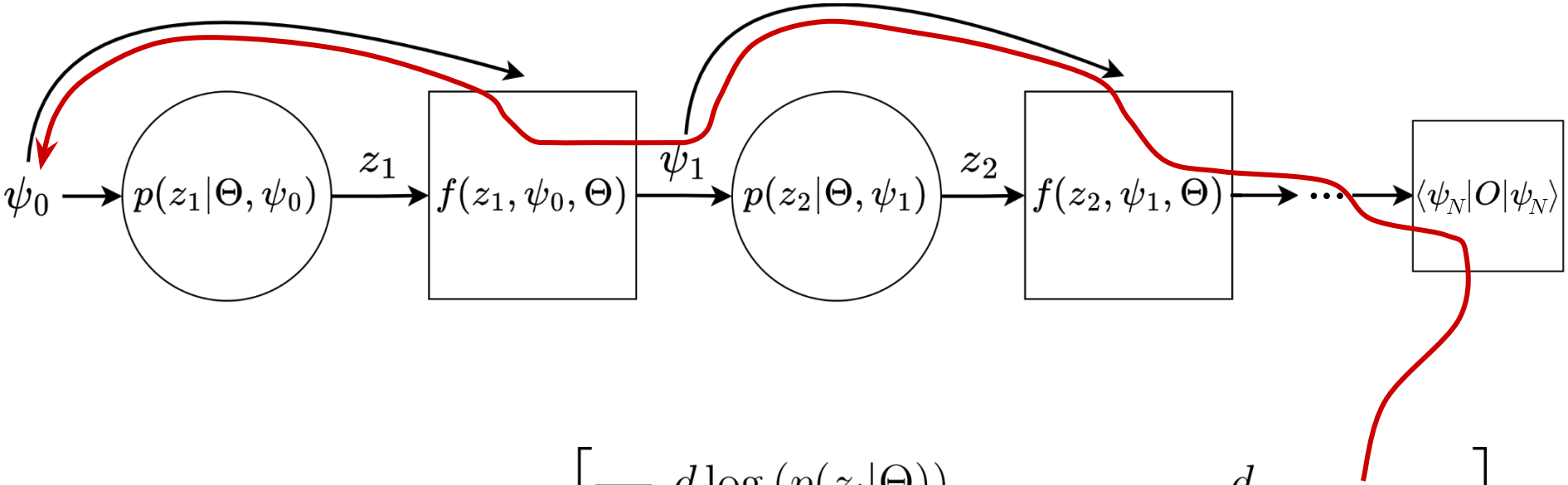
$$f(z, \psi, \Theta) = z \frac{U(\Theta)|\psi\rangle}{||U(\Theta)|\psi\rangle||} + (1 - z) \frac{C(\Theta)|\psi\rangle}{||C(\Theta)|\psi\rangle||}$$

Score based gradient for quantum trajectories



$$E\left[\langle\psi_N|O|\psi_N\rangle\right] = E_{p(z_i|\Theta)}\left[\sum_i \frac{d\log\left(p(z_i|\Theta)\right)}{d\Theta}\langle\psi_N|O|\psi_N\rangle + \frac{d}{d\Theta}\langle\psi_N|O|\psi_N\rangle\right]$$

Score based gradient for quantum trajectories



$$E\left[\langle\psi_N|O|\psi_N\rangle\right] = E_{p(z_i|\Theta)}\left[\sum_i \frac{d\log\left(p(z_i|\Theta)\right)}{d\Theta}\langle\psi_N|O|\psi_N\rangle + \frac{d}{d\Theta}\langle\psi_N|O|\psi_N\rangle\right]$$

Waiting time approach

1. Draw random number r between 0 and 1
2. Evolve $|\psi\rangle$ until $\langle\psi|\psi\rangle < r$ (without normalizing)

Crank-Nicolson

$$\left(1 + \frac{i}{2}\Delta t H_{\text{eff}}\right)\psi(t+\Delta t) = \left(1 - \frac{i}{2}\Delta t H_{\text{eff}}\right)\psi(t)$$

3. Perform Jump i with $p_i = \langle\psi|C_i^\dagger C_i|\psi\rangle / \sum_i p_i$
4. Normalize

Crank-Nicolson gradient

1. Deterministic H_{eff} evolution:

$$A\psi(t_{n+1}) = B\psi(t_n)$$

$$A\frac{d}{d\Theta}\psi(t_{n+1}) = -\frac{dA}{d\Theta}\psi(t_{n+1}) + \frac{dB}{d\Theta}\psi(t_n) + B\frac{d}{d\Theta}\psi(t_n)$$

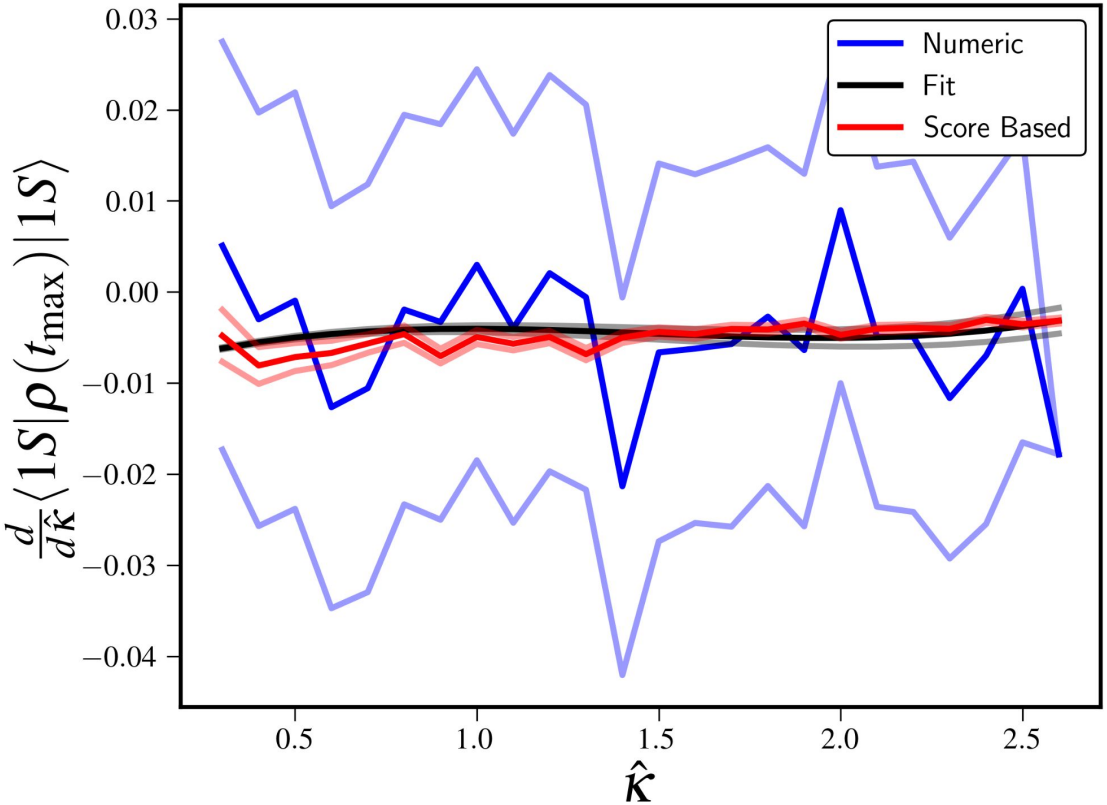
2. Discrete probability

$$p(z|\kappa) = \begin{cases} 1-\delta p & z=0 \\ \delta p\, p_1 & z=1 \\ \delta p\, p_2 & z=2 \\ \delta p\, p_3 & z=3 \\ \delta p\, p_4 & z=4 \end{cases}$$

δp now given by

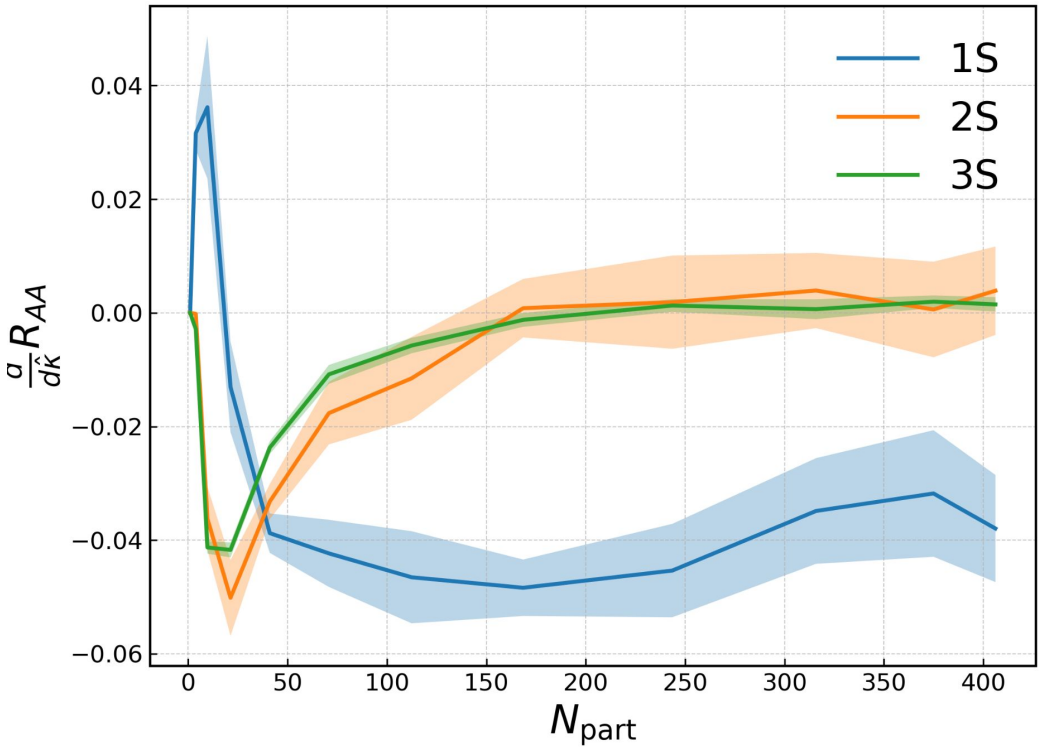
$$1 - \frac{\langle\psi_{n+1}|\psi_{n+1}\rangle}{\langle\psi_n|\psi_n\rangle}$$

