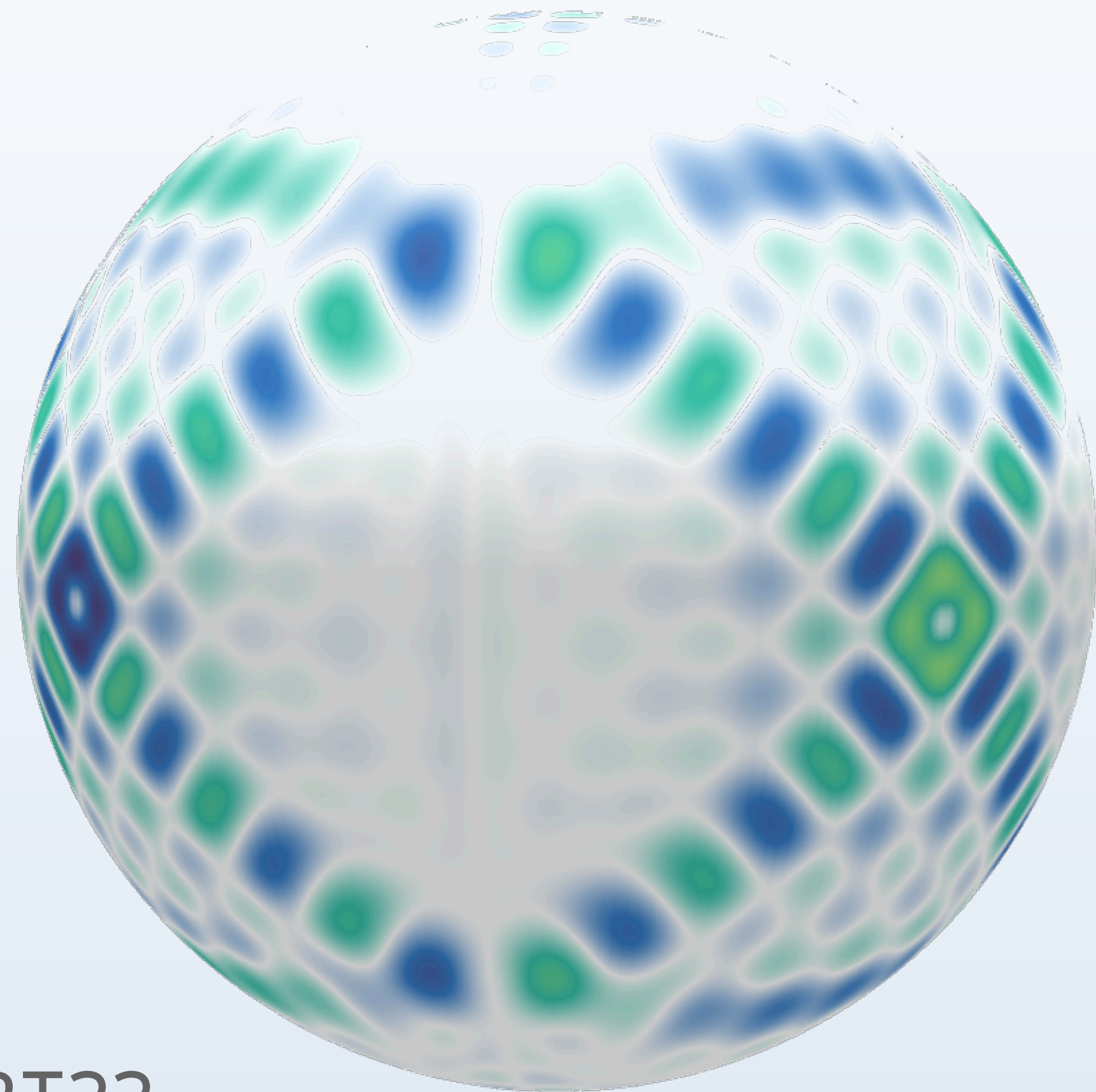


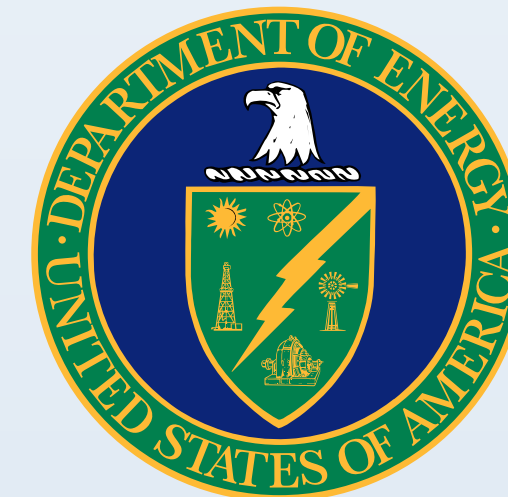
The two body density matrix of a Tomonaga-Luttinger liquid



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H. Radhakrishnan
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RPMBT22

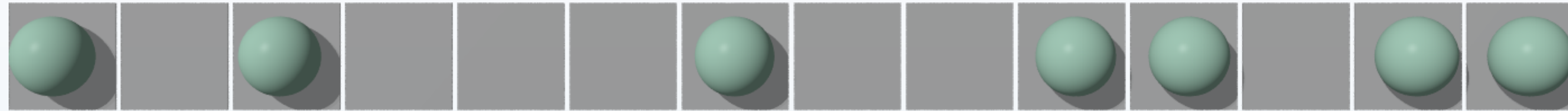
<http://delmaestro.org/adrian> • <https://github.com/DelMaestroGroup/>

M. Thamm, H. Radhakrishnan, H. Barghathi, B. Rosenow, AD, arXiv:2206.11301
H. Radhakrishnan, M. Thamm, H. Barghathi, B. Rosenow, AD, arXiv:2302.09093

*Can we understand the
interplay between
interactions and
(anti)symmetrization for
strongly correlated itinerant
particles?*

Description of Itinerant Particles

N indistinguishable fermions on L sites $|\mathcal{H}| = \binom{L}{N}$

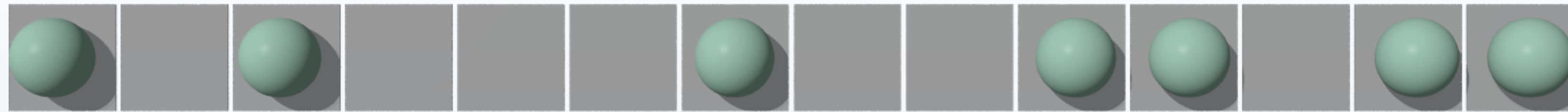


$$|\psi_\alpha\rangle = |10100010011011\rangle$$

$$= \frac{1}{\sqrt{7!}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} |2_1 3_2 7_3 10_4 11_5 13_6 14_7\rangle$$

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$$= \frac{1}{\sqrt{7!}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} |2_1 3_2 7_3 10_4 11_5 13_6 14_7\rangle$$

general state: $|\Psi\rangle = \sum_{\alpha} C_{\alpha} |\psi_{\alpha}\rangle$

1st quantization: $\Psi(i_1, \dots, i_N) = \langle i_1, \dots, i_N | \Psi \rangle$

$$i_{\alpha} \in \{1, L\}$$

$$\Psi(i_1, \dots, i_{\mu}, \dots, i_{\nu}, \dots, i_N) = -\Psi(i_1, \dots, i_{\nu}, \dots, i_{\mu}, \dots, i_N)$$



density matrix: $\rho = |\Psi\rangle \langle \Psi|$ dimension: $|\mathcal{H}| \times |\mathcal{H}|$ $\langle \mathcal{O} \rangle = \text{Tr}(\rho \mathcal{O})$
 $\text{Tr} \rho = 1$

Do we need the wavefunction?

REVIEWS OF MODERN PHYSICS

VOLUME 32, NUMBER 2

APRIL, 1960

Present State of Molecular Structure Calculations*

C. A. COULSON

Mathematical Institute, Oxford, England

(6) One of the most vigorously pursued lines of research during the last few years has been the density matrix. It has frequently been pointed out that a conventional many-electron wave function tells us more than we need to know. All the necessary information required for the energy and for calculating the properties of molecules is embodied in the first- and second-order density matrices. These may, of course, be obtained from the wave function by a process of integration. But this is aesthetically unpleasing, and so attempts have been made, by Löwdin, McWeeny, and others, to work directly with these matrices. There is an instinctive feeling that matters such as electron-correlation should show up in the two-particle density matrix. But here we are confronted by a serious lack of success. We do know the conditions that must be satisfied by the many-electron wave function $\psi(1,2,\dots,n)$, but we still do not know the conditions

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***N*-Representability** Problem

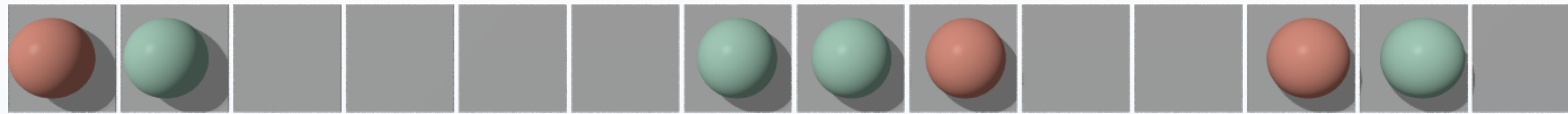
The n -particle density matrix must be constrained to represent a N -body density matrix (or wave function); otherwise, any minimized energy is unphysically below the ground-state energy for $N > 2$

A. J. Coleman, Rev. Mod. Phys. 35, 668 (1963)

D. A. Mazziotti, Phys. Rev. Lett. 108, 263002 (2011)

D. A. Mazziotti, Phys. Rev. Lett. 130, 153001 (2023)

n -Particle Reduced Density Matrix (n -RDM)

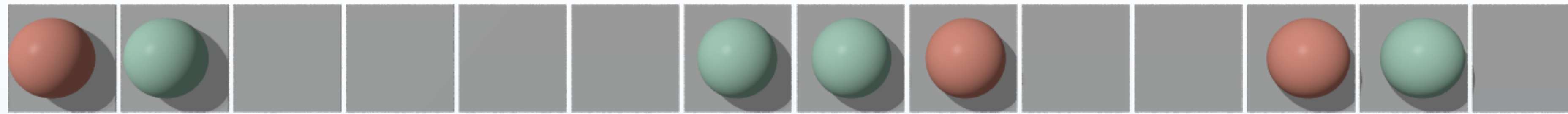


$$n = 3$$

$$N - n = 4$$

Maximum information which is available about n particles, irrespective of the state of other $N-n$ particles.

n -Particle Reduced Density Matrix (n -RDM)



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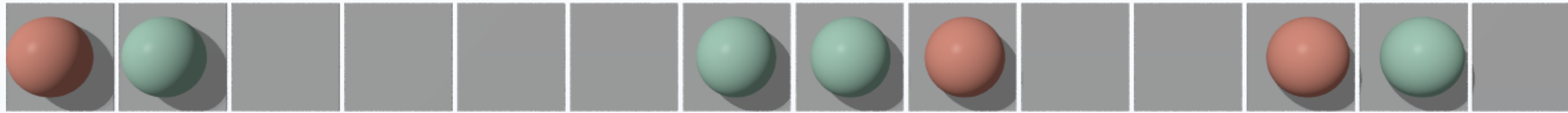
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$$n\text{-RDM: } \rho_n^{i_1, \dots, i_n, j_1, \dots, j_n} = \binom{N}{n}^{-1} \langle \Psi | c_{i_1}^\dagger \cdots c_{i_n}^\dagger c_{j_1} \cdots c_{j_n} | \Psi \rangle \quad \text{correlation function}$$

\swarrow $Tr \rho_n = 1$

n -Particle Reduced Density Matrix (n -RDM)



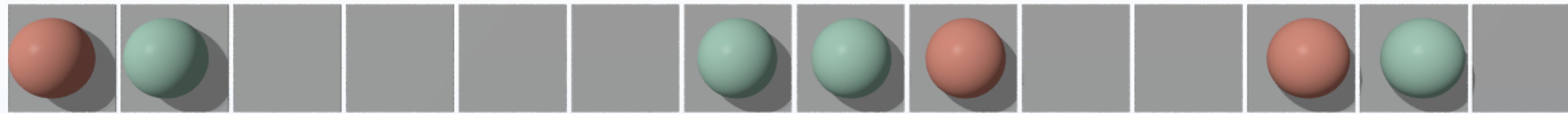
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$n = 3$

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 &\quad \searrow \text{integrate out}
 \end{aligned}$$

Any n -particle observable computable via n -particle reduced density matrix

$$\langle \mathcal{O}_{j_1, \dots, j_n} \rangle = \sum_{j_1, \dots, j_n} \left\{ \mathcal{O}_{j_1, \dots, j_n} \rho_n^{i_1, \dots, i_n, j_1, \dots, j_n} \right\} \Bigg|_{\forall \alpha=1, \dots, n}^{i_\alpha \rightarrow j_\alpha}$$

1-Particle Reduced Density Matrix



1-RDM: $\rho_1^{i_1, j_1} = \frac{1}{N} \langle \Psi | c_{i_1}^\dagger c_{j_1} | \Psi \rangle$

$$= \sum_{i_2, \dots, i_N} \psi^*(i_1, \overbrace{i_2, \dots, i_N}^{\text{integrate out}}) \psi(j_1, \overbrace{i_2, \dots, i_N}^{\text{integrate out}})$$

1-Particle Reduced Density Matrix



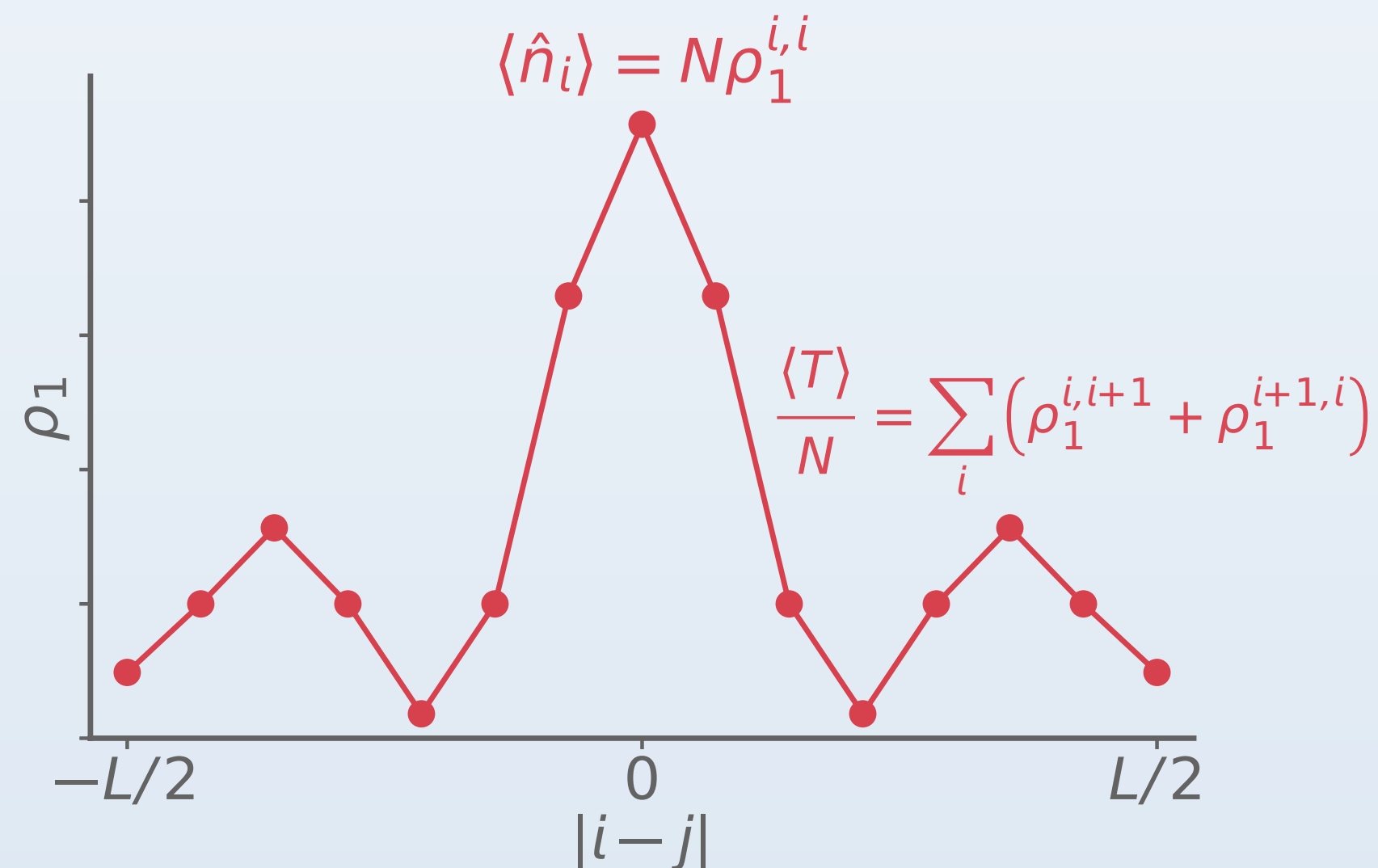
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integrate out

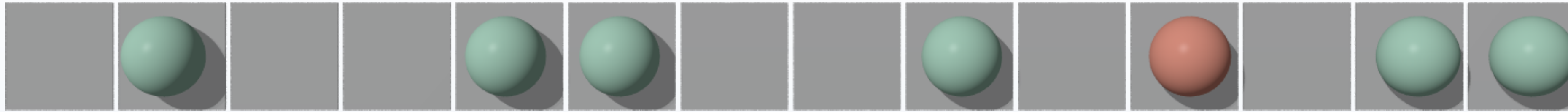
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Example: free fermions

$$\rho_1^{i,j} = \frac{1}{NL} \frac{\sin\left(\frac{\pi N}{L}|i-j|\right)}{\sin\left(\frac{\pi}{L}|i-j|\right)}$$



