High-precision numerical and simulation methods for ultraconfined hard disks.

Ana M. Montero
Universidad de Extremadura

Confined hard-disks system

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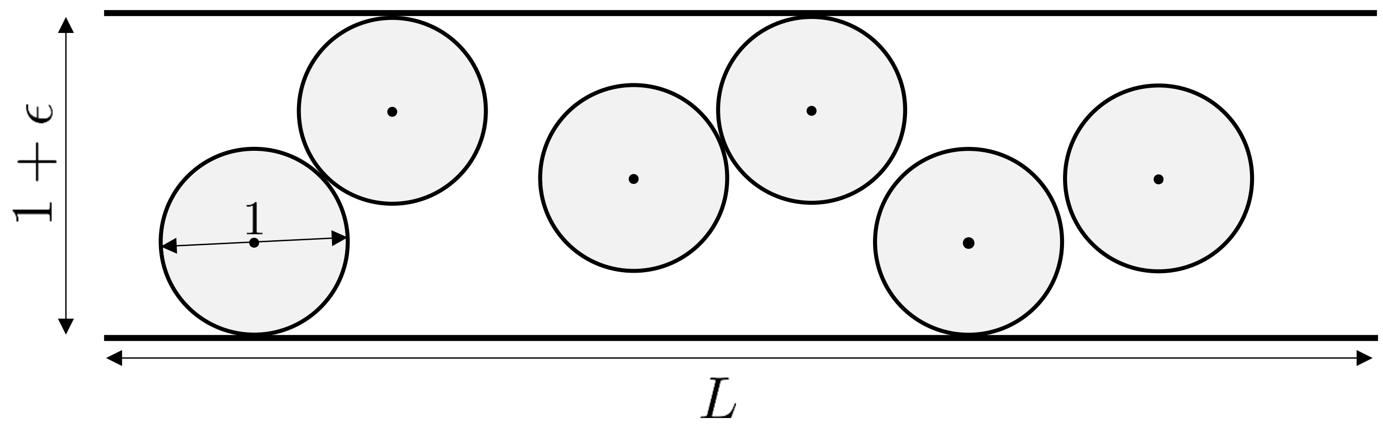

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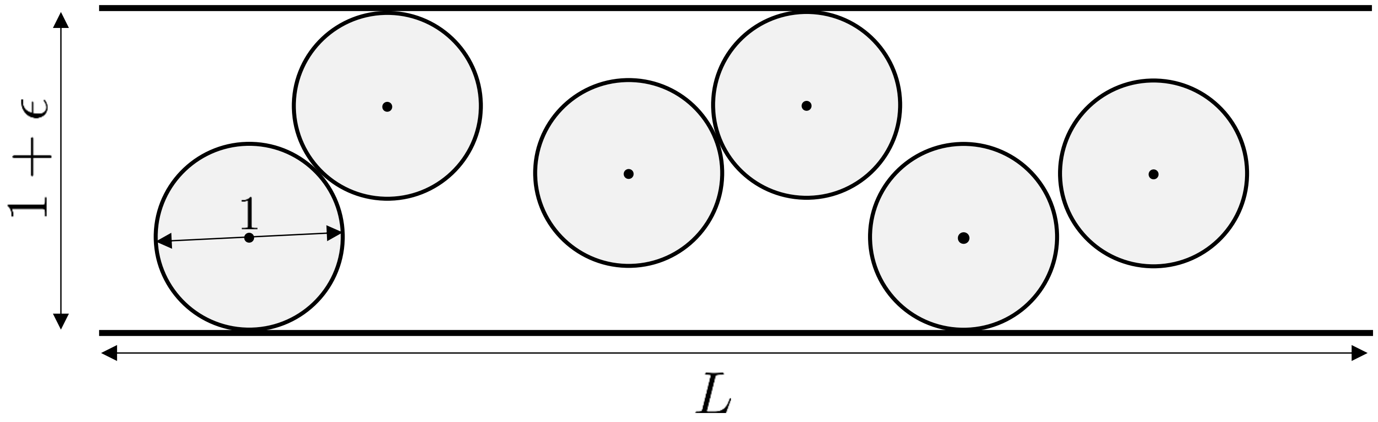

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nearest-neighbor interactions

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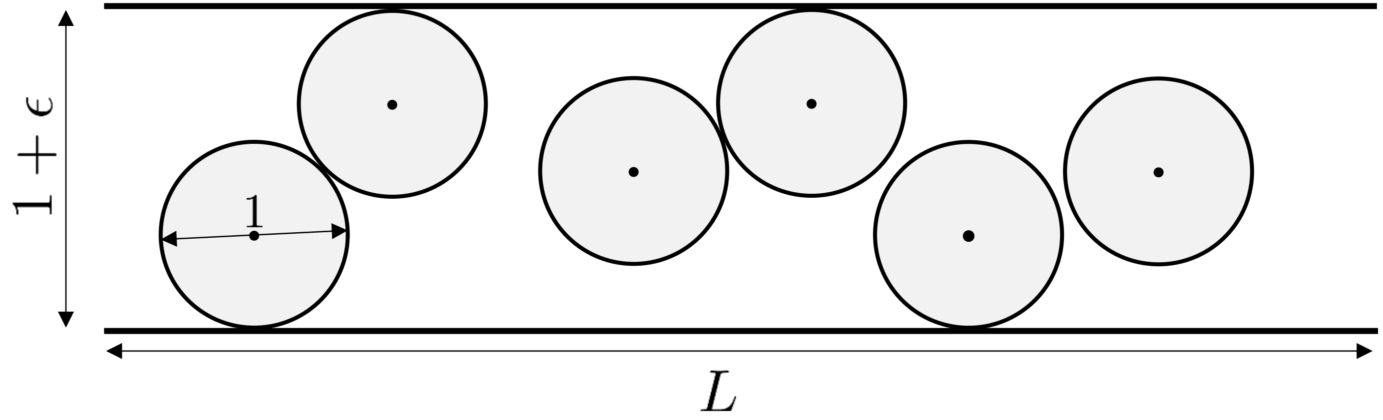

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high anisotropy

- Longitudinal: pressure (βp_x), longitudinal RDF ($g(x)$),...
- Transversal: pressure (βp_y), density profile,...
- Global: total RDF ($g(r)$), total pressure (βp),...

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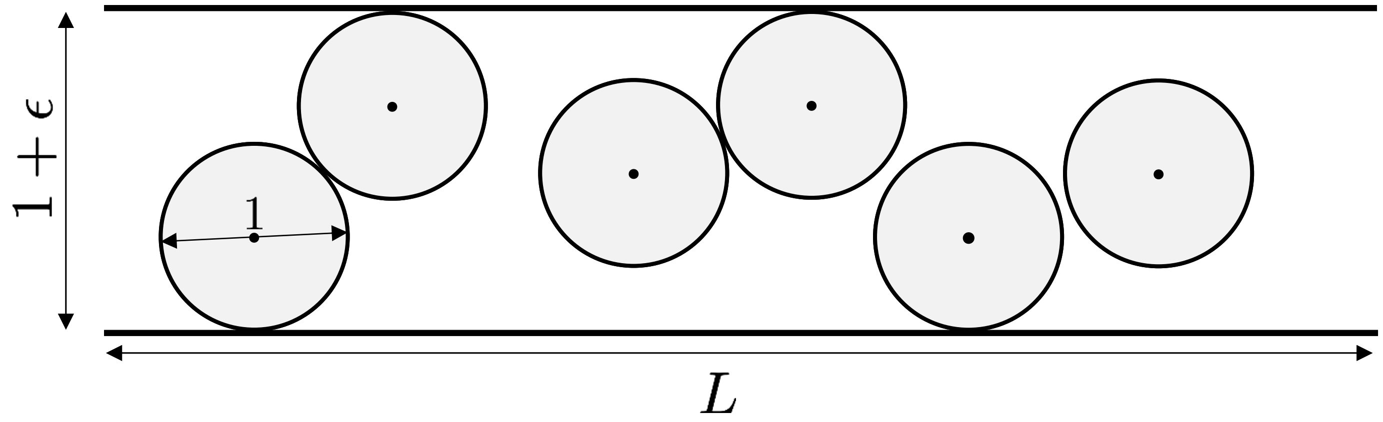

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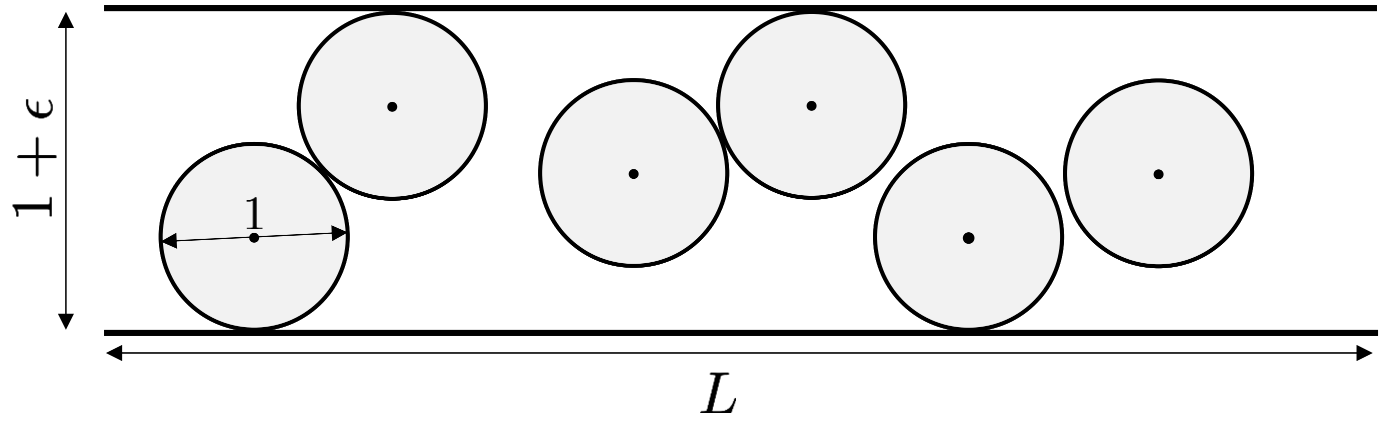
The main idea is map the transverse coordinate of the particles in the 2D system to different *species* in a 1D mixture



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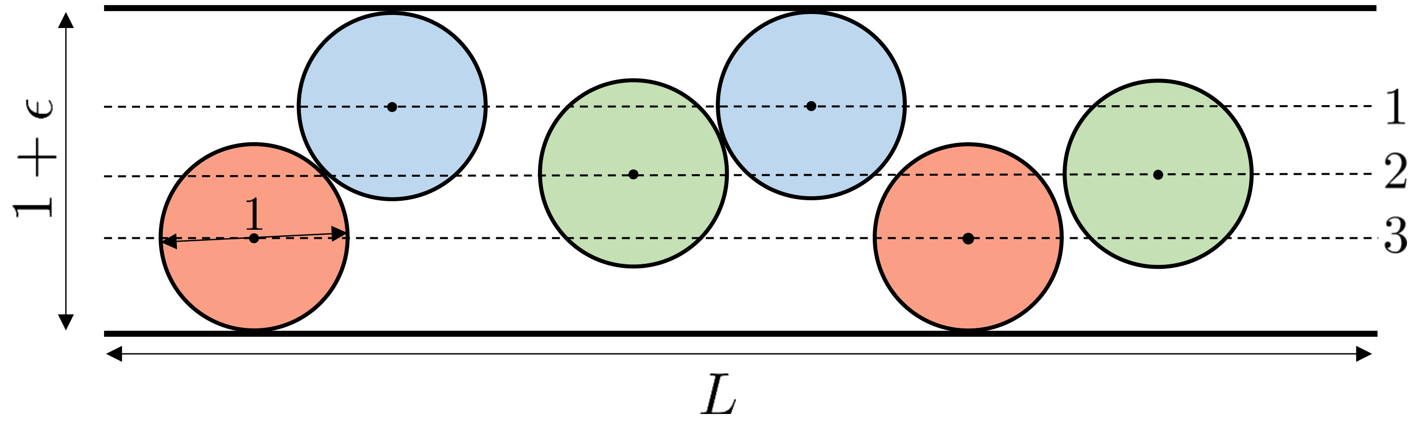

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- Here, $M = 3$ for simplicity
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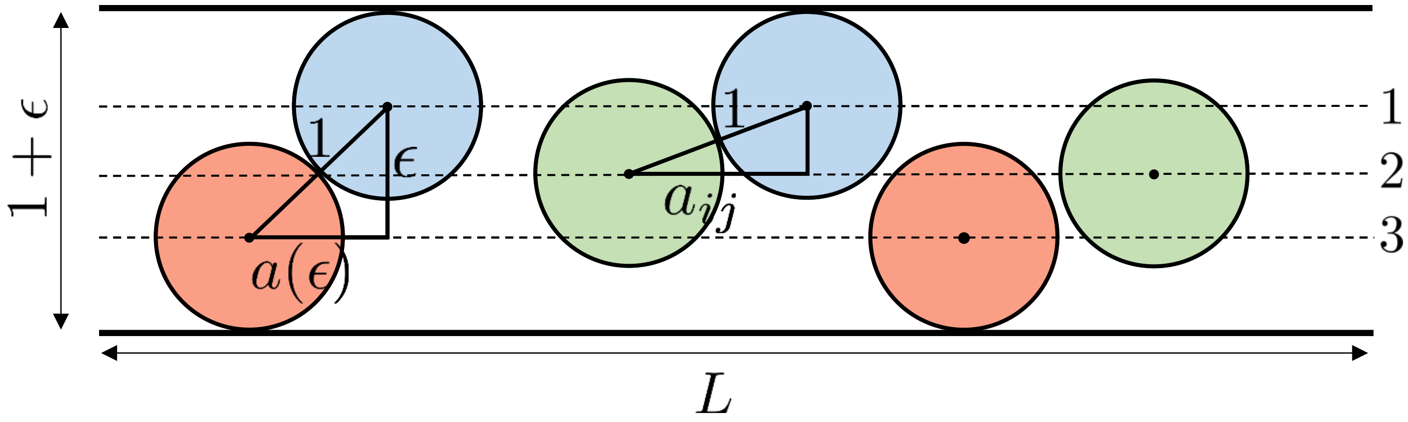

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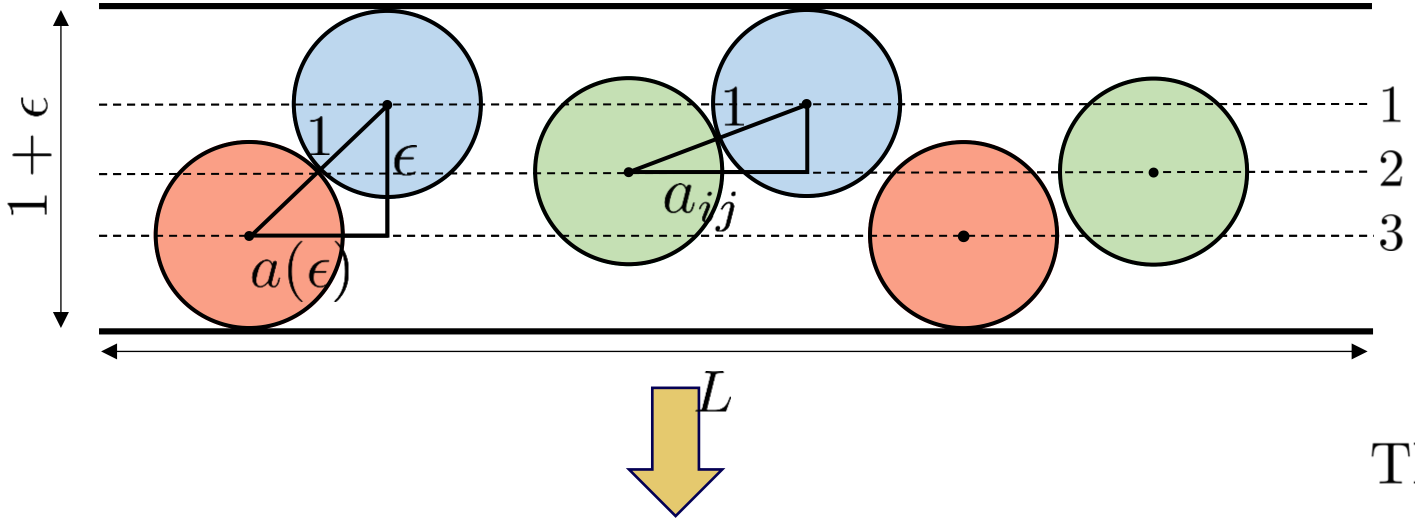

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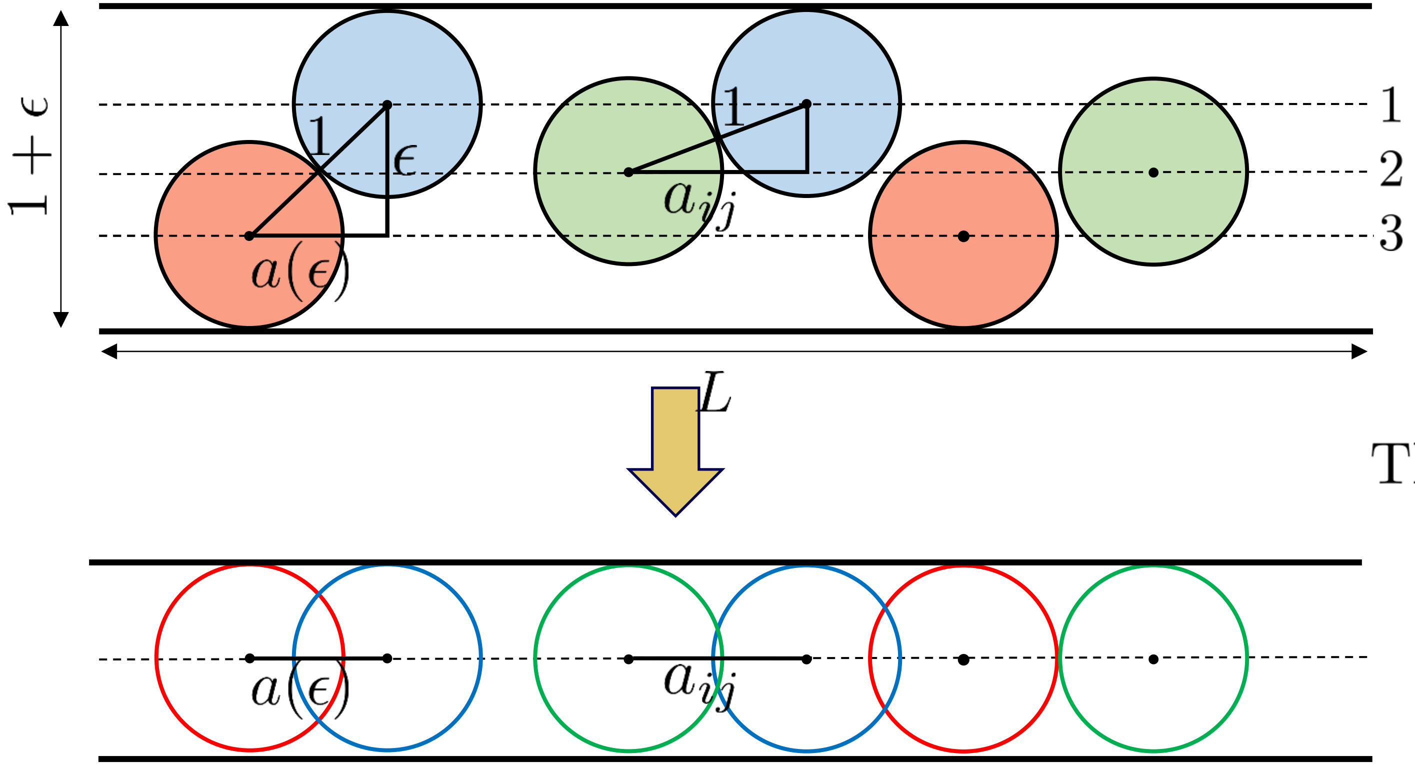

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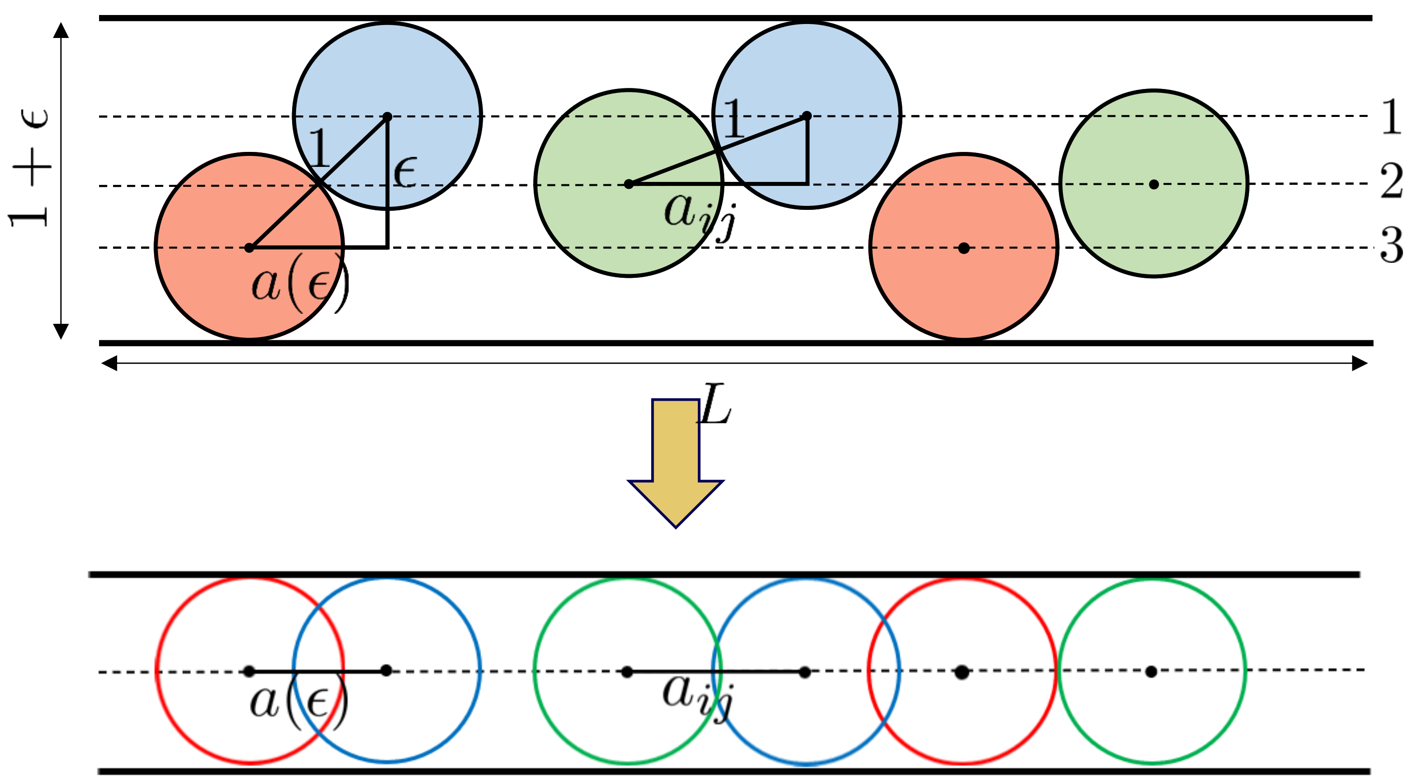