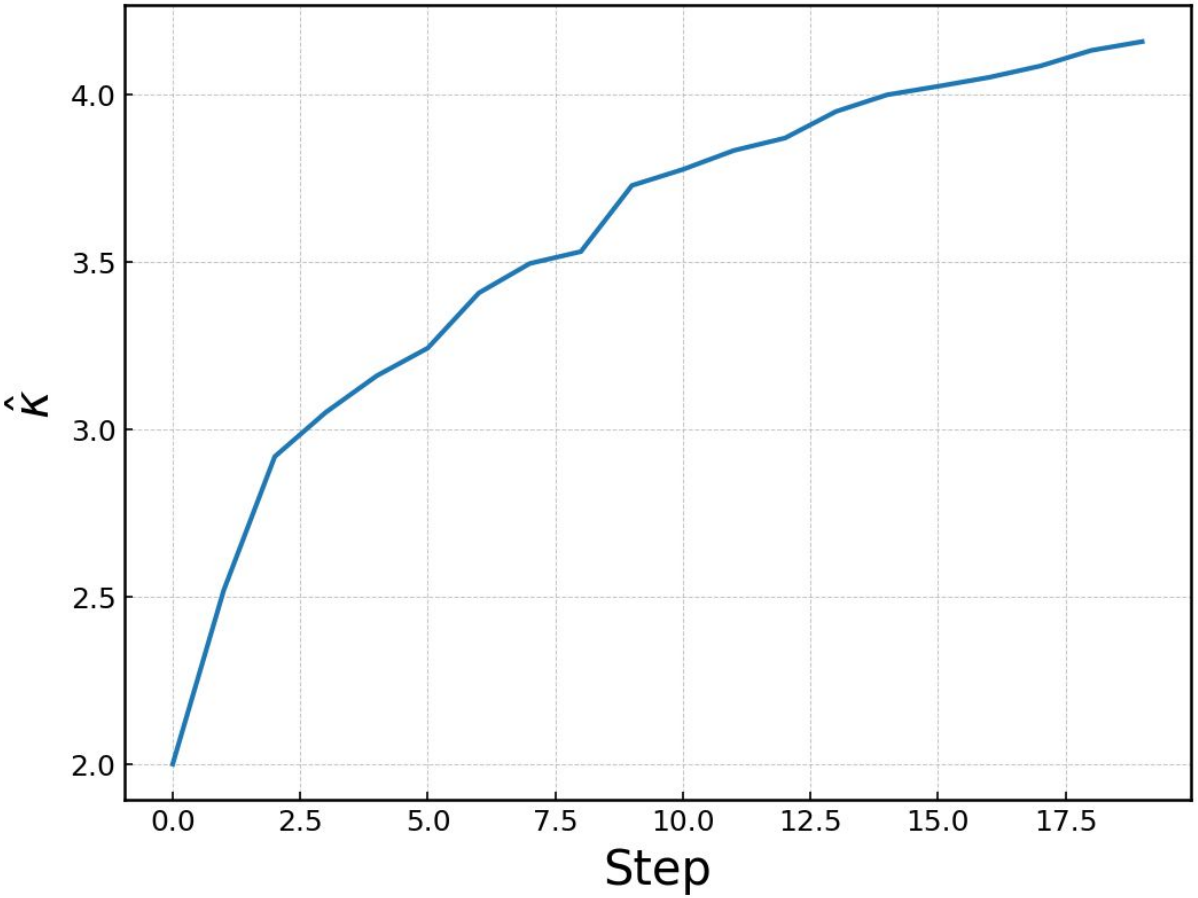
Score based gradient



Nuclear modification factor gradient

$\hat{\kappa} = 5$

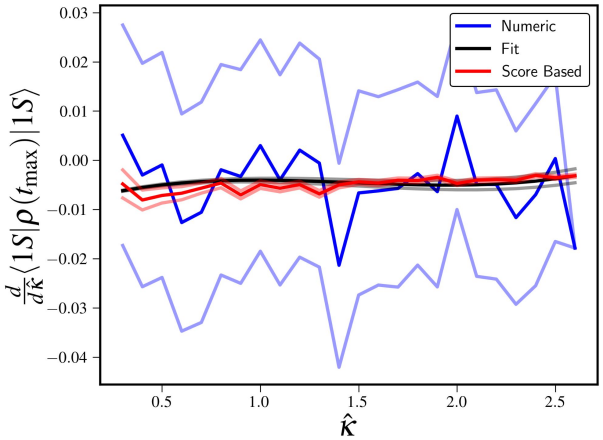


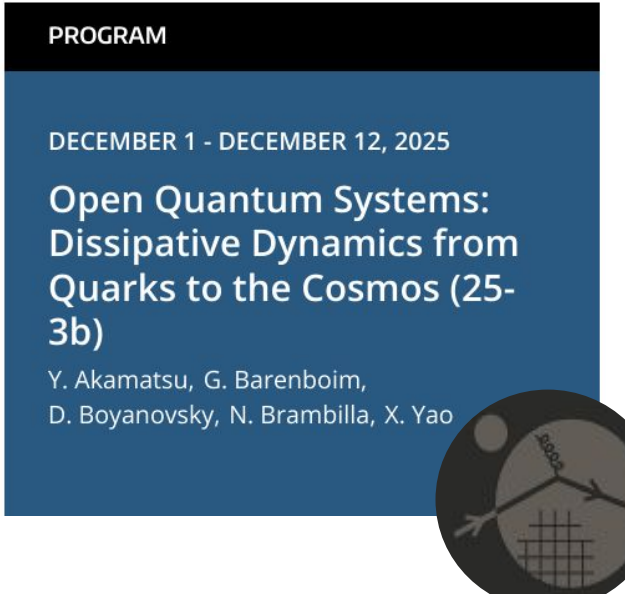

4.0
3.5
3.0
2.5
2.0
$\hat{K}$
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Step

Summary and outlook

1. Open Quantum System approach can provide phenomenological results for quarkonium suppression
2. Score based gradient estimation of Quantum trajectories for low variance gradients of input parameters

- December 2025: **INT Workshop**





Backup slides

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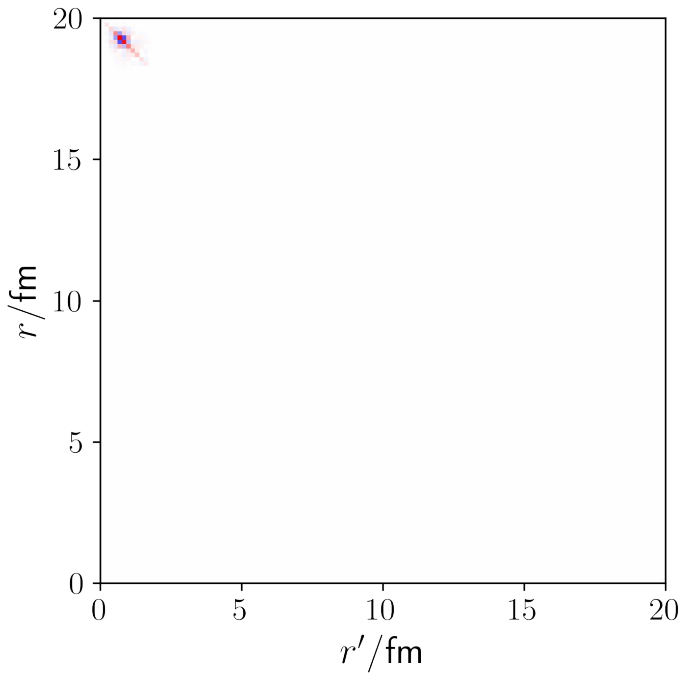

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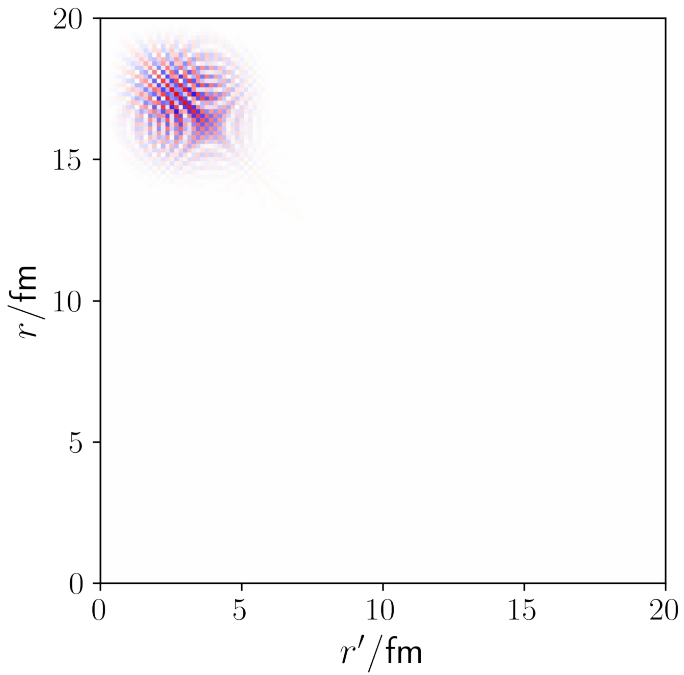

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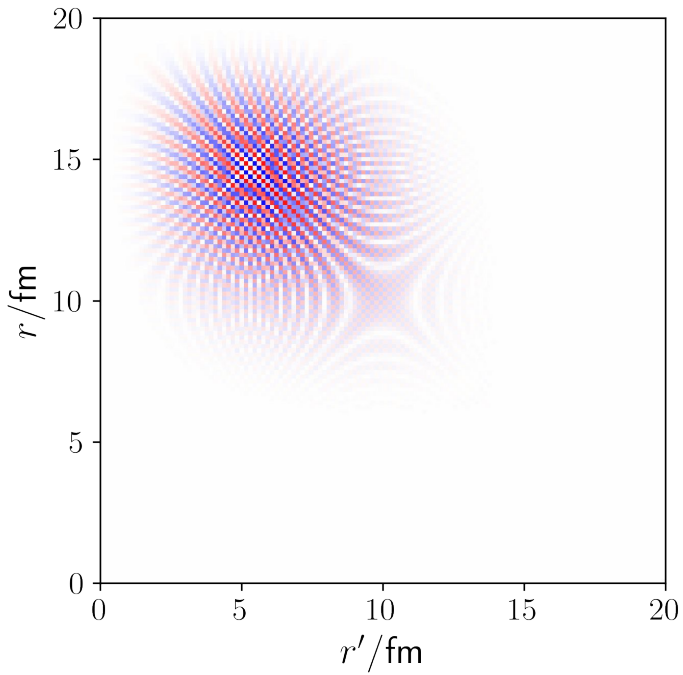