1-Particle Reduced Density Matrix



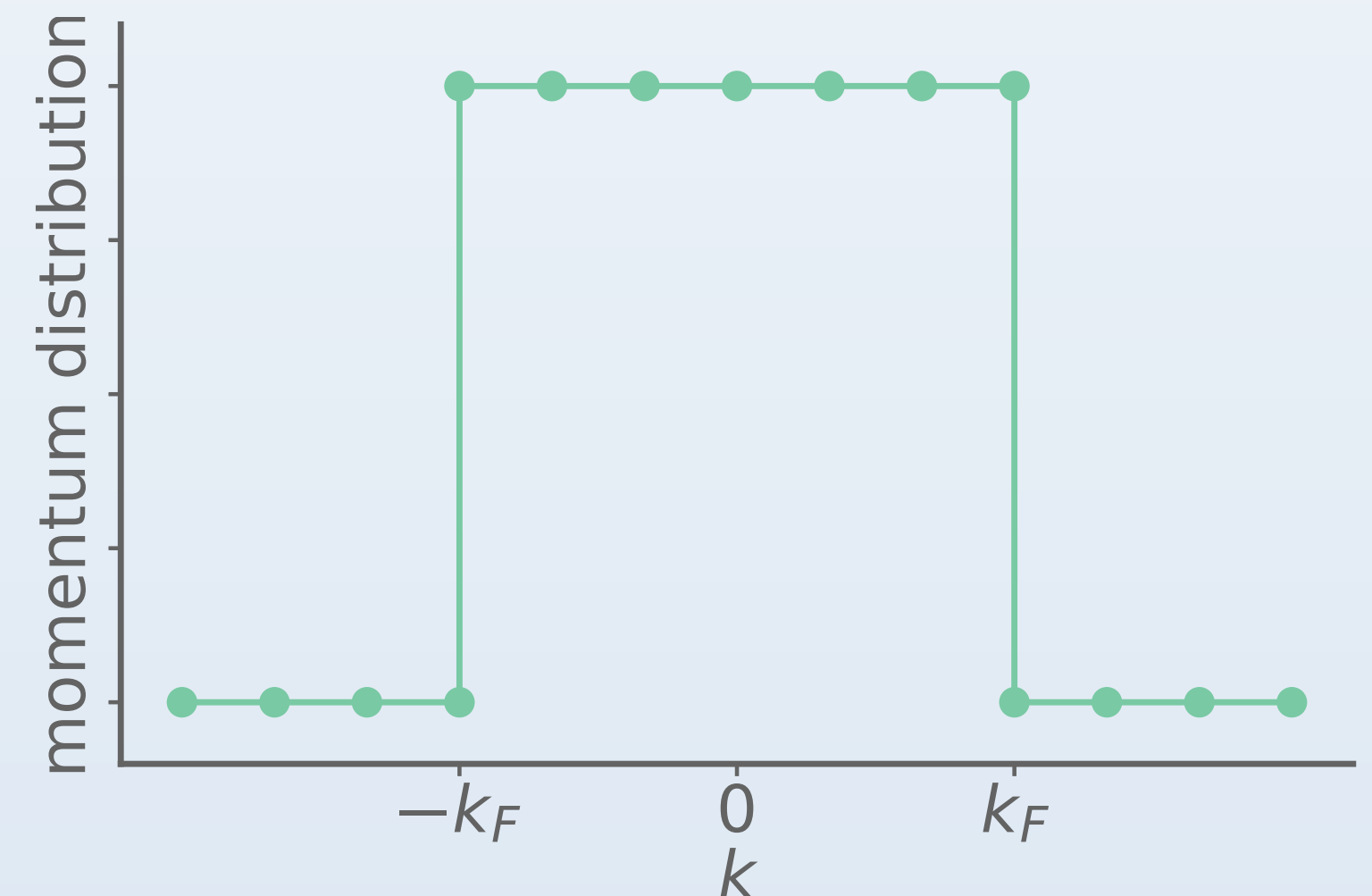
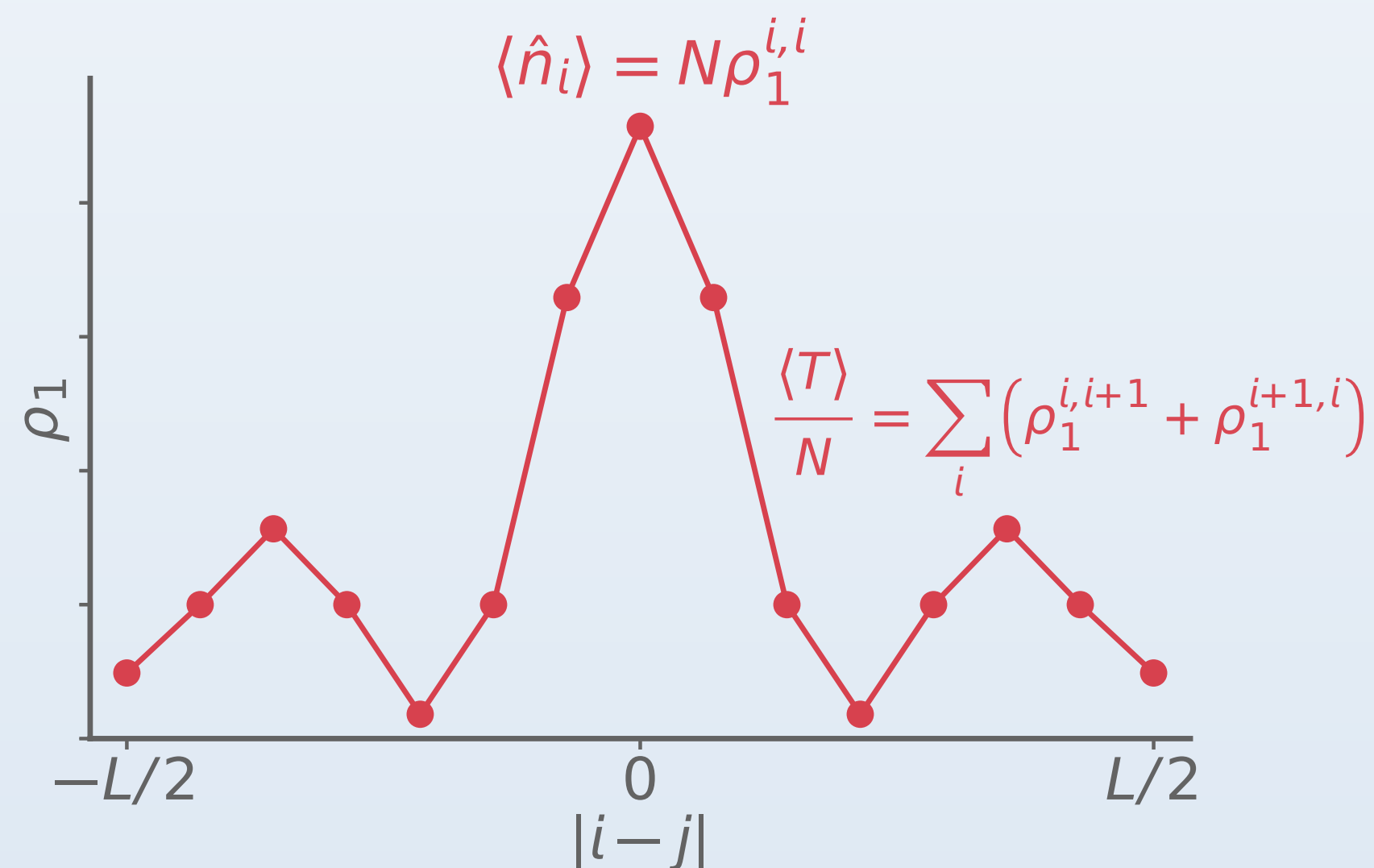
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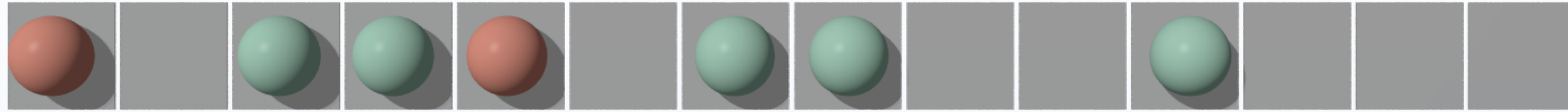
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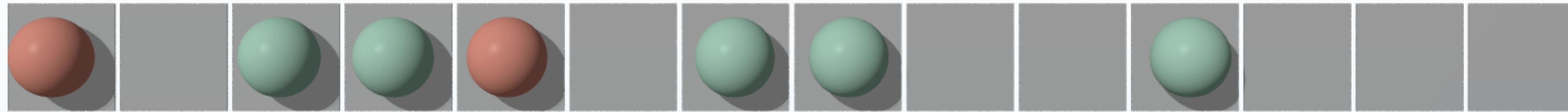


2-Particle Reduced Density Matrix



$$\begin{aligned} \text{2-RDM: } \rho_2^{i_1, i_2; j_1, j_2} &= \frac{(N-2)!}{N!} \langle \Psi | c_{i_1}^\dagger c_{i_2}^\dagger c_{j_1} c_{j_2} | \Psi \rangle \\ &= \sum_{i_3, \dots, i_N} \Psi^*(i_1, i_2, i_3, \dots, i_N) \Psi(j_1, j_2, i_3, \dots, i_N) \end{aligned}$$

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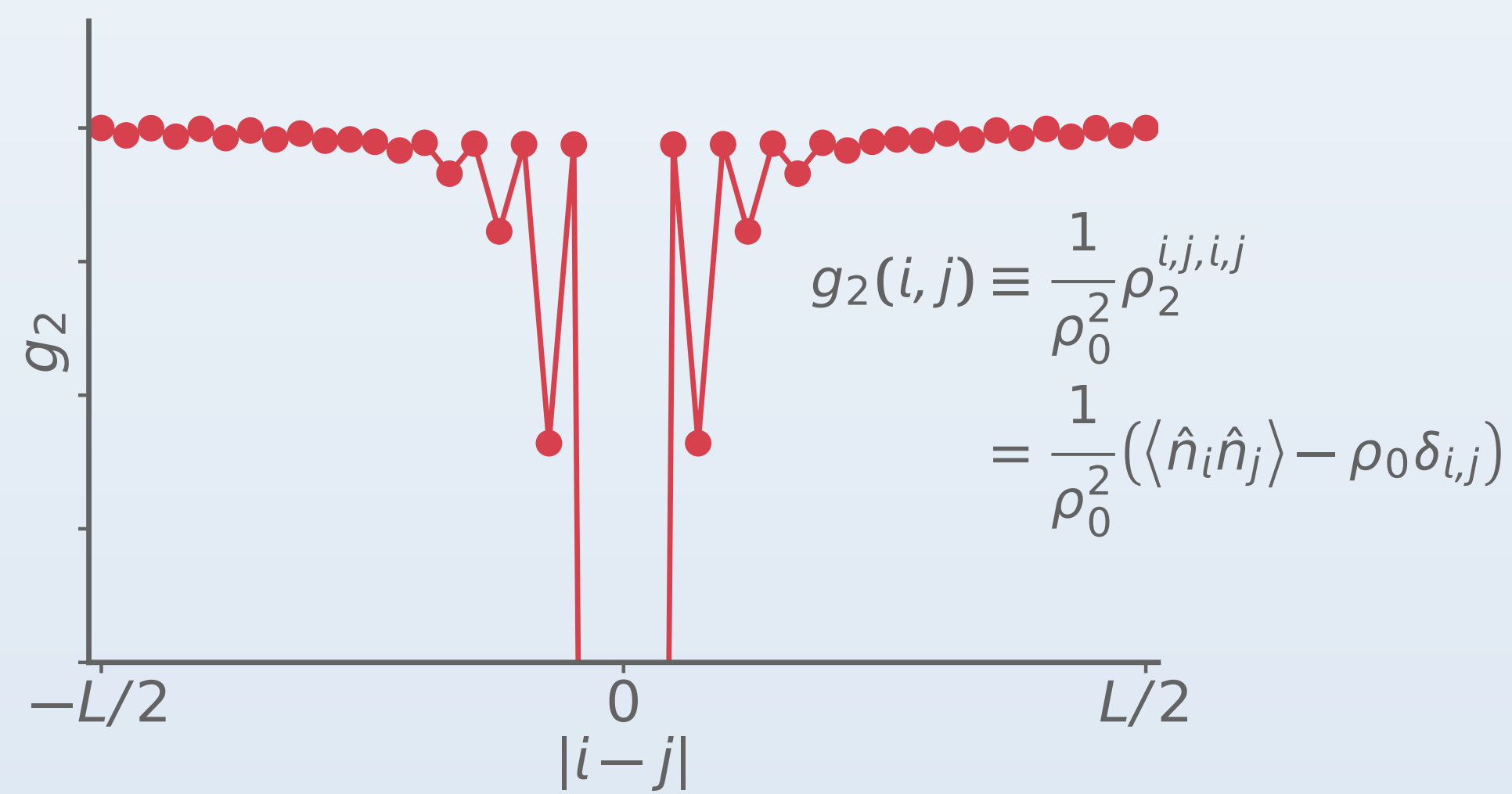


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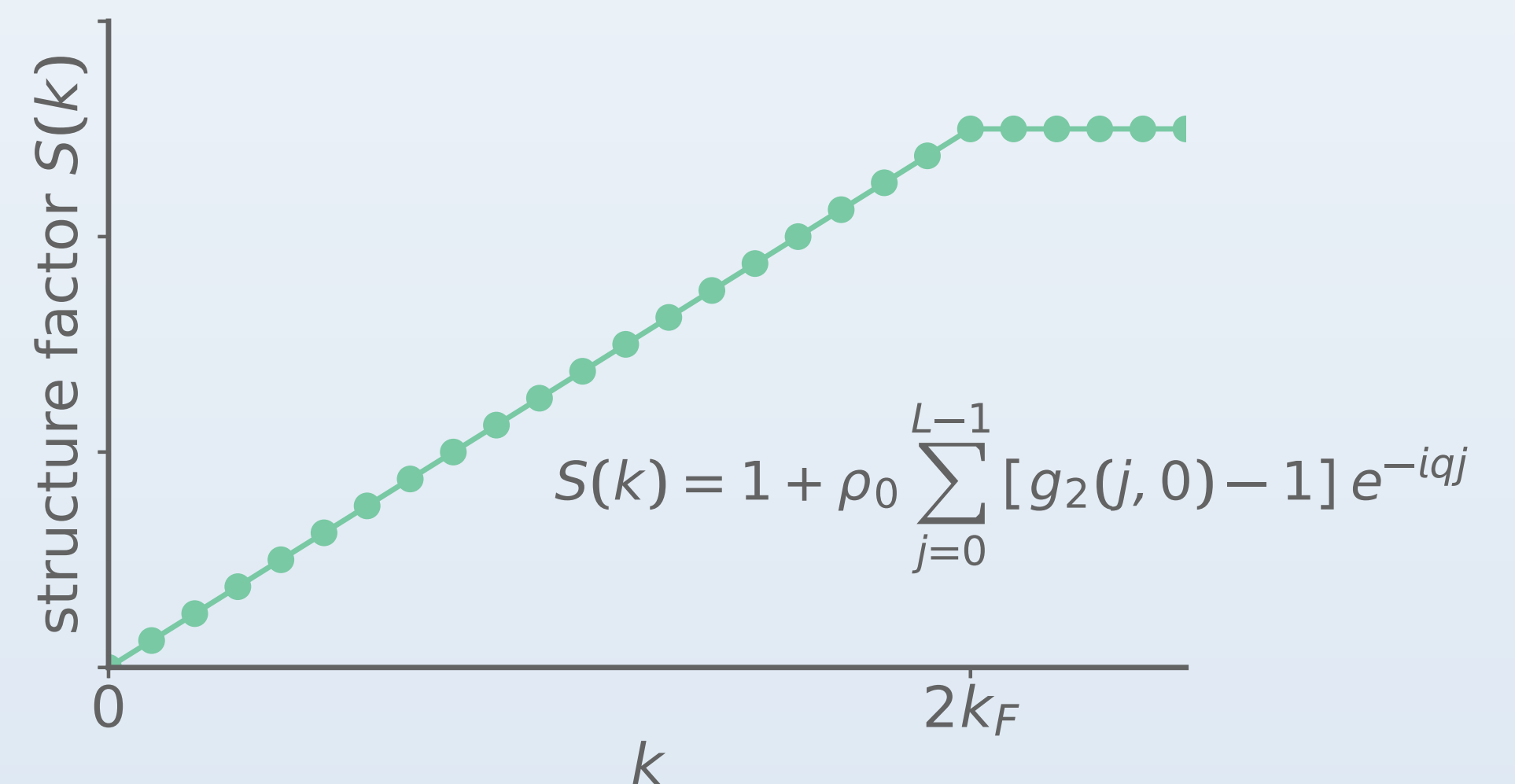
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Example: free fermions - diagonal elements

pair correlation function



structure factor



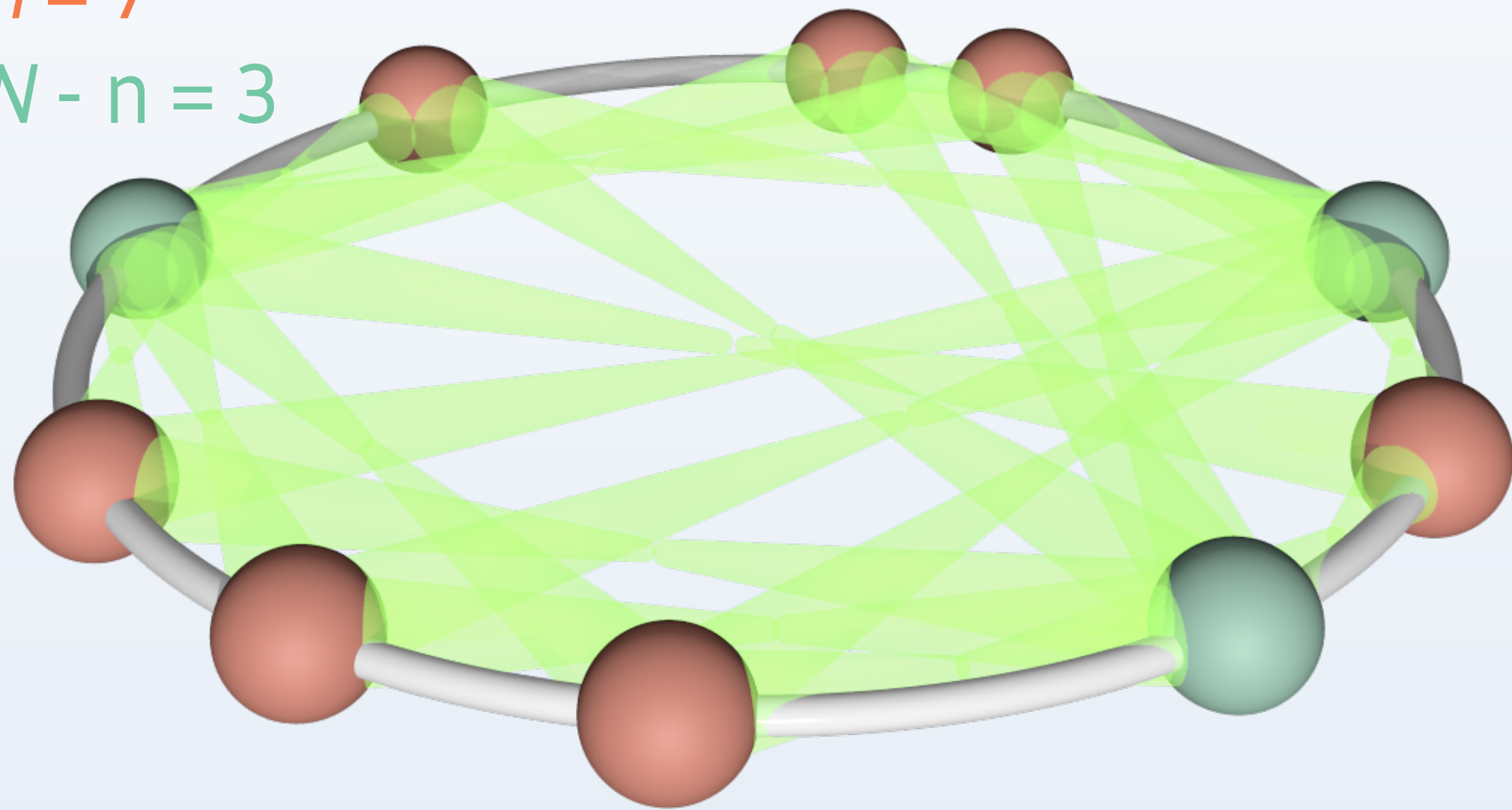
Particle Partition Entanglement

Non-classical information encoded **non-locally** in the n -particle state of a system quantified by von Neumann entropy of the n -RDM:

$$S(n) = -\text{Tr } \rho_n \ln \rho_n$$

$n = 7$

$N - n = 3$



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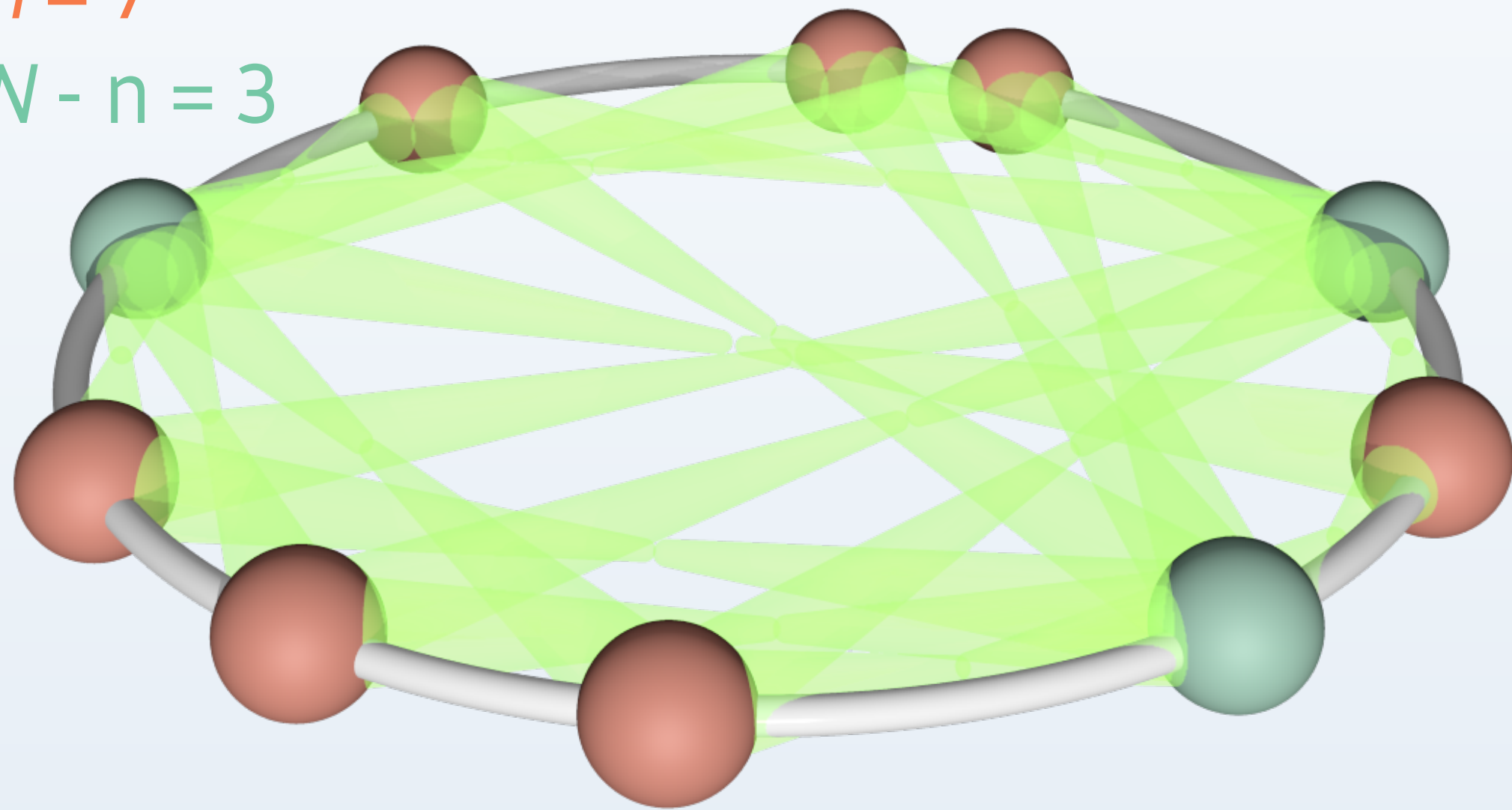
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Distinct/complementary to conventionally measured mode entanglement

- no imposed external length scale
- independent of modes
- strongly dependent on interactions
- sensitive to particle statistics at leading order!

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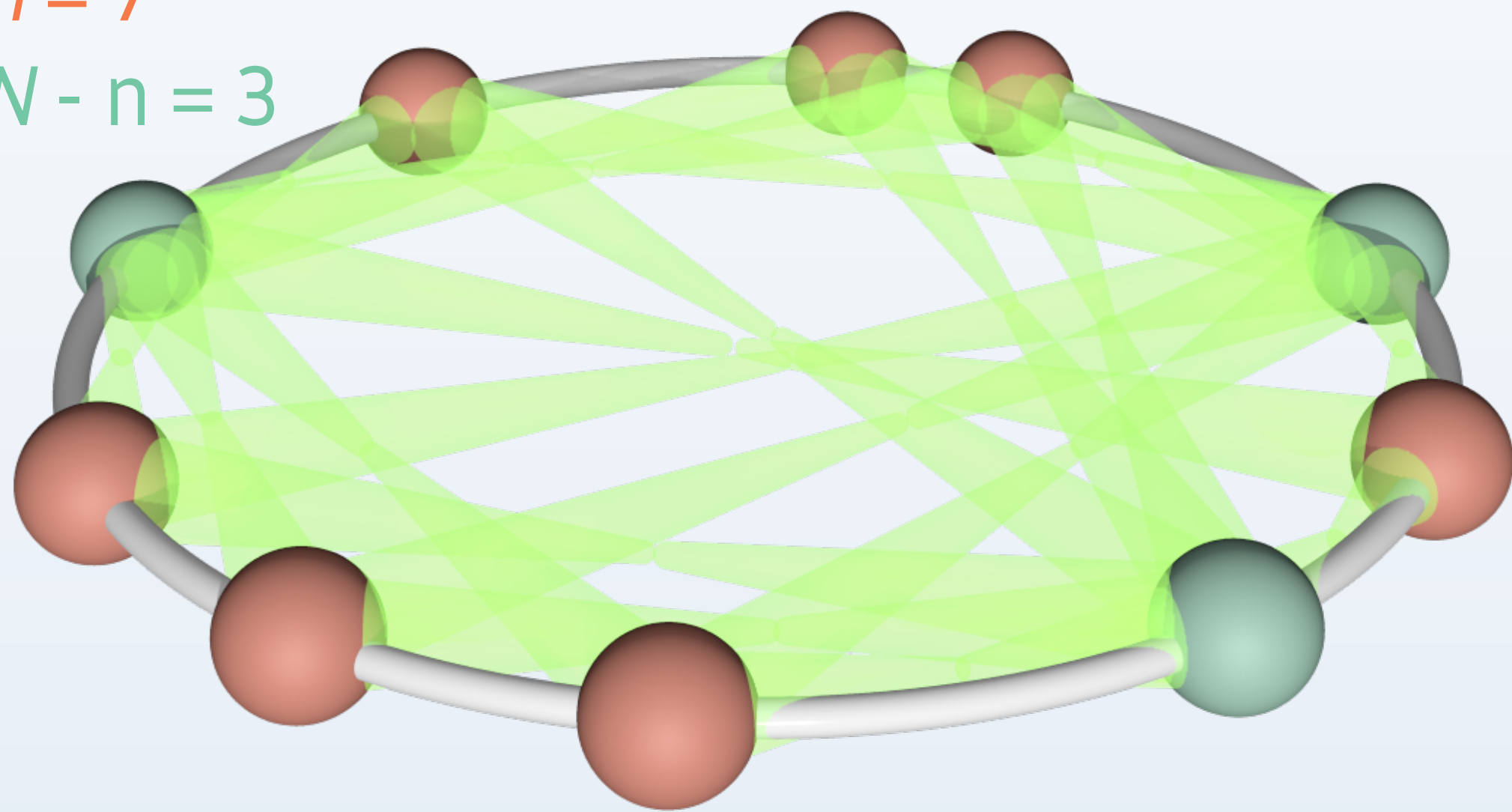
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non-interacting fermions: $S(n) = \ln \binom{N}{n}$

non-interacting bosons: $S(n) = 0$

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Lots to Learn About Particle Entanglement

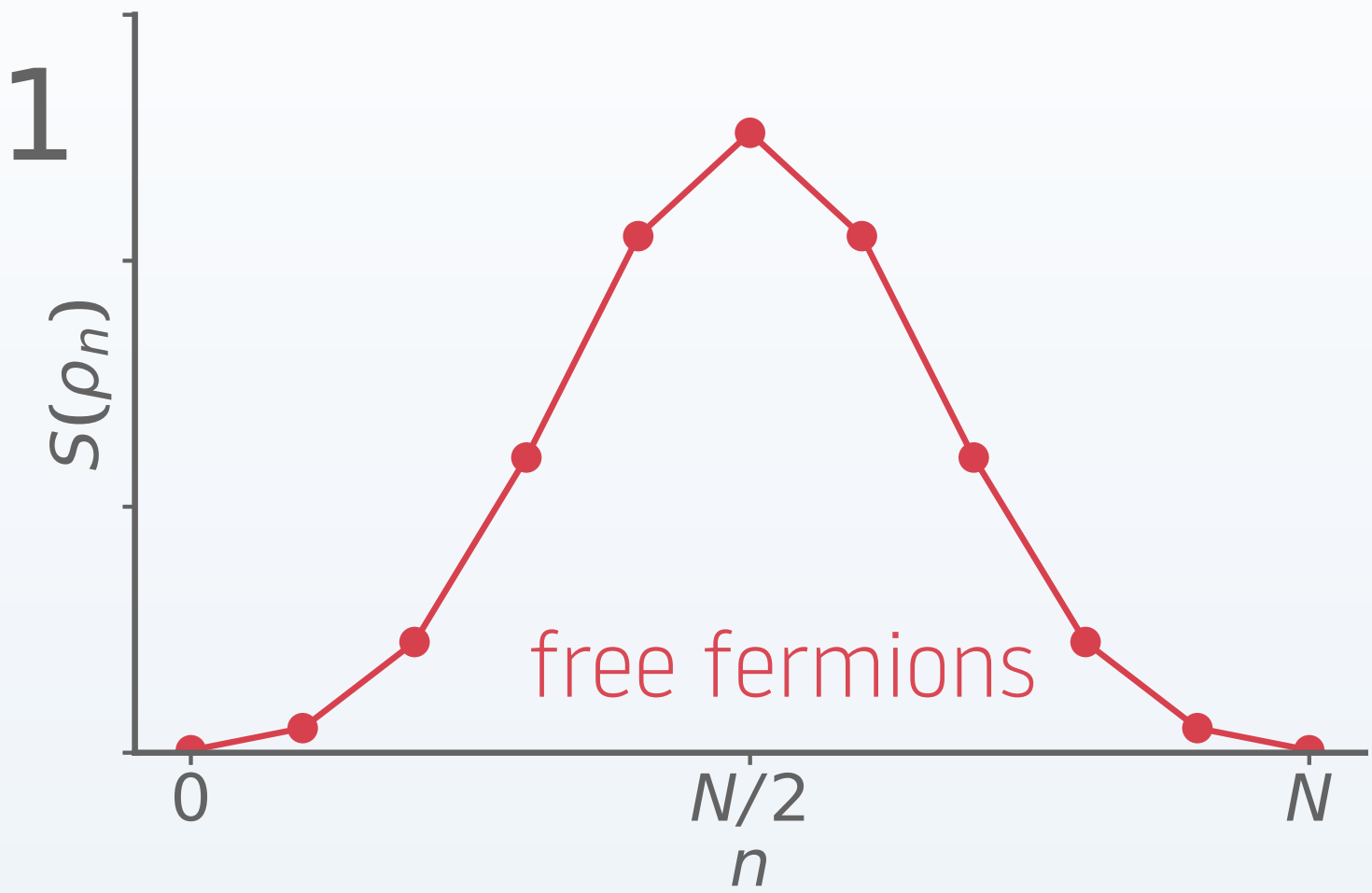
monotonicity: $S(\rho_n) \leq S(\rho_{n+1})$ for $1 \leq n \leq N/2 - 1$

reflection: $S(\rho_n) = S(\rho_{N-n})$

concavity: $S(\rho_n) \geq [S(\rho_{n+1}) + S(\rho_{n-1})]/2$

bounds $\ln N \leq S(\rho_1) \leq \ln L$

for fermions: $2S(\rho_1) - S(\rho_2) \geq \ln 2 - \ln(1 - e^{-S(\rho_1)})$



Lots to Learn About Particle Entanglement

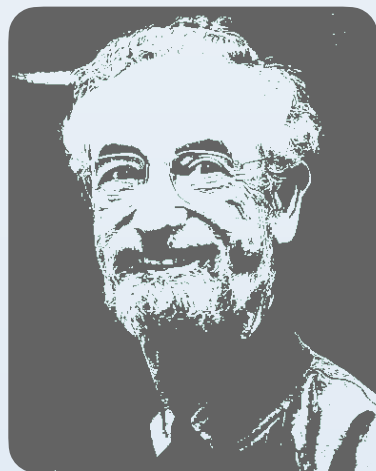
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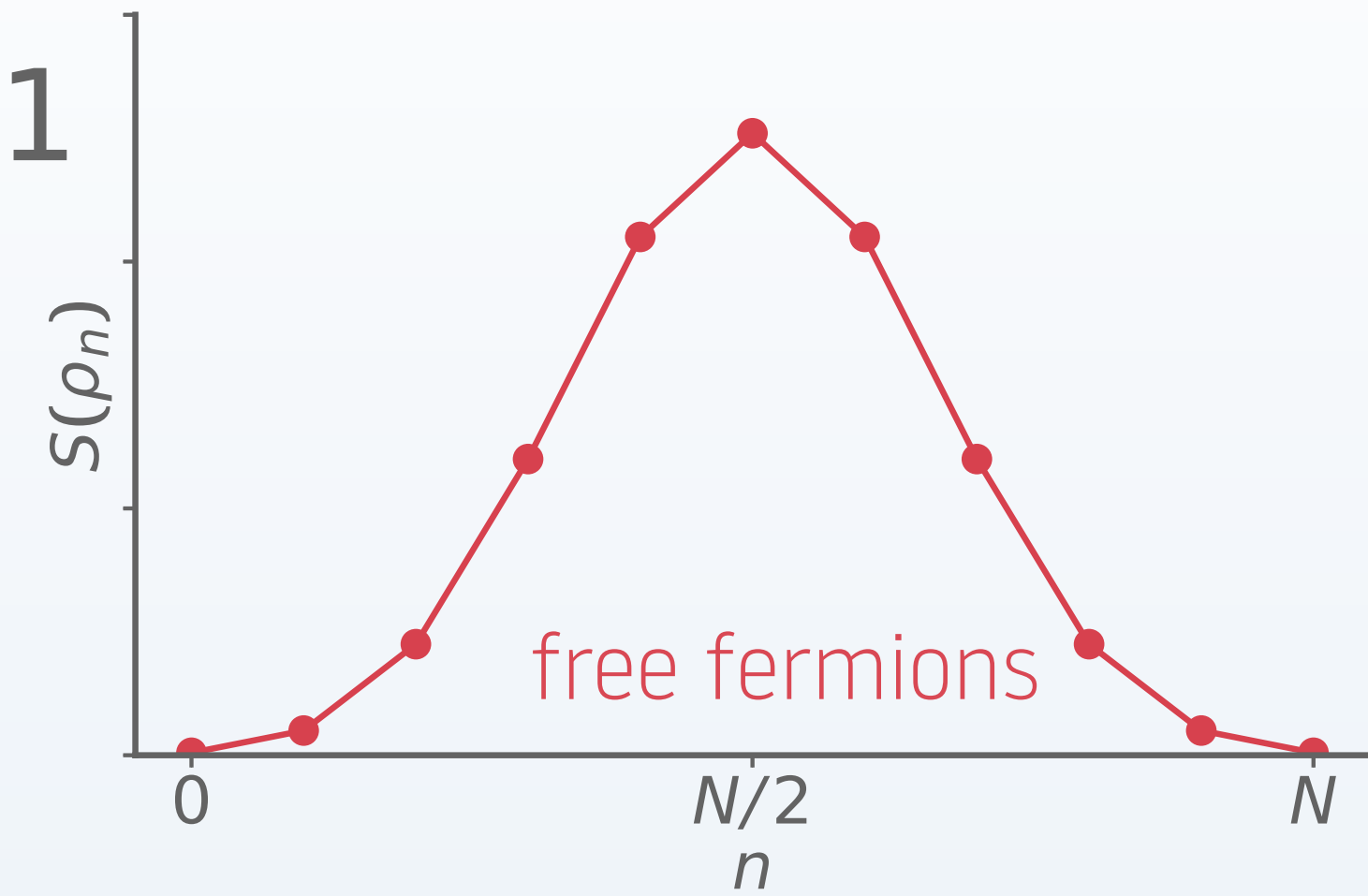
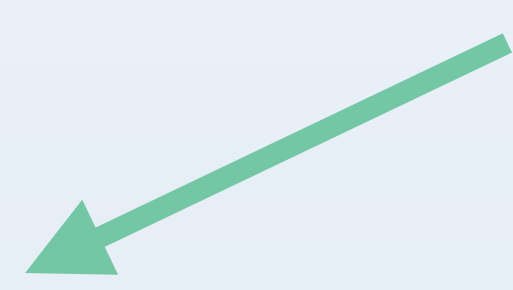
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 remains a conjecture!