2-dimensional confined disks

one-dimensional mixture of nonadditive rods

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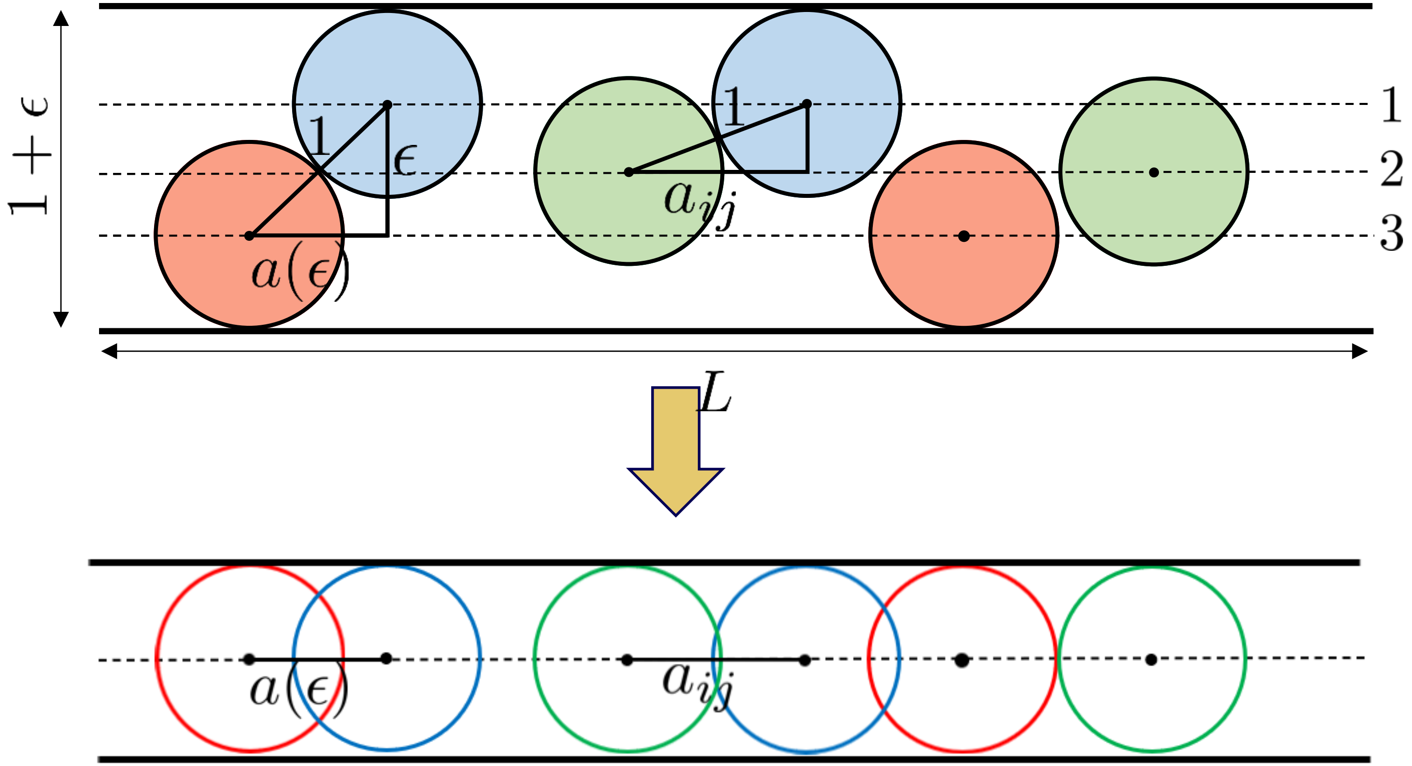

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Some mathematics

One-dimensional mixtures

Mathematics of mixtures: equal chemical potential

Working in the isothermal-isobaric ensemble. The nearest-neighbor probability distribution is given by

$$p_{ij}^{(1)}(x) = \frac{\phi_j}{\phi_i} A_i A_j e^{-\beta \varphi_{ij}(x)} e^{-\beta p_x x}$$

where

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- ϕ_k: molar fraction
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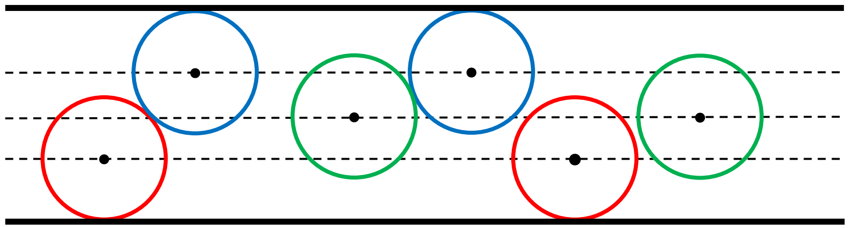

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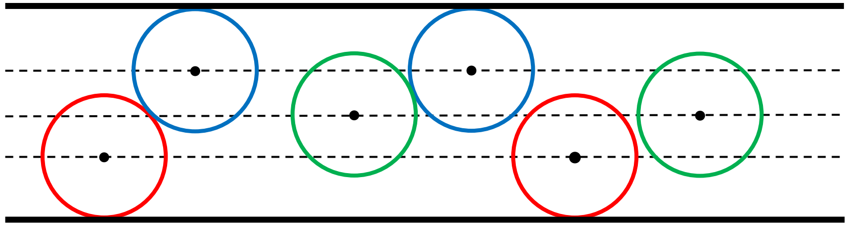

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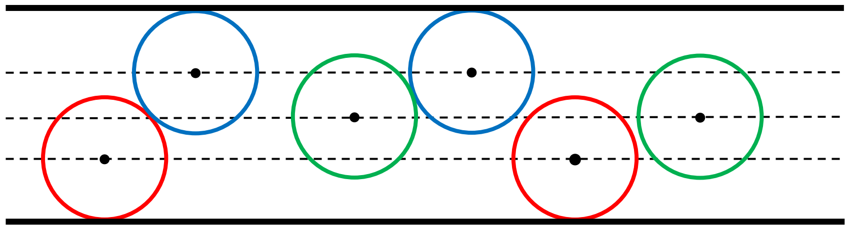

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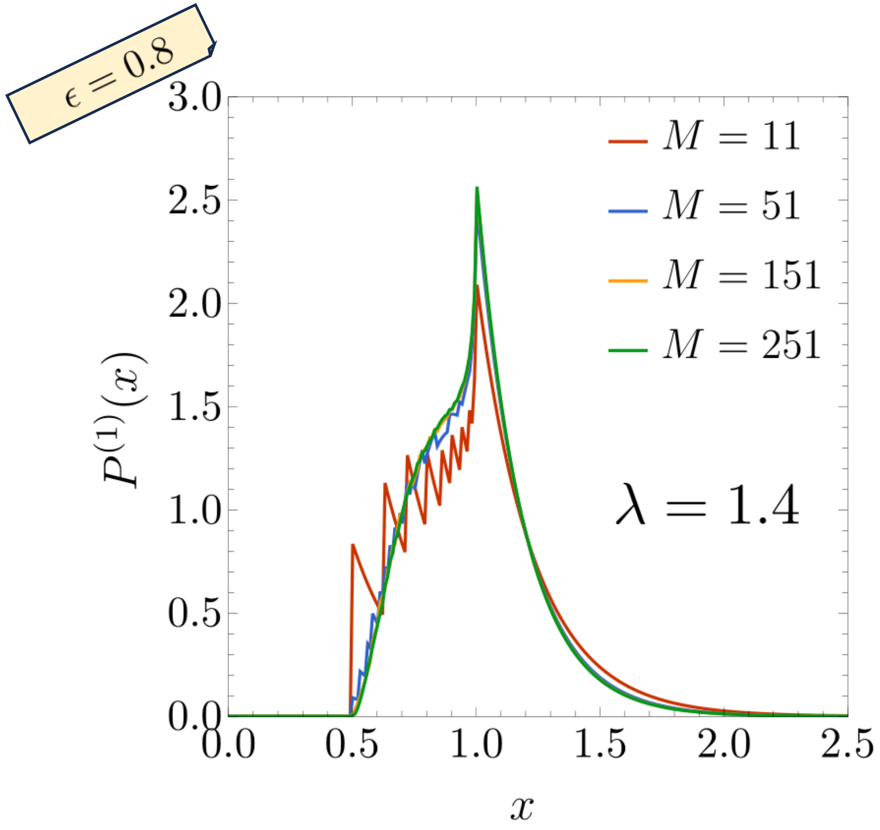

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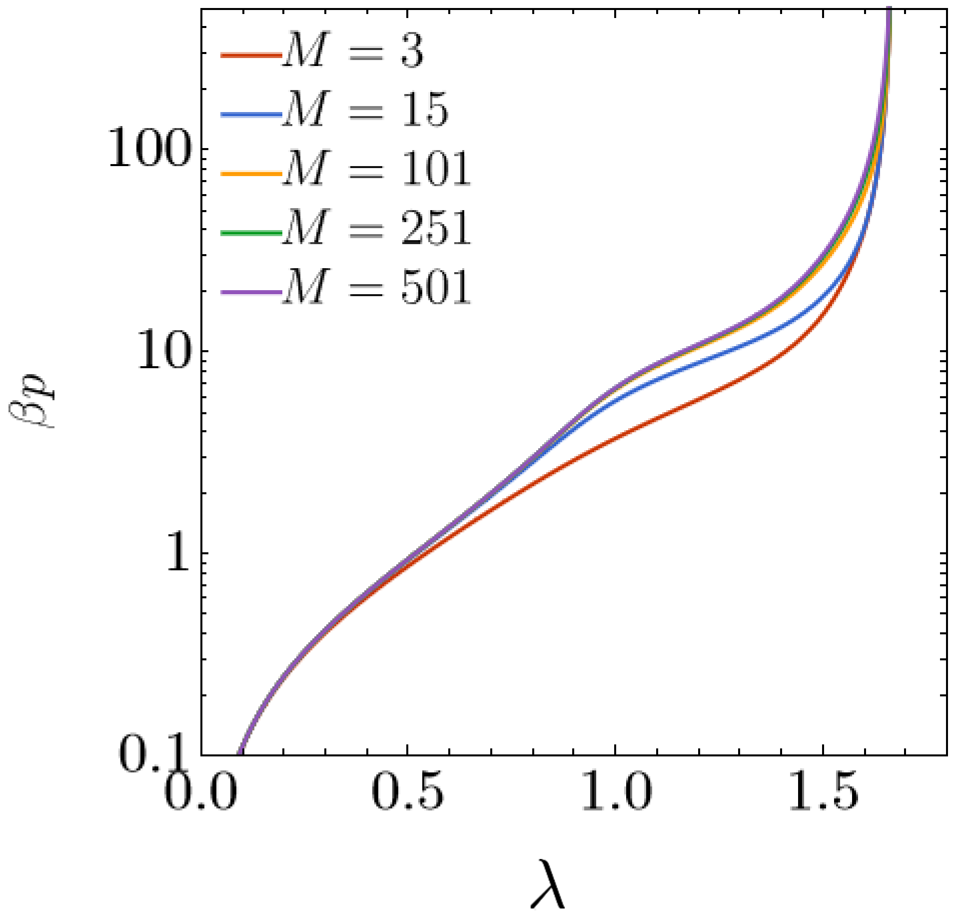

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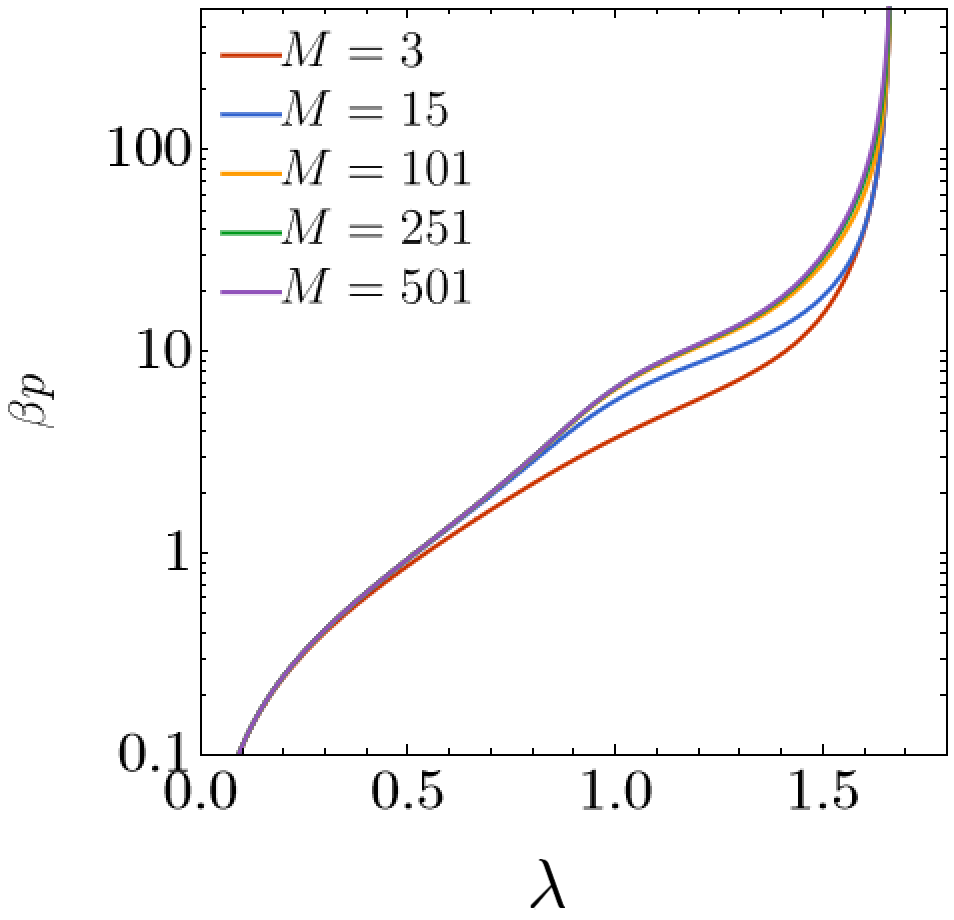

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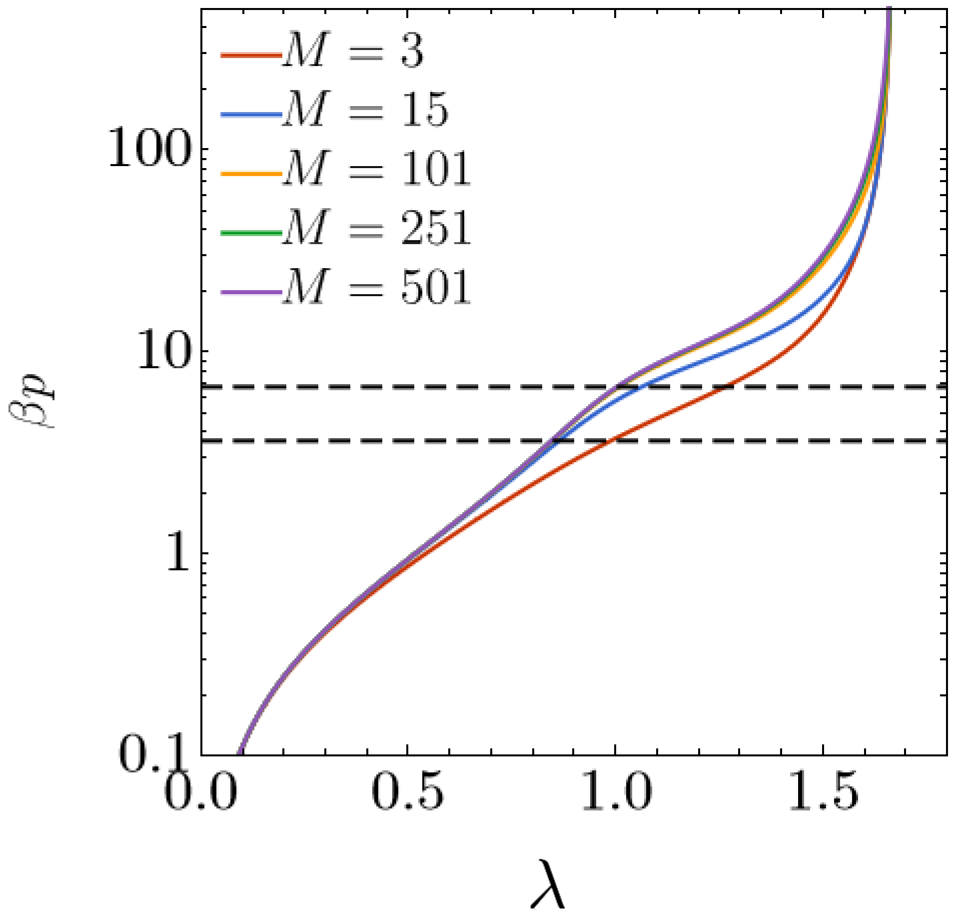

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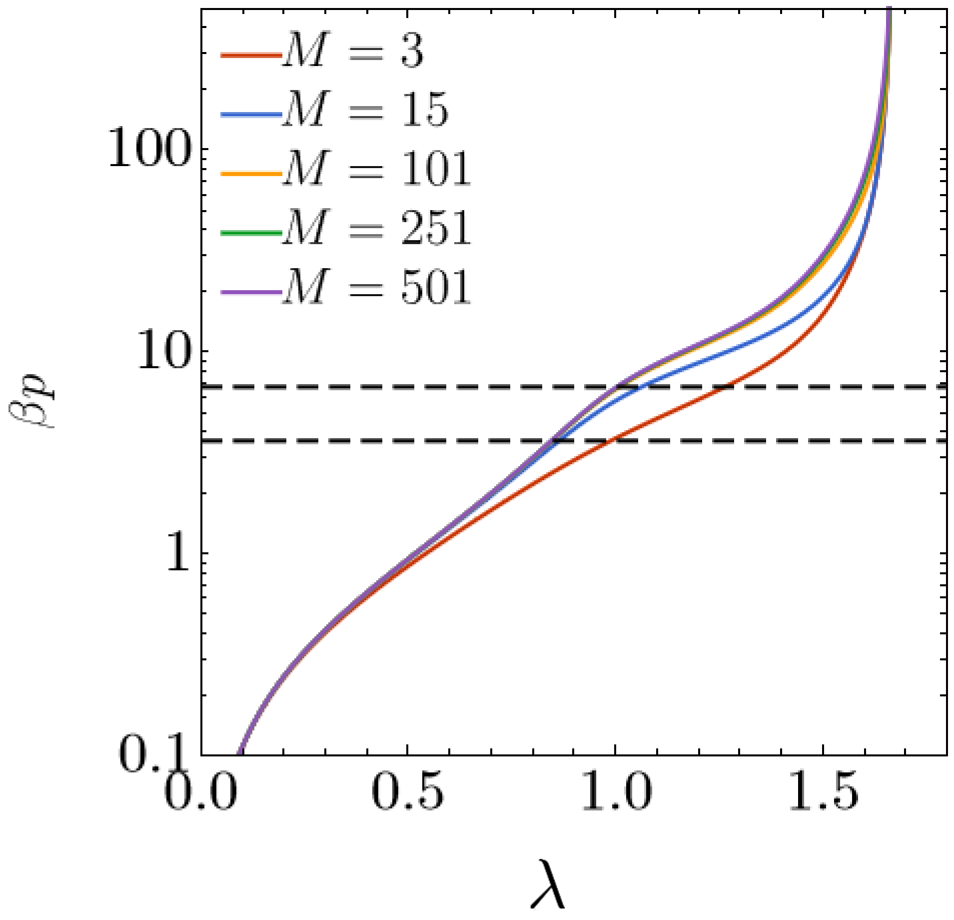

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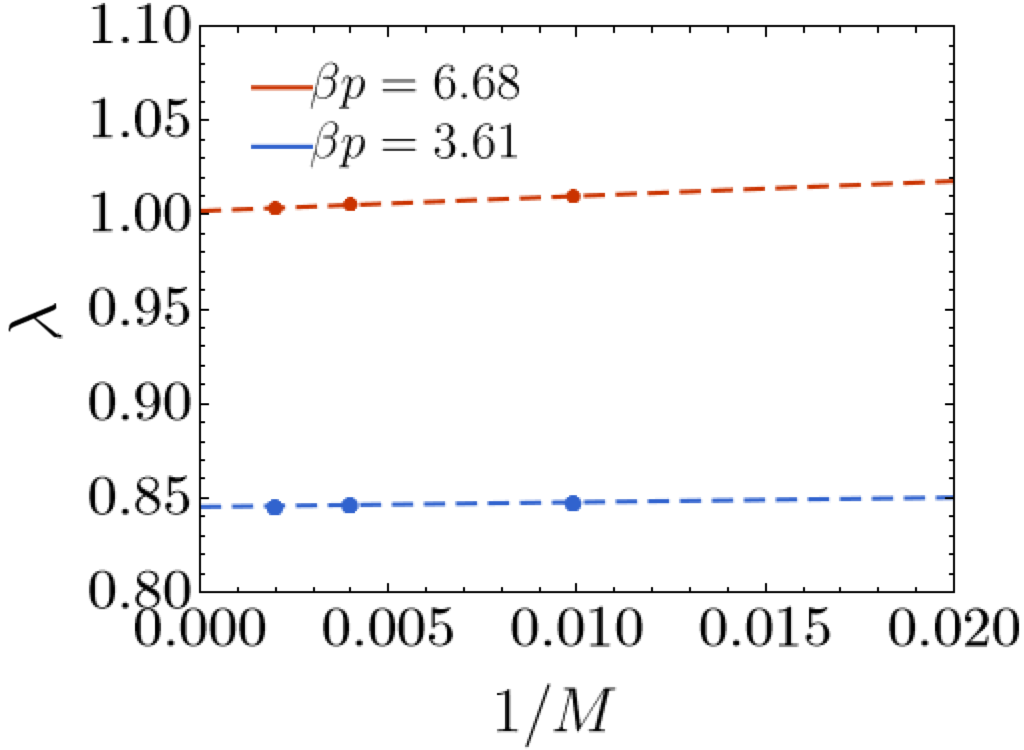