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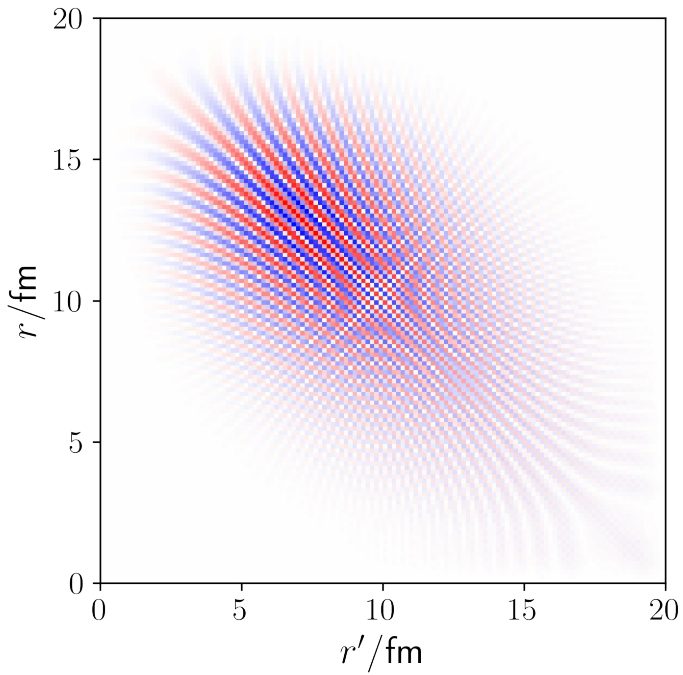

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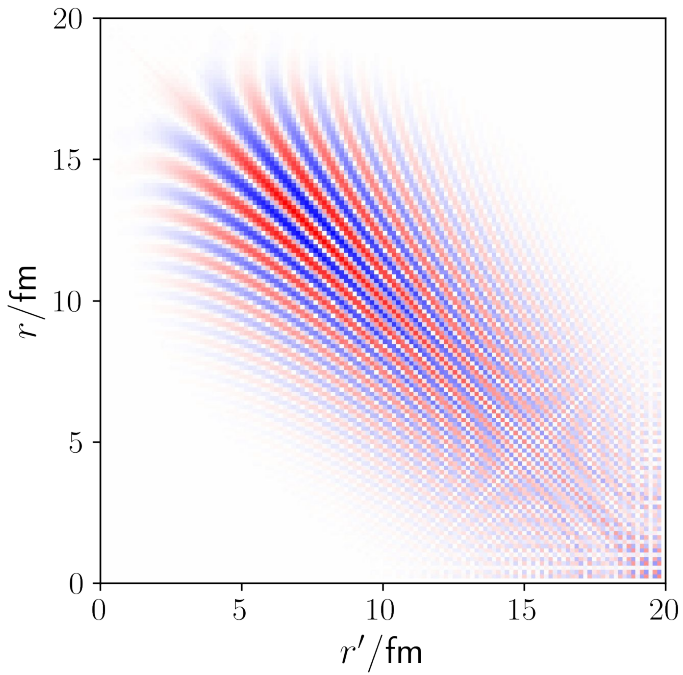

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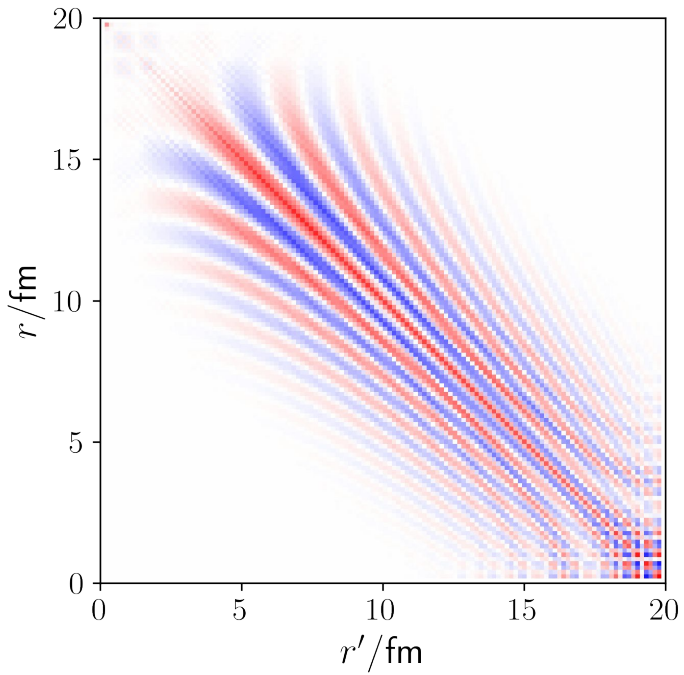

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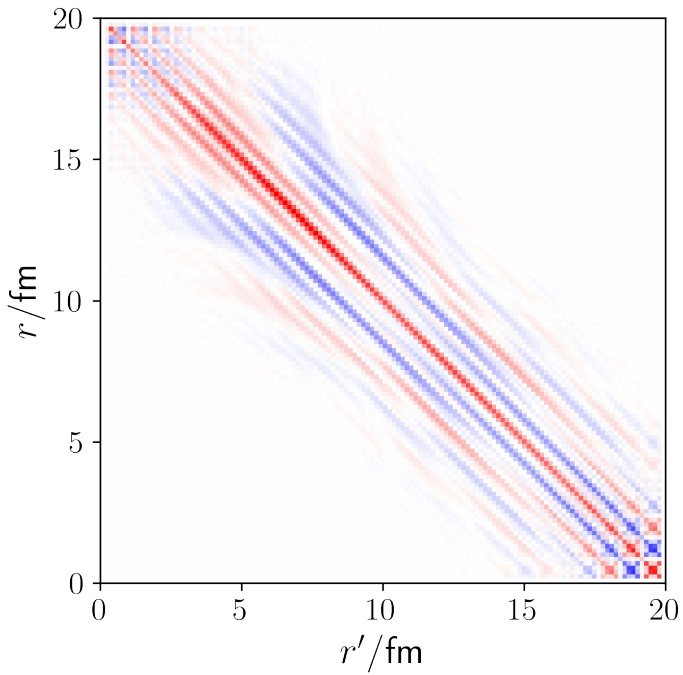

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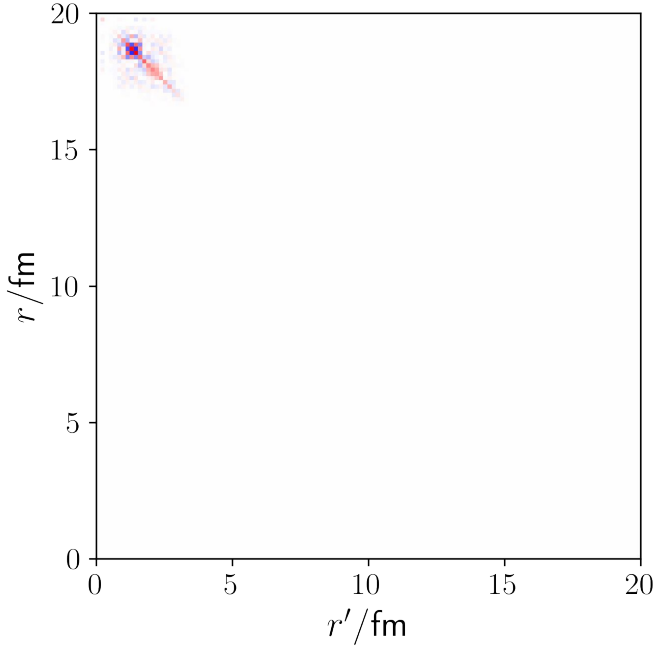

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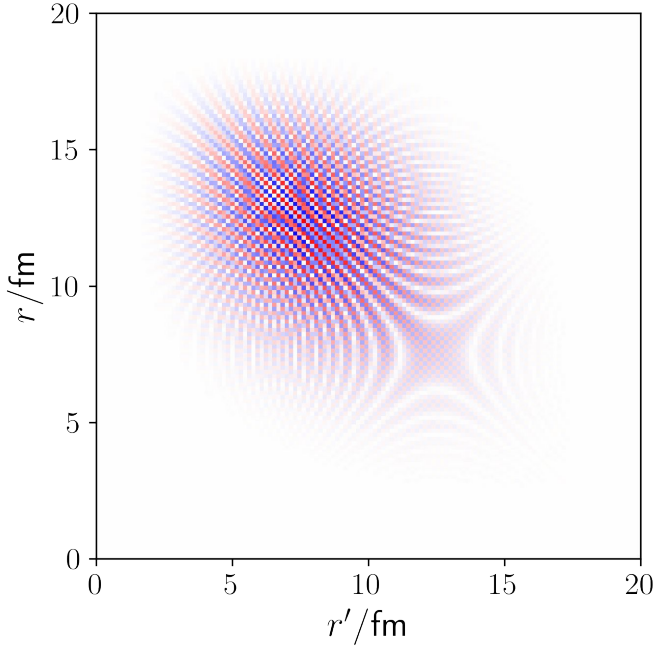

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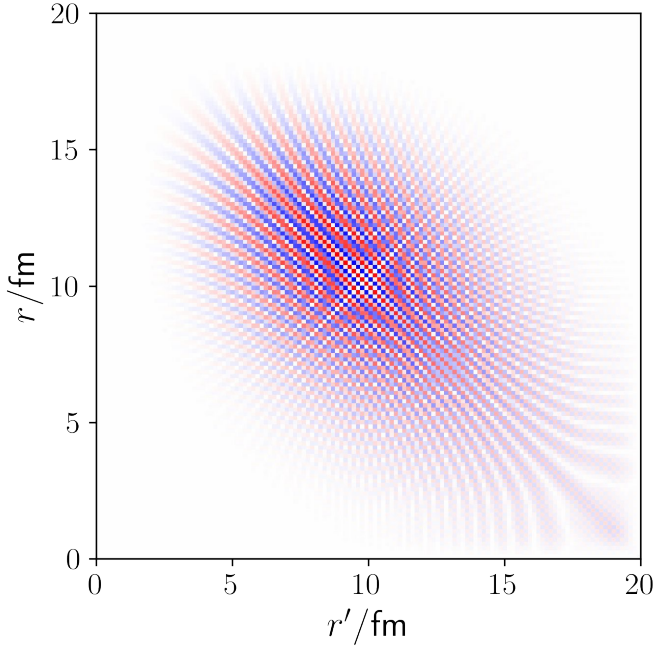