$$S(\rho_2) \stackrel{?}{\geq} \ln \binom{N}{2}$$



Lots to Learn About Particle Entanglement

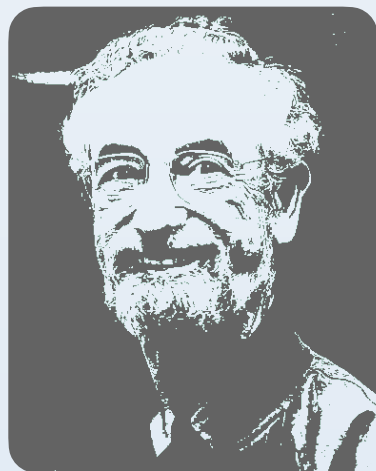
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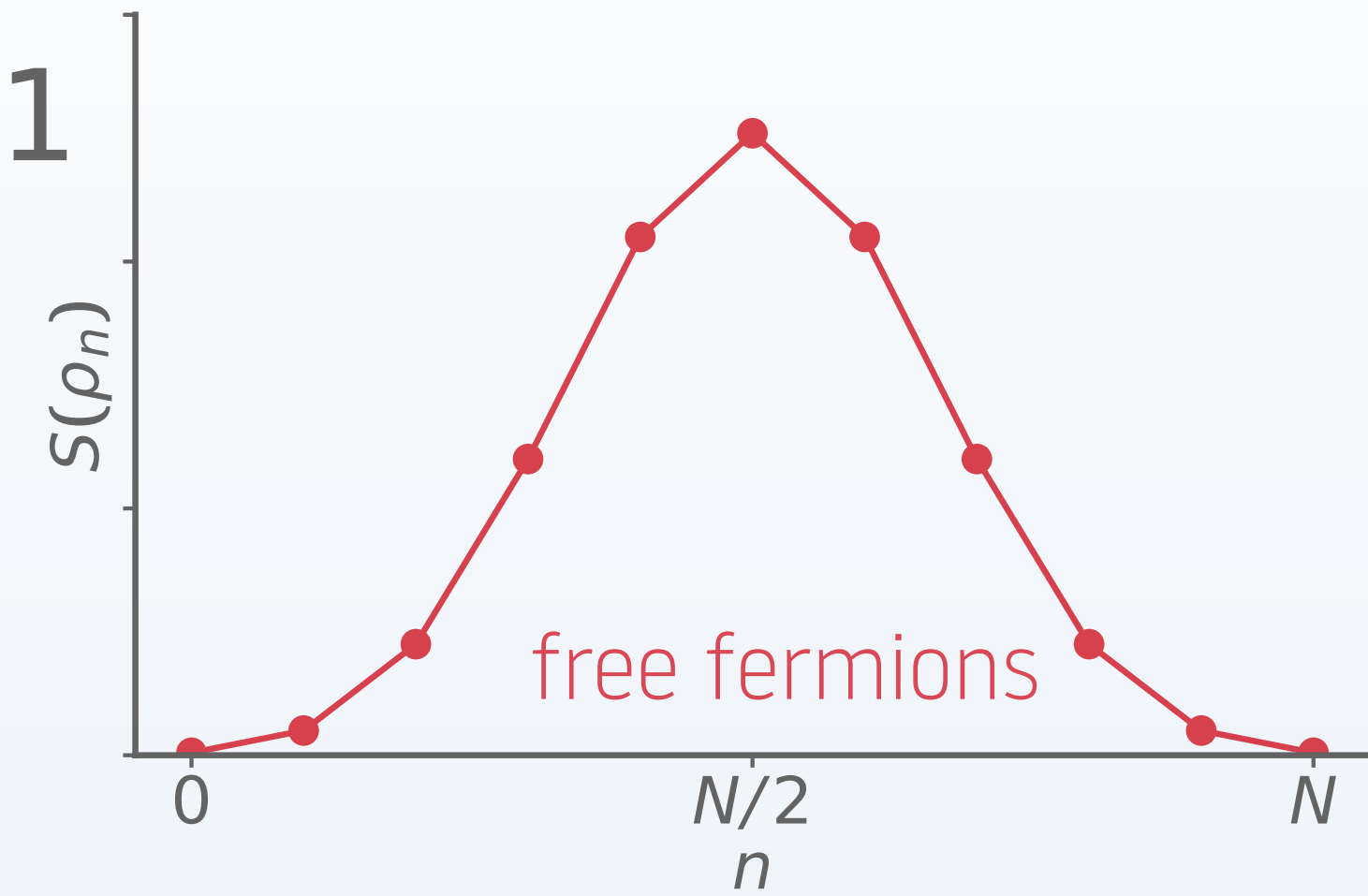
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$$S(\rho_2) \stackrel{?}{\geq} \ln \binom{N}{2}$$

Can a system of interacting fermions be **less entangled** than free fermions?



*How can we compute n -RDMs
for finite sized strongly
interacting Fermi systems?*

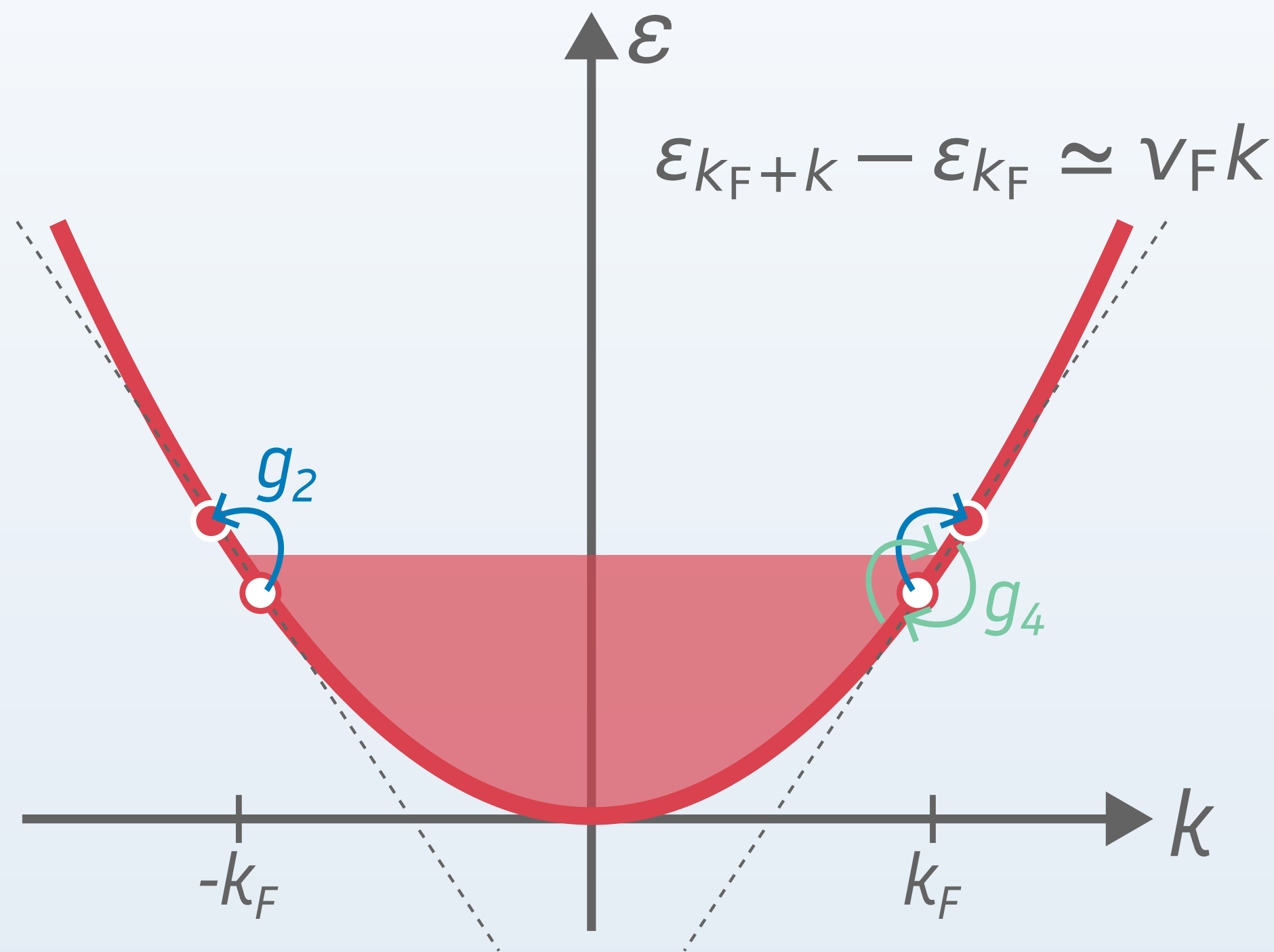


Tomonaga-Luttinger Model



Interacting fermions in 1D with forward scattering and a linearized dispersion

$$H = -\frac{1}{2M} \int dx \psi^\dagger(x) \nabla_x^2 \psi(x) + \int dx' \int dx \varrho(x') V(x' - x) \varrho(x) \longleftarrow \varrho(x) = \psi^\dagger(x) \psi(x)$$



- S. Tomonaga, Prog. Theor. Phys. 5, 544 (1950)
- J. M. Luttinger, J Math Phys. 4, 1154 (1963)
- D. C. Mattis and E. H. Lieb, J Math. Phys. 6, 304 (1965)
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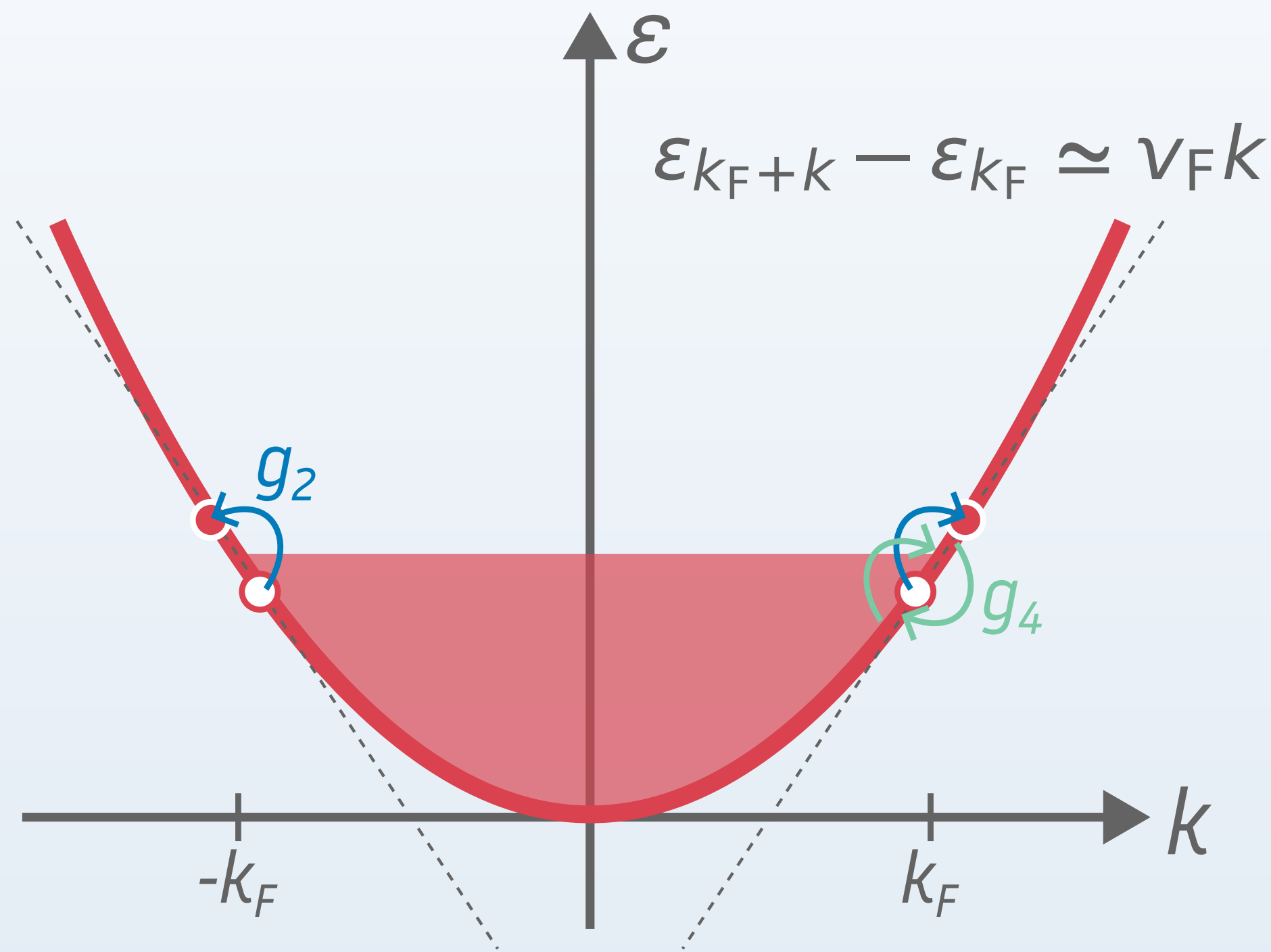


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Exactly solvable via bosonization!

$$\Psi(x) = e^{ik_F x} \Psi_L(x) + e^{-ik_F x} \Psi_R(x)$$

$$\Psi_\alpha(x) = \frac{\chi_\alpha}{\sqrt{2\pi\eta}} e^{i(\varphi_{0,\alpha} + \alpha \frac{2\pi x}{L} N_\alpha)} e^{-i\phi_\alpha(x)}$$

$$\varrho_\alpha(x) = \frac{N_\alpha}{L} + \frac{\alpha}{2\pi} \partial_x \varphi_\alpha(x)$$

↑
exponentiated
boson field

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J. von Delft, H. Schoeller, Ann. Phys. 7 225, (1998)

Constructive Bosonization

$$\phi_\alpha(x) = - \sum_{q>0} \sqrt{\frac{2\pi}{qL}} e^{-q\eta/2} \left[e^{i\alpha qx} b_{\alpha q} + e^{-i\alpha qx} b_{\alpha q}^\dagger \right] \leftarrow \text{mode decomposition}$$

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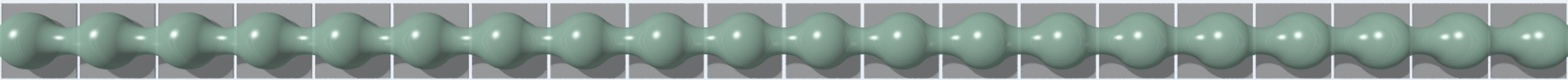
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$$= \text{z.m.} + \sum_{q \neq 0} v|q| a_q^\dagger a_q \quad \rightarrow \quad H = \frac{v}{2\pi} \int dx \left[\frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right]$$

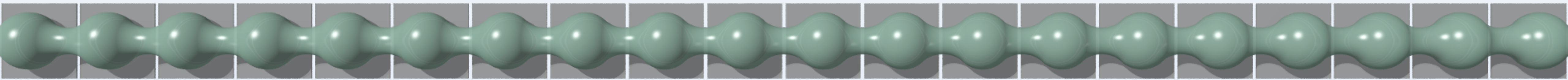


Constructive Bosonization

$$\phi_\alpha(x) = - \sum_{q>0} \sqrt{\frac{2\pi}{qL}} e^{-q\eta/2} \left[e^{i\alpha qx} b_{\alpha q} + e^{-i\alpha qx} b_{\alpha q}^\dagger \right] \quad \leftarrow \text{mode decomposition}$$

$$H = \sum_{q \neq 0} [\omega_0(q) + m(q)] b_q^\dagger b_q + \frac{1}{2} \sum_{q \neq 0} g_2(q) (b_q b_{-q} + b_q^\dagger b_{-q}^\dagger)$$

$$= \text{z.m.} + \sum_{q \neq 0} v|q| a_q^\dagger a_q \quad \rightarrow \quad H = \frac{v}{2\pi} \int dx \left[\frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right]$$



Can compute any fermionic correlation function via Bose-cumulant formula

$$\langle e^{i(\phi_\alpha(x) - \phi_\alpha(0))} \rangle = e^{-\frac{1}{2} \langle (\phi_\alpha(x) - \phi_\alpha(0))^2 \rangle}$$

well known, see, e.g. Giamarchi Appendix C

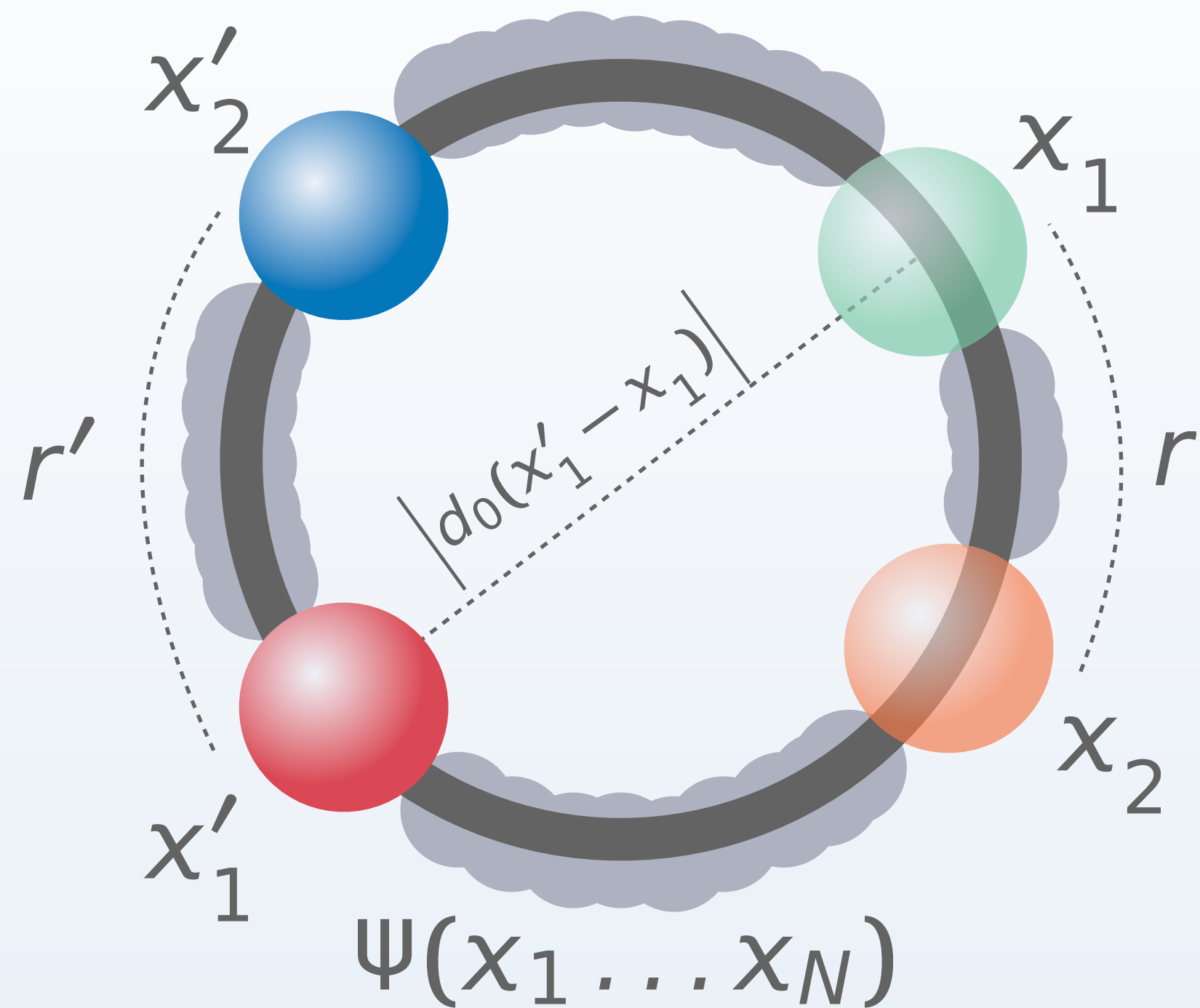
Vl. S. Dotsenko and V. A. Fateev, Nucl. Phys. B 240, 312 (1984)

or Tsvetlik Chap. 26-27

$$e^{-\frac{1}{2} \sum_{i < j} [-A_i A_j K - B_i B_j K^{-1}] F_1(r_i - r_j) + [A_i B_j + B_i A_j] F_2(r_i - r_j)} \quad (\text{C.38})$$

$$\langle A(1) \cdots A(4) \rangle = \left(\left| \frac{z_{13} z_{24}}{z_{12} z_{14} z_{23} z_{34}} \right| \right)^{4\Delta} G(x, \bar{x}) \quad (26.30)$$