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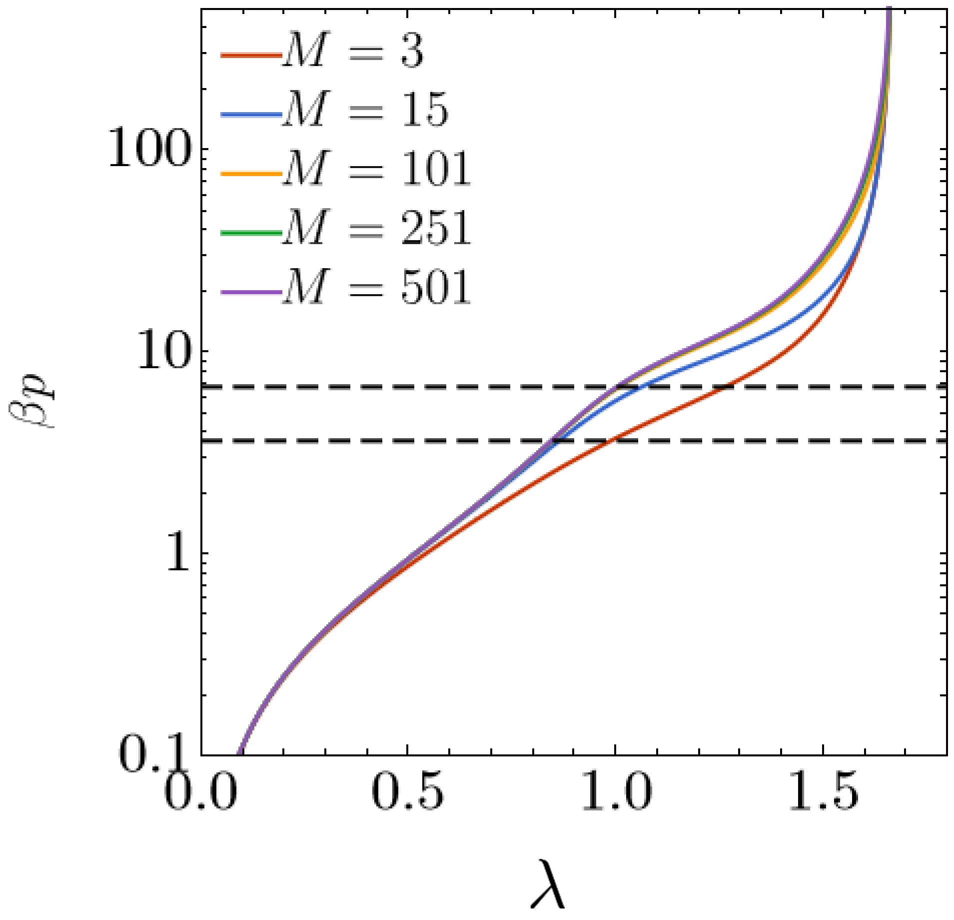

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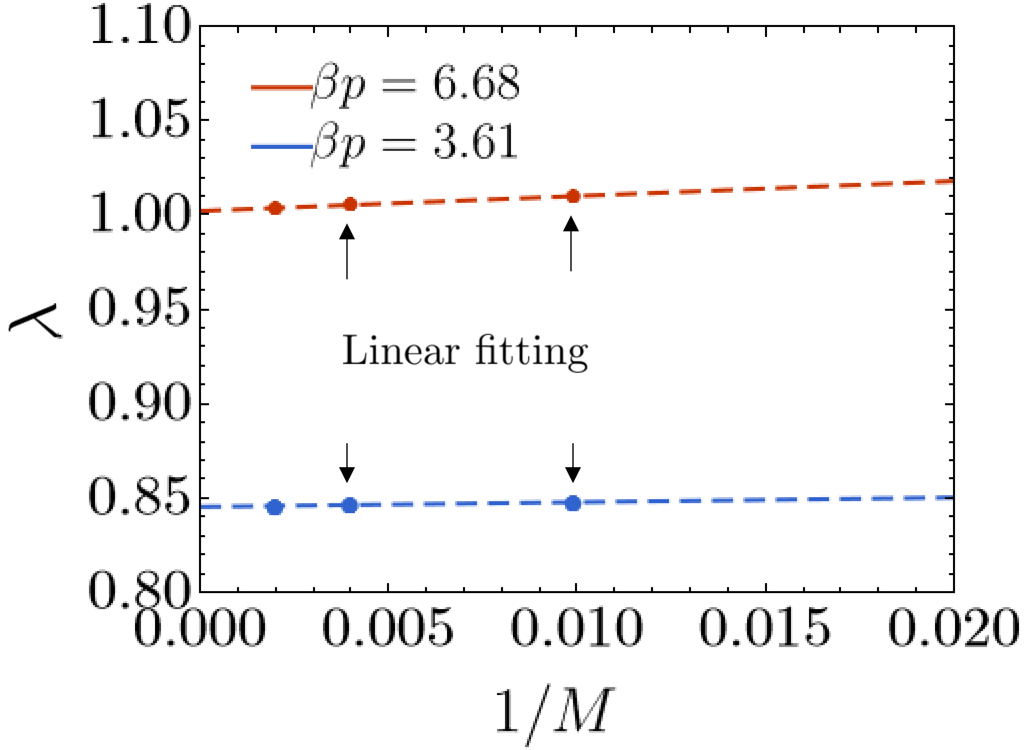

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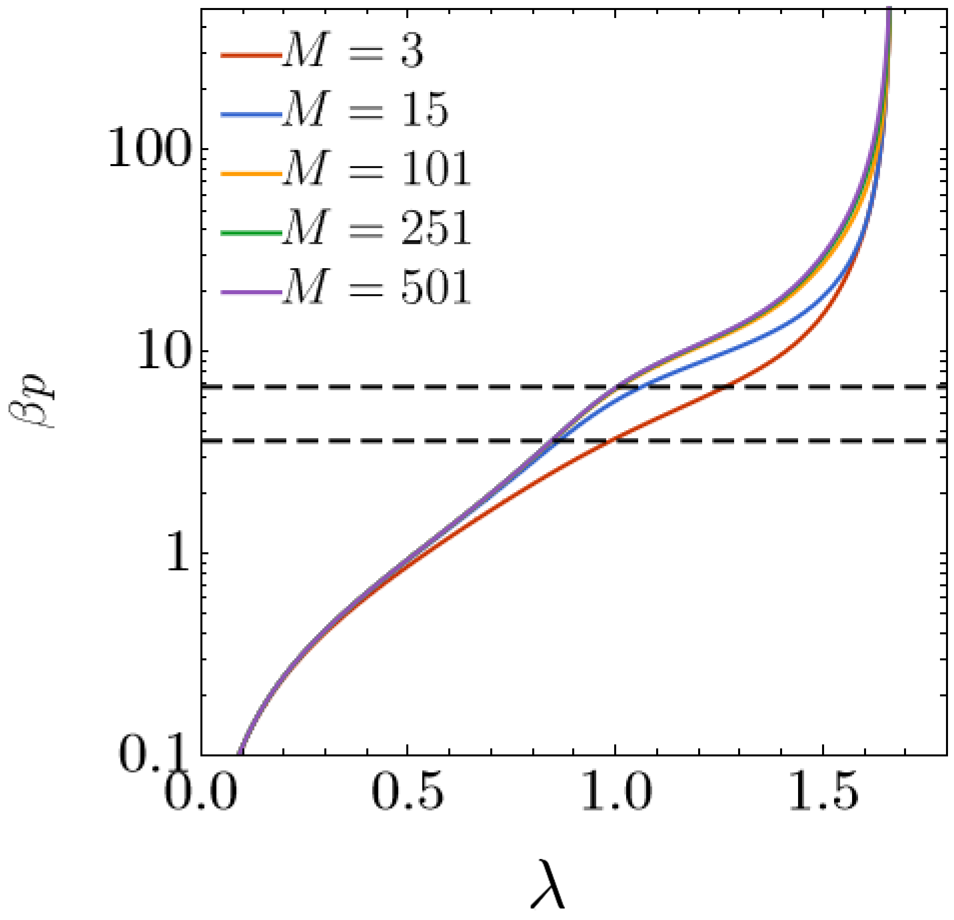

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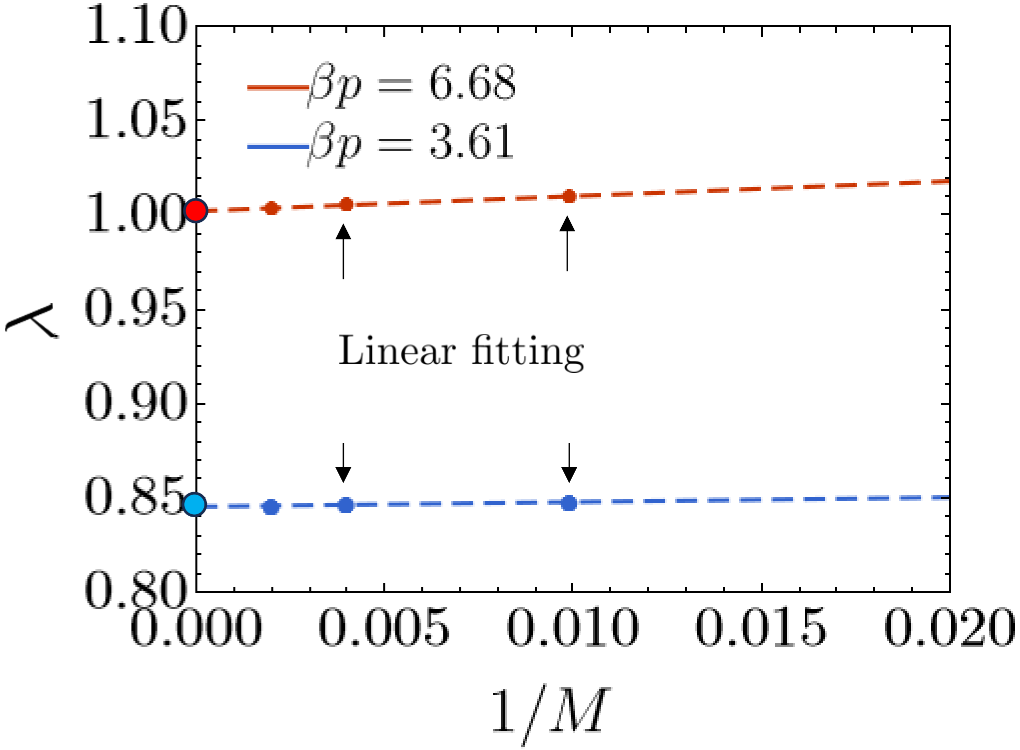

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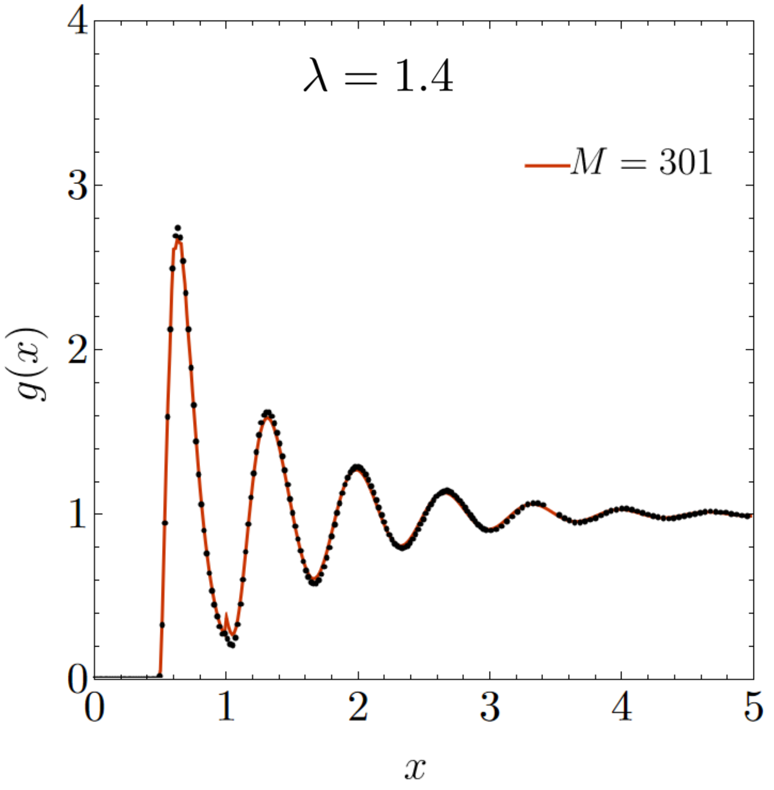

S Varga *et al J. Stat. Mech.* (2011) P11006

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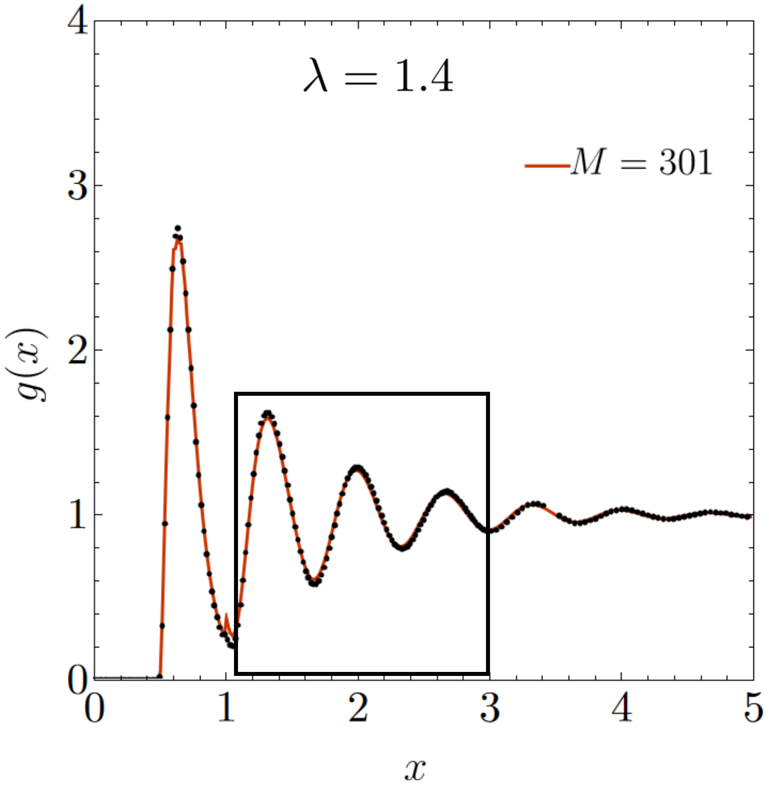

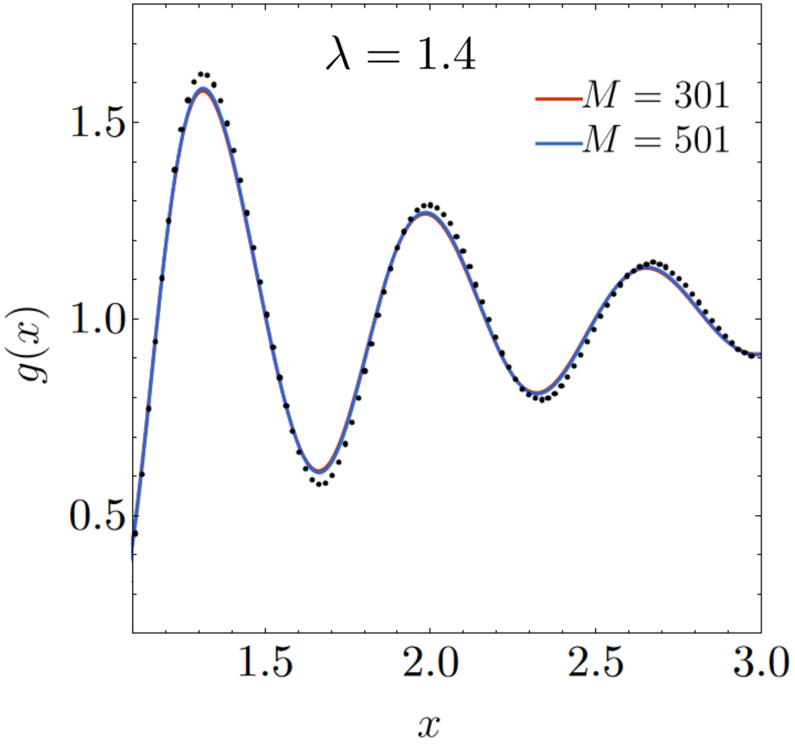

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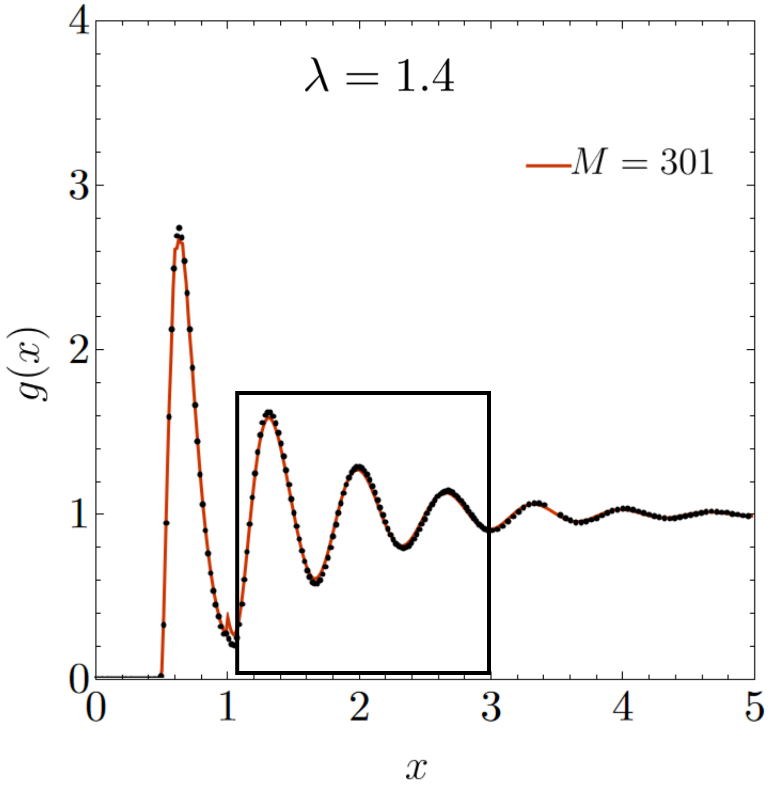

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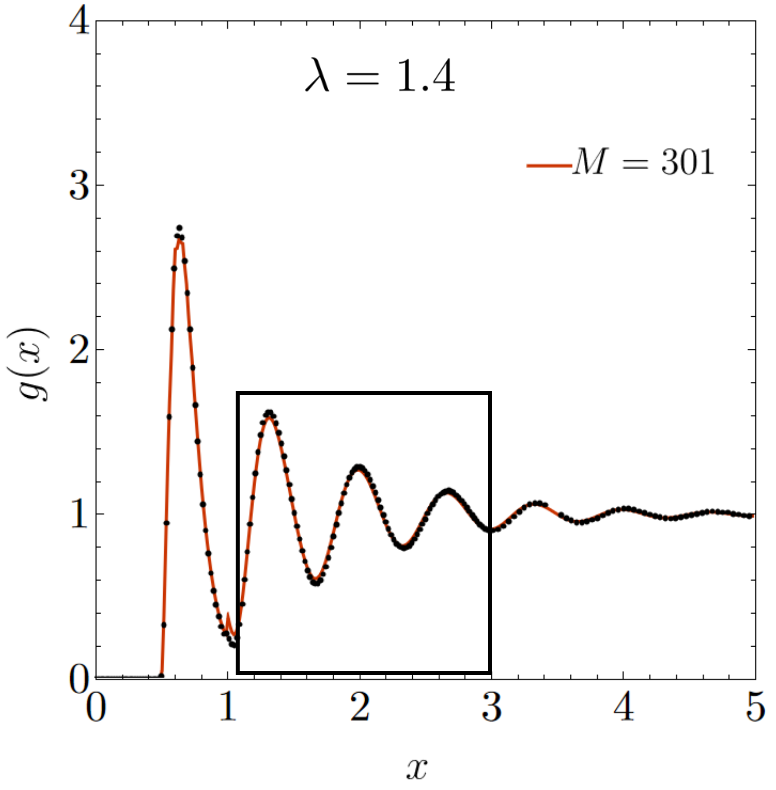