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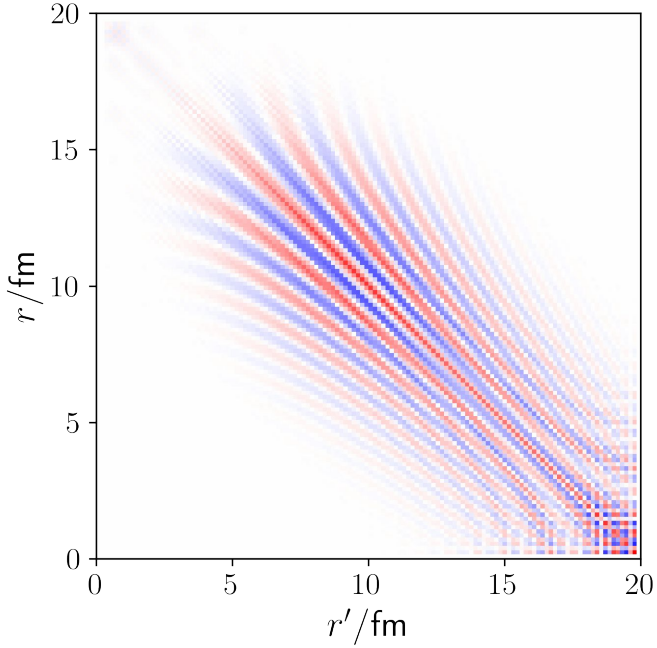

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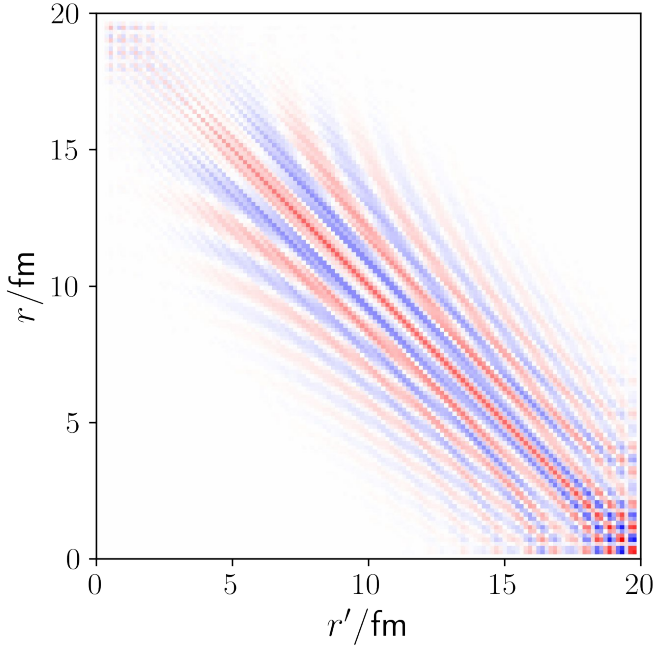

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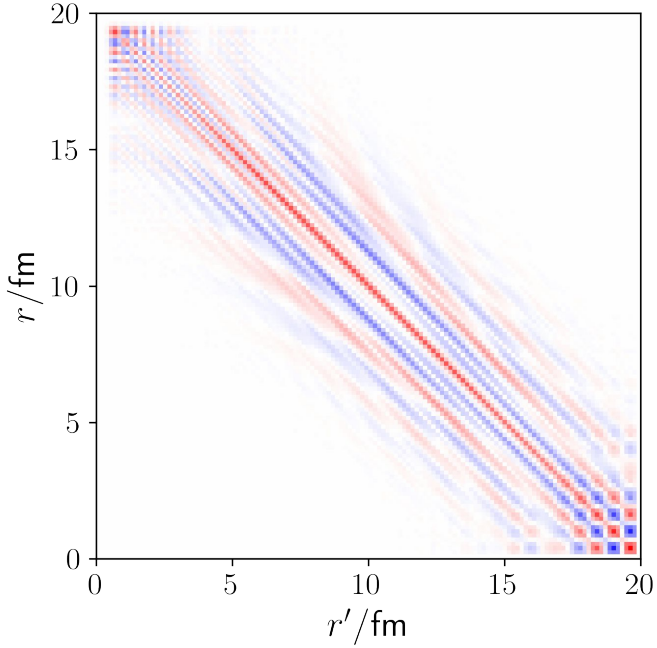
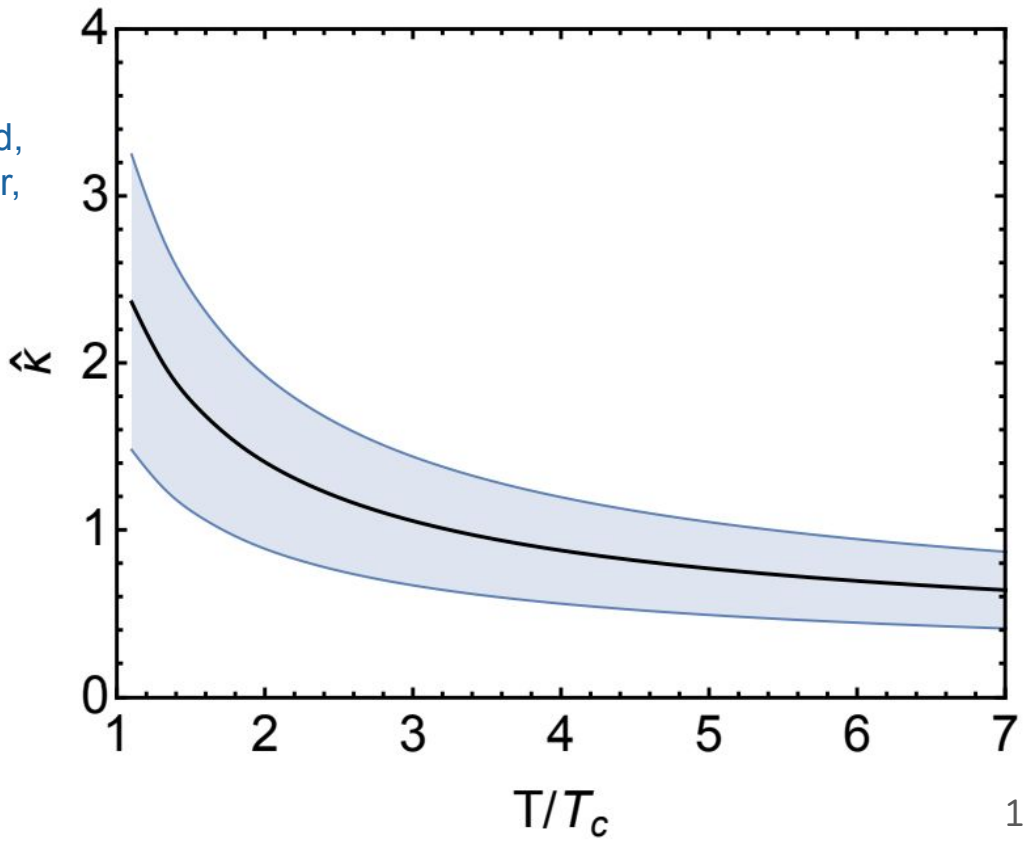


Non perturbative correction

N. Brambilla, M. A. Escobedo, M. Strickland, A. Vairo, P. Vander Griend, and J. H. Weber, JHEP 05, 136 (2021), 2012.01240



Heavy quark diffusion coefficient

$$V_s^{\text{non-pert}}(r) = -i\frac{g^2 T_F}{3N_c} r^2 \int_0^\infty dt \langle E^a(t)\Omega(t,0)^{ab} E^b(0)\rangle$$

$$\gamma = \frac{g^2}{3N_c} \text{Im} \int_0^\infty dt \, \langle E^a(t)\Omega(t,0)^{ab} E^b(0)\rangle$$

Determination of transport coefficients

- Indirectly determine $\hat{\kappa}$ and $\hat{\gamma}$ from lattice measurements of the **in medium width** Γ and **mass shift** δm

$$\kappa = \hat{\kappa} T^3$$

no vacuum part

$$\gamma = \gamma(T=0) + \hat{\gamma} T^3$$

- Assume simple model for the vacuum part $\gamma(T=0)$

$$\langle E^a(t)\Omega(t,0)^{ab}E^b(0)\rangle = \langle E^2(0)\rangle \mathrm{e}^{-i\Lambda_E t}$$

G. S. Bali and A. Pineda, Physical Review D 69 (2004)

$\langle g^2 E^2(0)\rangle = -0.2\mathrm{GeV}^4$

$\Lambda_E = 1.25\mathrm{GeV}$

S. Narison, Qcd parameters and sm-high precisions from e+e-→hadrons :Summary(2023),2309.05342

EFTs for Quarkonium Suppression

- Use NREFTs to exploit hierarchy of scales

$$M \gg 1/a_0 \gg \pi T \gg E$$

- Inverse radius:

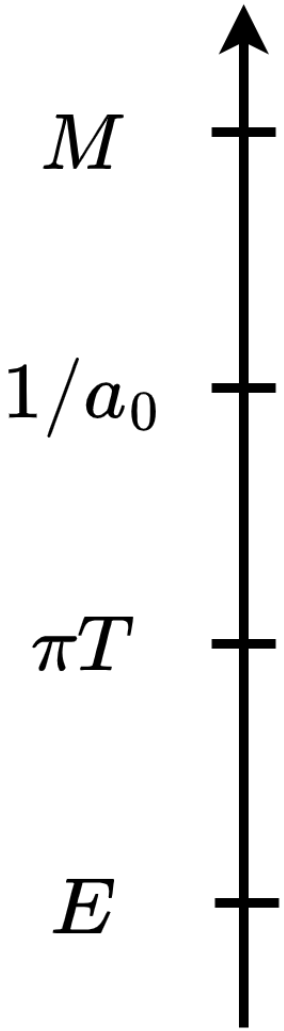
$$1/a_0 \approx 1.2\mathrm{GeV}$$

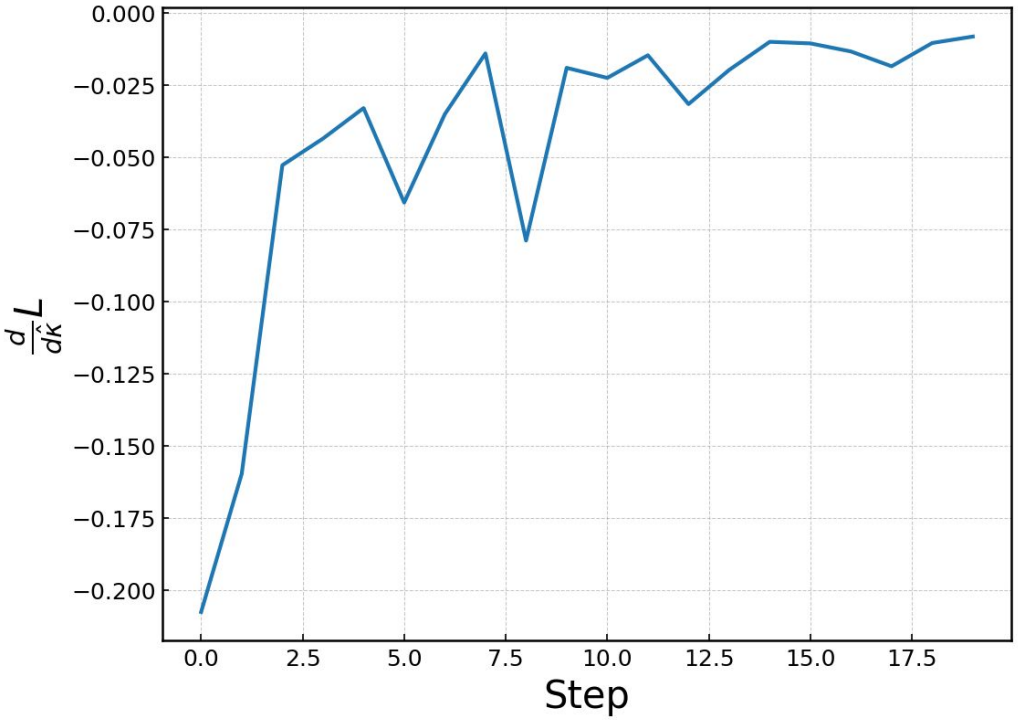
- Temperature regime:

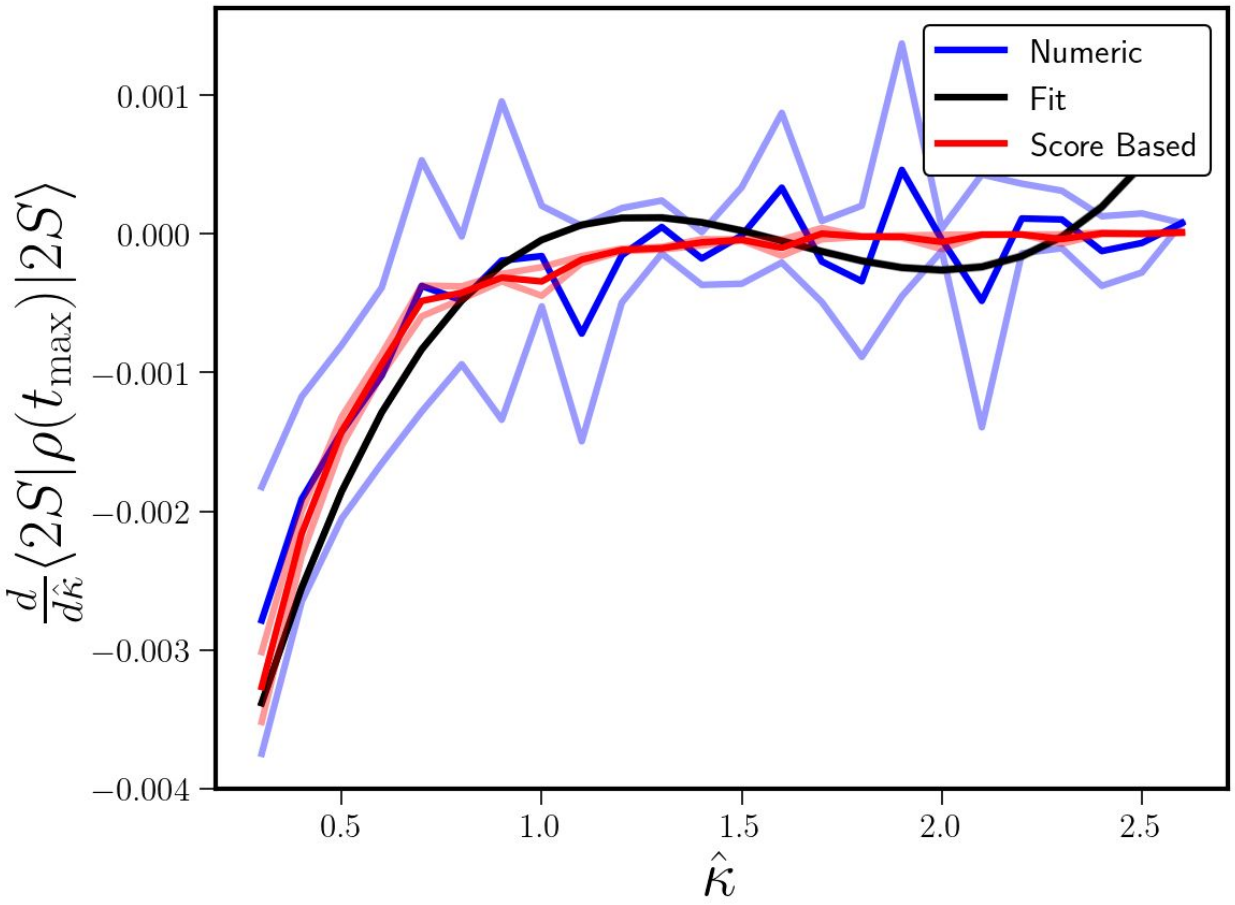
$$250\mathrm{MeV} < T < 425\mathrm{MeV}$$

- Binding Energy:

$$E \sim 0.4\mathrm{GeV}$$

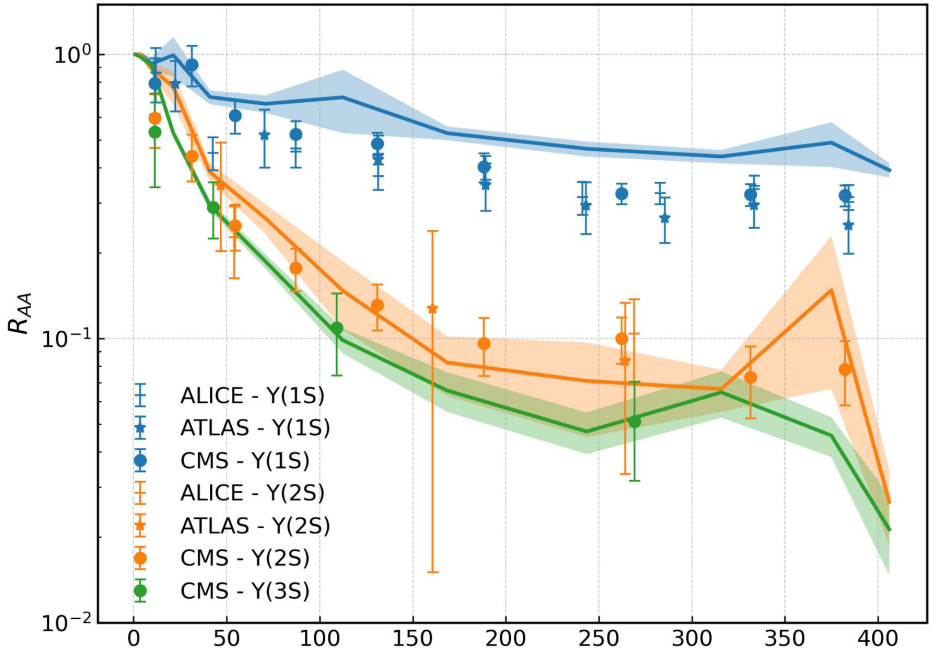



0.000
−0.025
−0.050
−0.075
−0.100
−0.125
−0.150
−0.175
−0.200
$\frac{d}{d\hat{\kappa}}L$
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Step

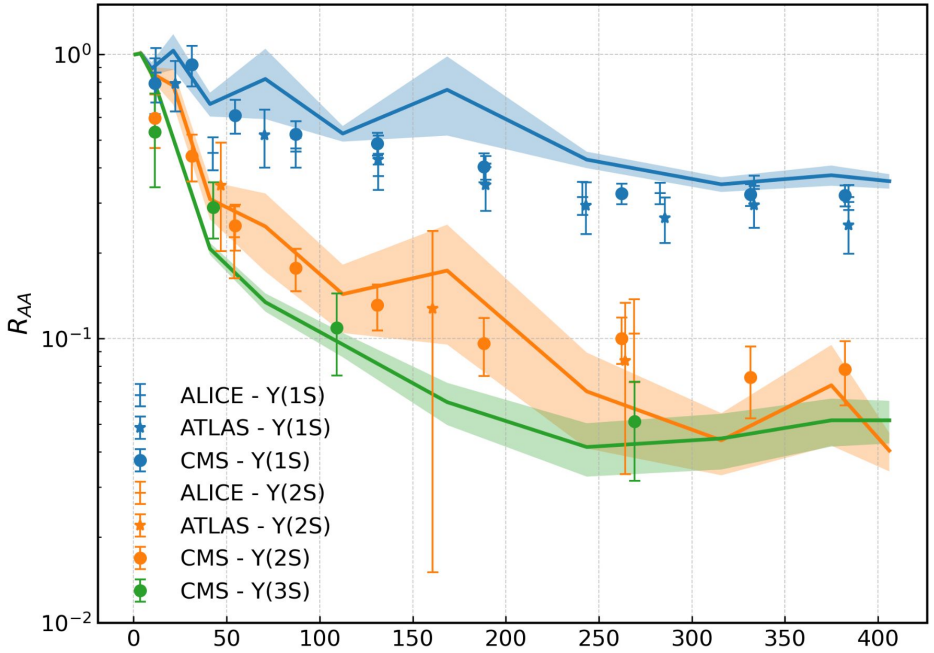

Numeric
Fit
Score Based
0.001
0.000
−0.001
−0.002
−0.003
−0.004
0.5
1.0
1.5
2.0
2.5
$\frac{d}{d\hat{\kappa}}\langle 2S|\rho(t_{\max})|2S\rangle$
$\hat{\kappa}$

