Interacting Rods in Heterogeneous Environment

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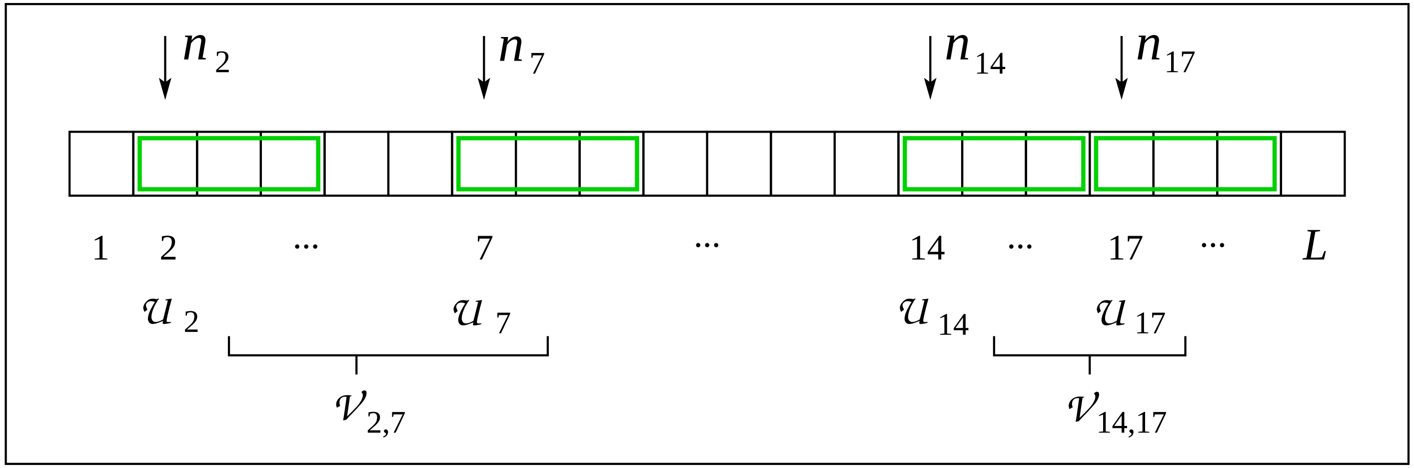
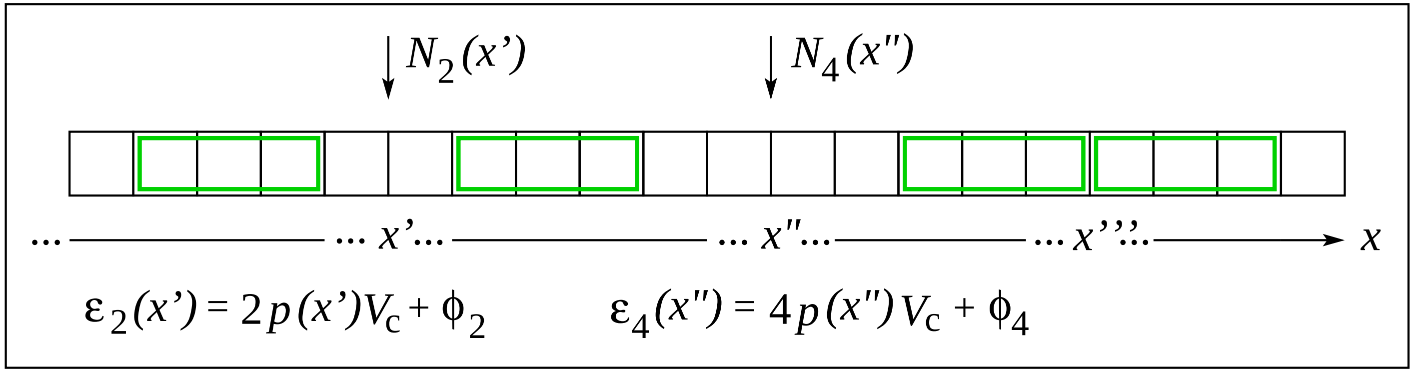
Interacting Rods