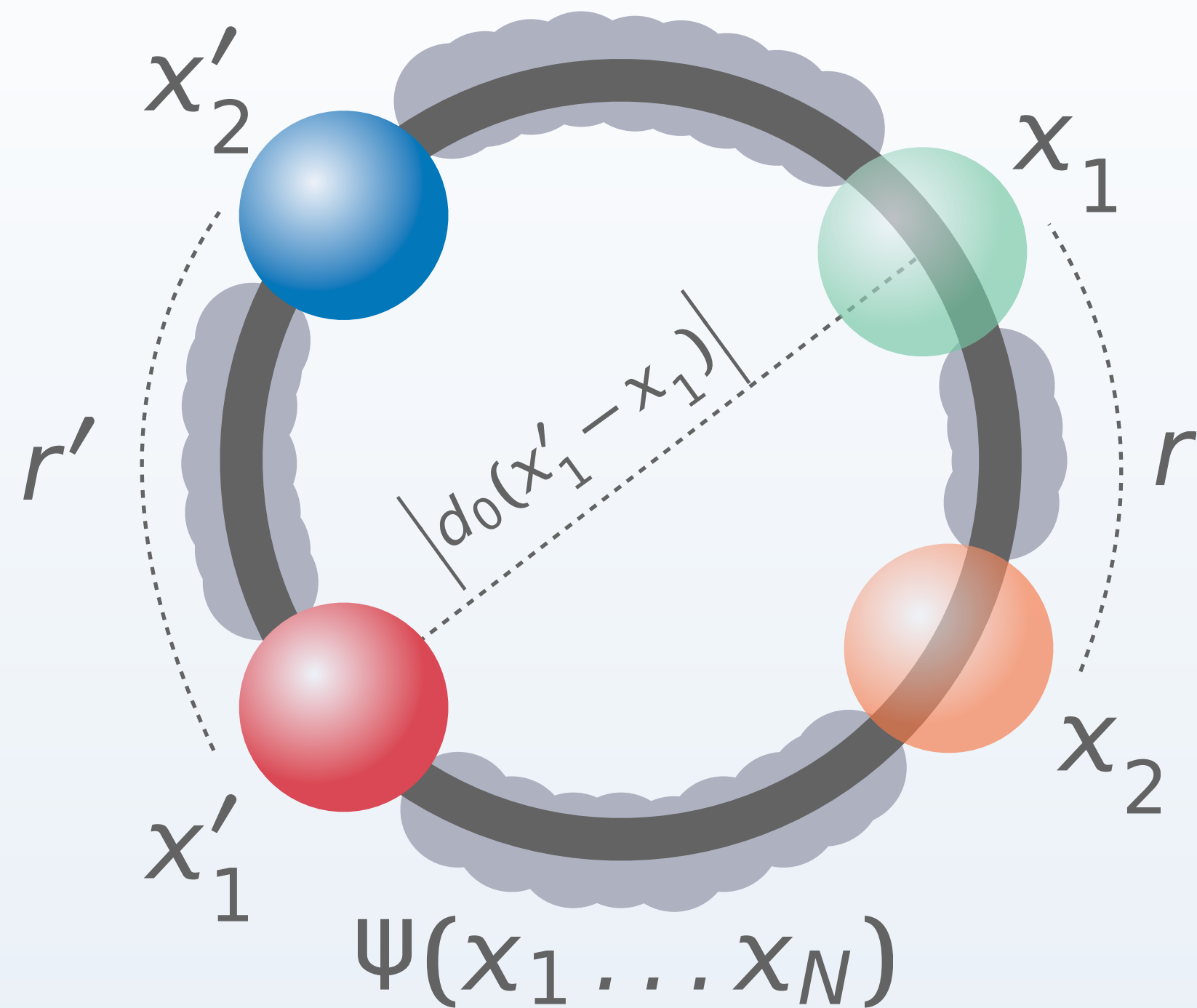
2-Particle Density Matrix: Bosonization



$$\rho_2(x'_2, x'_1, x_2, x_1) = \langle \Psi^\dagger(x'_2) \Psi^\dagger(x'_1) \Psi(x_1) \Psi(x_2) \rangle$$

Finite size L , periodic boundary conditions

2-Particle Density Matrix: Bosonization



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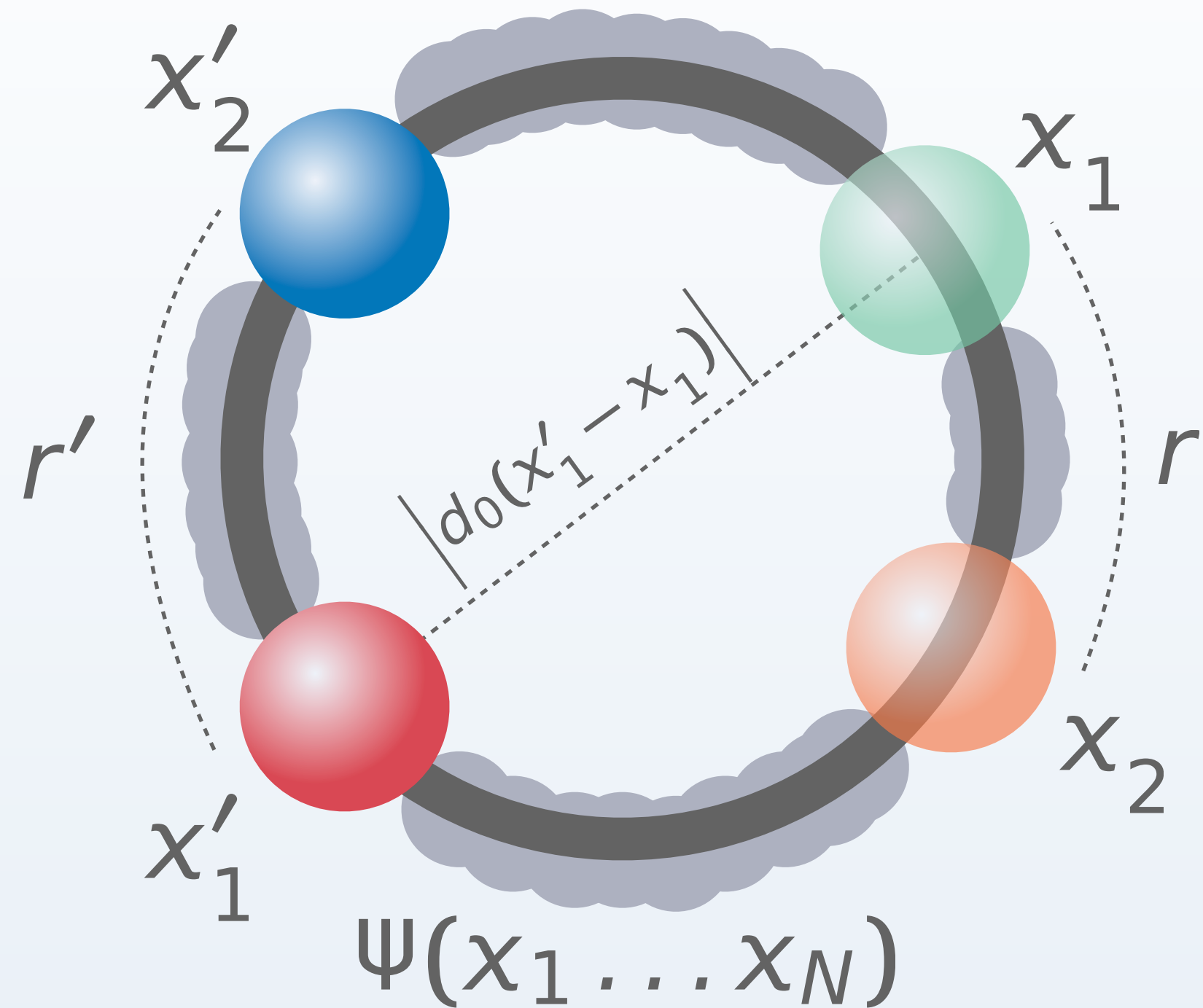
$$\langle \Psi_\alpha^\dagger(x'_2) \Psi_\alpha^\dagger(x'_1) \Psi_\alpha(x_1) \Psi_\alpha(x_2) \rangle$$

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6 surviving terms

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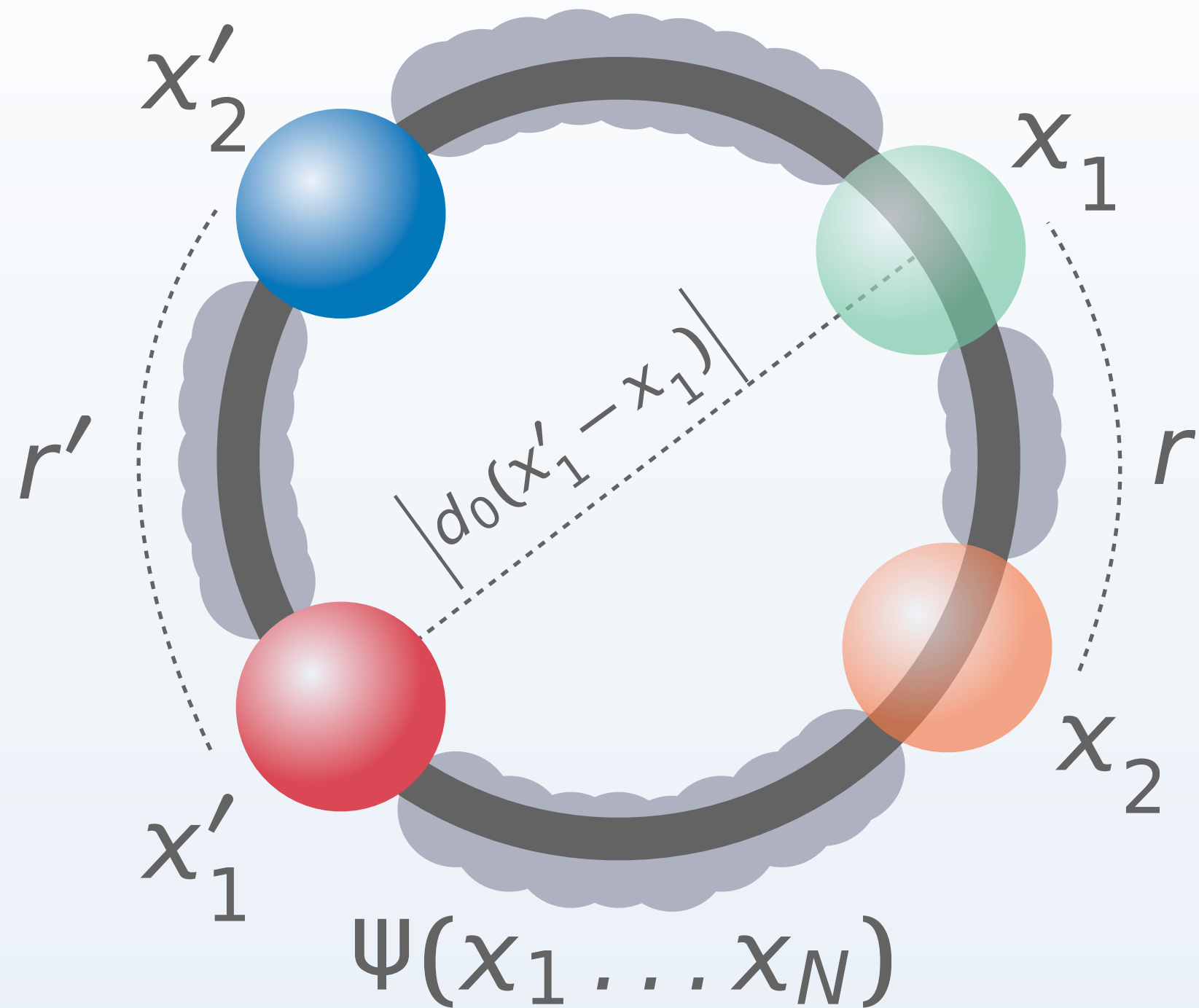
6 surviving terms

$$d_\epsilon(x) = \frac{L}{\pi} \sin \left[\frac{\pi}{L} (x + i\epsilon) \right]$$

$$h_\epsilon(x, y) = d_\epsilon(x) d_\epsilon(y)$$

$$\begin{aligned} \langle \Psi^\dagger(x'_2) \Psi^\dagger(x'_1) \Psi(x_1) \Psi(x_2) \rangle &= \frac{\cos(k_F(x'_2 + x'_1 - x_2 - x_1))}{2\pi^2} \left[\frac{h_0(x'_2 - x'_1, x_2 - x_1)}{h_0(x'_2 - x_2, x'_1 - x_1) h_0(x'_2 - x_1, x'_1 - x_2)} \right] \left| \frac{h_\epsilon(0, 0) h_\epsilon(x'_2 - x'_1, x_2 - x_1)}{h_\epsilon(x'_2 - x_2, x'_1 - x_1) h_\epsilon(x'_2 - x_1, x'_1 - x_2)} \right|^{\gamma^2} \\ &+ \frac{\cos(k_F(x'_2 - x'_1 - x_2 + x_1))}{2\pi^2} \left[\frac{1}{h_0(x'_2 - x_2, x'_1 - x_1)} \right] \left| \frac{h_\epsilon(0, 0)}{h_\epsilon(x'_2 - x_2, x'_1 - x_1)} \right|^{\gamma^2} \left| \frac{h_\epsilon(x'_2 - x'_1, x_2 - x_1)}{h_\epsilon(x'_2 - x_1, x'_1 - x_2)} \right|^\lambda \\ &- \frac{\cos(k_F(x'_2 - x'_1 + x_2 - x_1))}{2\pi^2} \left[\frac{1}{h_0(x'_2 - x_1, x'_1 - x_2)} \right] \left| \frac{h_\epsilon(0, 0)}{h_\epsilon(x'_2 - x_1, x'_1 - x_2)} \right|^{\gamma^2} \left| \frac{h_\epsilon(x'_2 - x'_1, x_2 - x_1)}{h_\epsilon(x'_2 - x_2, x'_1 - x_1)} \right|^\lambda \end{aligned}$$

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Finite size L , periodic boundary conditions