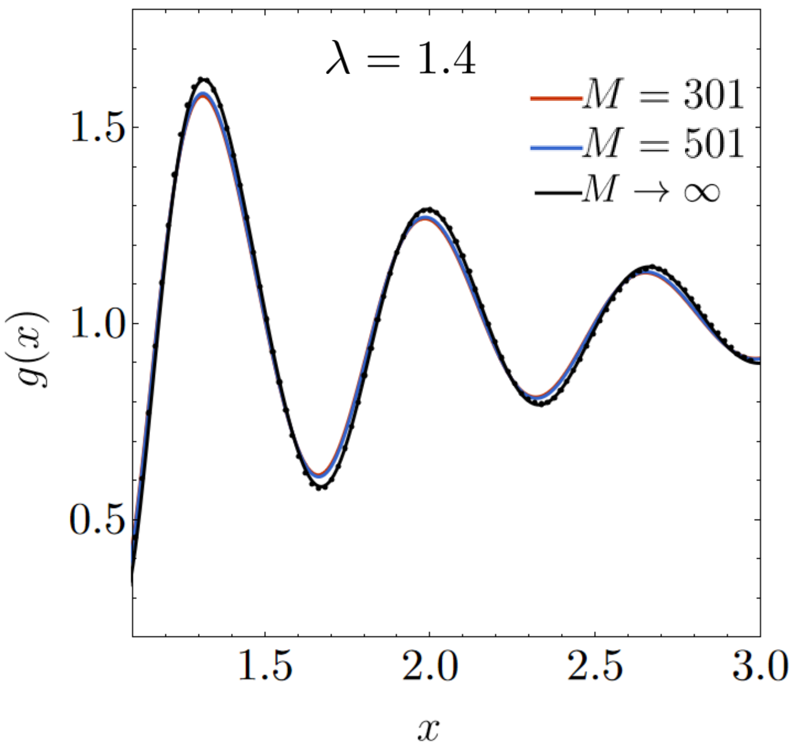

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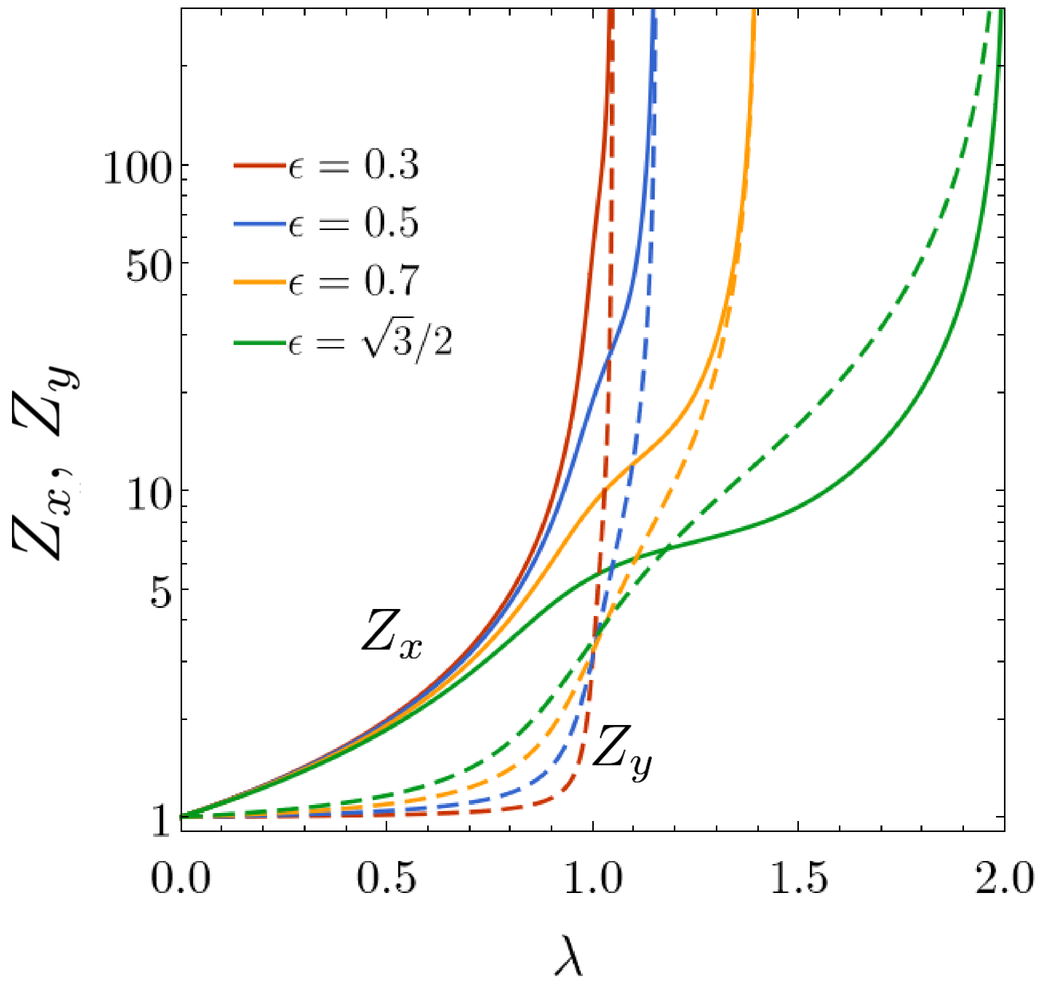
Equation of state: theoretical result



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$\xrightarrow{\text{inverse Laplace transform}}$ RDF $g(x)$

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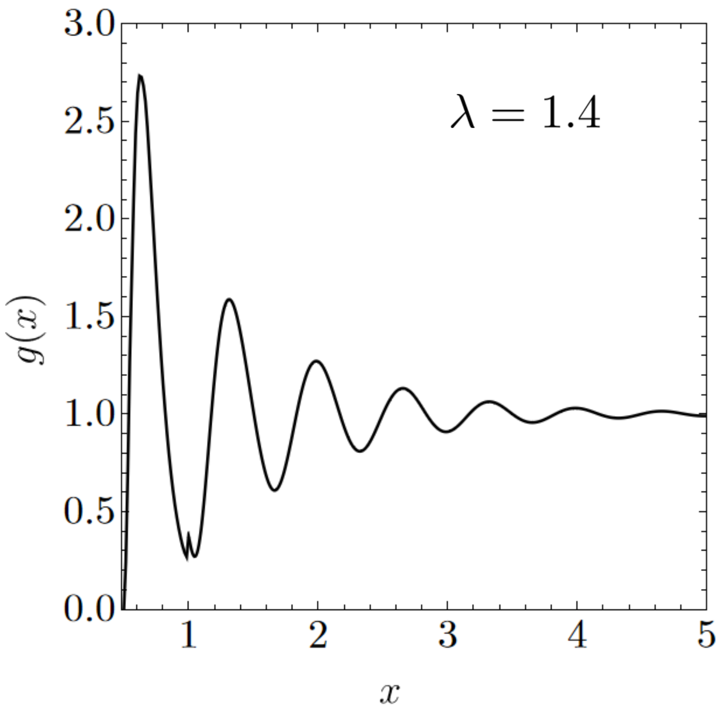

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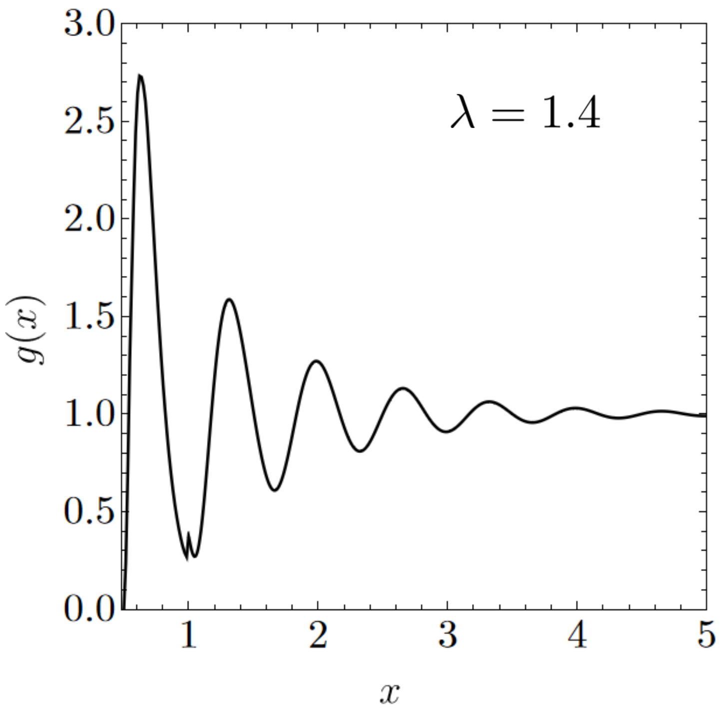
inverse
Laplace transform

RDF $g(x)$

analytical inversion



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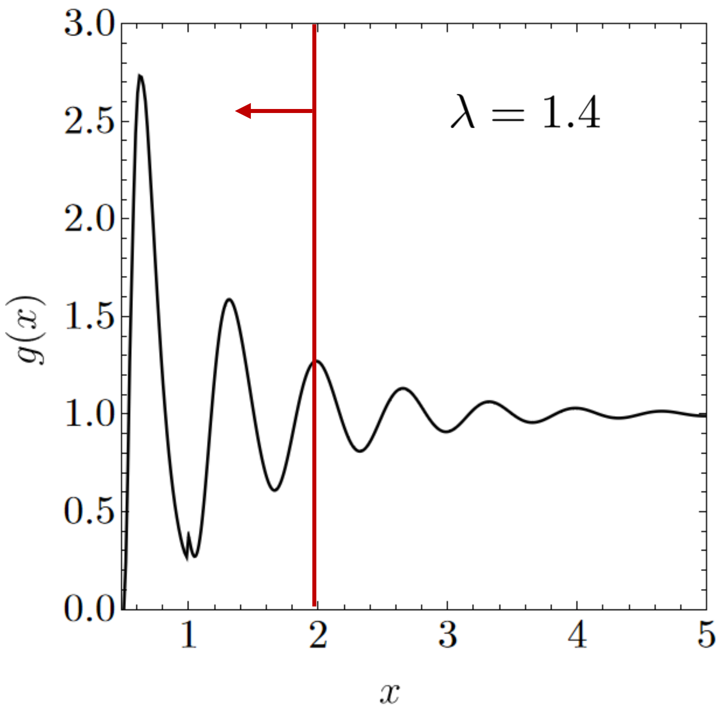
inverse
Laplace transform

RDF $g(x)$

analytical inversion



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inverse Laplace transform → RDF $g(x)$

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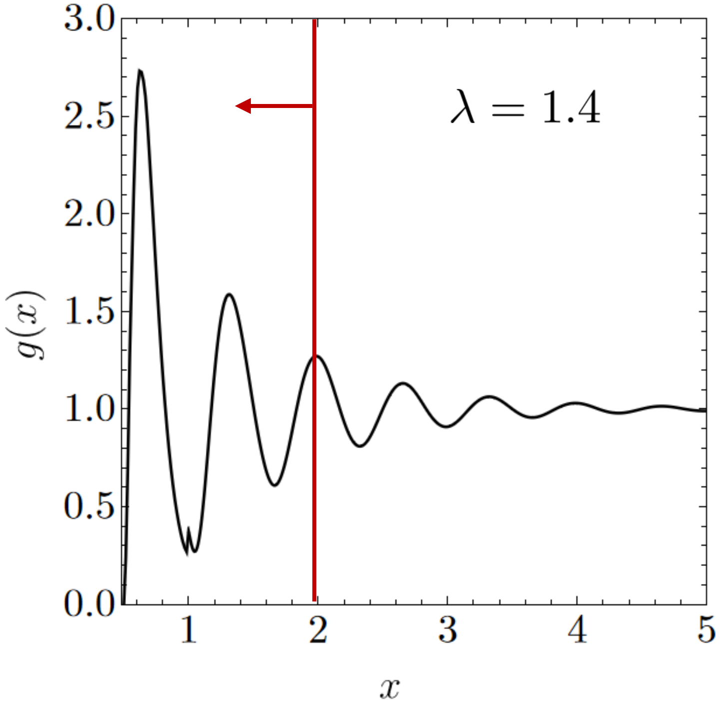

$$g(x) = \frac{1}{\lambda} \sum_{n=1}^{\infty} A^{2n} \sum_i^M \sum_j^M \phi_i \phi_j Q_{ij}^{(n)}(x).$$

where

$$Q_{ij}^{(n)}(x) = \sum_{k_1} \sum_{k_2} \cdots \sum_{k_{n-1}} R^{(n)}(x; a_{ik_1} + a_{k_1 k_2} + \cdots + a_{k_{n-1} j}),$$

with

$$R^{(n)}(x;\alpha) \equiv \frac{e^{-\beta p x}}{(n-1)!} (x-\alpha)^{n-1} \Theta(x-\alpha).$$

Longitudinal RDF: numerical details

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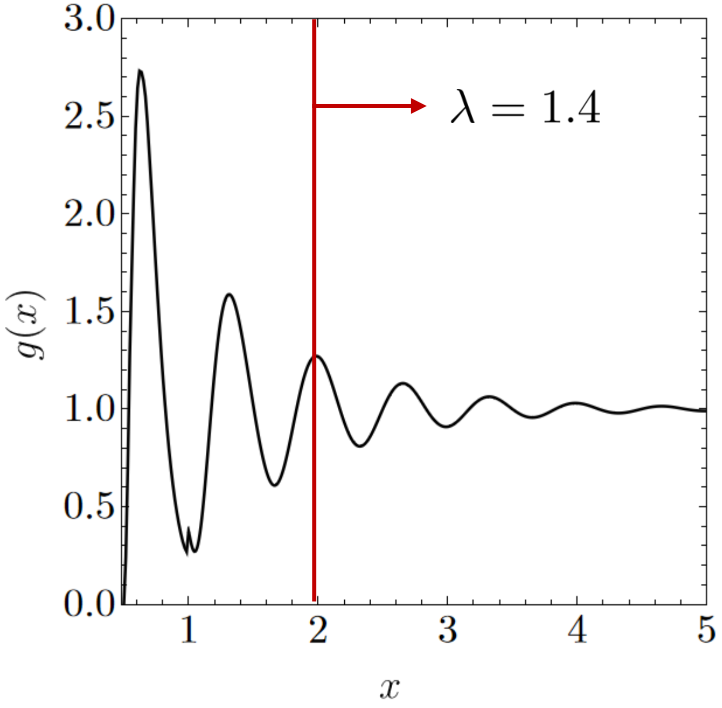

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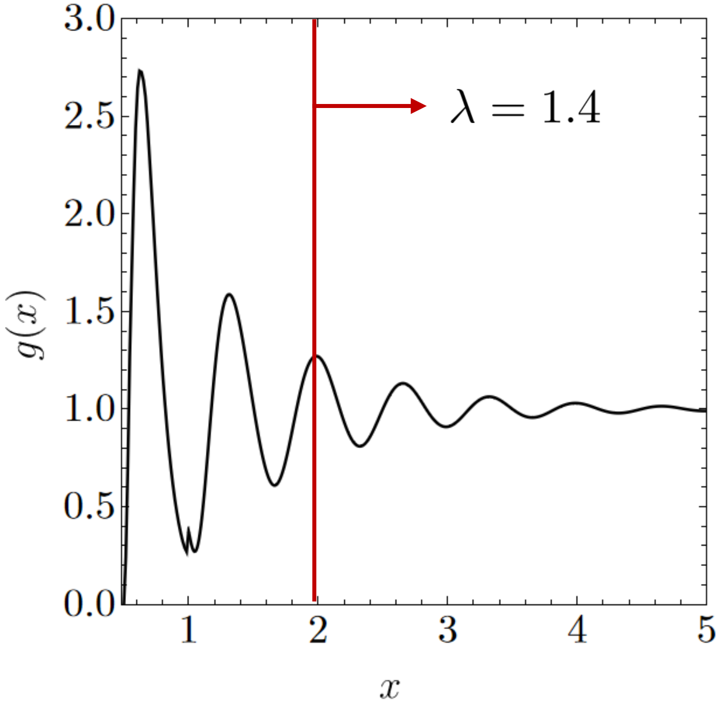

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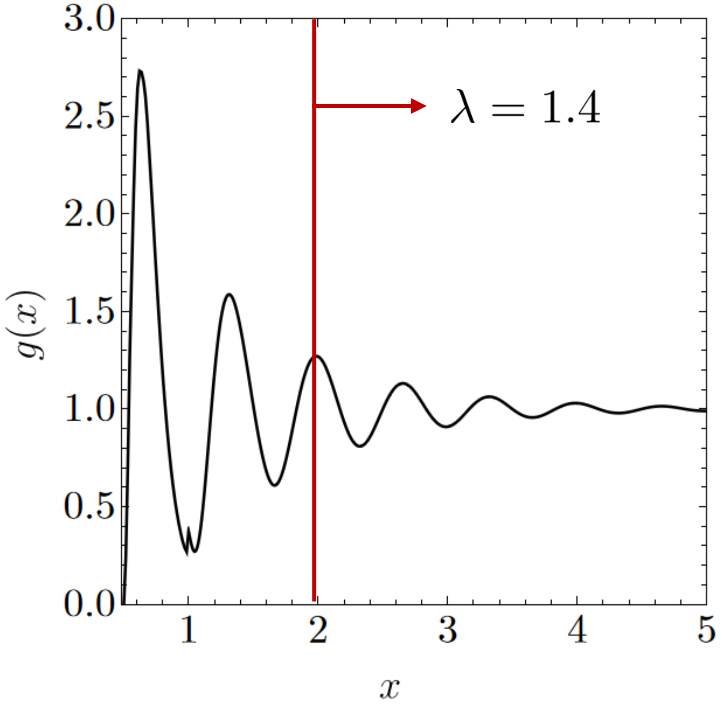

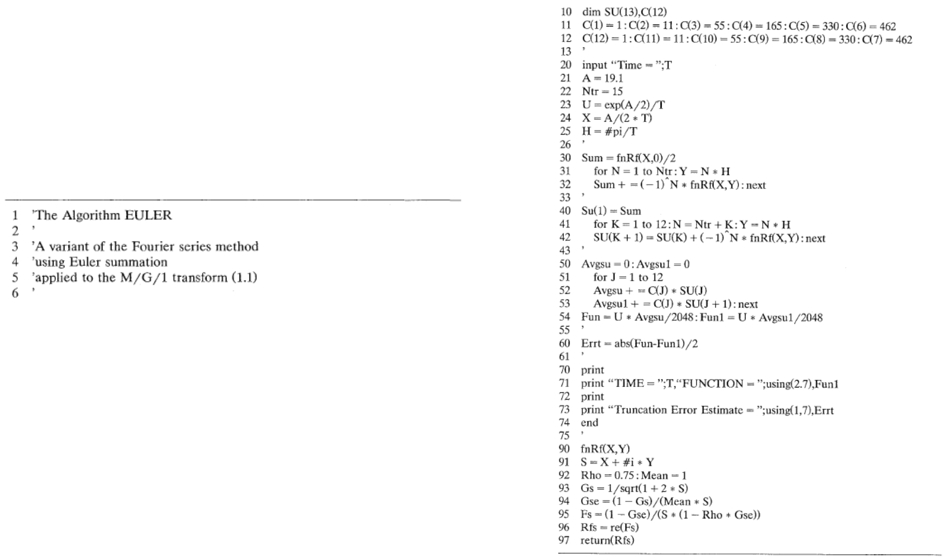

```
1  'The Algorithm EULER
2  '
3  'A variant of the Fourier series method
4  'using Euler summation
5  'applied to the M/G/1 transform (1.1)
6  '
10 dim SU(13),C(12)
11 C(1) = 1 : C(2) = 11 : C(3) = 55 : C(4) = 165 : C(5) = 330 : C(6) = 462
12 C(12) = 1 : C(11) = 11 : C(10) = 55 : C(9) = 165 : C(8) = 330 : C(7) = 462
13 '
20 input "Time = ";T
21 A = 19.1
22 Ntr = 15
23 U = exp(A/2)/T
24 X = A/(2 * T)
25 H = #pi/T
26 '
30 Sum = fnRf(X,0)/2
31    for N = 1 to Ntr : Y = N * H
32    Sum + = (-1)^N * fnRf(X,Y) : next
33 '
40 Su(1) = Sum
41    for K = 1 to 12 : N = Ntr + K : Y = N * H
42    SU(K + 1) = SU(K) + (-1)^N * fnRf(X,Y) : next
43 '
50 Avgsu = 0 : Avgsu1 = 0
51    for J = 1 to 12
52    Avgsu + = C(J) * SU(J)
53    Avgsu1 + = C(J) * SU(J + 1) : next
54 Fun = U * Avgsu/2048 : Fun1 = U * Avgsu1/2048
55 '
60 Errt = abs(Fun-Fun1)/2
61 '
70 print
71 print "TIME = ";T,"FUNCTION = ";using(2.7),Fun1
72 print
73 print "Truncation Error Estimate = ";using(1,7),Errt
74 end
75 '
90 fnRf(X,Y)
91 S = X + #i * Y
92 Rho = 0.75 : Mean = 1
93 Gs = 1/sqrt(1 + 2 * S)
94 Gse = (1 - Gs)/(Mean * S)
95 Fs = (1 - Gse)/(S * (1 - Rho * Gse))
96 Rfs = re(Fs)
97 return(Rfs)
```

Abate, J., Whitt, W. *Queueing Syst* **10**, 5–87 (1992).