- Linear array of cells with volume V_c
- One size of rods: $\sigma V_c, \sigma = 1, 2, 3, \ldots$
- Occupation numbers: $n_2 = n_7 = n_{14} = n_{17} = 1$
- Hardcore exclusion interaction: $n_3 = n_4 = 0, \ldots$
- Interaction potential: $\mathcal{V}_{ij}$
- External potential: $\mathcal{U}_i$
- Open system: number of rods controlled by chemical potential
- Continuum limit: $\sigma \to \infty, \quad V_c \to 0$

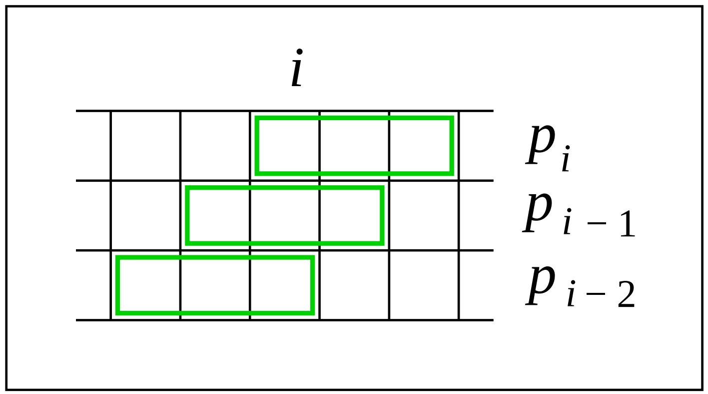
Noninteracting Vacancies



- Linear array of cells and rods of one size as before.
- Vacancies of variable size $mV_c, m = 1, 2, \ldots$ between rods.
- Population densities of vacancies at (mesoscopic) position x: $N_m(x)$
- Closed system: number of rods fixed at N_r
- Activation energy of vacancies: $\epsilon_m(x) = mV_c p(x) + \phi_m$
- Hardcore repulsion accounted for naturally
- Interaction potential $\mathcal{V}_{ij}$ contained in ϕ_m
- External potential $\mathcal{U}_i$ contained in $p(x)$

Exact Density Functionals (1)

- Hamiltonian: $\mathcal{H}(n_1,\ldots,n_L) = \sum_{i<j} \mathcal{V}_{i,j} n_i n_j + \sum_i \mathcal{U}_i n_i$
- Densities and correlators: $p_i = \langle n_i \rangle, \quad C_{i,j} \doteq \langle n_i n_j \rangle = f_{ij}(\{p_k\})$
- Free-energy functional: $F[p_1,\ldots,p_L]$ independent of $\mathcal{U}_i$
- Grand potential: $\Omega[p_1,\ldots,p_L] = F[p_1,\ldots,p_L] + \sum_{i=1}^{L} (\mathcal{U}_i - \mu) p_i$
- Extremum condition: $\frac{\delta}{\delta p_i} \Omega[p_1,\ldots,p_L] = 0, \quad i = 1,\ldots,L$
- Cell occupancy (mass density): $\rho_i \doteq \sum_{j=i-\sigma+1}^{i} p_i$



Exact Density Functionals (2)

$$\beta F[p_1,\ldots,p_L] = \sum_{i,j}\beta\mathcal{V}_{i,j}C_{i,j} + \sum_{s=1}^{L}\Bigg\{\Phi\Big(p_s - \sum_{i=s-\xi}^{s-\sigma}C_{s,i}\Big) + \Phi\Big(1-\sum_{i=s-\xi}^{s}p_i + \sum_{i=s-\xi+\sigma}^{s}\sum_{j=s-\xi}^{i-\sigma}C_{i,j}\Big)$$

$$-\Phi\Big(1-\sum_{i=s-\xi}^{s-1}p_i + \sum_{i=s-\xi+\sigma}^{s-1}\sum_{j=s-\xi}^{i-\sigma-1}C_{i,j}\Big)$$

$$+\sum_{i=s-\xi}^{s-\sigma}\Big\{\Phi\Big(C_{s,i}\Big) + \Phi\Big(p_i - \sum_{j=i+\sigma}^{s}C_{j,i}\Big) - \Phi\Big(p_i - \sum_{j=i+\sigma}^{s-1}C_{j,i}\Big)\Big\}\Bigg\}$$