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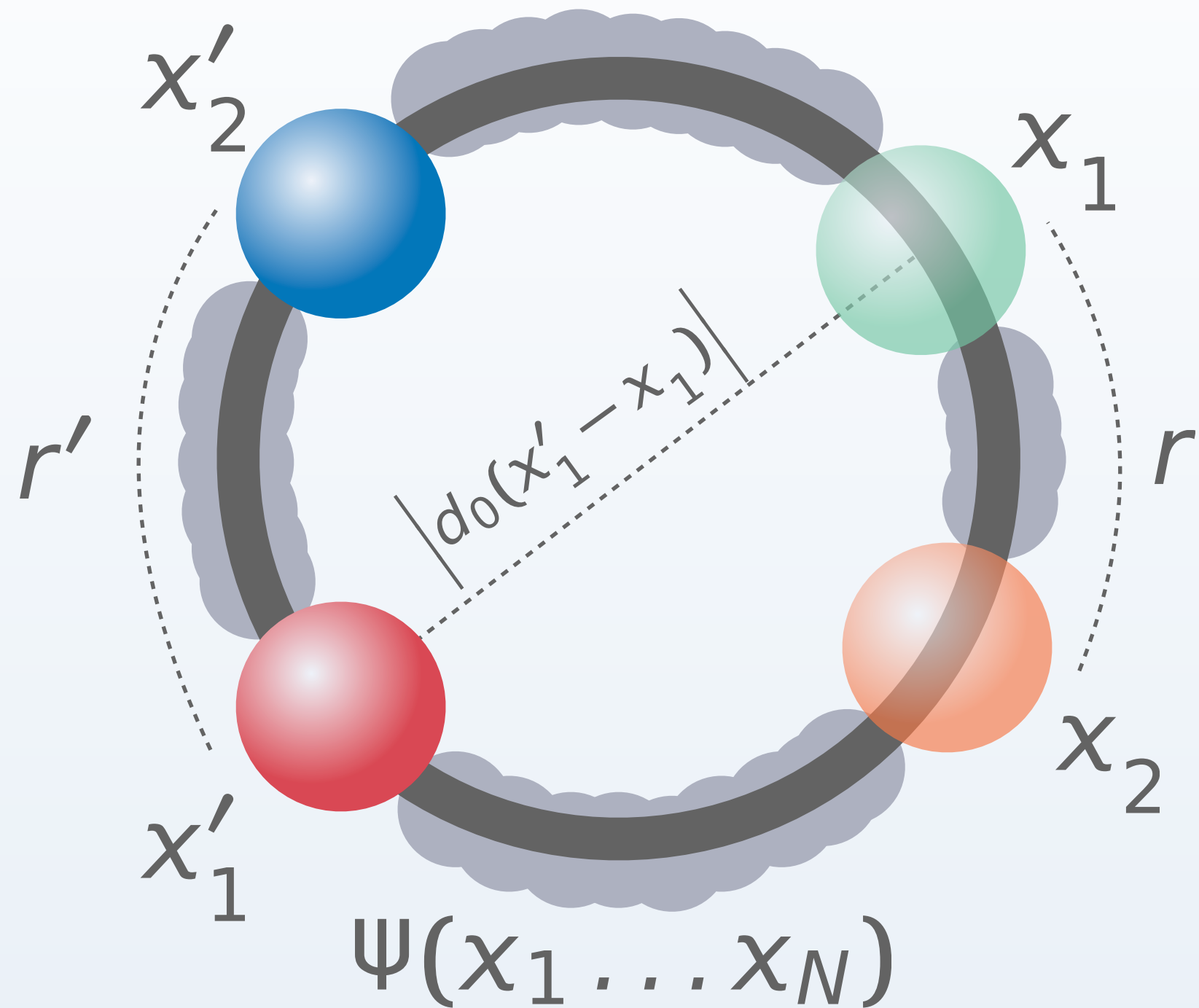
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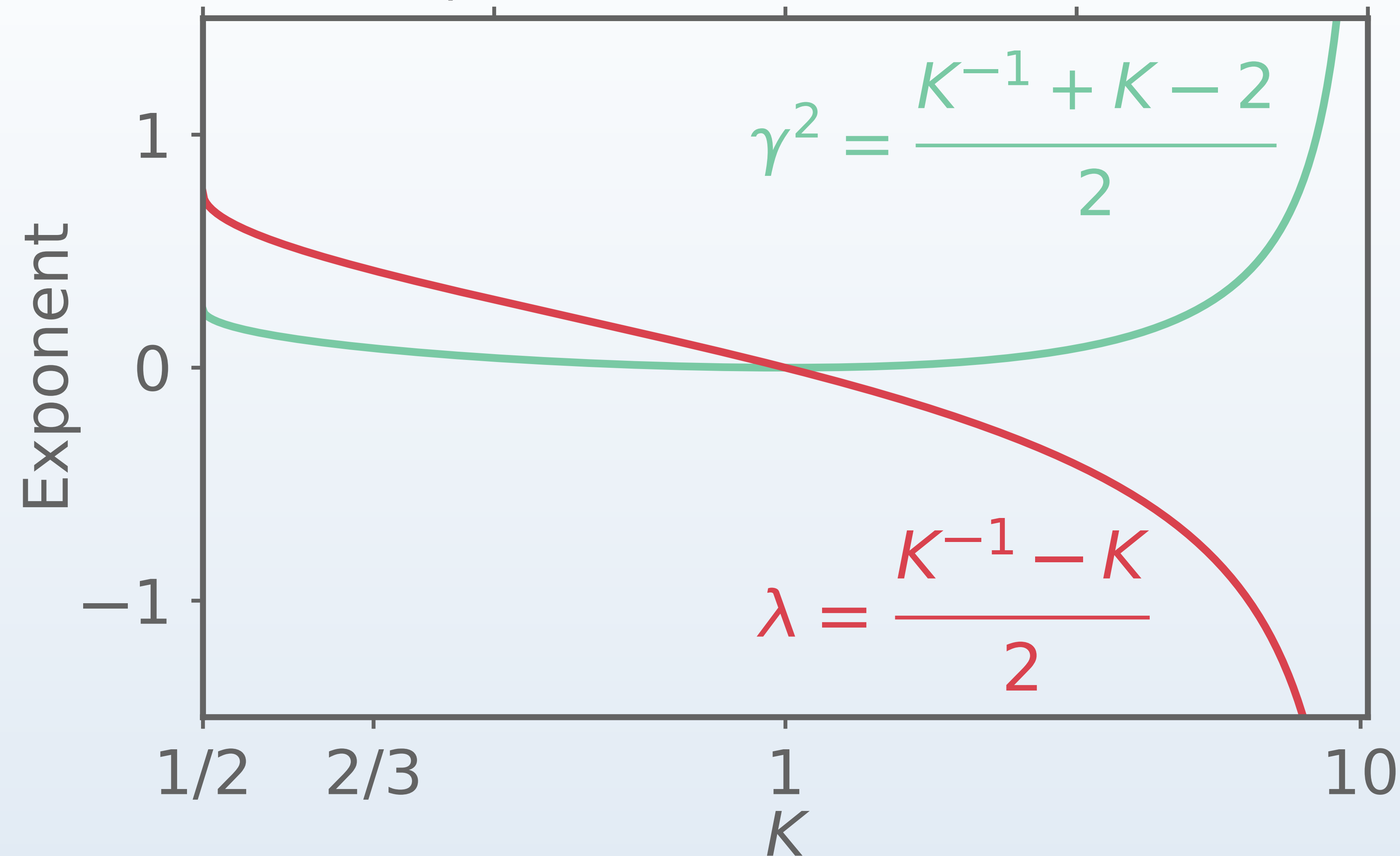
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new!

2-RDM: Interaction Exponents

repulsive

attractive



$$\rho_2(x'_2, x'_1, x_1, x_2) \Big|_{\substack{K=1 \\ \gamma^2=\lambda=0}} = \langle \Psi^\dagger(x'_2) \Psi(x_2) \rangle_0 \langle \Psi^\dagger(x'_1) \Psi(x_1) \rangle_0 - \langle \Psi^\dagger(x'_2) \Psi(x_1) \rangle_0 \langle \Psi^\dagger(x'_1) \Psi(x_2) \rangle_0$$

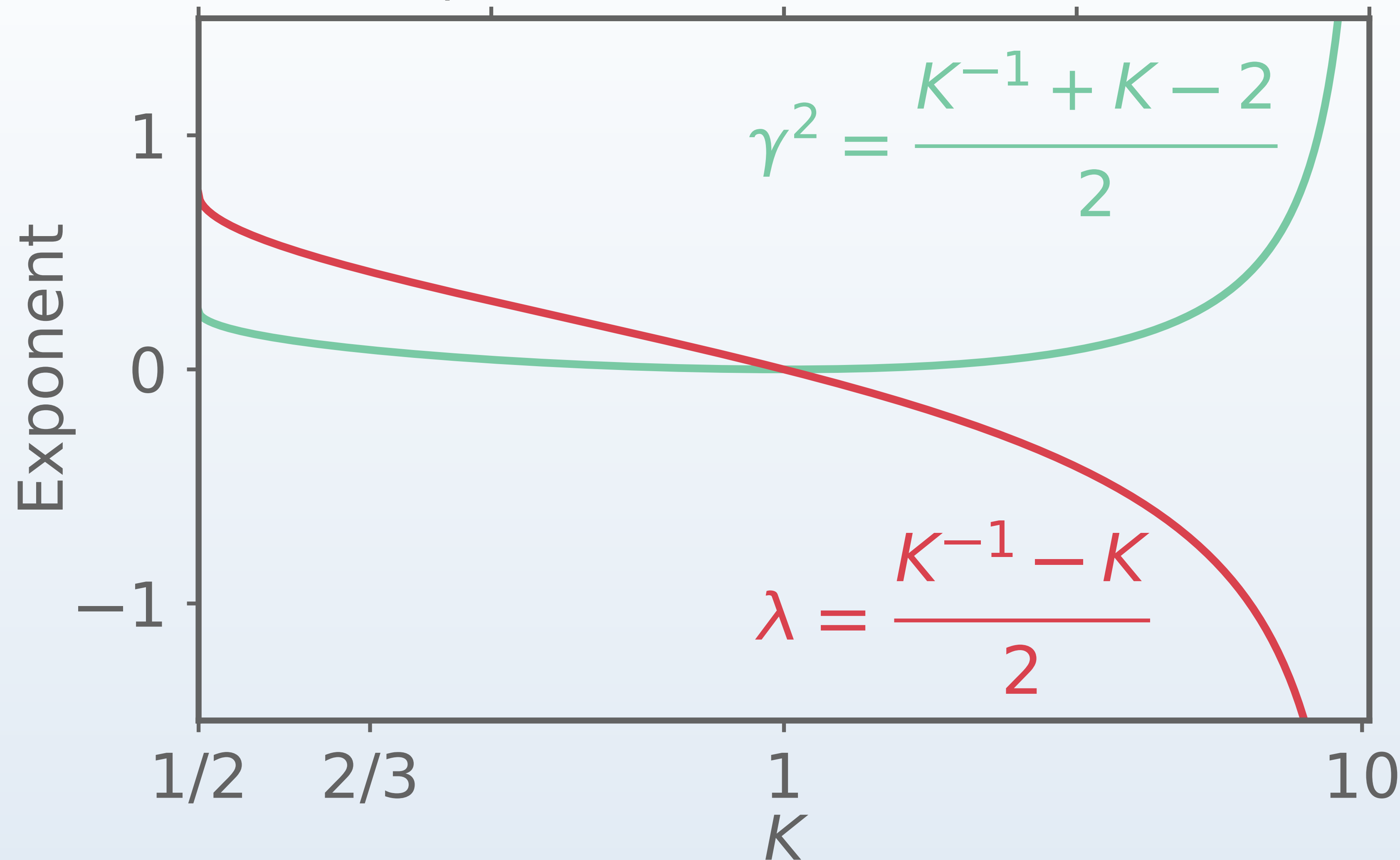
2-RDM: Interaction Exponents

repulsive

attractive

$$\gamma^2 = \frac{K^{-1} + K - 2}{2}$$

$$\lambda = \frac{K^{-1} - K}{2}$$



γ^2 appears in 1-RDM

$$\rho_1(x'_1, x_1) = \rho_{1,FF}(x'_1, x_1) \left| \frac{\sin(\pi i \epsilon / L)}{d_\epsilon(x'_1 - x_1)} \right|^{\gamma^2}$$

M. A. Cazalilla, Phys Rev Lett 97, 156403 (2006).

M. Thamm, H. Radhakrishnan, H. Barghathi, B. Rosenow, AD, Phys. Rev. B 106, 165116 (2022)

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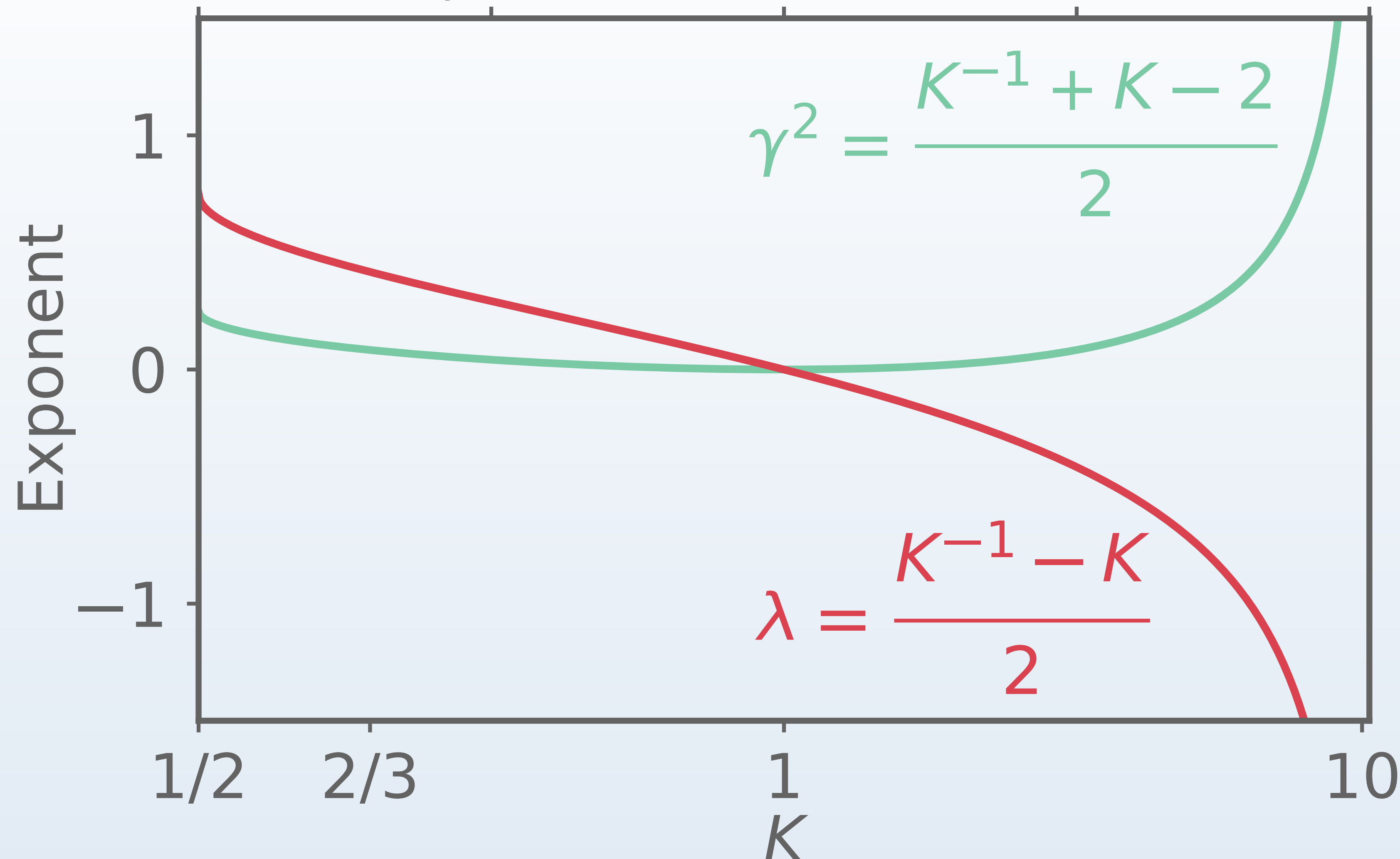
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Explore **interaction effects** related to λ

$$\rho_2(x'_2, x'_1, x_1, x_2) \Big|_{\substack{K=1 \\ \gamma^2=\lambda=0}} = \langle \Psi^\dagger(x'_2) \Psi(x_2) \rangle_0 \langle \Psi^\dagger(x'_1) \Psi(x_1) \rangle_0 - \langle \Psi^\dagger(x'_2) \Psi(x_1) \rangle_0 \langle \Psi^\dagger(x'_1) \Psi(x_2) \rangle_0$$

2-RDM: Coordinates & Structure

$$\rho_2(x'_2, x'_1, x_2, x_1) = \langle \Psi^\dagger(x'_2) \Psi^\dagger(x'_1) \Psi(x_1) \Psi(x_2) \rangle$$

$$\Sigma R \equiv R' + R = \frac{1}{2}(x'_2 + x'_1 + x_2 + x_1) = \text{const.}$$

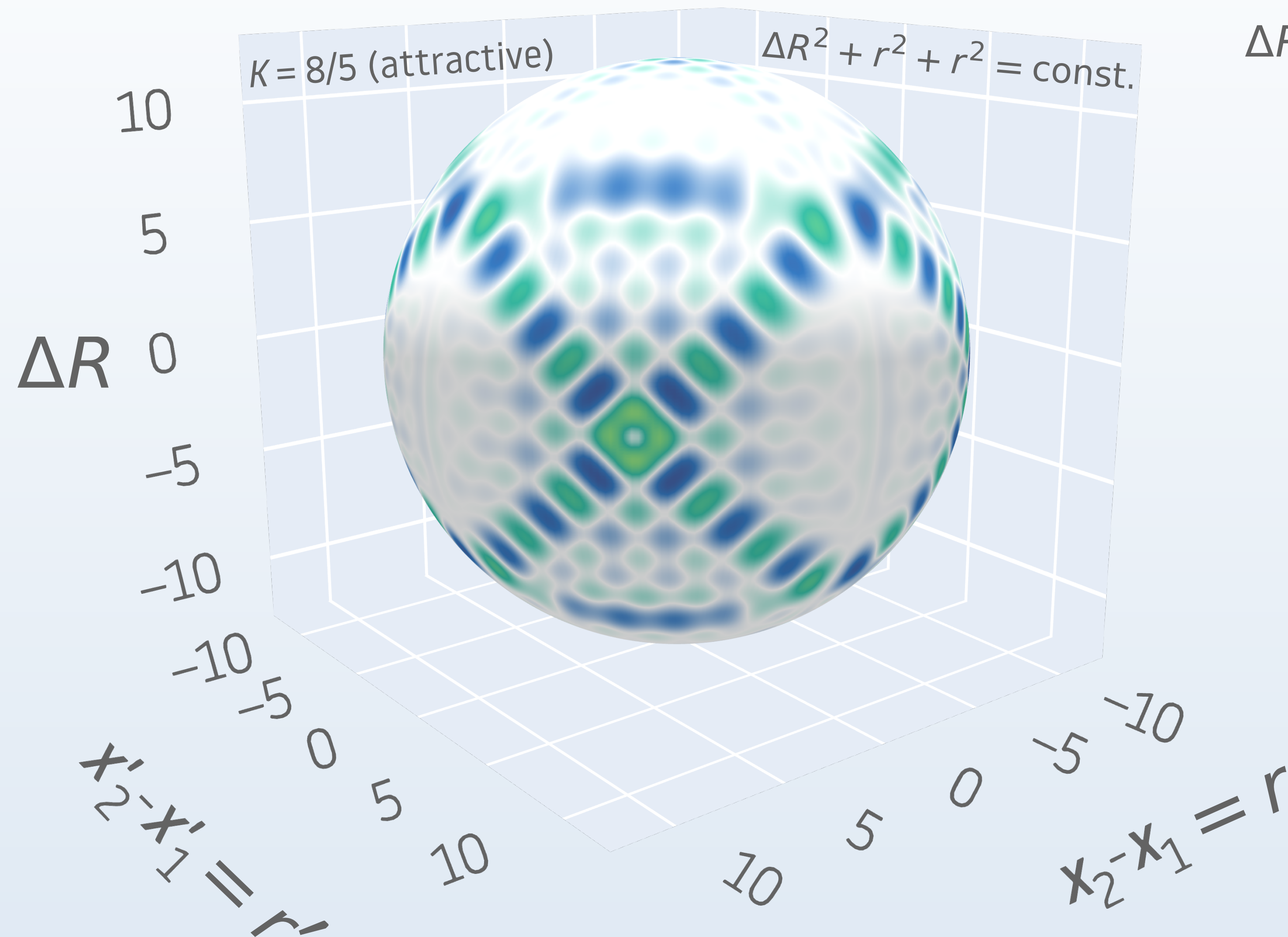
$$\Delta R = R' - R = \frac{1}{2}(x'_2 + x'_1 - x_2 - x_1)$$