Longitudinal RDF: numerical details

$$\hat{G}(s) = \sum_{i}^{M} \sum_{j}^{M} \phi_j^2 \phi_i^2 \hat{G}_{ij}(s)$$

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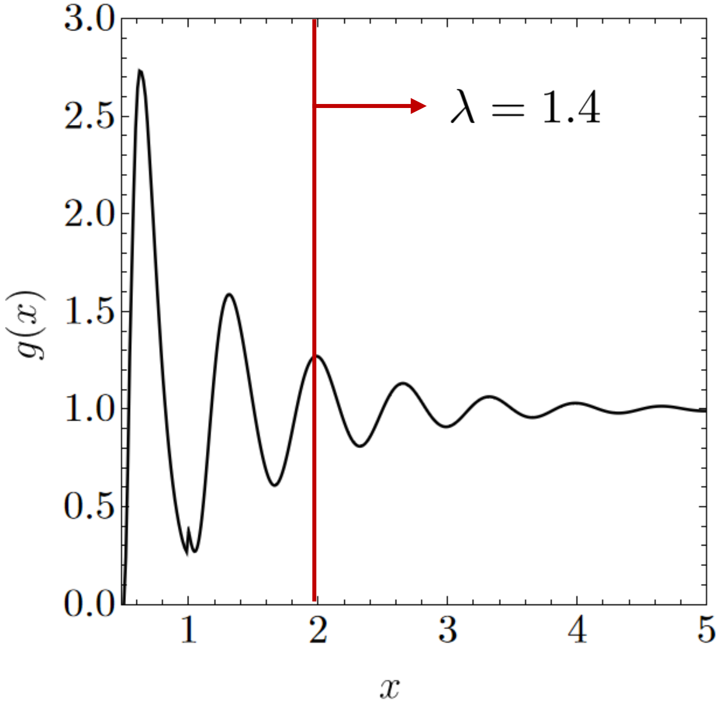
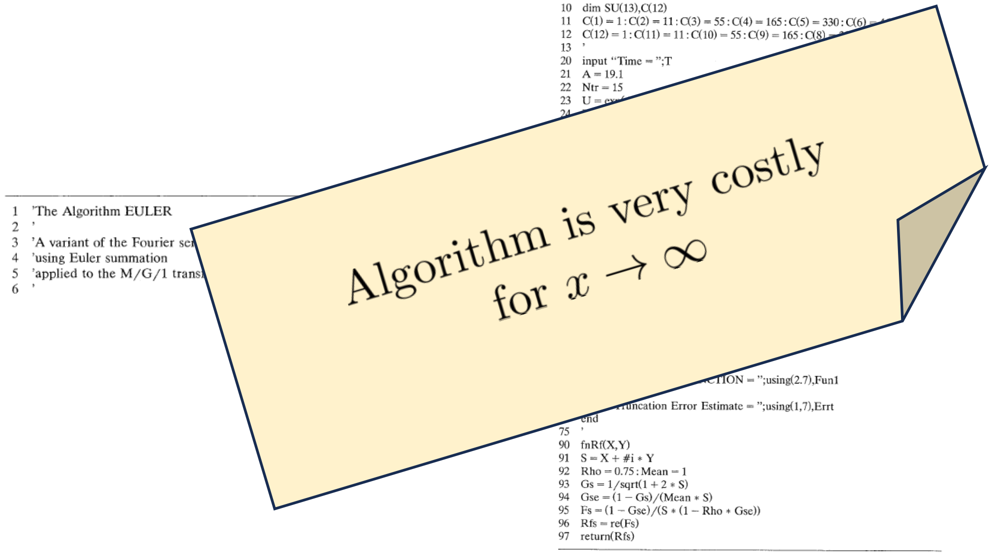
inverse Laplace transform → RDF $g(x)$

numerical inversion ↓





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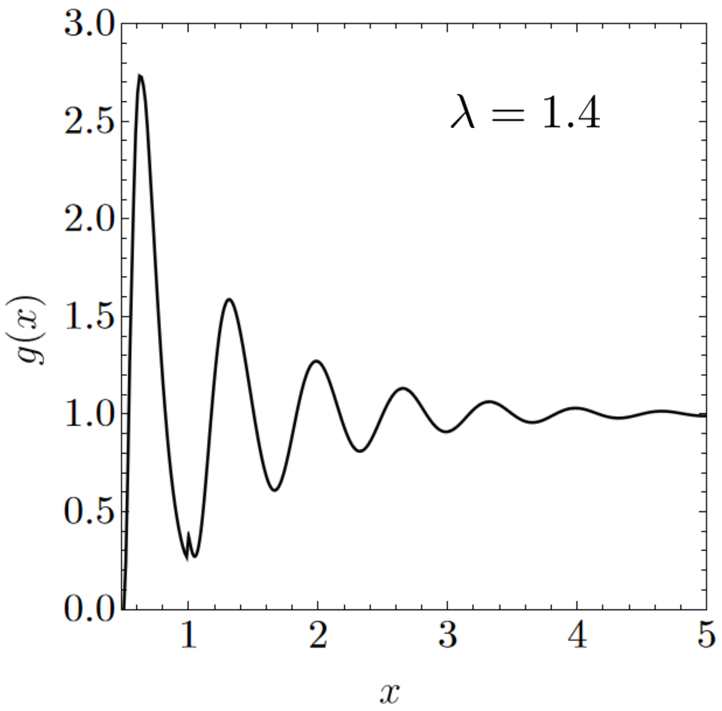
inverse
Laplace transform → RDF $g(x)$



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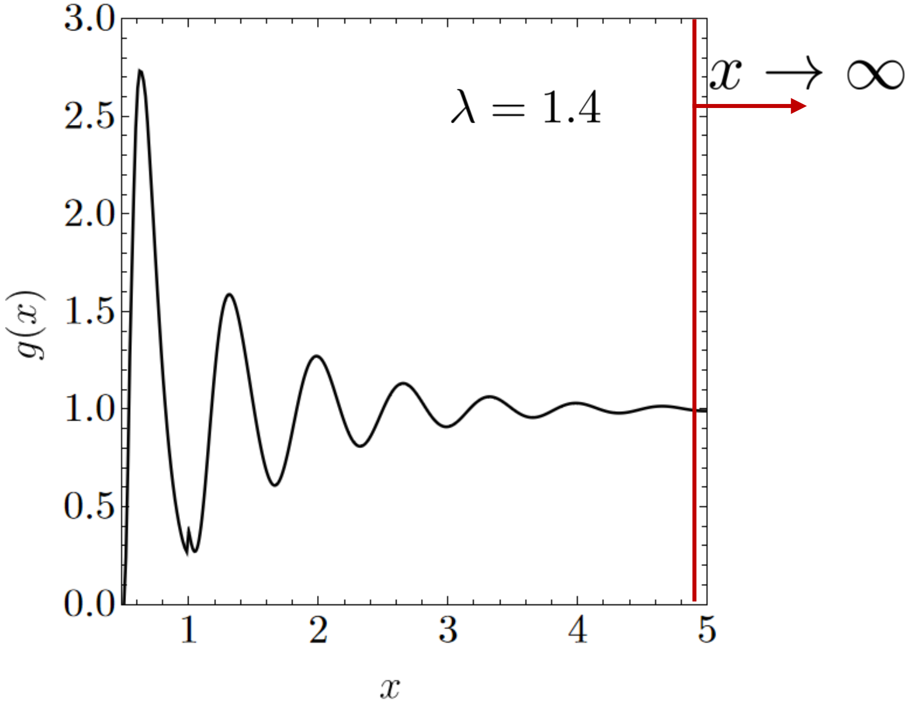

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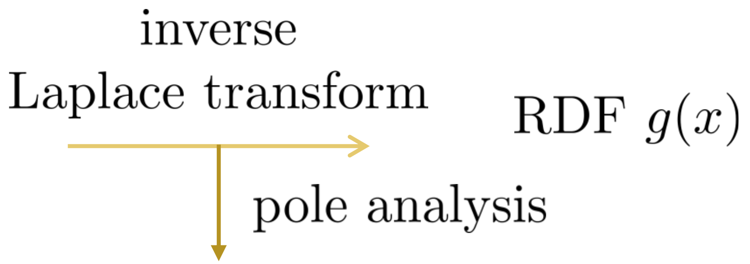

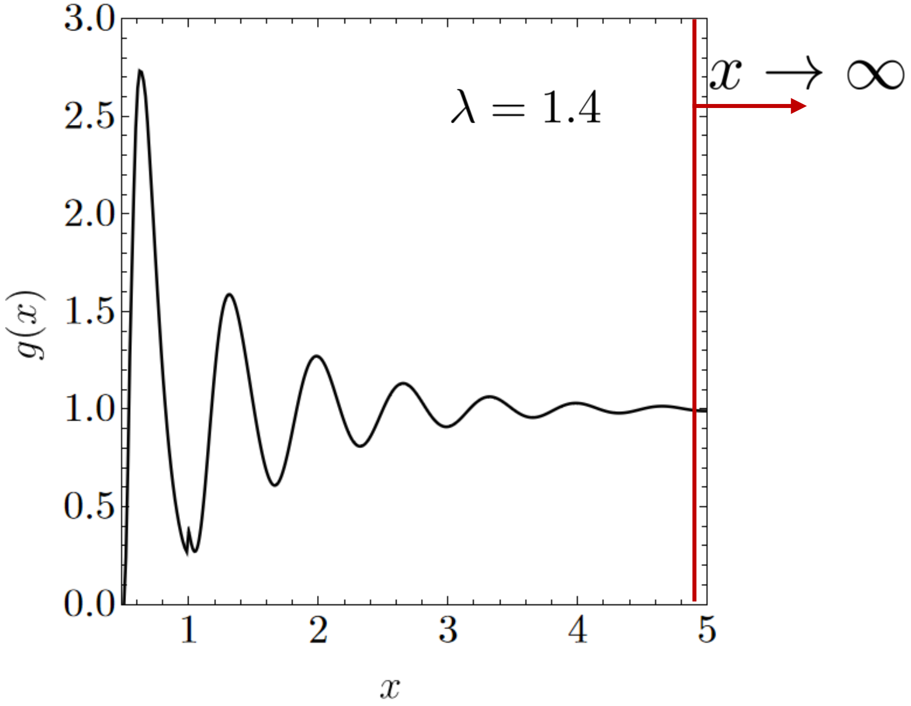

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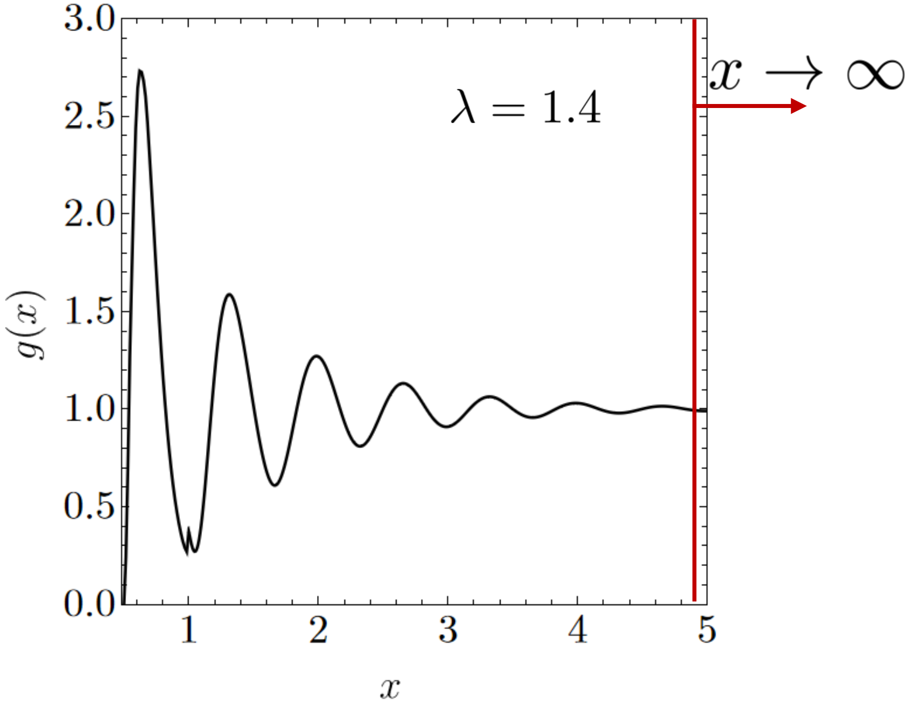
inverse Laplace transform → RDF $g(x)$

pole analysis ↓



Compute the poles of $\hat{G}_{ij}(s)$ $\quad \det\left[\mathbf{I} - A^2 \mathbf{\Omega}(s+\beta p)\right] = 0$

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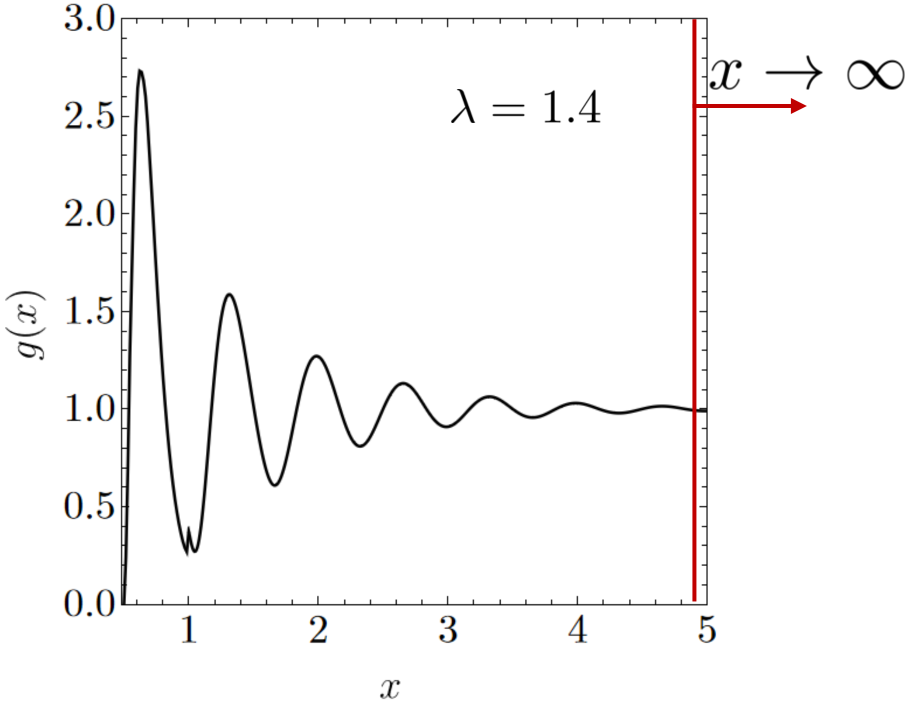
inverse Laplace transform → RDF $g(x)$

↓ pole analysis



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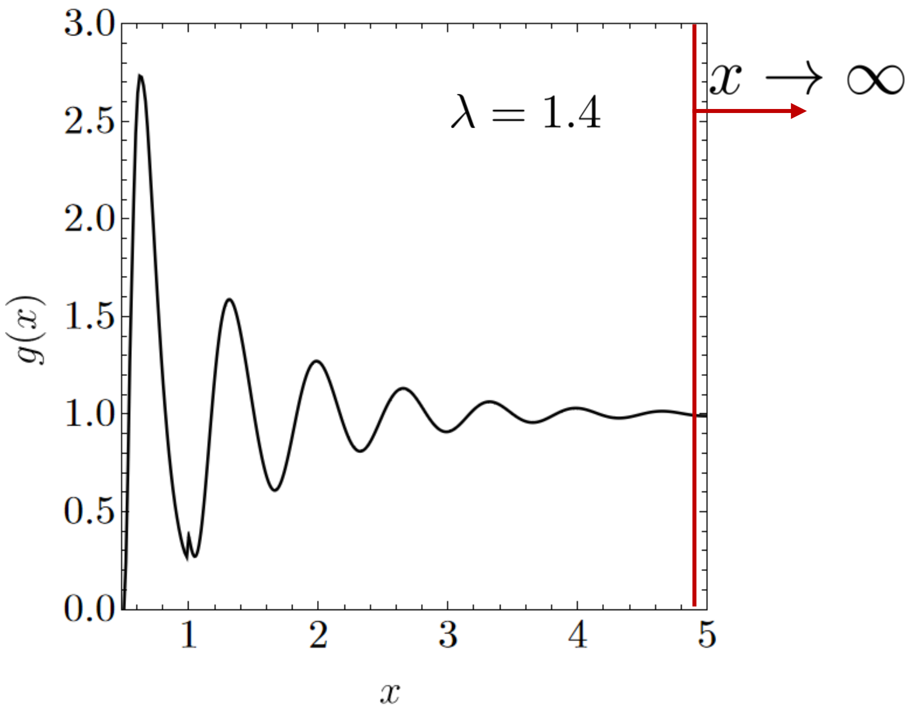

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For $x \to \infty$ only s_1 is important:

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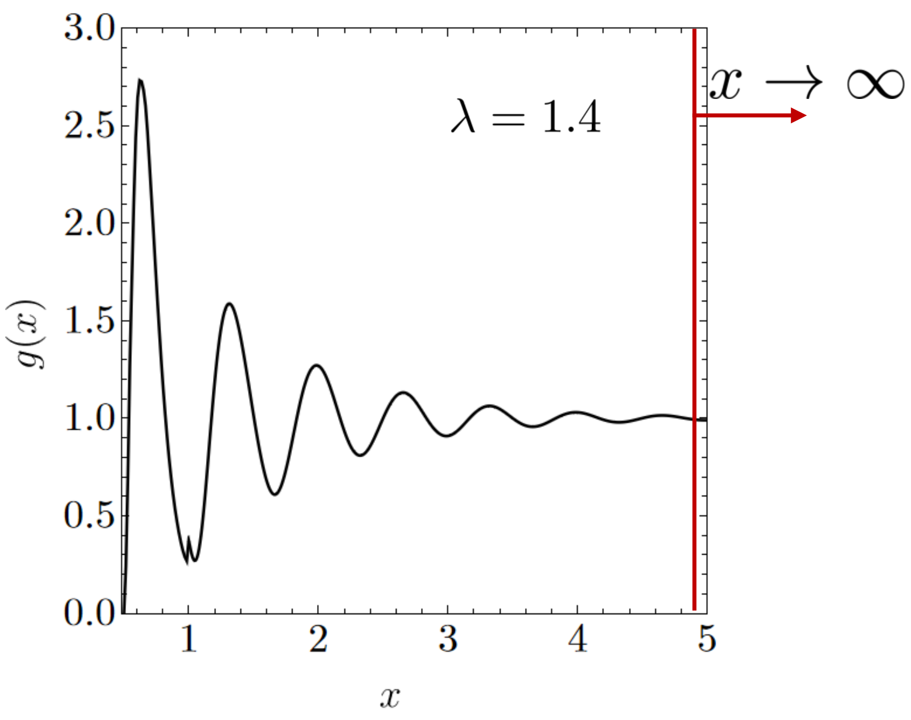

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For $x \to \infty$ only s_1 is important:

$$g_{ij}(x) \approx 1 + \mathcal{A}_{ij} e^{-\kappa x}, \qquad s_1 = -\kappa$$

$$g_{ij}(x) \approx 1 + 2|\mathcal{A}_{ij}| e^{-\kappa x} \cos(\omega x + \delta_{ij}), \qquad s_1 = -\kappa \pm \imath\omega$$

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inverse
Laplace transform → RDF $g(x)$

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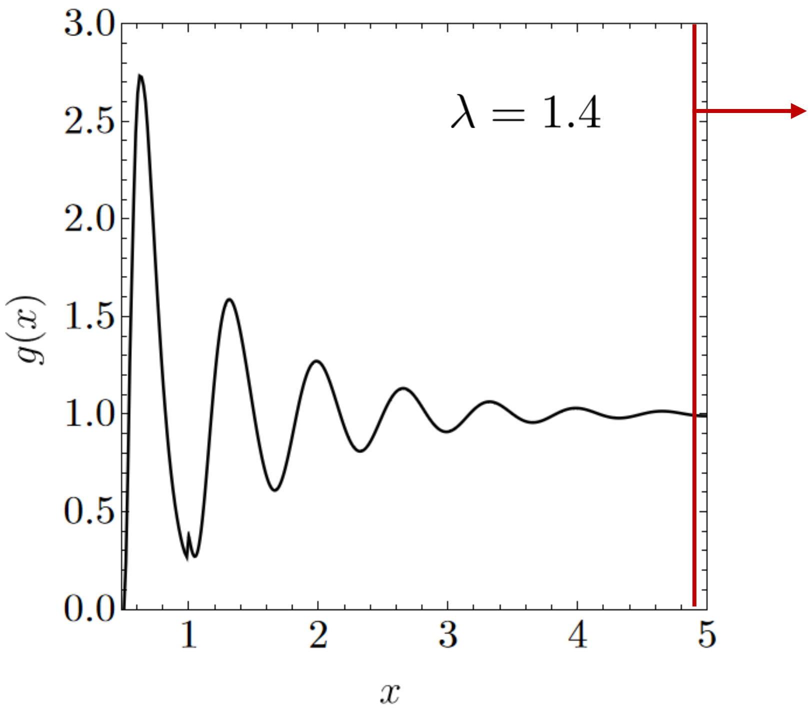

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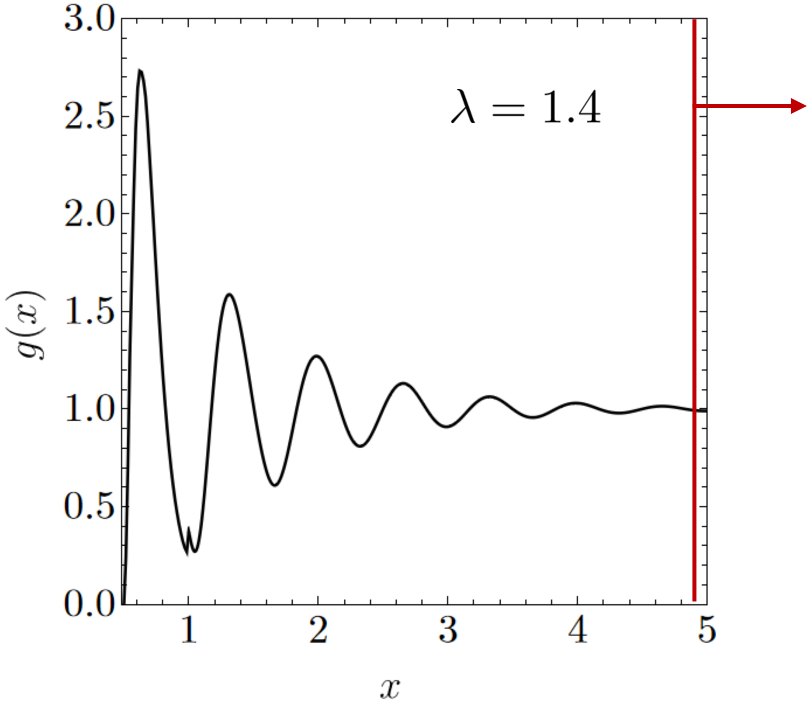

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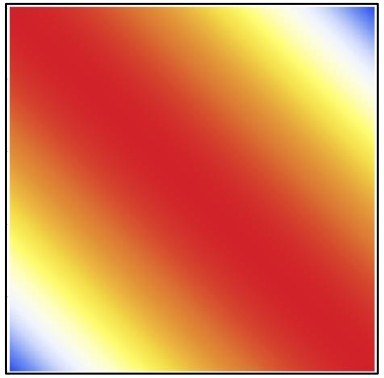
$M \times M$



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inverse Laplace transform → RDF $g(x)$

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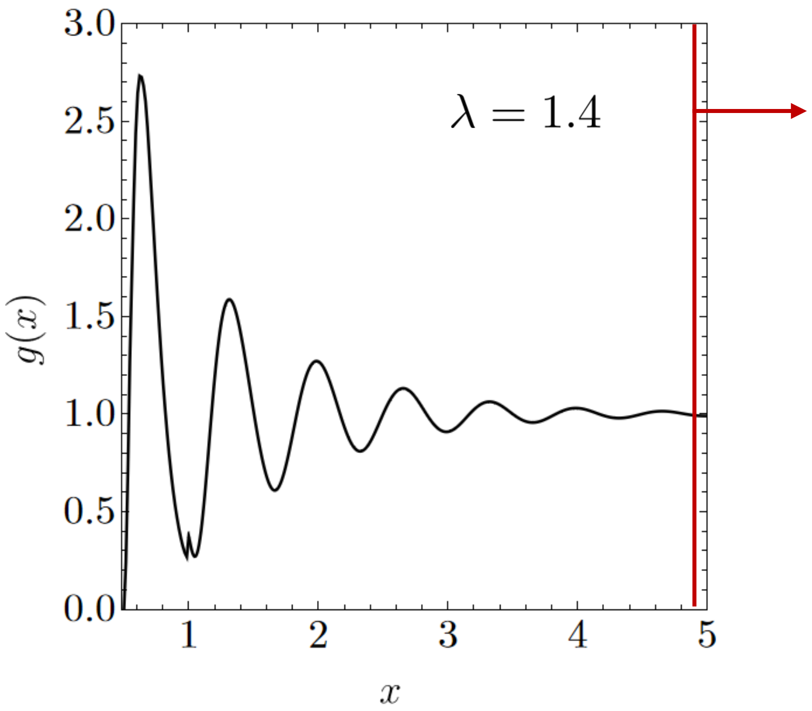

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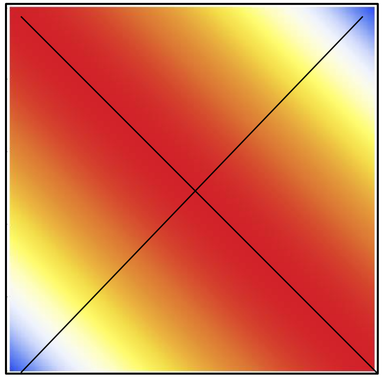