$$C_{i,j} = \frac{\phi_i(1_i,0)\phi_i(0,1_j)}{\phi_i(0,0)}\left[\prod_{s=i+1}^{j+\xi}\frac{\phi_s(0,1_j)}{\tilde{\phi}_s(0,1_j)}\frac{\tilde{\phi}_s(0,0)}{\phi_s(0,0)}\right]e^{-\beta\mathcal{V}_{i,j}}, \quad \Phi(x)\doteq x\ln x$$

$$\phi_s(0,0) = 1-\sum_{k=s-\xi}^{s}p_k + \sum_{i=s-\xi+\sigma}^{s}\sum_{j=s-\xi}^{i-\sigma}C_{i,j}, \quad \phi_s(1_i,0) = p_i - \sum_{j=s-\xi}^{i-\sigma}C_{i,j}$$

$$\phi_s(0,1_j) = p_j - \sum_{i=j+\sigma}^{s}C_{i,j}, \quad \phi_s(1_i,1_j) = C_{i,j}, \quad \tilde{\phi}(\ldots) : \sum^{s} \rightarrow \sum^{s-1}$$

Generalized Exclusion Statistics

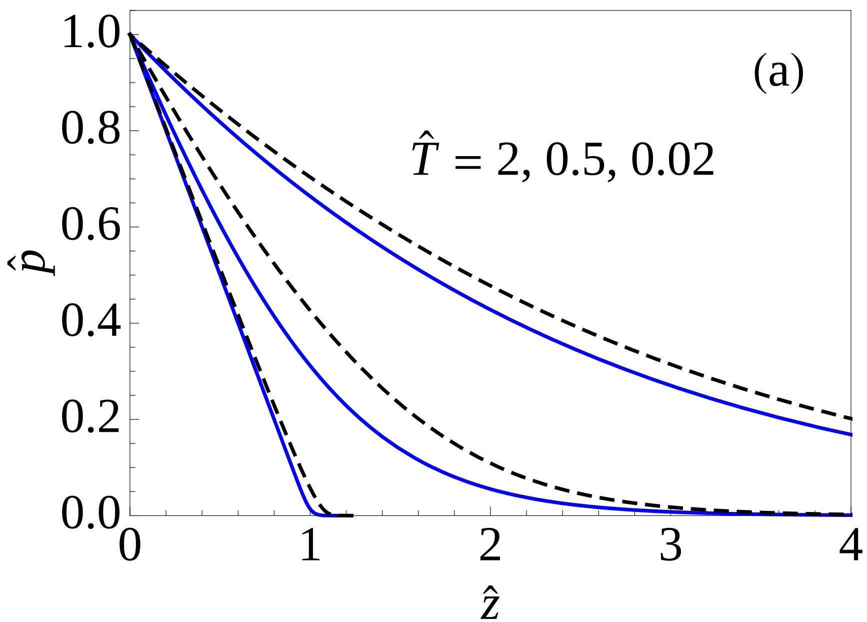
- Statistically interacting vacancy particles: compacts of size mV_c
- Specifications for combinatorial analysis: $A_m = N-1, \quad g_{mm'} = \begin{cases} 1 & : \; m' \geq m \\ 0 & : \; m' < m \end{cases}$
- Activation energies: $\epsilon_m(p) = mV_\mathrm{c}p + \phi_m$ with $p = p(x)$
- Statistical mechanical analysis yields $B_{lk}(T,p) \doteq \displaystyle\sum_{m=0}^{\infty} m^l \left[\beta\epsilon_m(p)\right]^k e^{-\beta\epsilon_m(p)}$
- Free-energy density: $\beta\bar{G}(T,p) = -\ln\Big(1 + B_{00}(T,p)\Big)$
- Density of vacant cells: $\bar{N}_\mathrm{v} \doteq \displaystyle\sum_{m=1}^{\infty} m\bar{N}_m = \frac{B_{10}(T,p)}{B_{00}(T,p)}$
- Density of occupied cells: $\rho = \dfrac{\sigma}{\sigma + \bar{N}_\mathrm{v}}$
- Local pressure from differential relation $V_\mathrm{c}dp = -\rho d\mathcal{U}$
- Separation of variables: $V_\mathrm{c}\displaystyle\int_{p_0}^{p}\frac{dp'}{\rho(p')} = \mathcal{U}(x_0) - \mathcal{U}(x)$