Optimization results

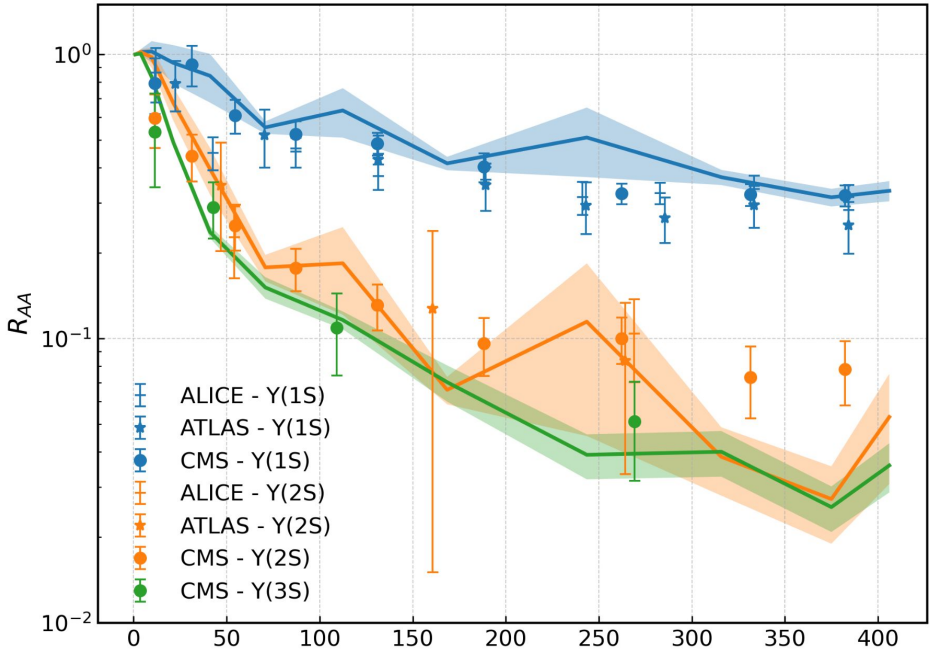
$$\hat{\kappa} = 2$$



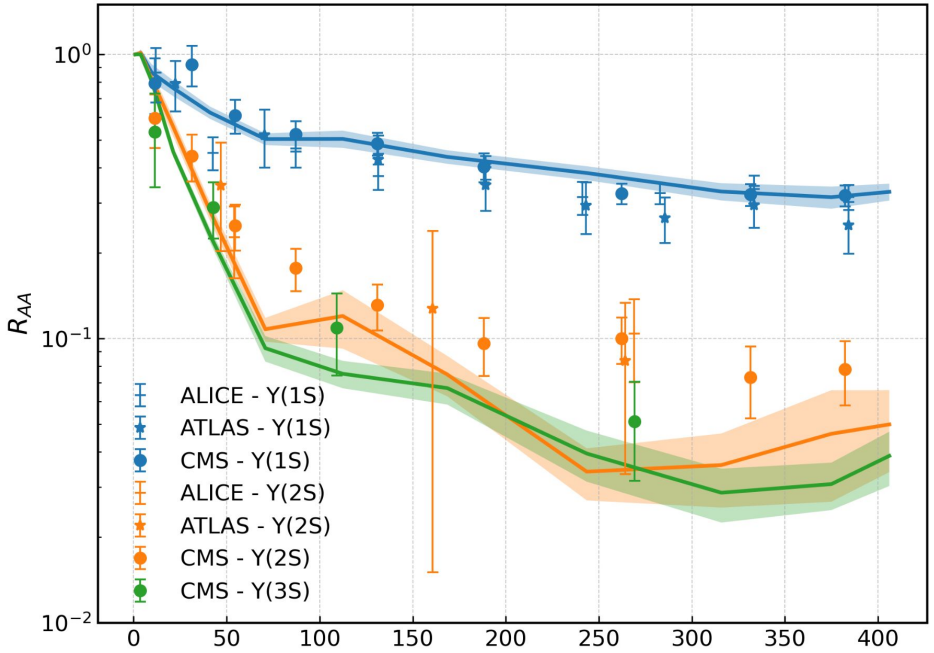
Optimization results



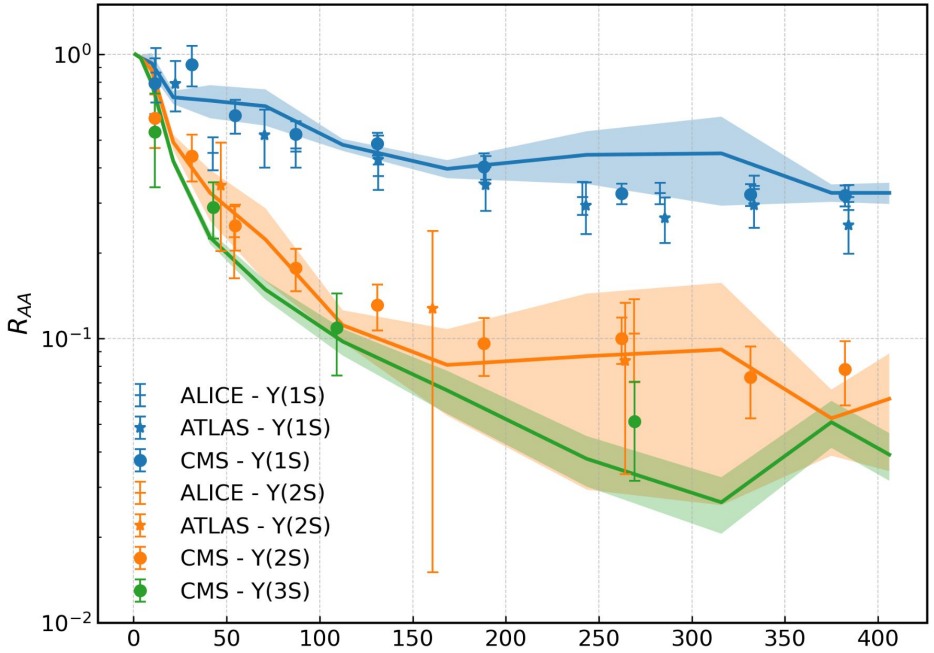
Optimization results



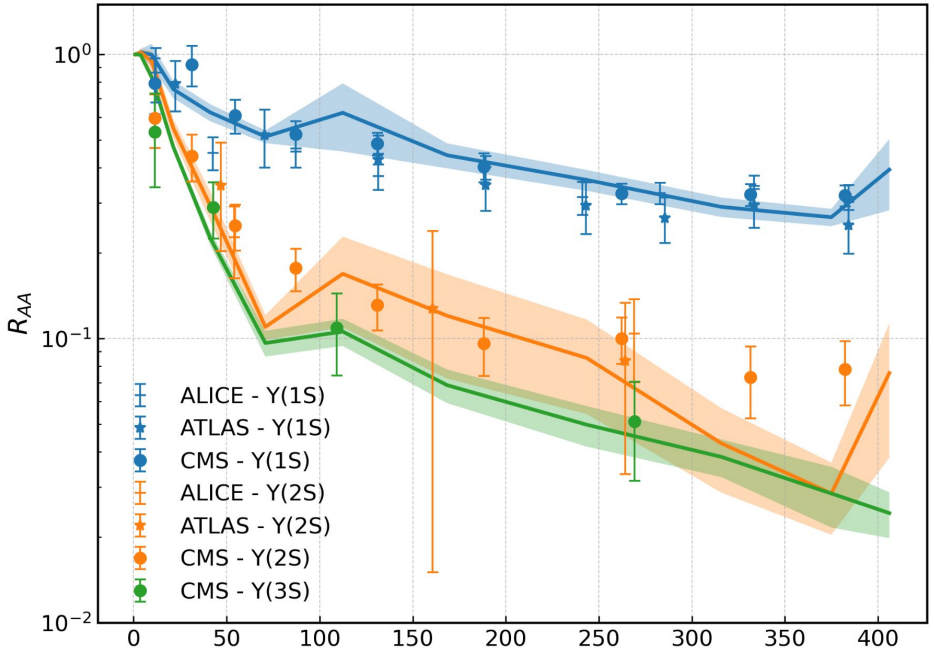
Optimization results



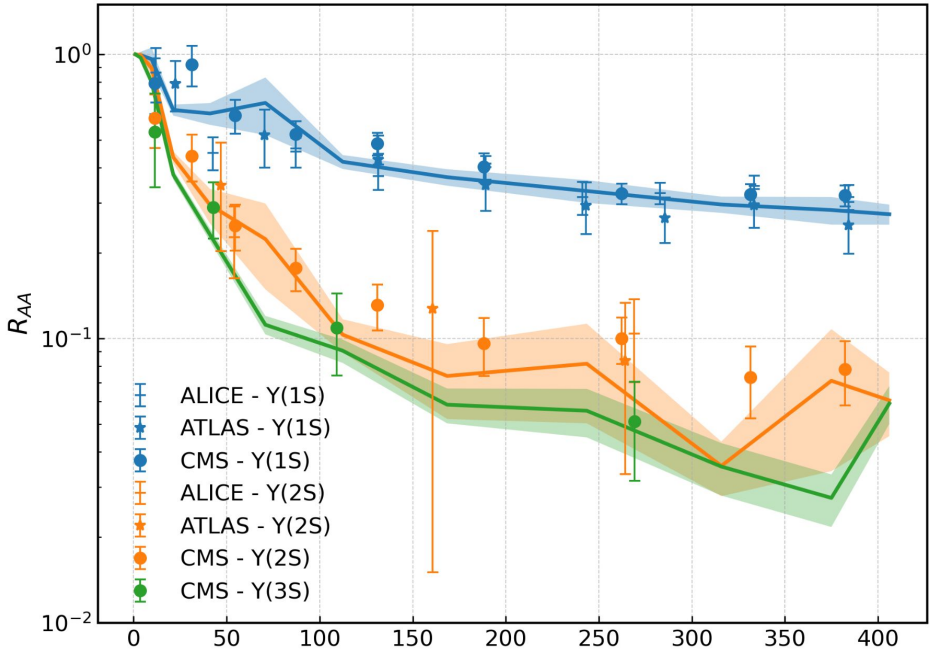
Optimization results



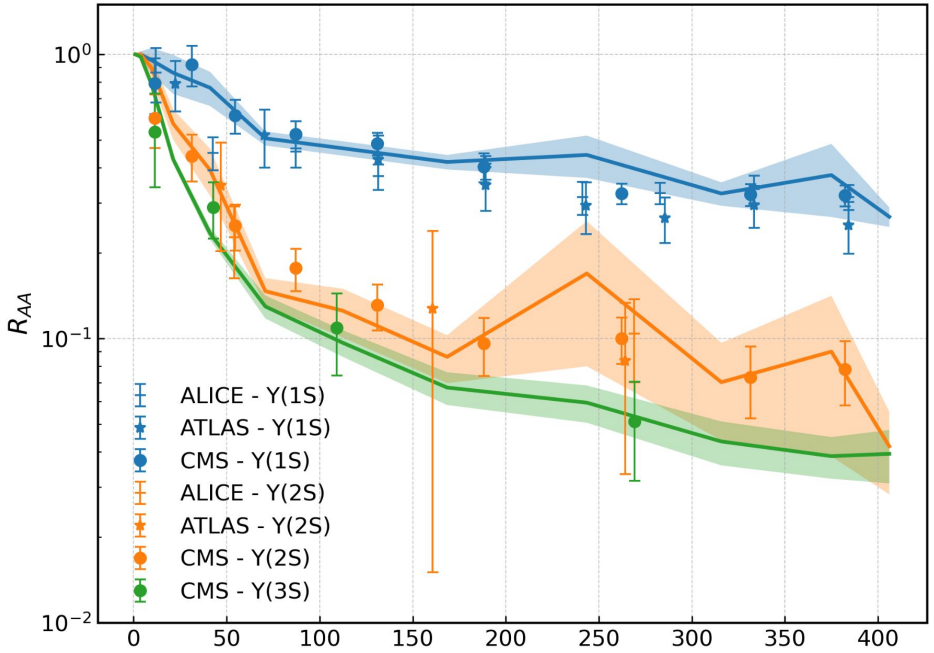