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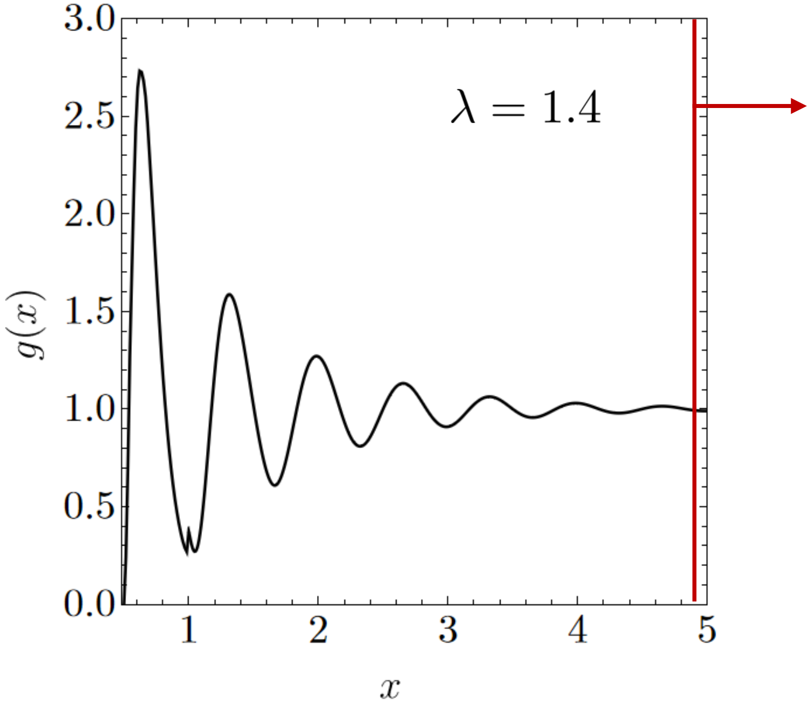

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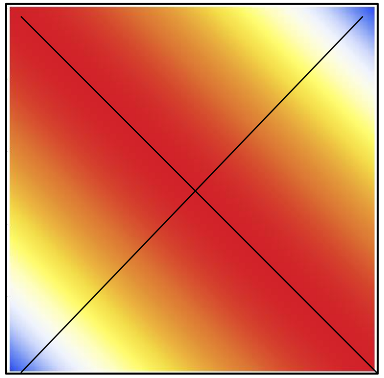
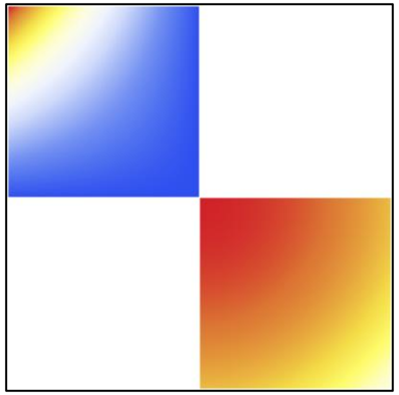


$\mathbf{I} - A^2 \mathbf{\Omega}(s+\beta p)$

$$\mathbf{X} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{I} & \bar{\mathbf{R}} \\ -\bar{\mathbf{R}} & \mathbf{I} \end{pmatrix} \longrightarrow$$



$\mathbf{X}^T (\mathbf{I} - A^2 \mathbf{\Omega}(s+\beta p)) \mathbf{X}$

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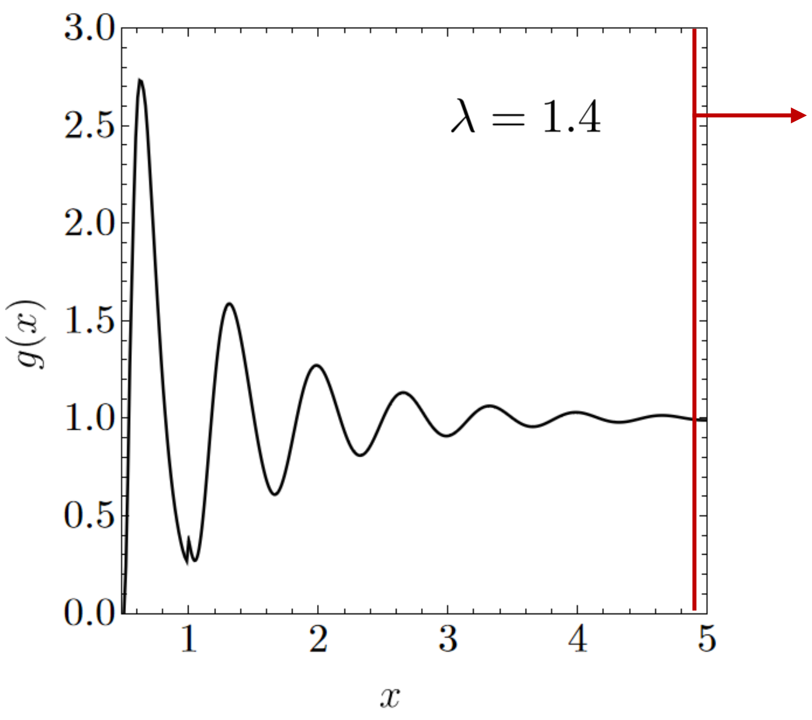

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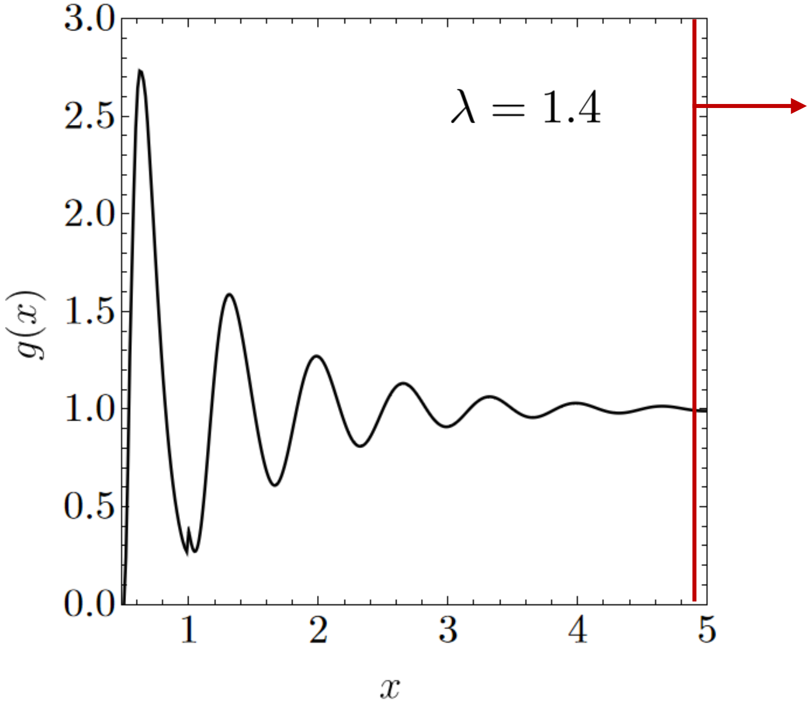

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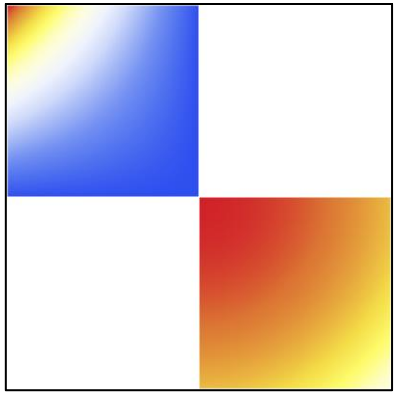

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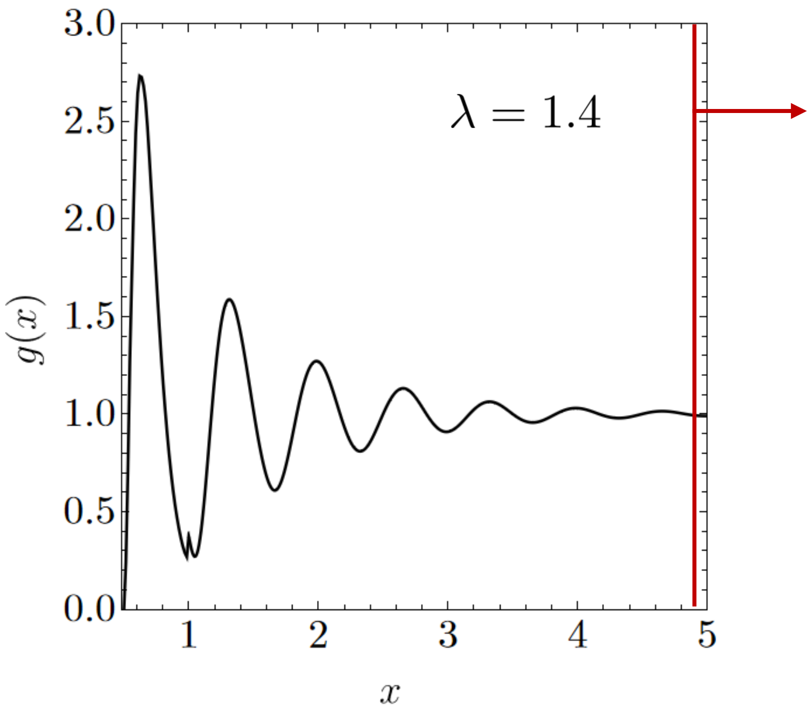

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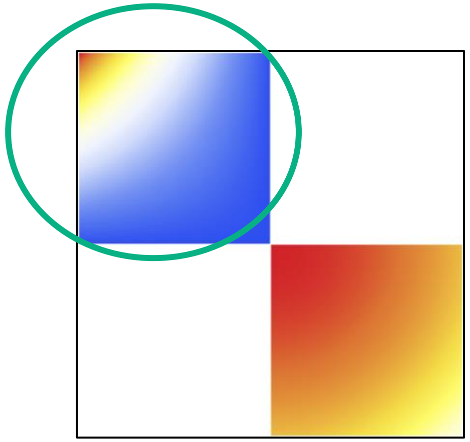

$\mathcal{A}_{ij,n} \equiv \mathrm{Res}[\hat{G}_{ij}(s)]_{s_n}$ anti-symmetric

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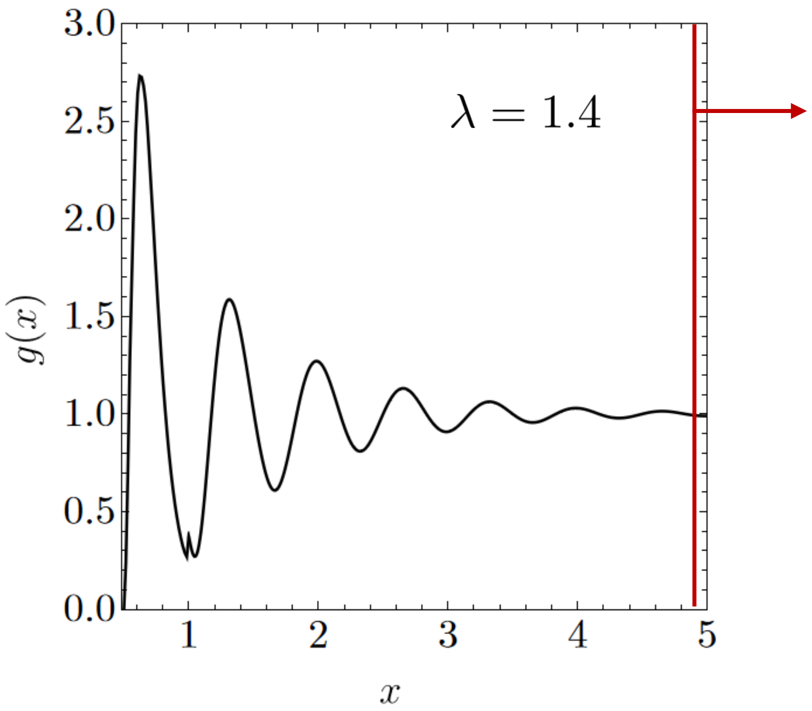

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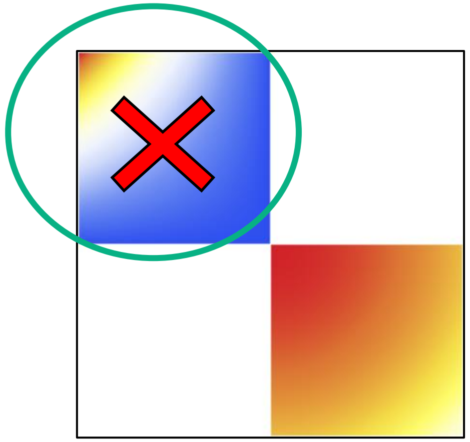


$\mathcal{A}_{ij,n} \equiv \mathrm{Res}[\hat{G}_{ij}(s)]_{s_n}$ anti-symmetric

$\mathbf{X}^T (\mathbf{I} - A^2 \mathbf{\Omega}(s+\beta p)) \mathbf{X}$

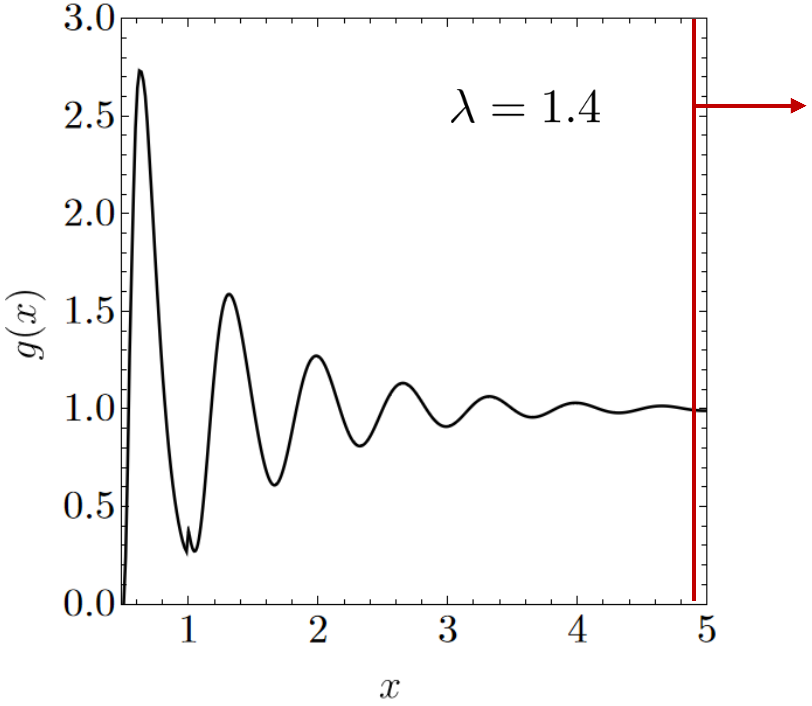
Longitudinal RDF: numerical details

$$\hat{G}(s) = \sum_{i}^{M} \sum_{j}^{M} \phi_j^2 \phi_i^2 \hat{G}_{ij}(s)$$

$$\hat{G}_{ij}(s) = \frac{A^2}{\lambda \phi_j \phi_i} \left(\mathbf{\Omega}(s+\beta p) \cdot \left[\mathbf{I} - A^2 \mathbf{\Omega}(s+\beta p) \right]^{-1} \right)_{ij}$$

inverse
Laplace transform → RDF $g(x)$

↓ pole analysis



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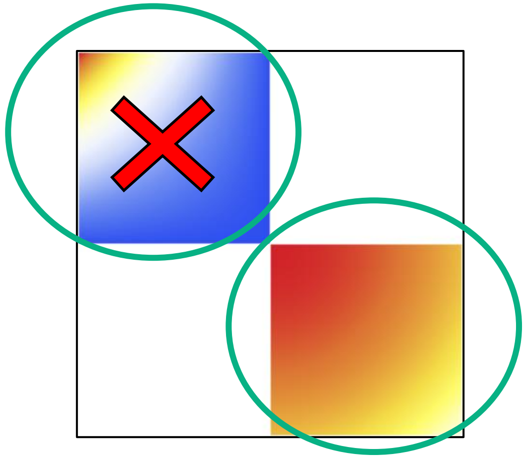

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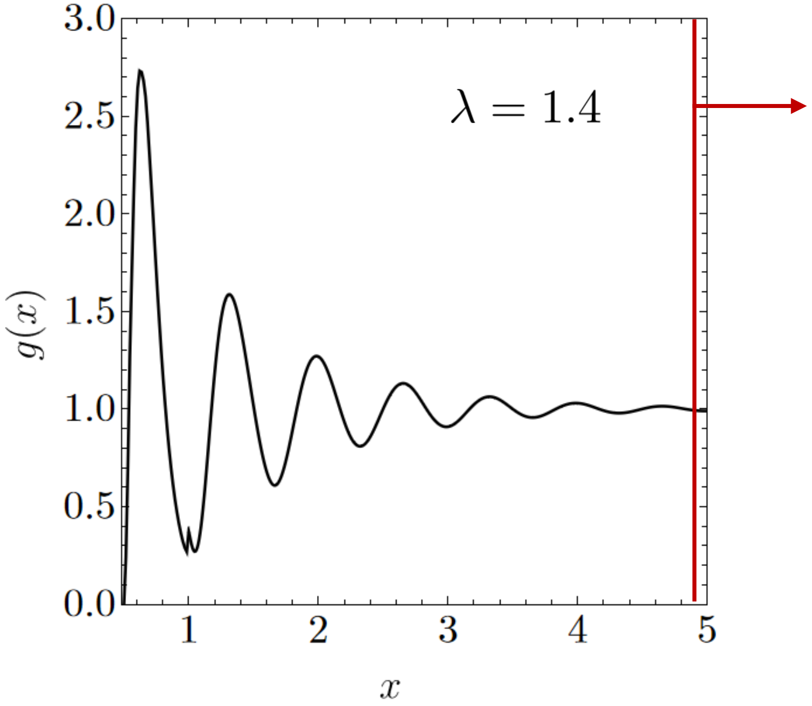

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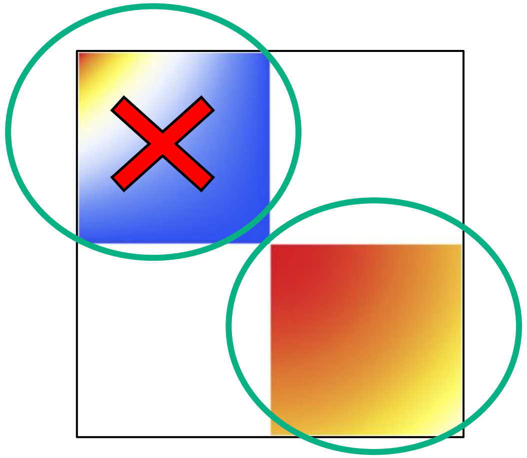

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inverse
Laplace transform

RDF $g(x)$

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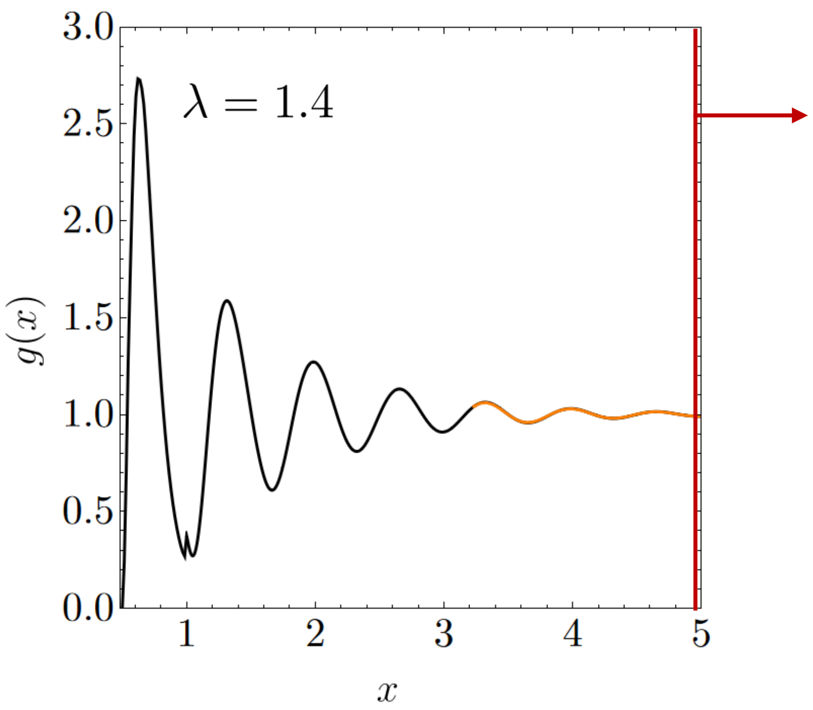

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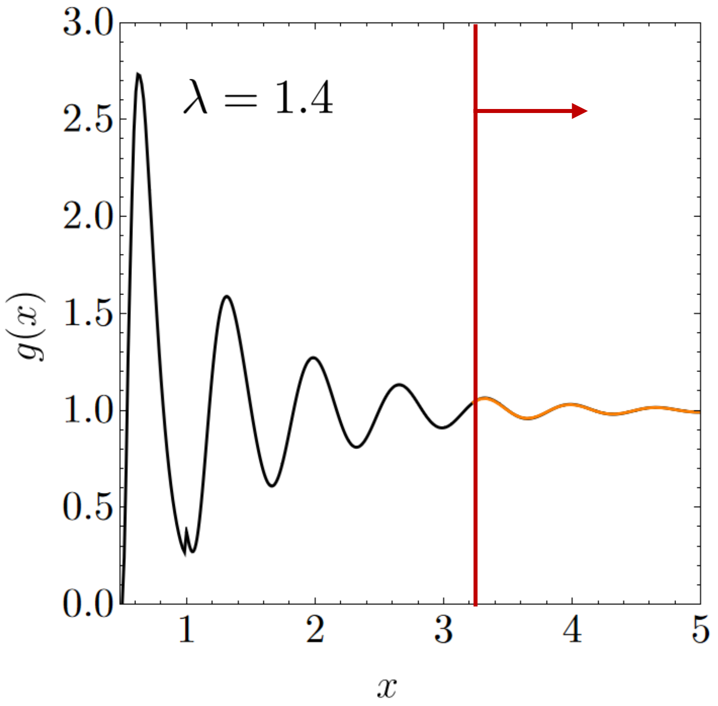