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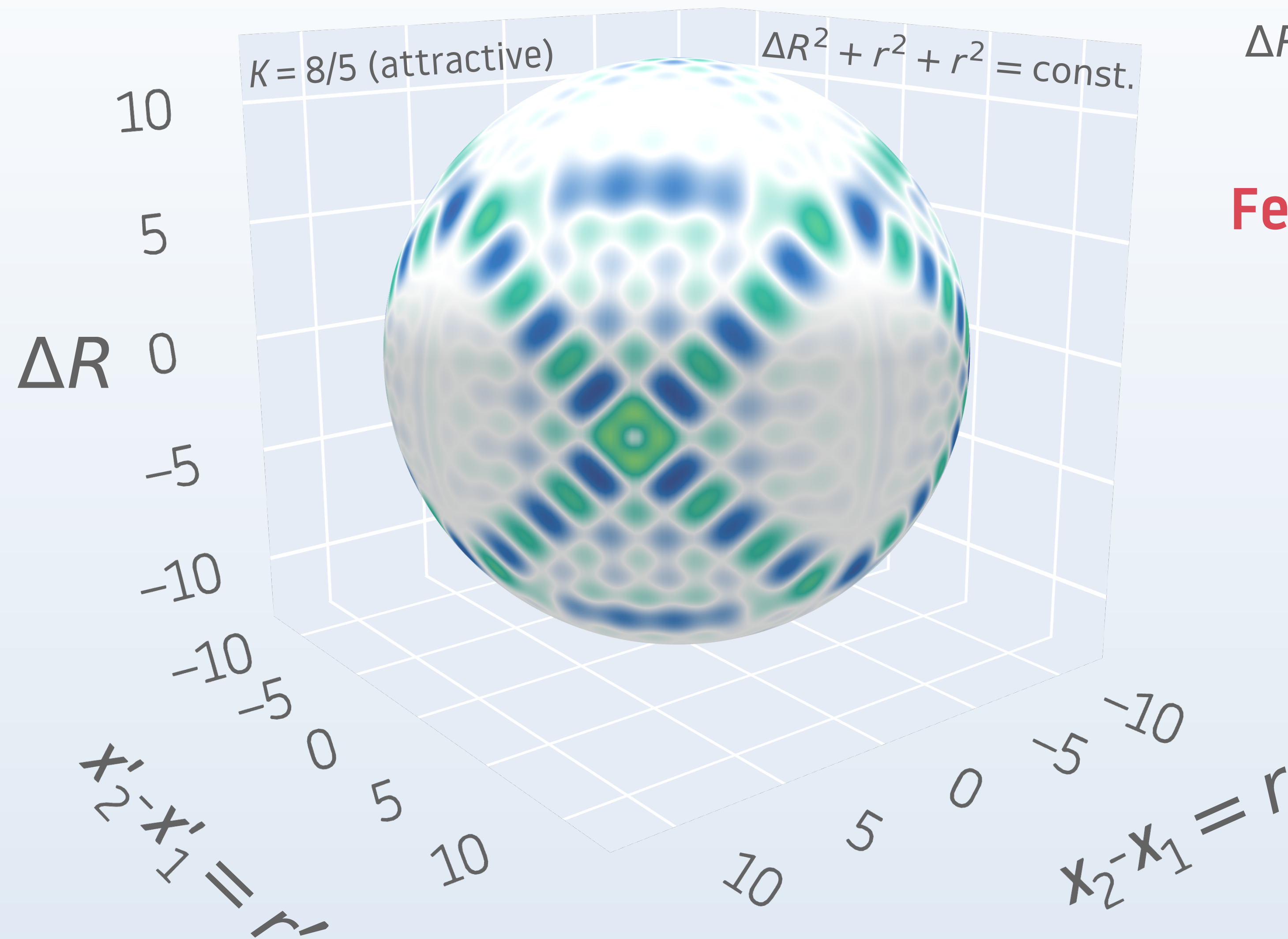


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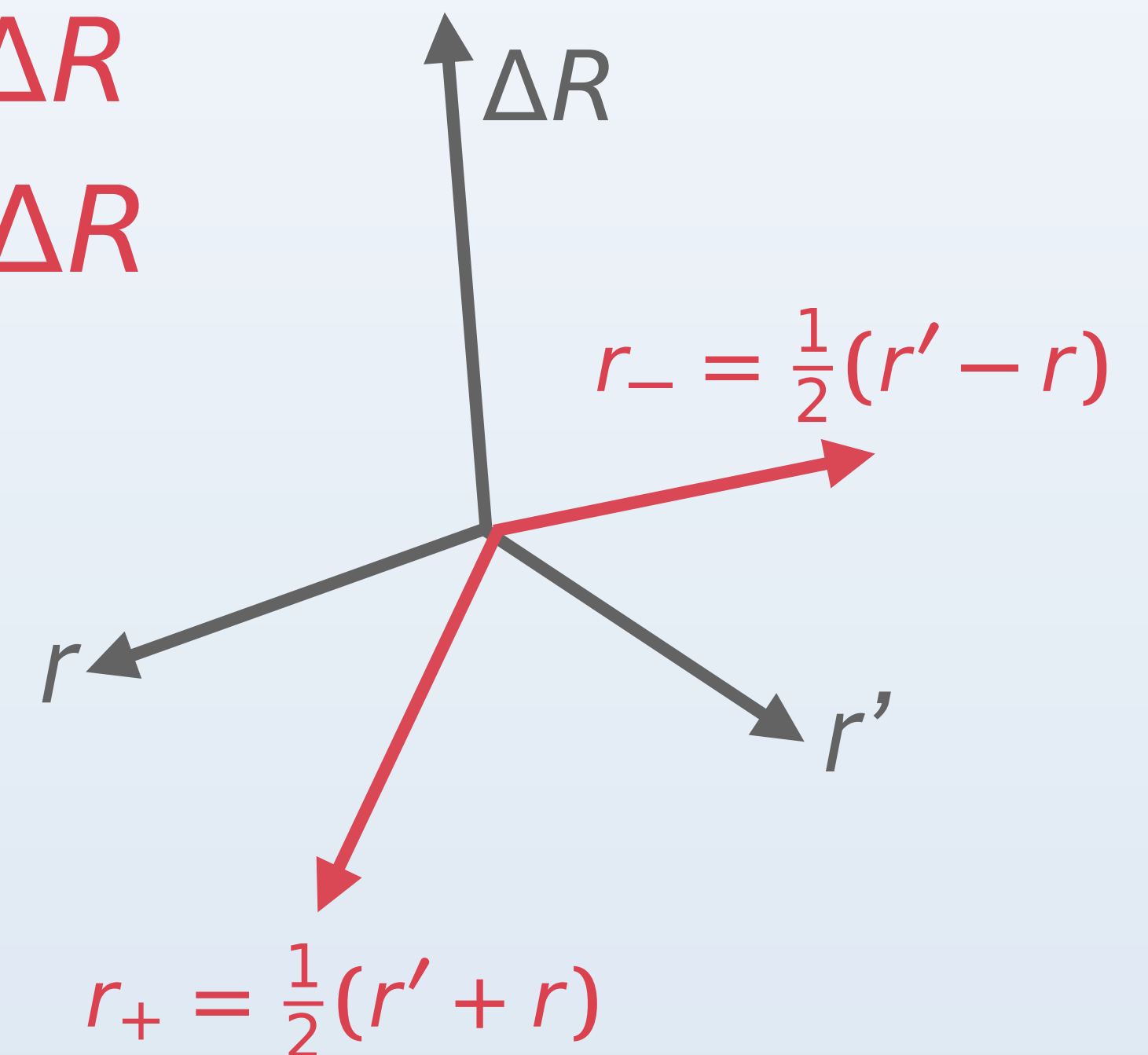
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Features: intersections of 4 hyperplanes