Optimization results



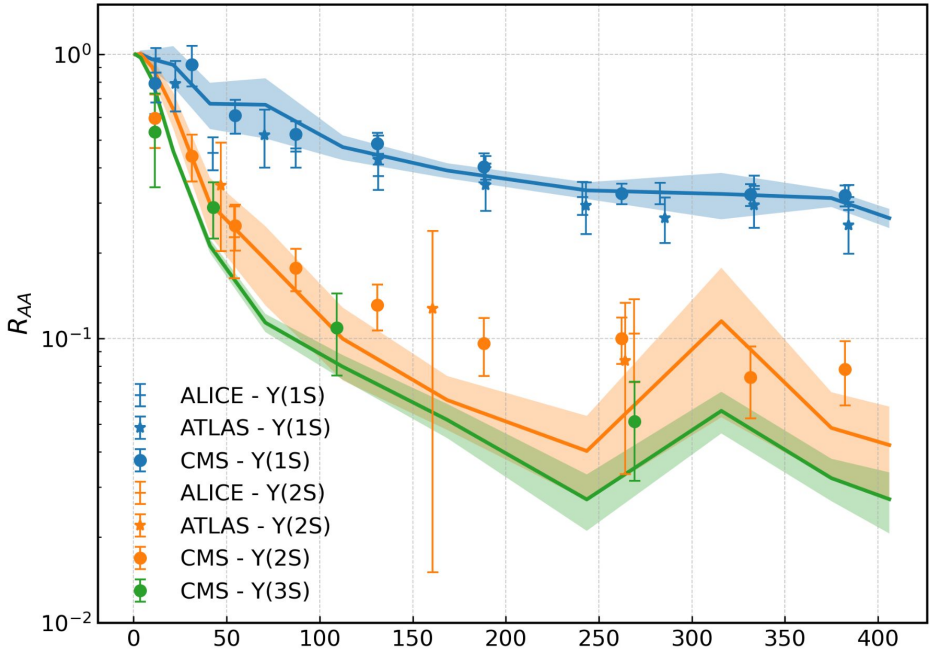
Optimization results



Optimization results



Optimization results



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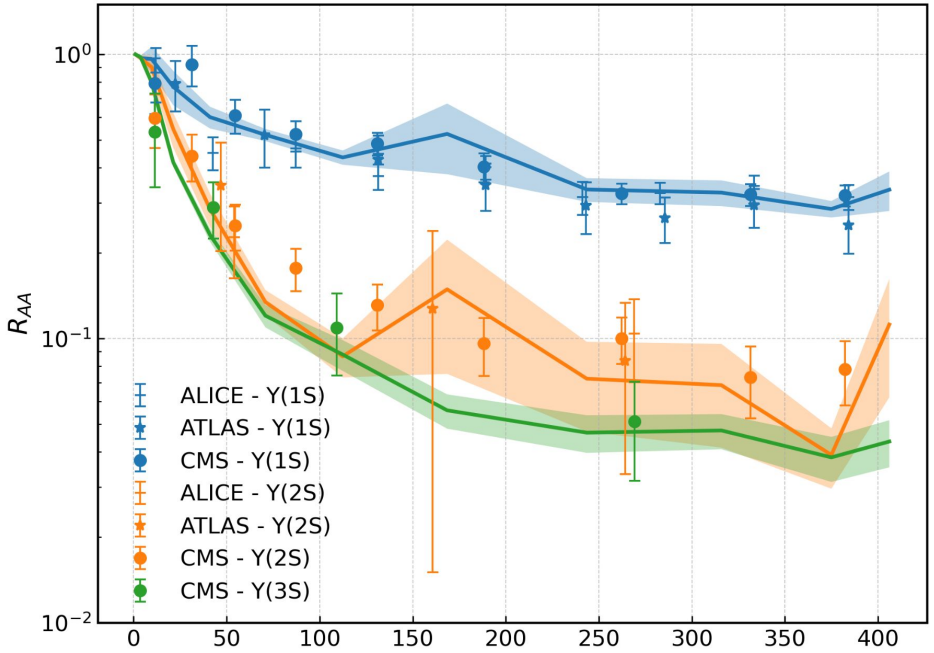

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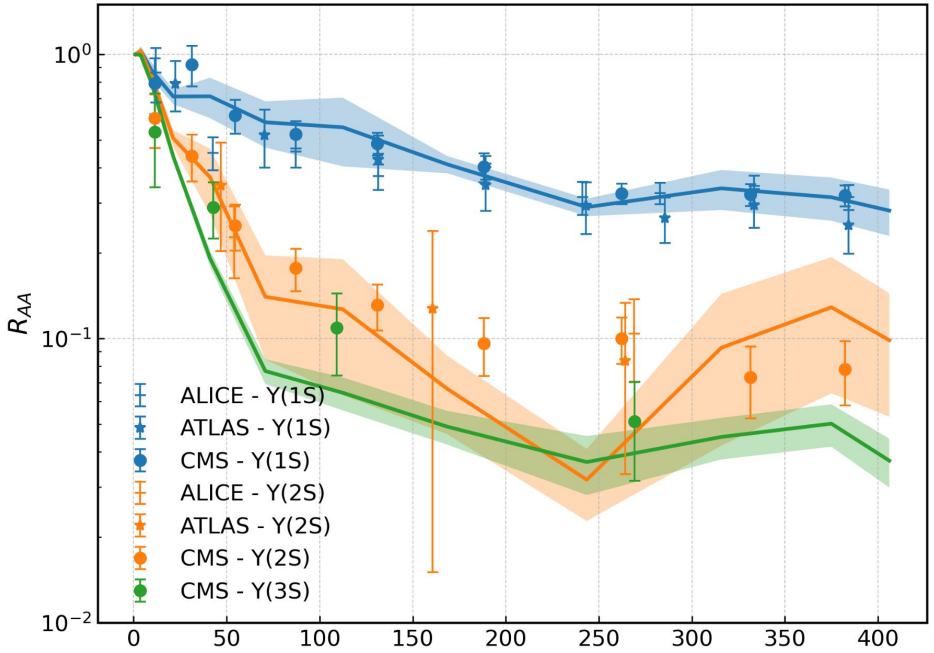
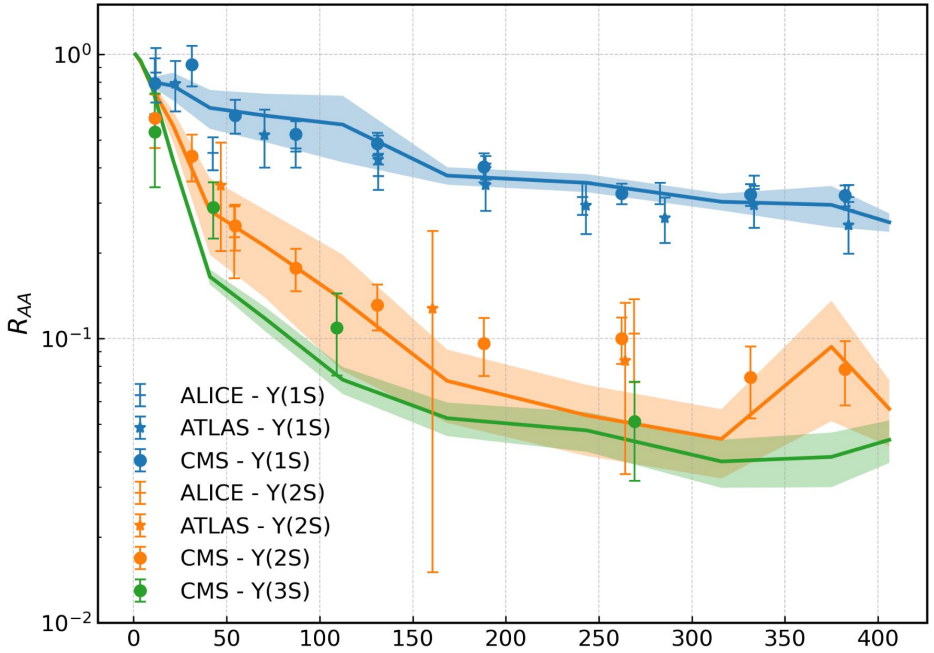
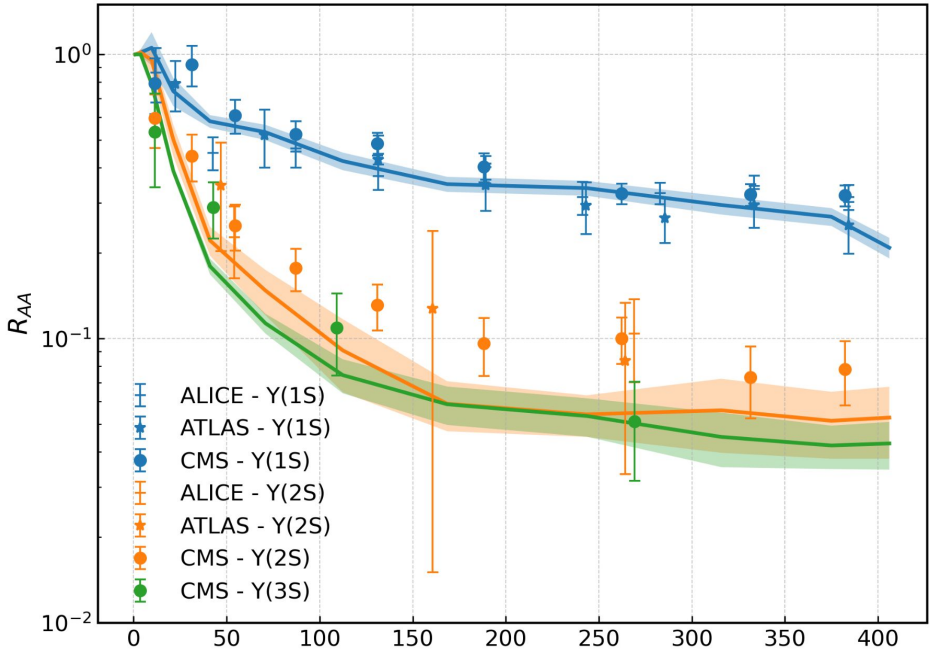