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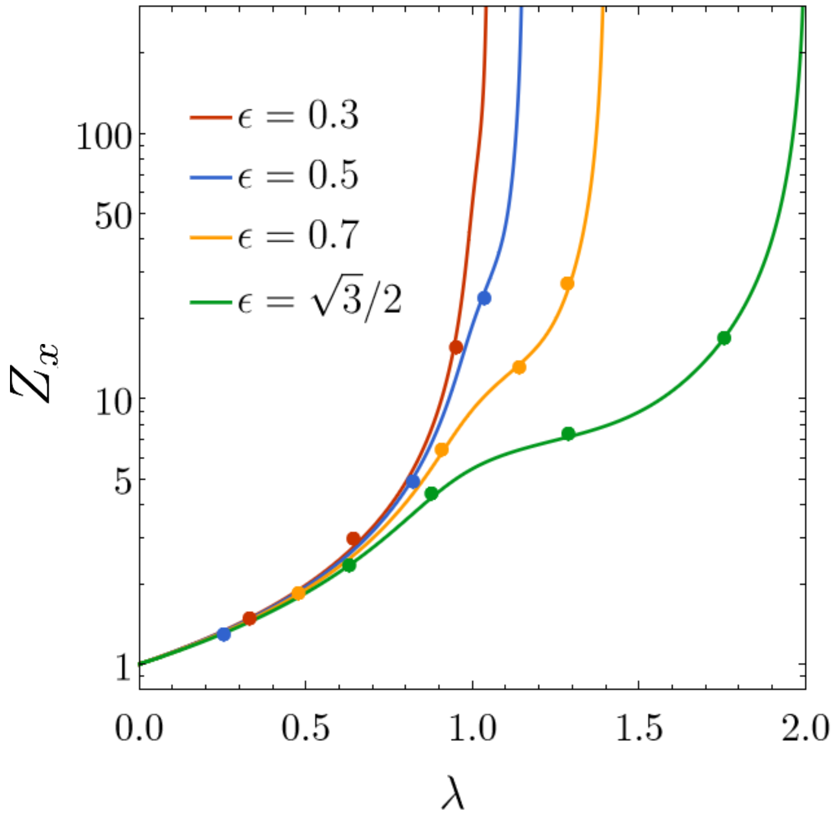
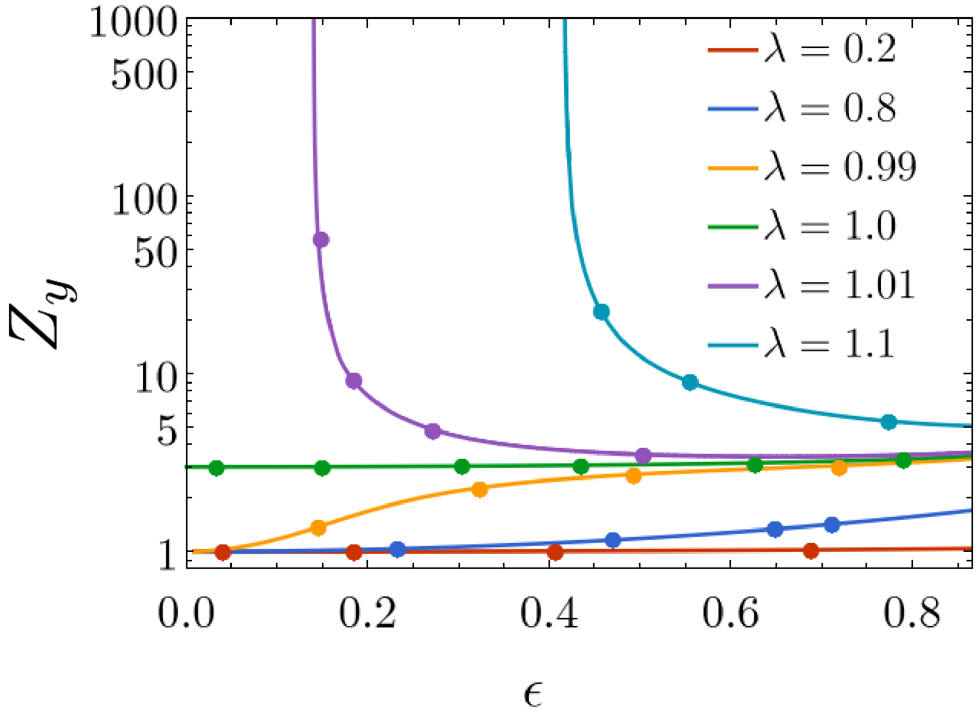
Simulations

Equation of state: simulations





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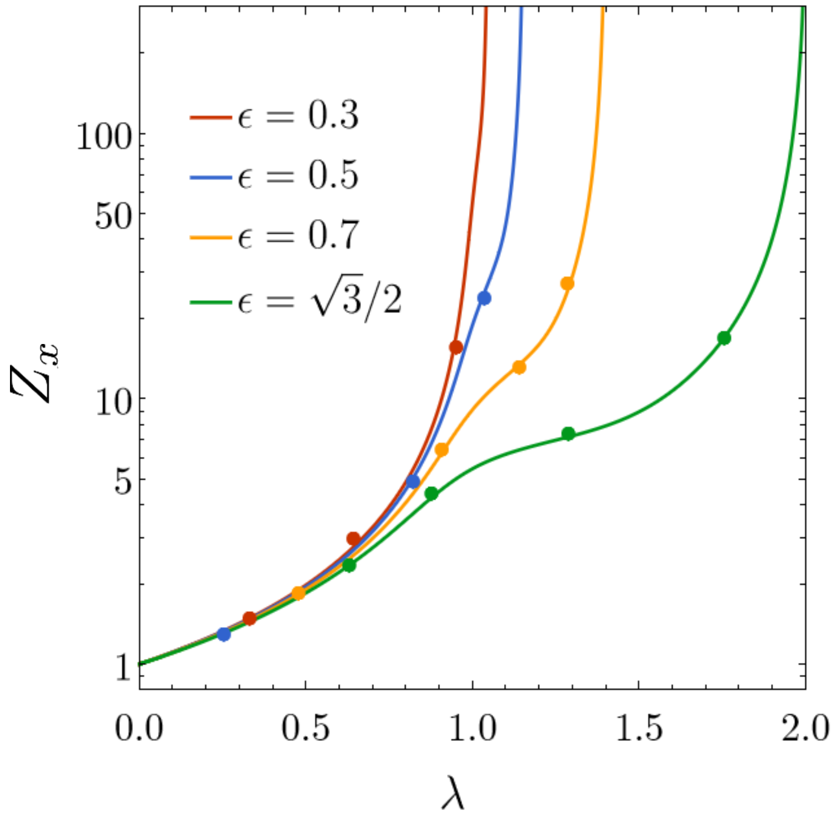
Equation of state: simulations



Simulations done in the $\{N, p_x, \epsilon, T\}$ ensemble.

$$\lambda = N/L_x$$

Simulations in the $\{N, L_x, \epsilon, T\}$ ensemble are problematic to compute the equation of state:

$$Z = \frac{1 - \lambda \int_{a(\epsilon)}^{1} dx\, g(x)}{1 - \lambda \left[1 - \lambda \int_{a(\epsilon)}^{1} dx\, (1-x) g(x)\right]}.$$

High sensitivity

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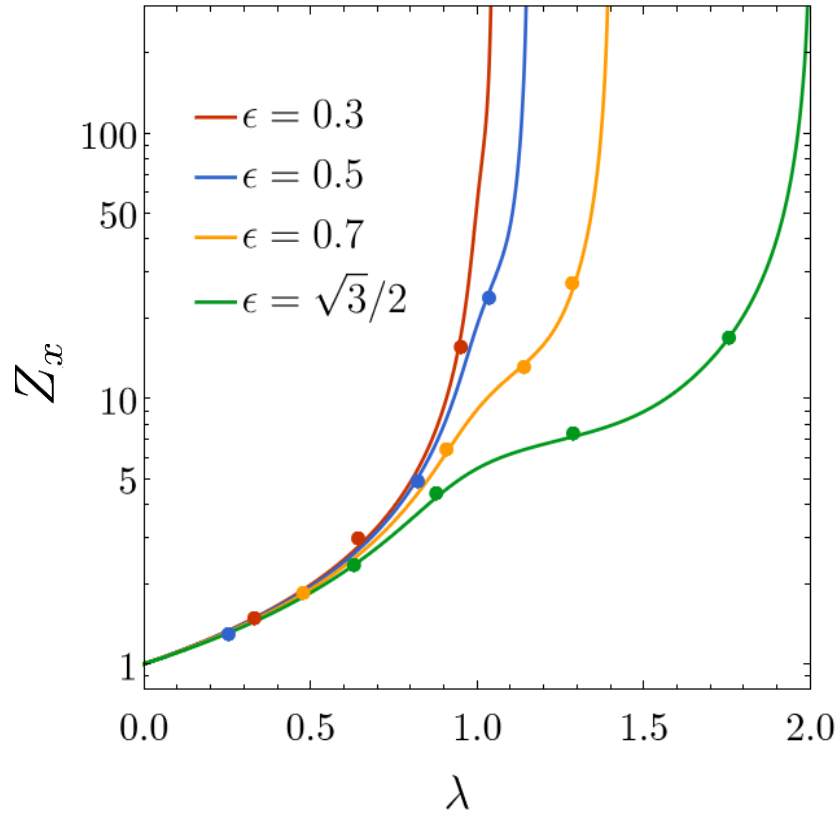
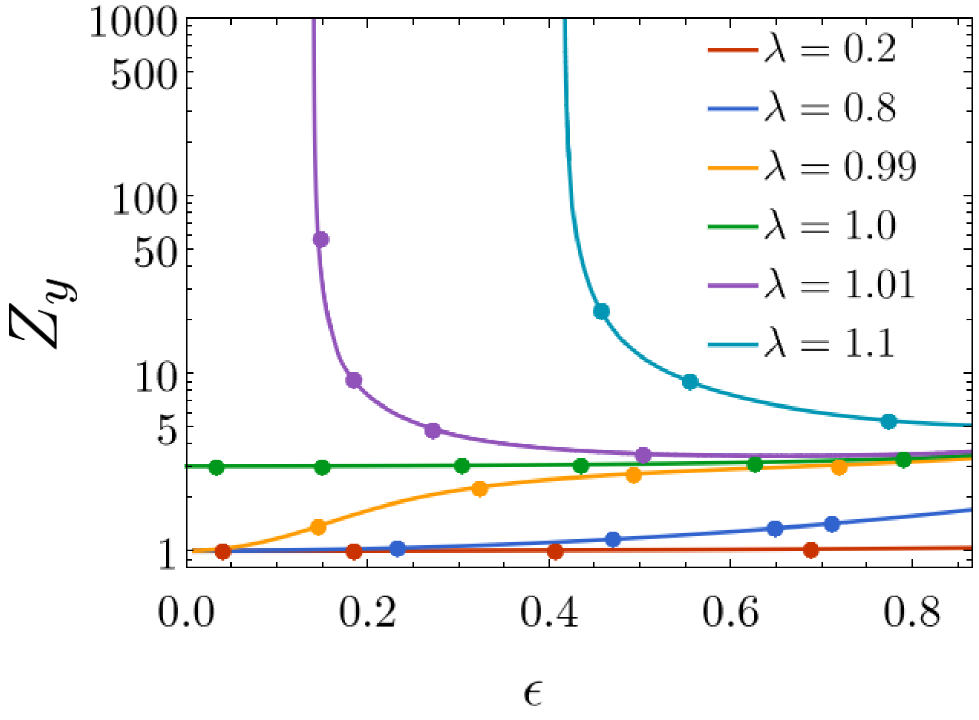
Equation of state: simulations





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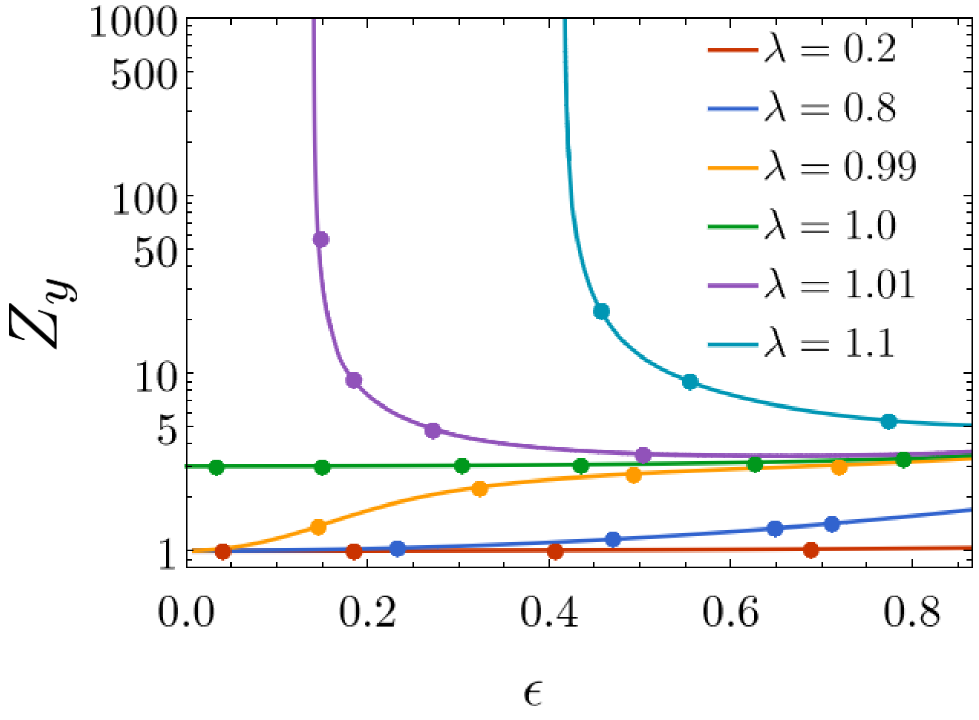
Equation of state: simulations

Simulations done in the $\{N, p_y, L_x, T\}$ ensemble.

$$\lambda = N/L_x$$

Simulations in the $\{N, L_x, \epsilon, T\}$ ensemble are also problematic



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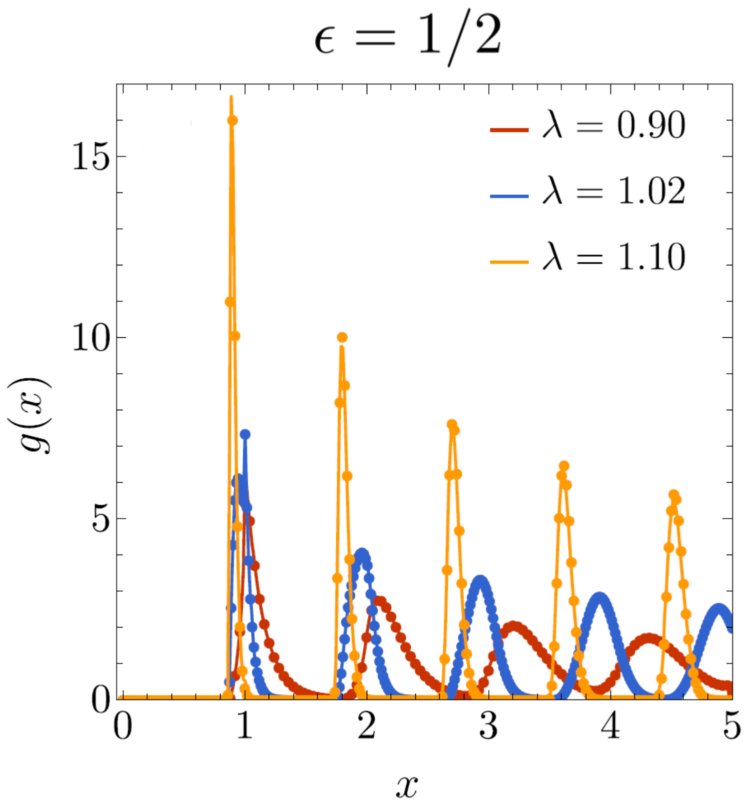
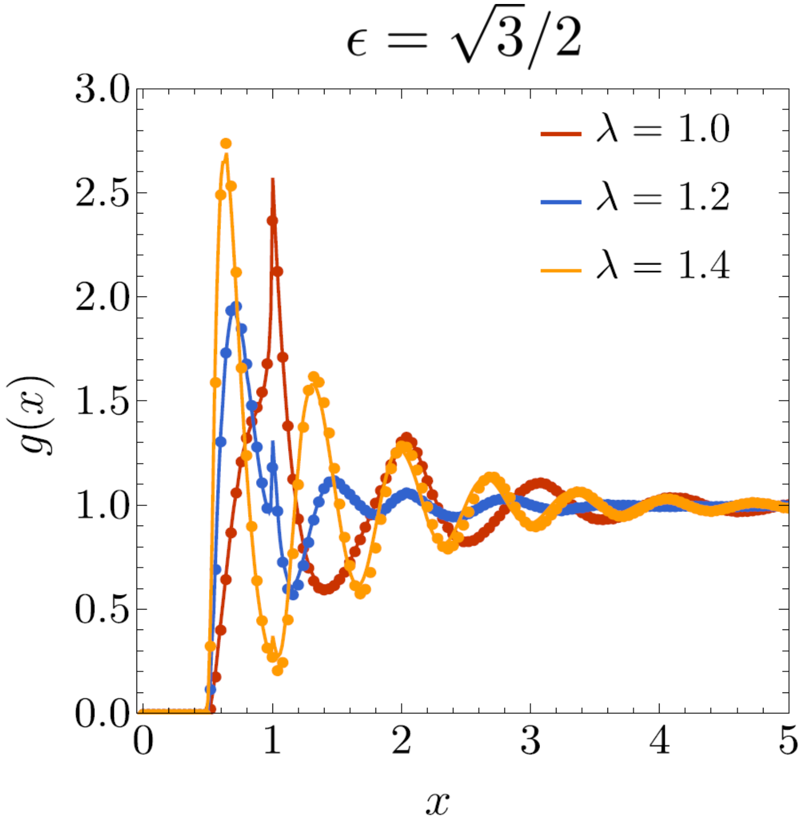
RDF: simulations

RDF simulation can be done in the $\{N, L_x, \epsilon, T\}$ ensemble.





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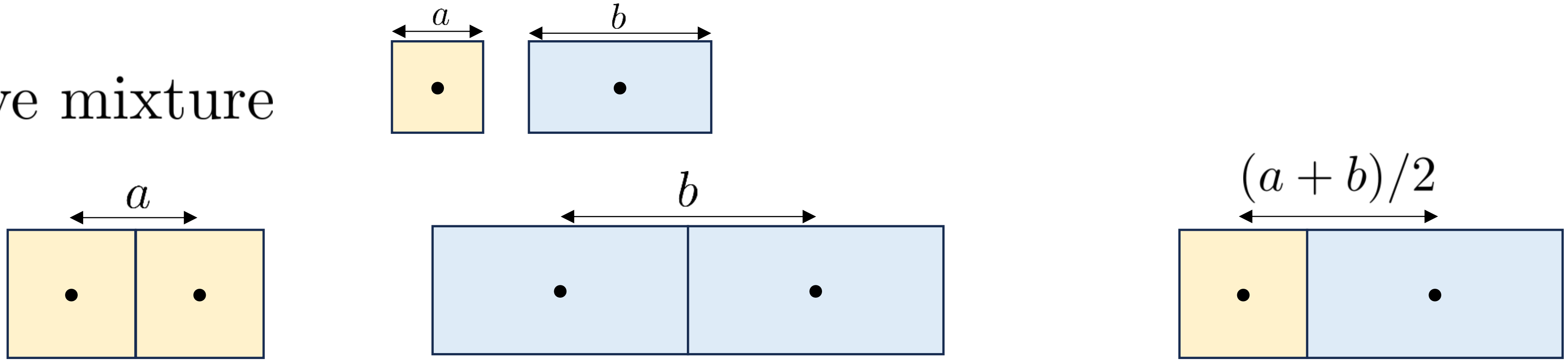
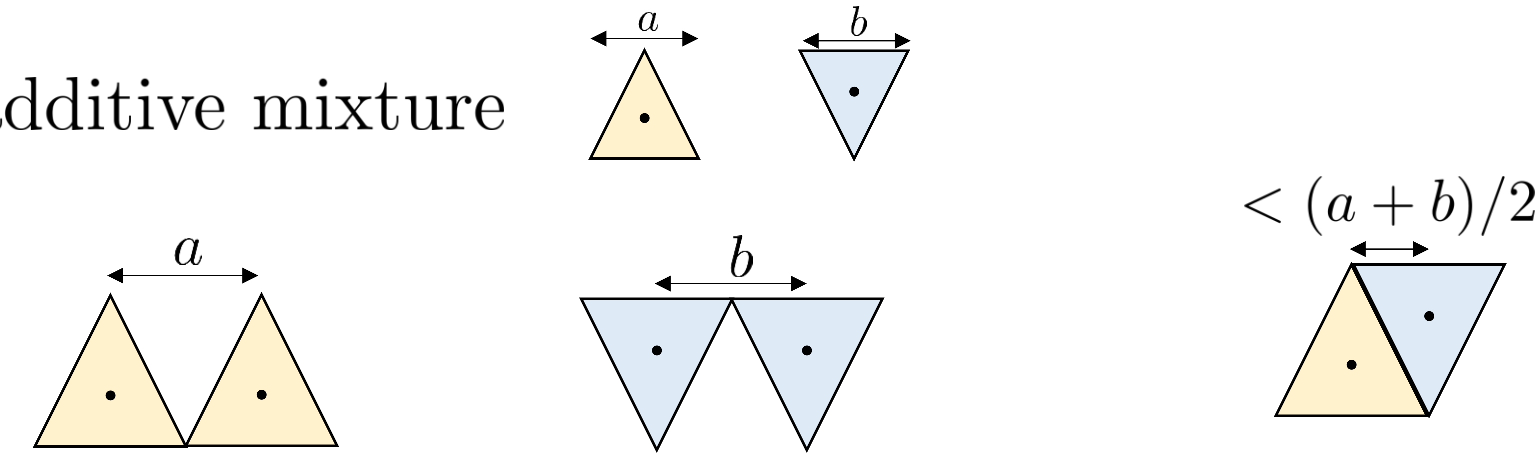
Thank you for your attention