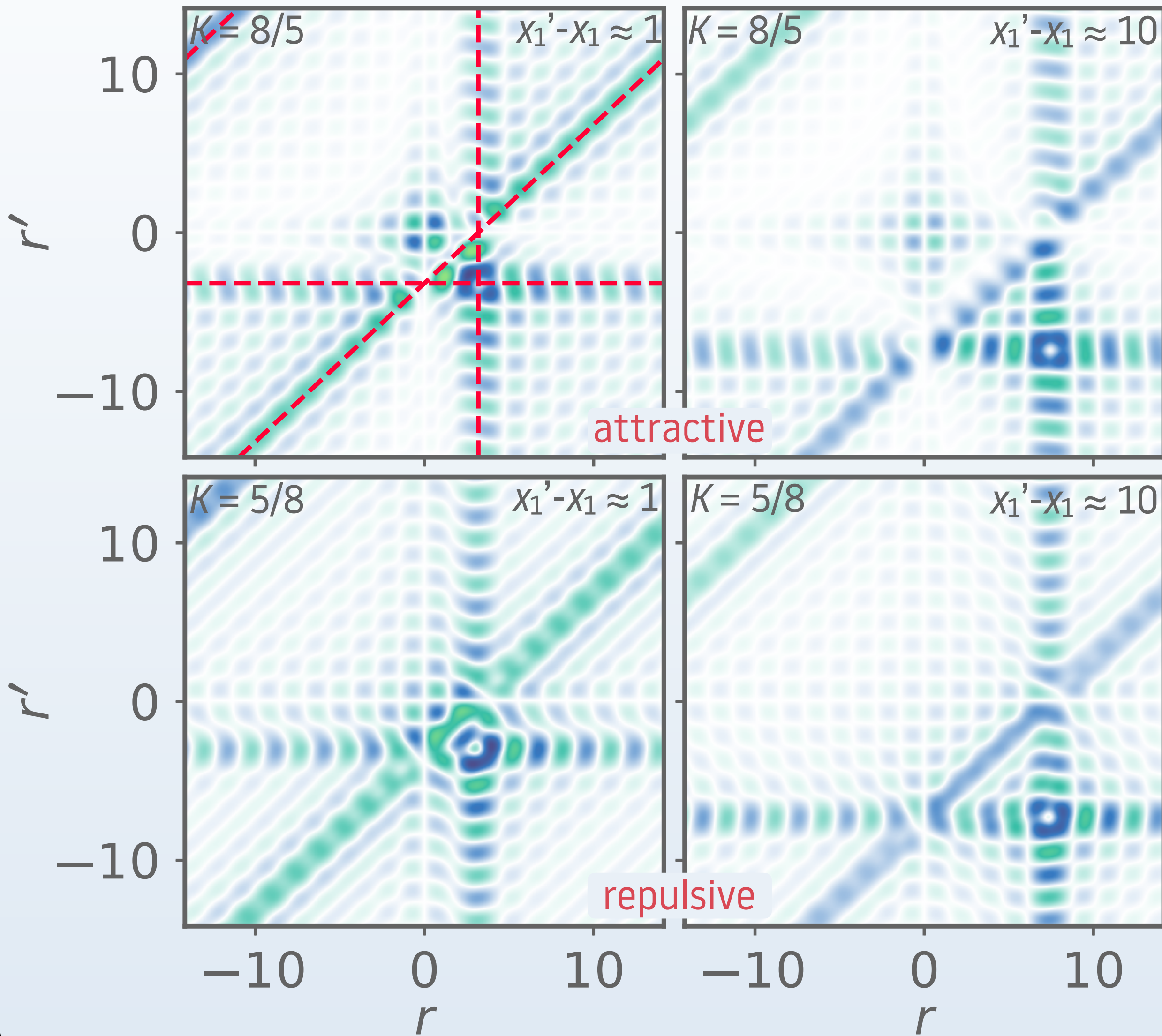
$$r_+ = \pm \Delta R$$

$$r_- = \pm \Delta R$$



2-RDM: Interaction Effects

$$\rho_2(x'_2, x'_1, x_2, x_1) - \rho_{2,FF}(x'_2, x'_1, x_2, x_1)$$

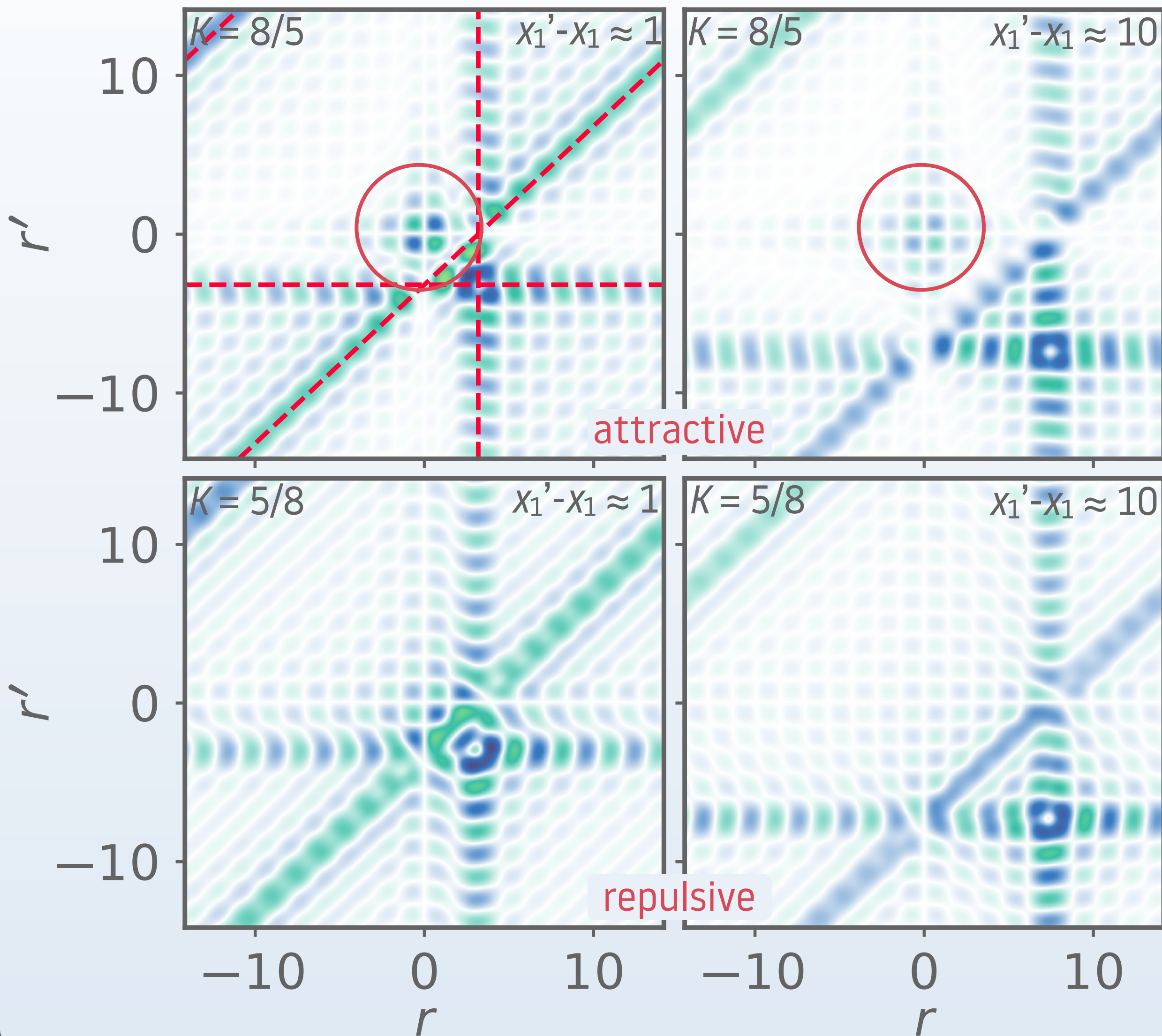


Explore: cut // to $x'_1 - x_1 = 0$

- Intersections w/ 3 other planes

2-RDM: Interaction Effects

$$\rho_2(x'_2, x'_1, x_2, x_1) - \rho_{2,FF}(x'_2, x'_1, x_2, x_1)$$

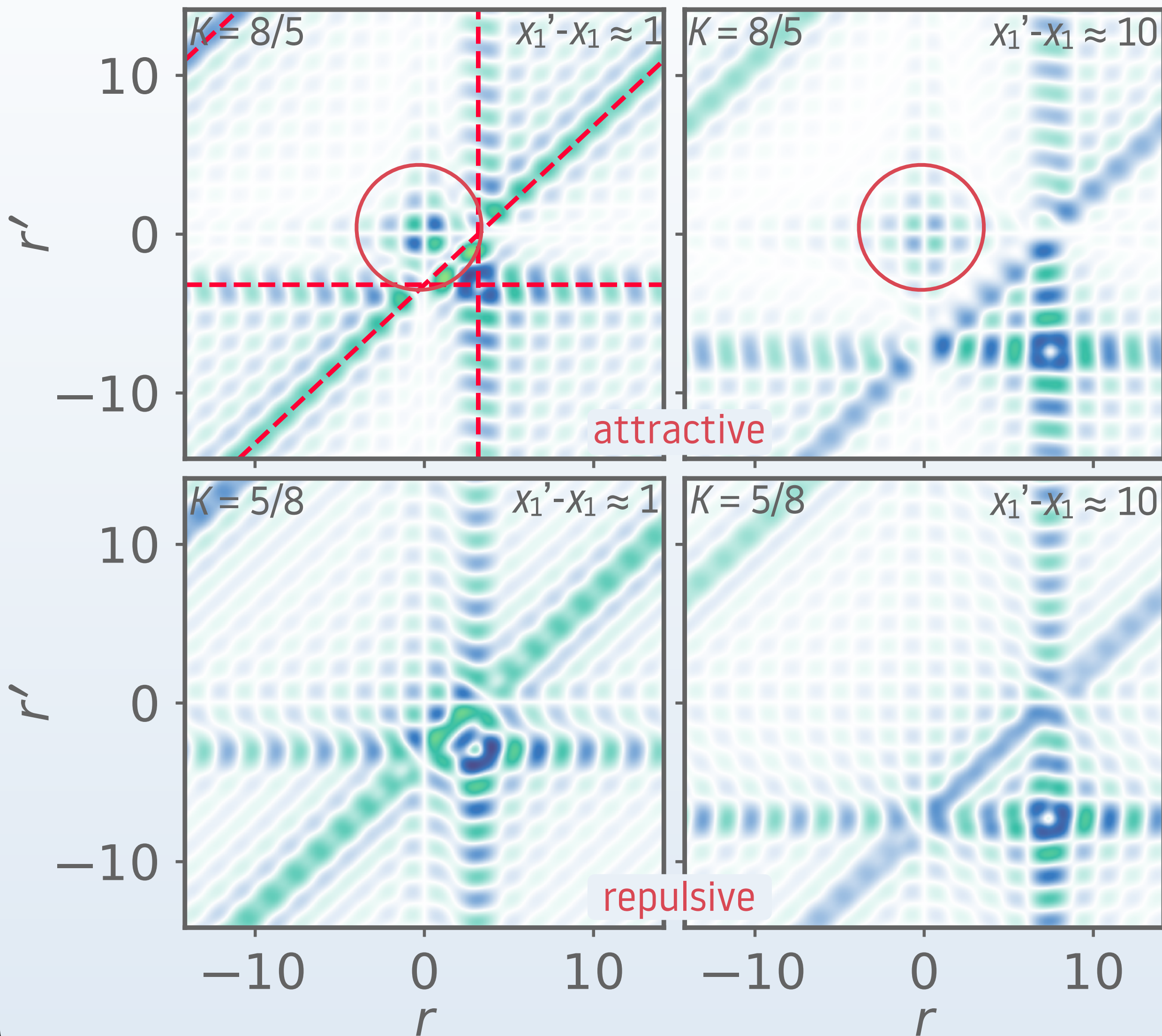


Explore: cut // to $x'_1 - x_1 = 0$

- Intersections w/ 3 other planes
- Strong signals of **clustering / pairing**

2-RDM: Interaction Effects

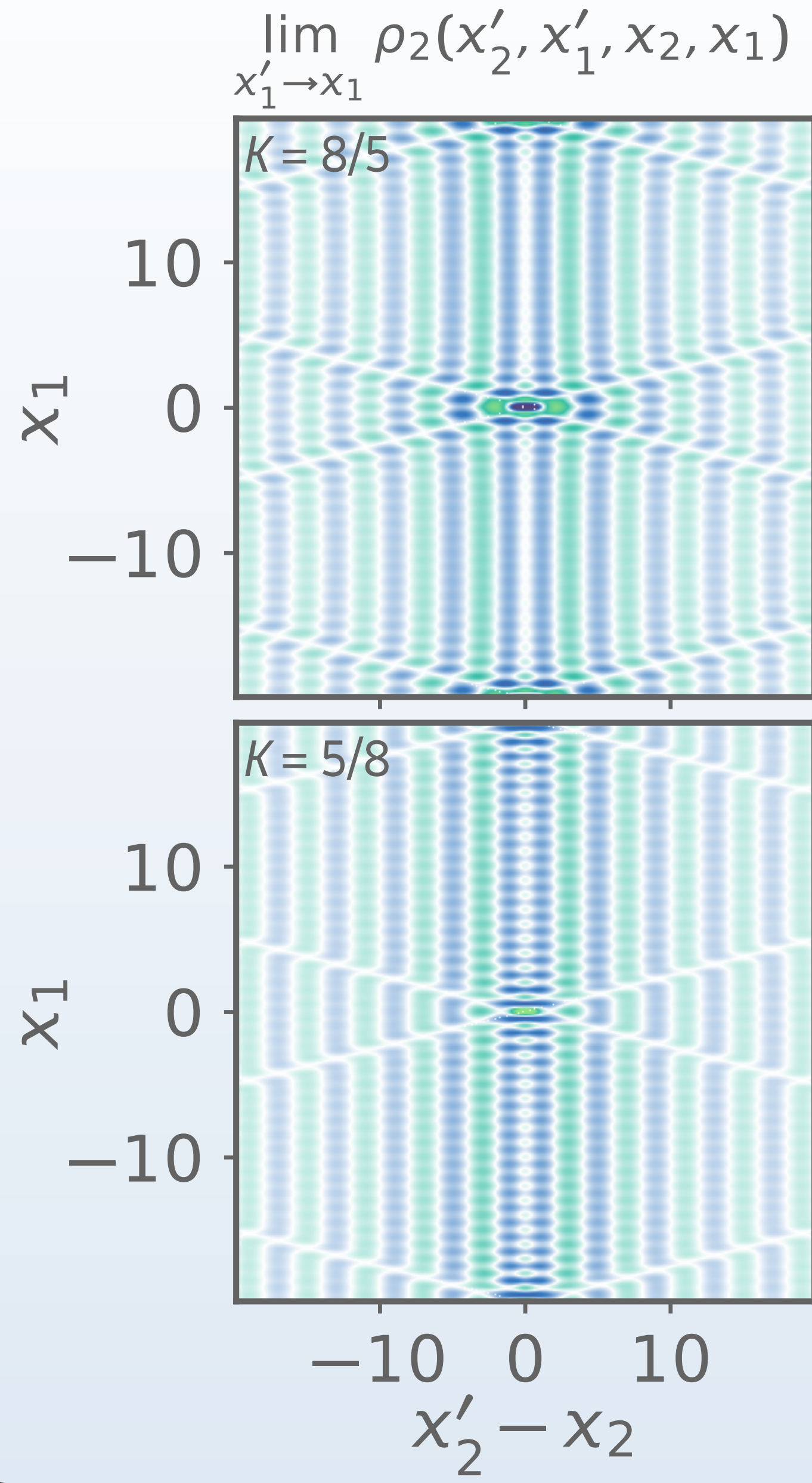
$$\rho_2(x'_2, x'_1, x_2, x_1) - \rho_{2,FF}(x'_2, x'_1, x_2, x_1)$$



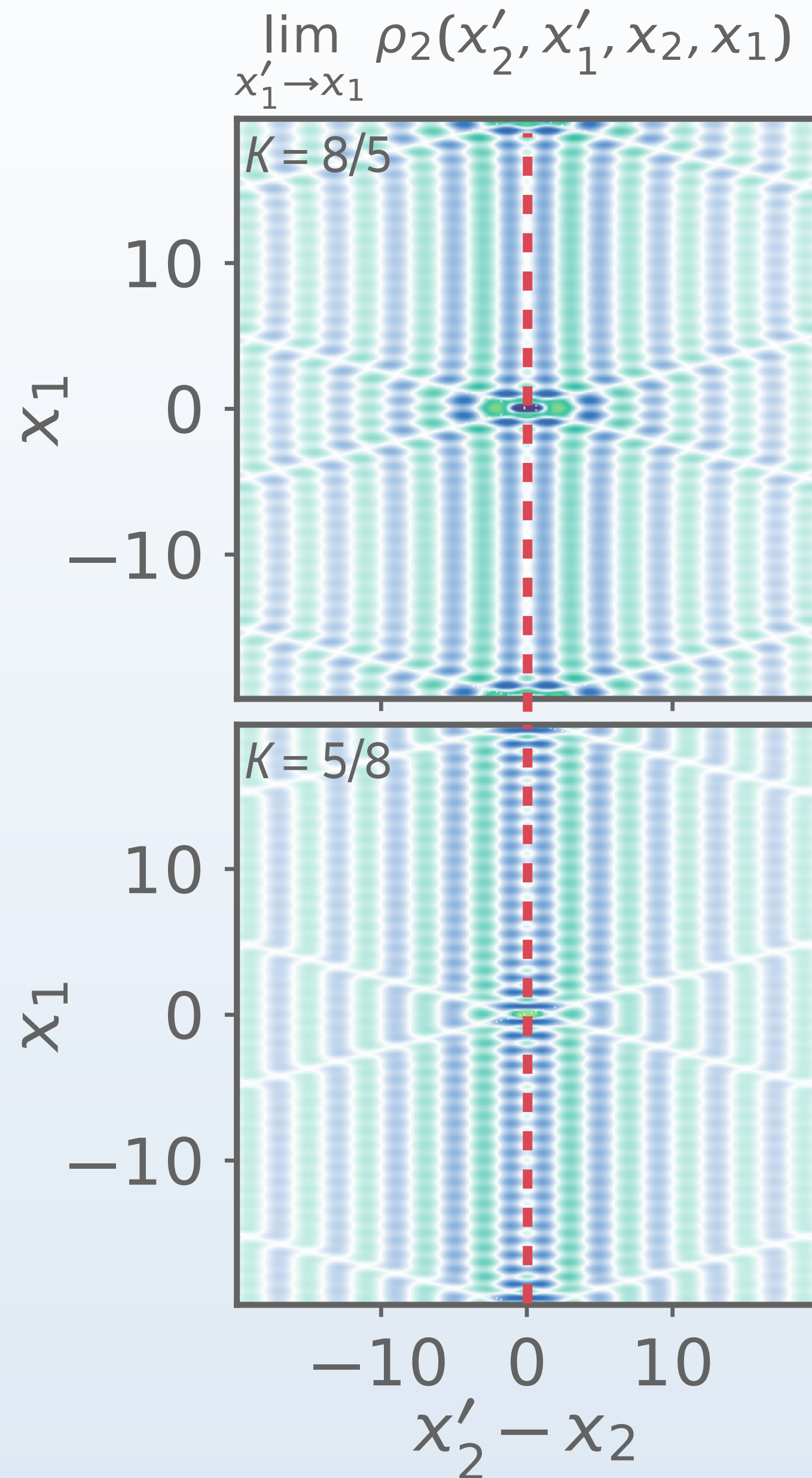
Explore: cut // to $x'_1 - x_1 = 0$

- Intersections w/ 3 other planes
- Strong signals of **clustering / pairing**
- Observe **negative copy** of diagonal elements (due to antisymmetrization)

2-RDM: Diagonal Elements



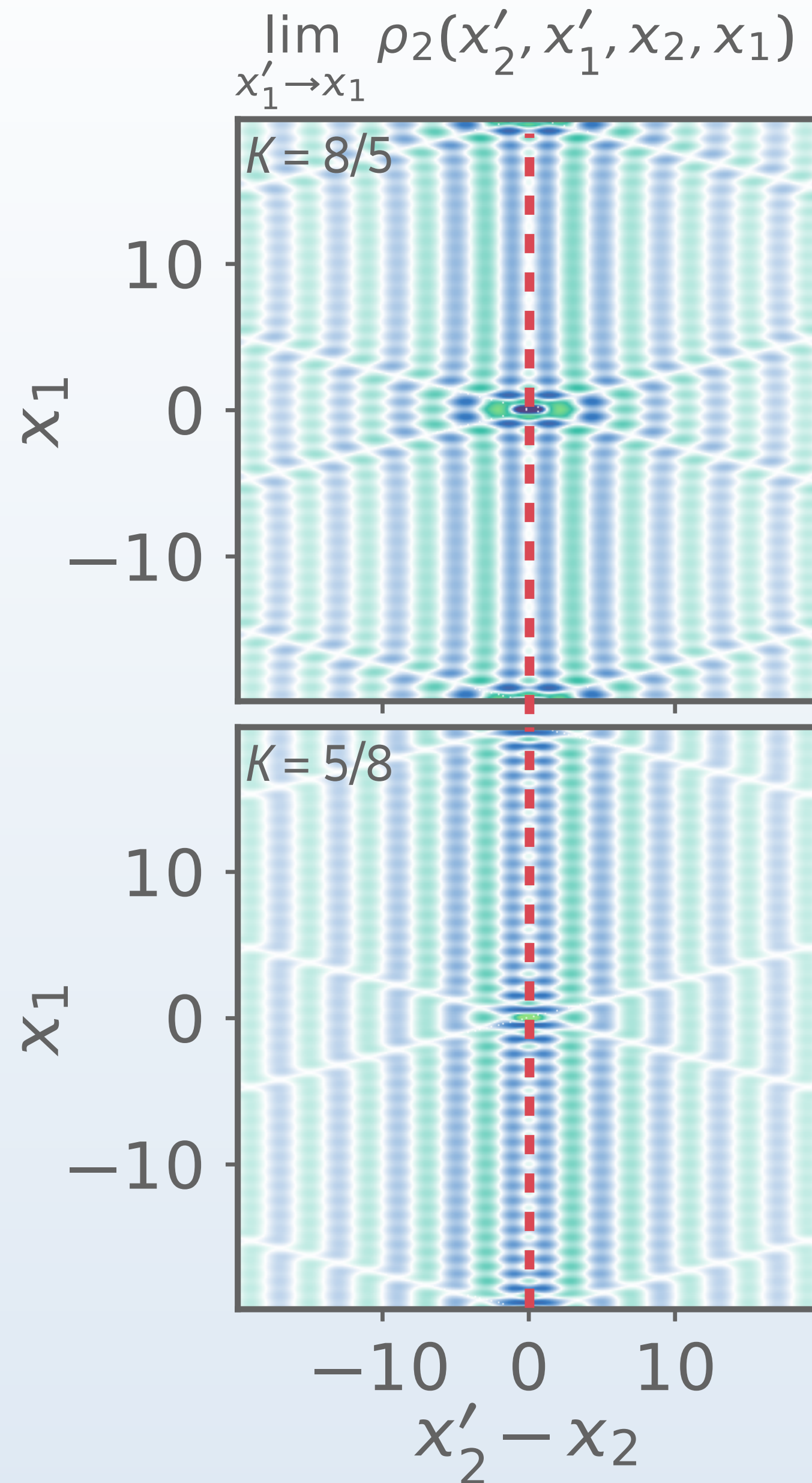
2-RDM: Diagonal Elements



Density-Density correlations

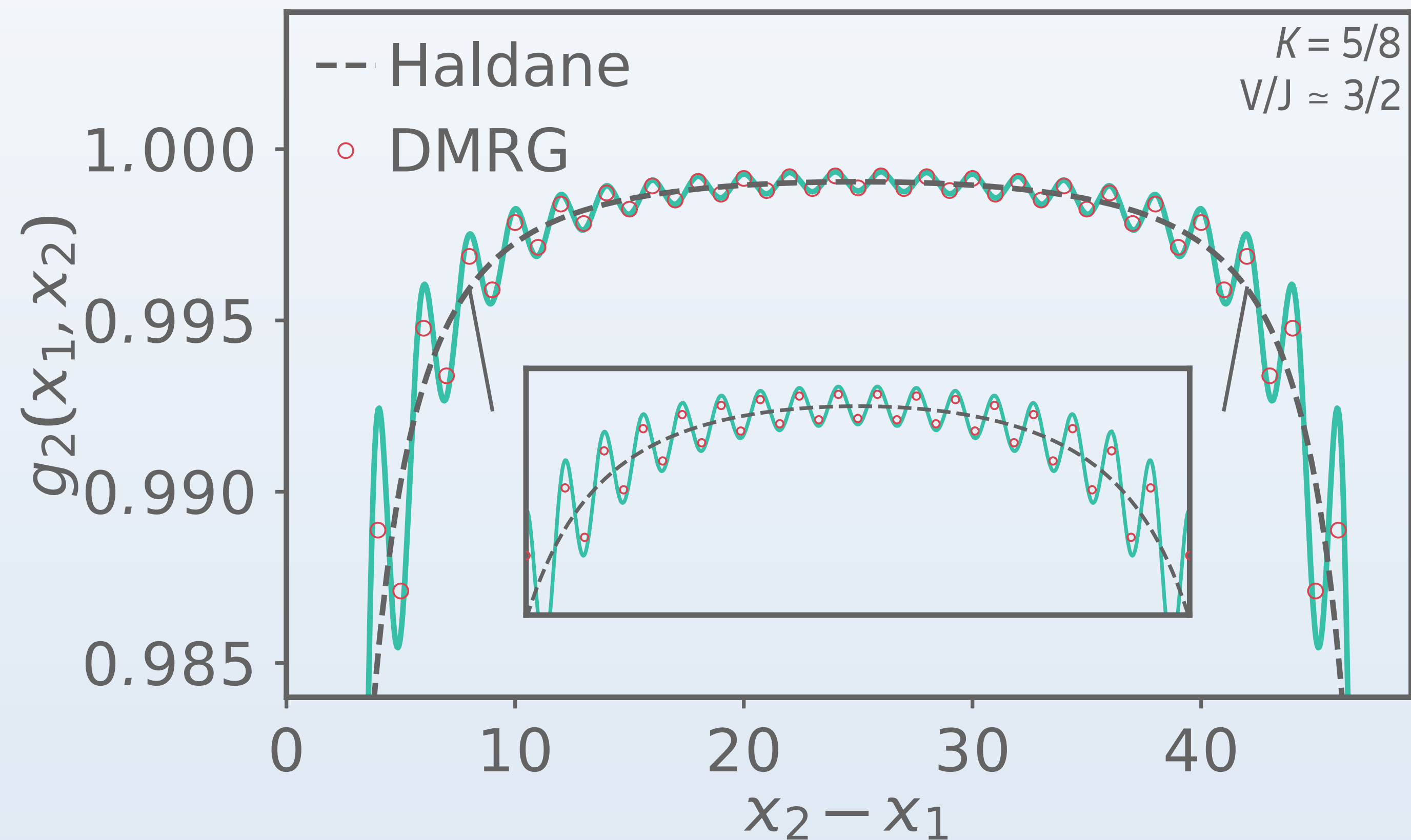
$$\begin{aligned}
 \lim_{x'_2 \rightarrow x_2} \lim_{x'_1 \rightarrow x_1} \rho_2(x'_2, x'_1, x_2, x_1) &= \rho_0^2 g_2(x_2, x_1) \\
 &= \langle \hat{\rho}(x_2) \hat{\rho}(x_1) \rangle - \rho_0 \delta(x_1 - x_2)
 \end{aligned}$$

2-RDM: Diagonal Elements



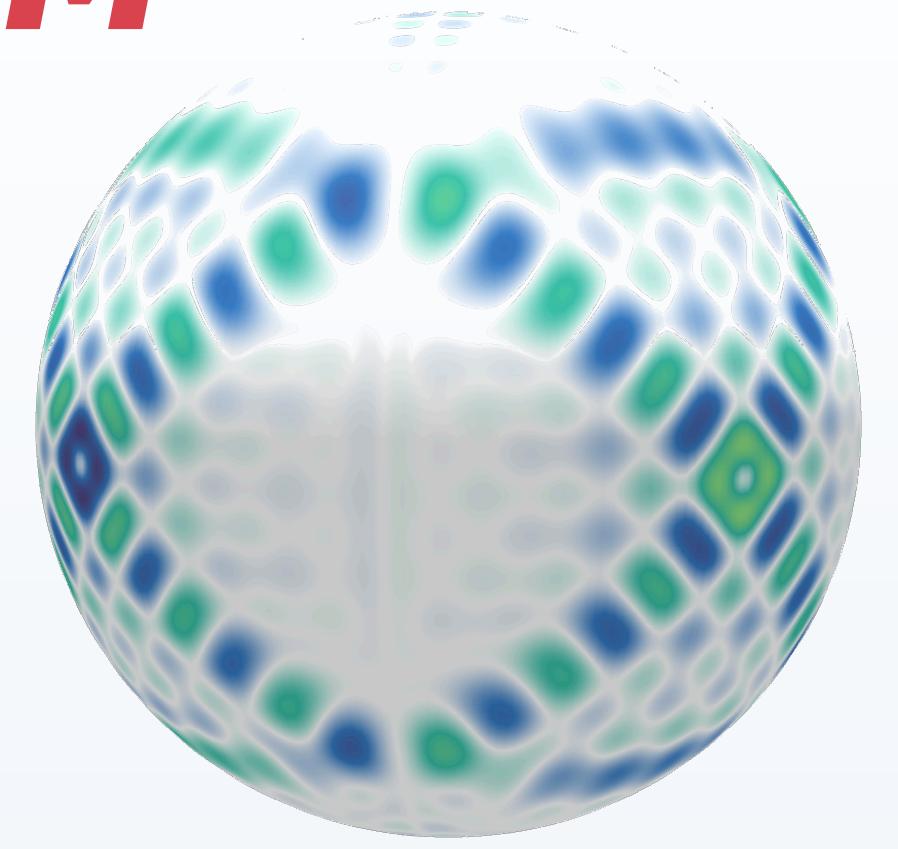
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A Finite Size LL Expression for the 2-RDM

A theoretical playground for probing interaction effects in the quantum liquid regime of a 1D interacting system (e.g. deviation from Wick's theorem, pairing signatures, ...)



Open Questions & Future Prospects

- Particle entanglement: DMRG results hint at the possibility of universal scaling with N .
- Use ρ_2 to probe the Carlen-Lieb-Reuvers conjecture.
- ...