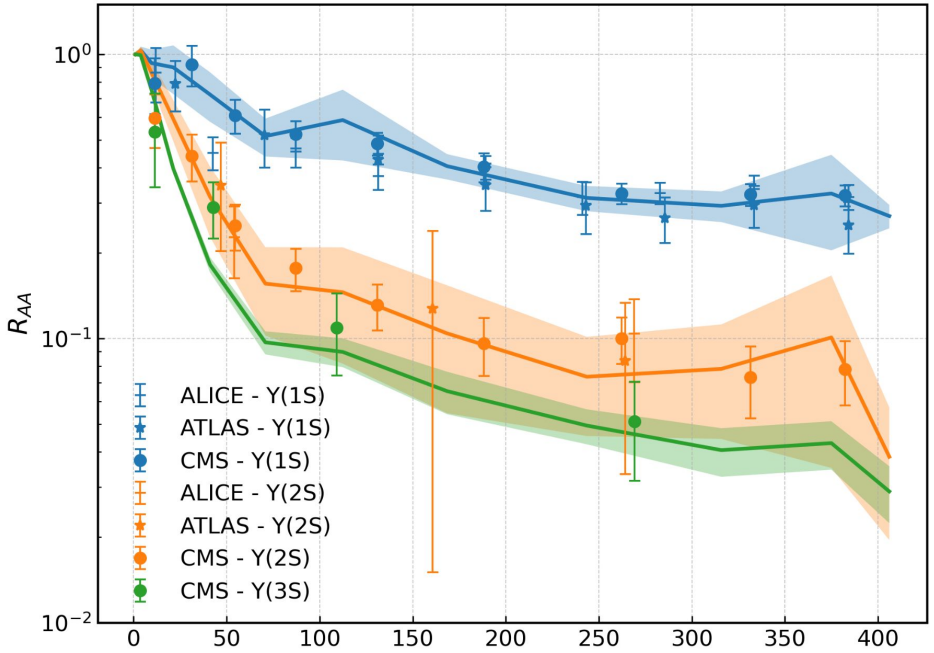
Optimization results



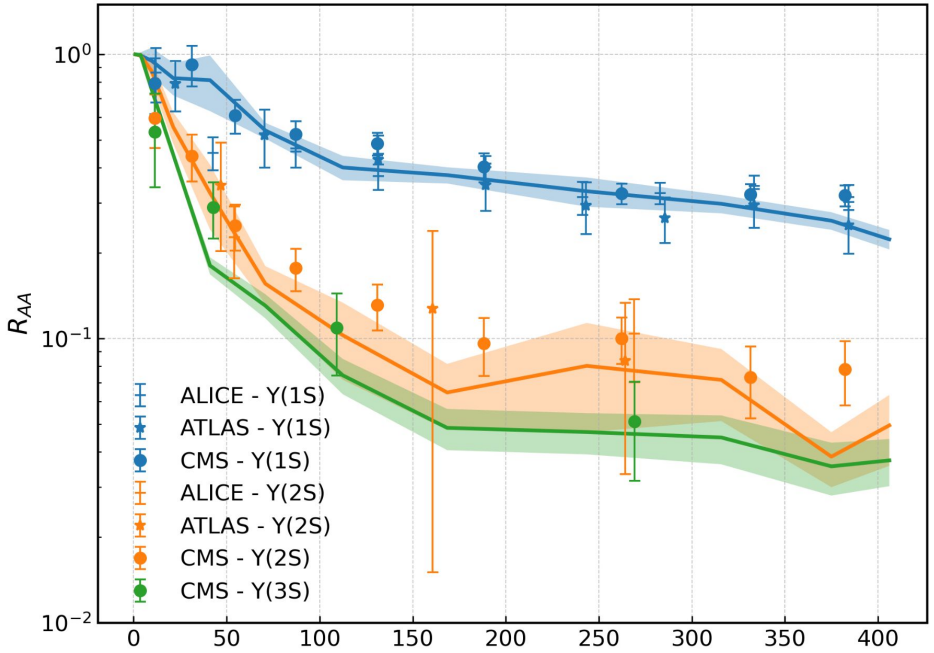
Optimization results



Optimization results



Optimization results



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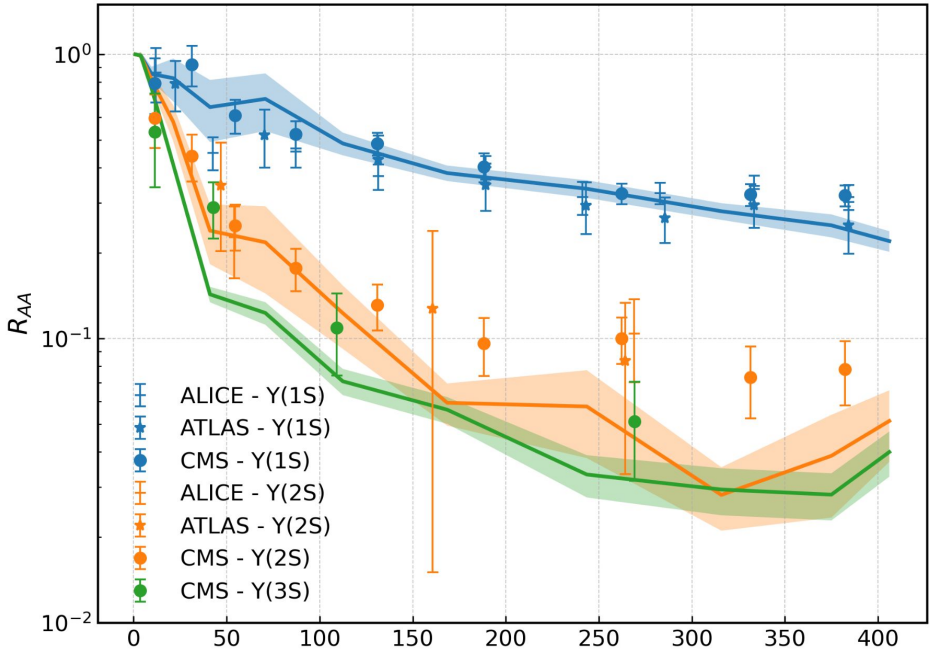
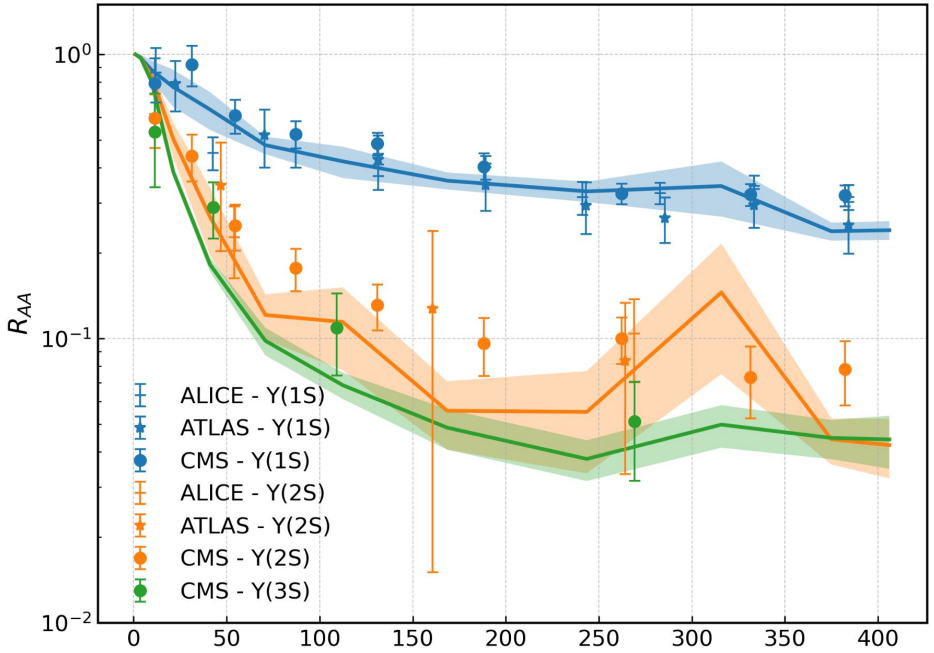
Optimization results