Additivity in the mixtures

Additive mixture



Non-additive mixture



Extrapolating M to infinity

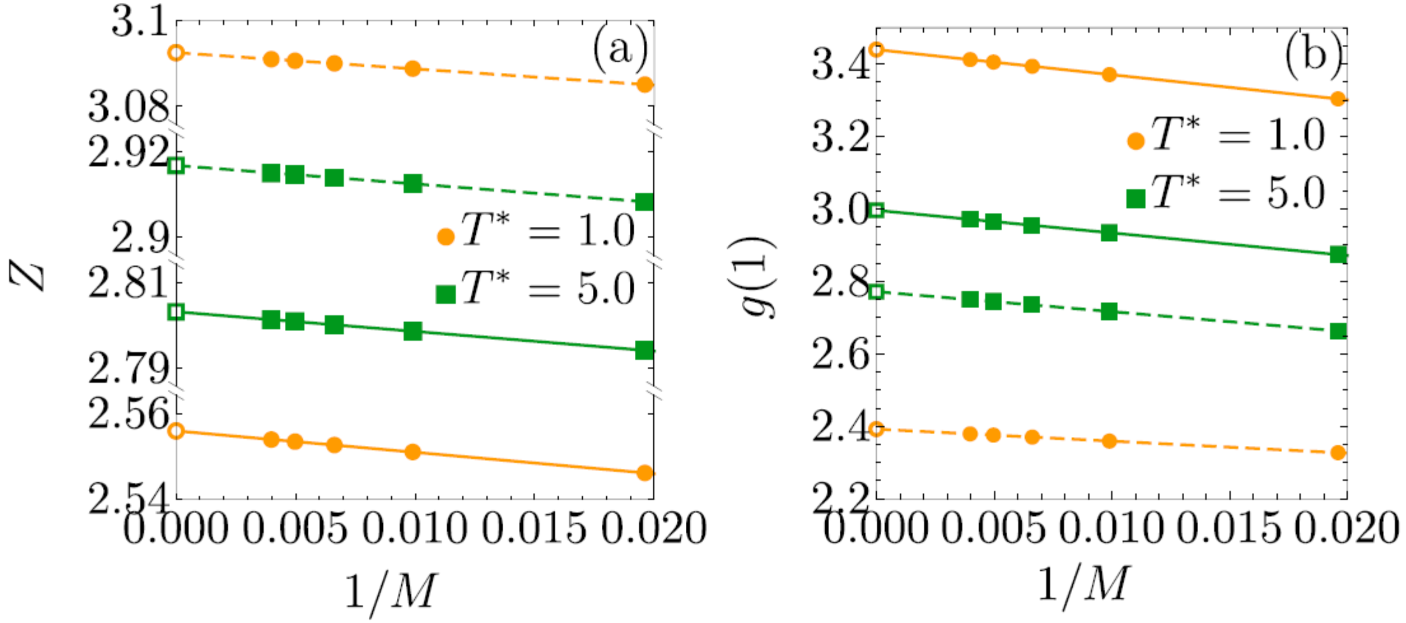
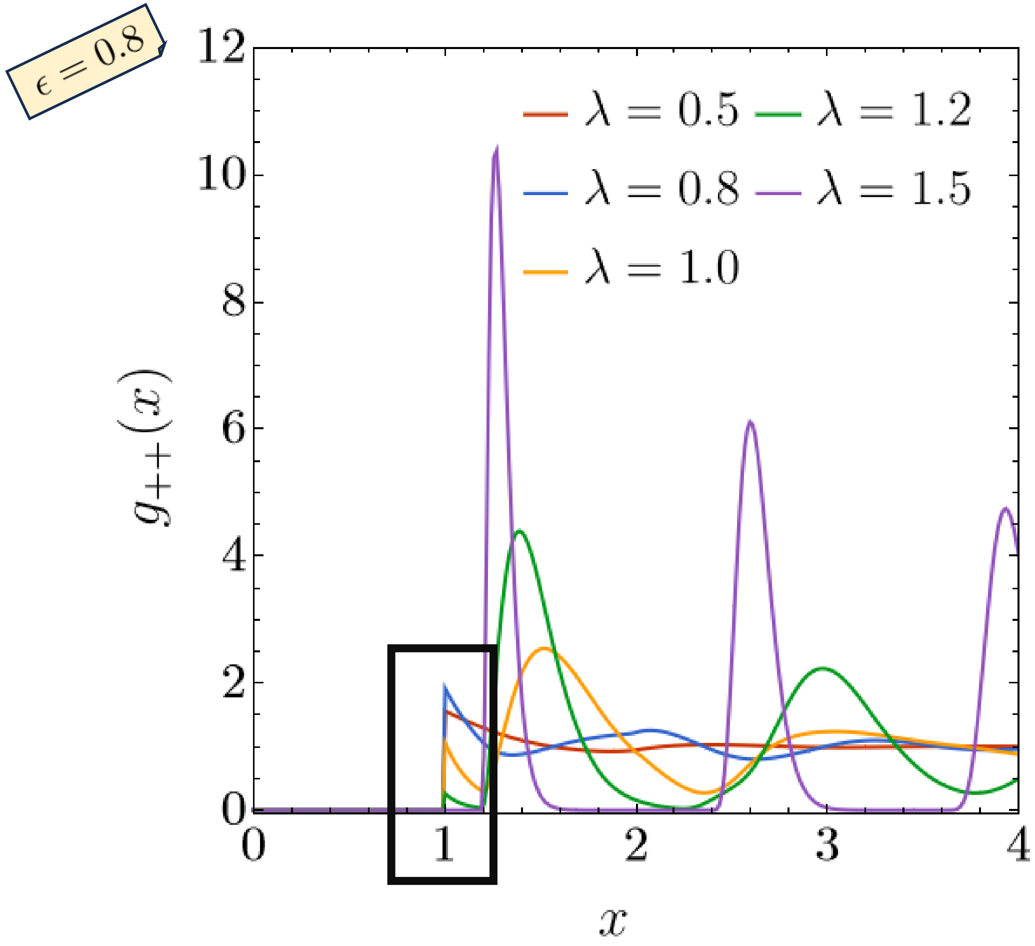


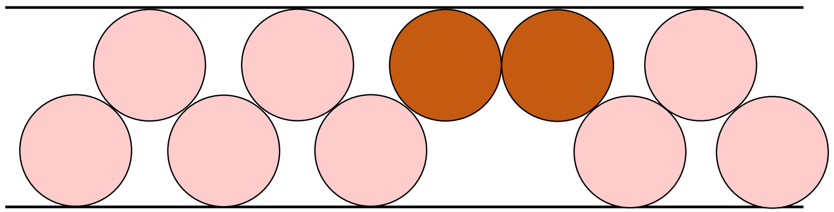
FIG. 3. Plot of (a) Z and (b) $g(1)$ versus $1/M$ for $T^* = 1$ (circles) and $T^* = 5$ (squares), in both cases with $\lambda = 1$. The lines (solid for SW and dashed for SS) are linear fits to the numerical data. The open symbols at $1/M$ denote the extrapolations to $M \to \infty$.

Structural properties: defects

Structural properties: defects

At high density, a zig-zag structure is favoured, but defects might appear in the structure





- $g_{++}(x)$ measures correlations between particles in the uppermost part of the channel.
- The disappearance of defects in the structure evolves as

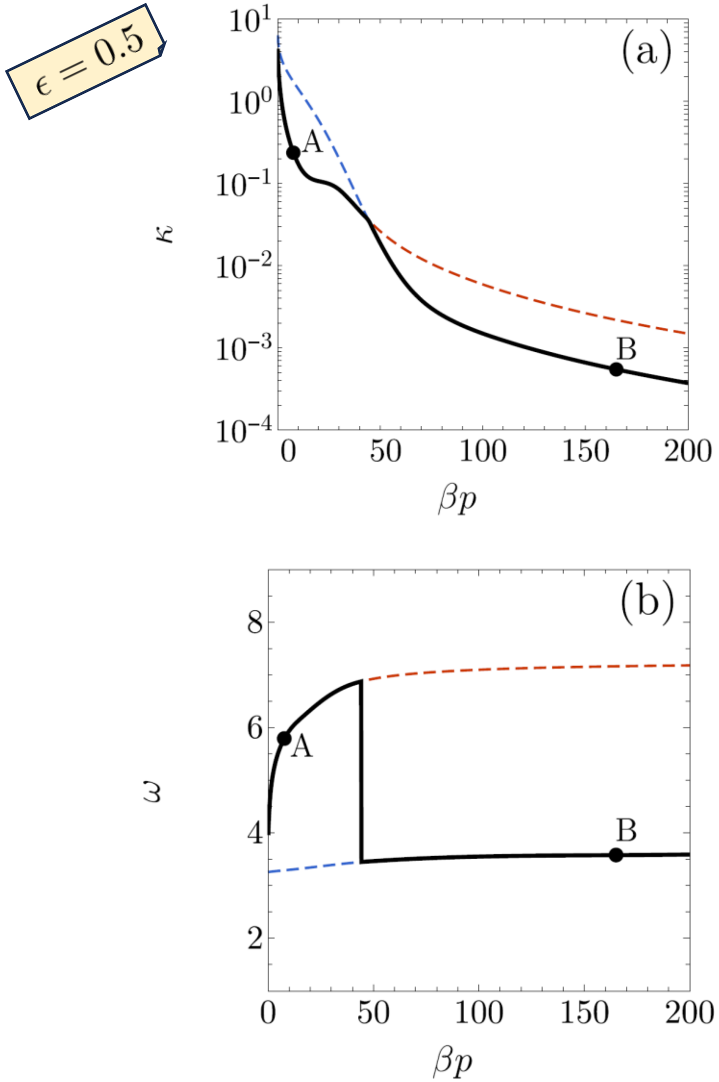
$$g_{++}(1^+) \propto \beta p_x e^{-\beta p_x}$$

Structural properties: asymptotic behavior

Structural properties: asymptotic behavior

$$\begin{cases} g_{ij}(x) \approx 1 + 2|\mathcal{A}_{ij}|e^{-\kappa x}\cos(\omega x + \delta_{ij}) \\ g_{ij}(x) \approx 1 + \mathcal{A}_{ij}e^{-\kappa x} \end{cases}$$

Structural properties: asymptotic behavior



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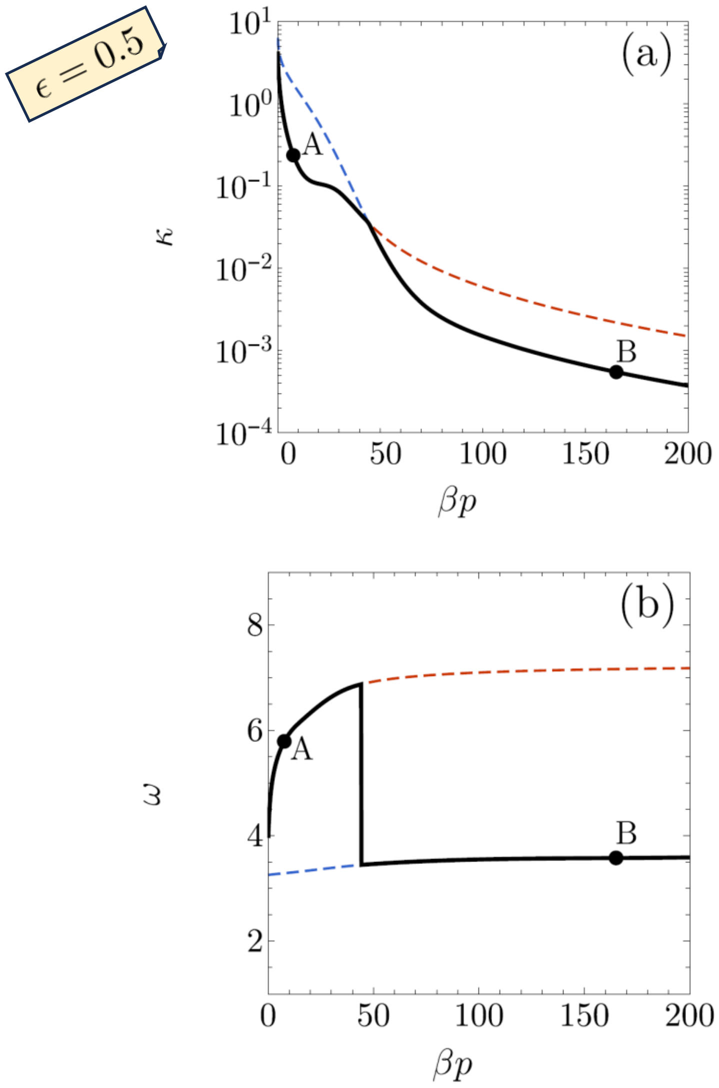

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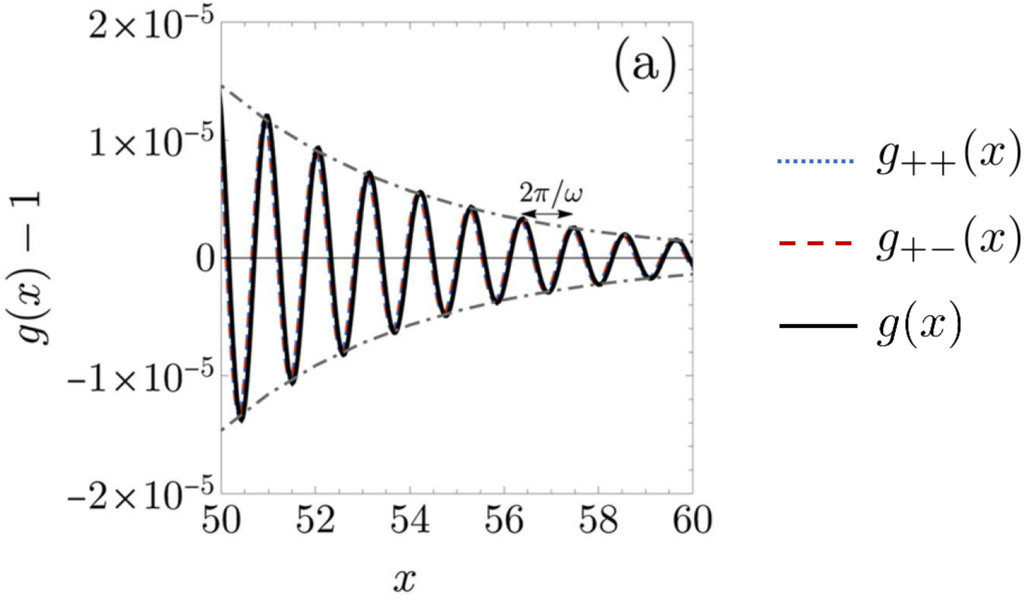
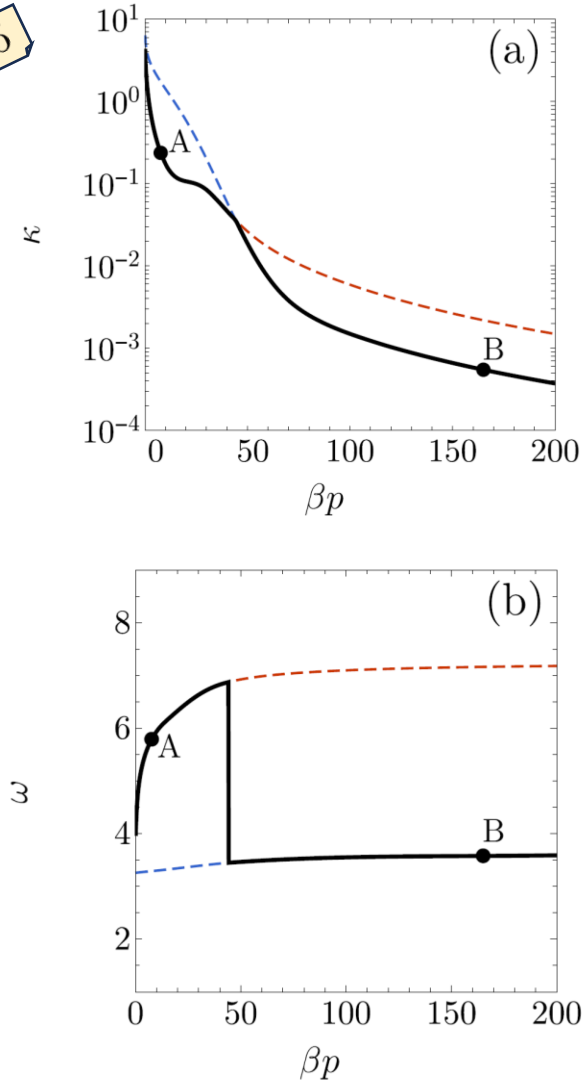


Structural properties: asymptotic behavior

$\epsilon = 0.5$



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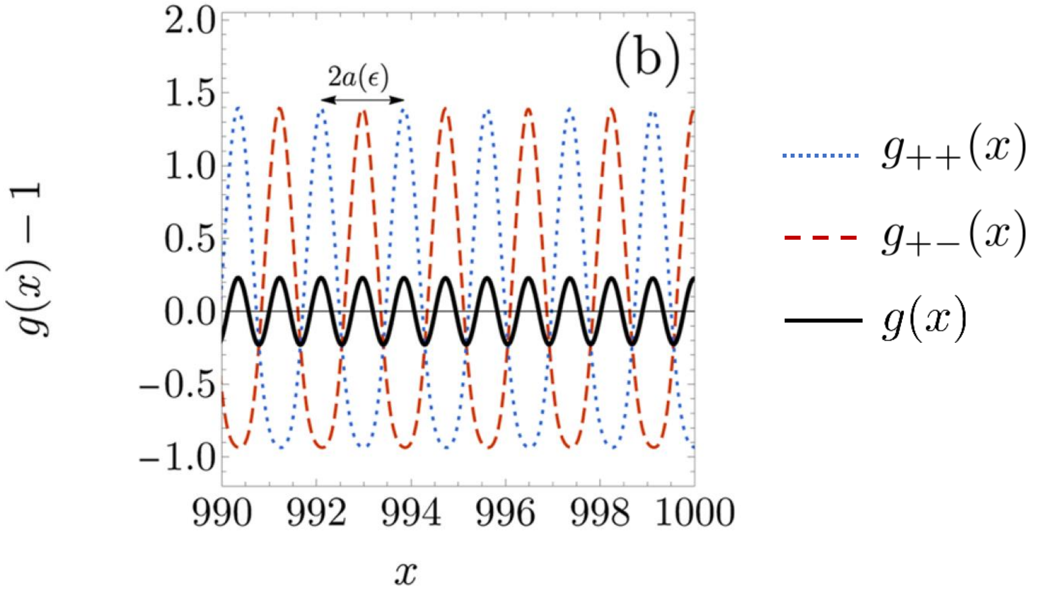
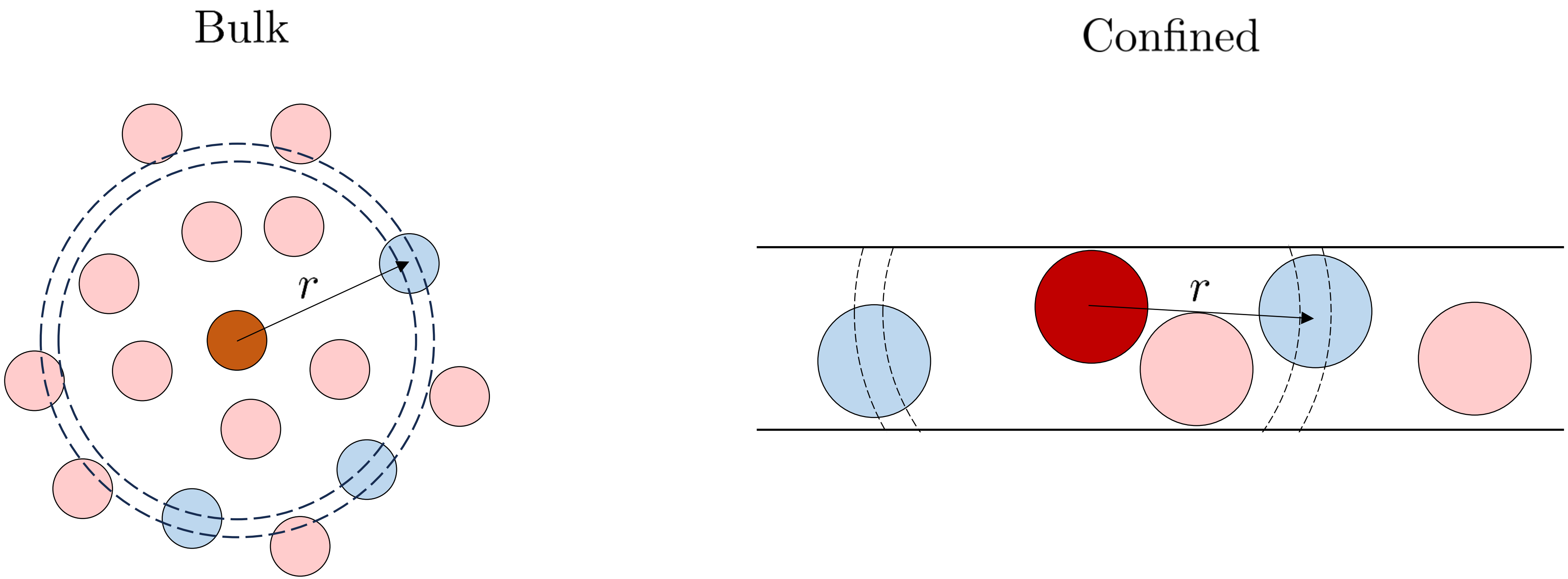


Structural properties

In confined liquids, defining a global RDF, $g(r)$, proves less straightforward compared to bulk systems due to the loss of rotational invariance in the fluid.



Structural properties

We start by defining the pair correlation function $g(\mathrm{r}_1, \mathrm{r}_2)$

$$n_2(\mathbf{r}_1, \mathbf{r}_2) = n_1(\mathbf{r}_1) n_2(\mathbf{r}_2) g(\mathbf{r}_1, \mathbf{r}_2) = n_1(\mathbf{r}_1) n_2(\mathbf{r}_2) g_{i,j}(|x_1 - x_2|)$$

Define $\hat{n}(r)\mathrm{d}r$ as the average number of particles at a distance between r and $r + \mathrm{d}r$

$$\hat{n}(r) = 2\lambda r \int_\epsilon \mathrm{d}y_1 \int_\epsilon \mathrm{d}y_2 \, \phi_{y_1}^2 \phi_{y_2}^2 \, \frac{g_{y_1,y_2}(\sqrt{r^2 - y_{12}^2})}{\sqrt{r^2 - y_{12}^2}}$$

$$\hat{n}^{\mathrm{nc}}(r) = 2\lambda r \int_\epsilon \mathrm{d}y_1 \int_\epsilon \mathrm{d}y_2 \, \phi_{y_1}^2 \phi_{y_2}^2 \, \frac{1}{\sqrt{r^2 - y_{12}^2}}$$

no correlations

$$\hat{n}^{\mathrm{id}}(r) = 2\lambda r \frac{1}{\epsilon^2} \int_\epsilon \mathrm{d}y_1 \int_\epsilon \mathrm{d}y_2 \, \frac{1}{\sqrt{r^2 - y_{12}^2}}$$

ideal gas

Structural properties

- One can define $g(r) = \hat{n}(r)/\hat{n}^{\mathrm{nc}}(r)$
- What is measured in simulations is $\hat{n}(r)$