Uniform Gravitational Field (1): Vacancy Particles

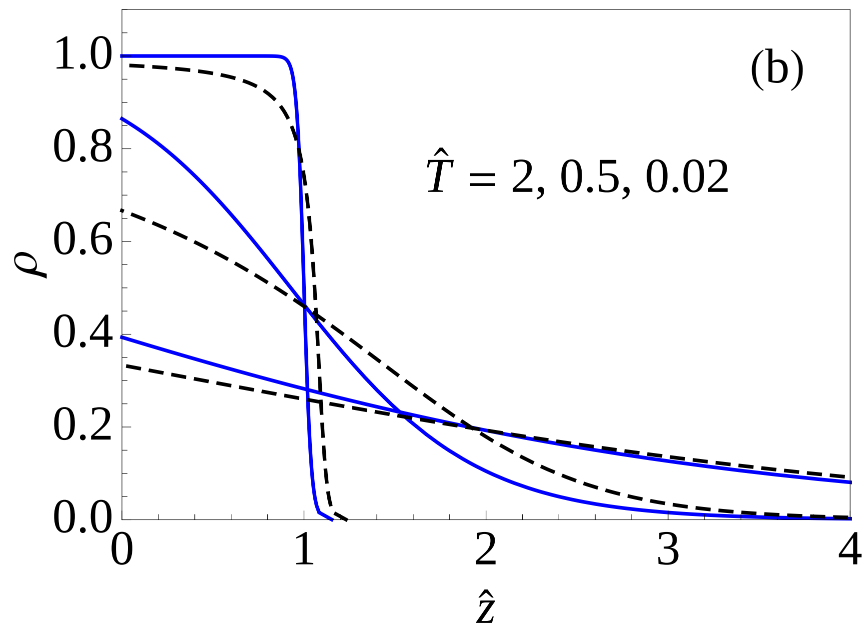
- Gravitational potential: $\mathcal{U}(z) = \dfrac{m_\mathrm{r}}{\sigma} g z$
- Mesoscopic length scale: $z_\mathrm{s} = N_\mathrm{r} V_\mathrm{r}, \quad V_\mathrm{r} = \sigma V_\mathrm{c}, \quad N_\mathrm{r} \gg 1$
- Pressure at $z = 0$: $p_\mathrm{s} = N_\mathrm{r} m_\mathrm{r} g$ (independent of T)
- Scaled variables: $\hat{z} \doteq \dfrac{z}{z_\mathrm{s}}, \quad \hat{p} \doteq \dfrac{p}{p_\mathrm{s}}, \quad \hat{T} \doteq \dfrac{k_\mathrm{B} T}{p_\mathrm{s} V_\mathrm{r}}$
- Density of vacant cells: $\bar{N}_\mathrm{v} = \left[\exp\left(\dfrac{\hat{p}}{\sigma \hat{T}}\right) - 1\right]^{-1}$
- Mass density: $\rho = \dfrac{\exp\left(\frac{\hat{p}}{\sigma\hat{T}}\right) - 1}{\exp\left(\frac{\hat{p}}{\sigma\hat{T}}\right) - 1 + \frac{1}{\sigma}}$
- Pressure profile from $V_\mathrm{c} \displaystyle\int_{p_\mathrm{s}}^{p} \frac{dp'}{\rho(p')} = -mgz$: $\exp\left(\dfrac{(\sigma-1)(\hat{p}-1)}{\sigma\hat{T}}\right) \dfrac{e^{\hat{p}/\sigma\hat{T}} - 1}{e^{1/\sigma\hat{T}} - 1} = e^{-\hat{z}/\hat{T}}$
- Continuum limit from $\sigma \to \infty, V_\mathrm{c} \to 0$: $\rho = \dfrac{\hat{p}/\hat{T}}{\hat{p}/\hat{T} + 1}, \quad \hat{p} - 1 + \hat{T} \ln \hat{p} = \hat{z}$

Uniform Gravitational Field (2): Vacancy Particles

pressure profile



density profile



- $\sigma = 2$ (solid curves)
- $\sigma = \infty$ (dashed curves)
- Atmospheric pressure for $\hat{T} \gg 1$: $\hat{p} \rightsquigarrow e^{-\hat{z}/\hat{T}}$
- Hydrostatic pressure for $\hat{T} \to 0$: $\hat{p} \rightsquigarrow (1-\hat{z})\theta(1-\hat{z})$

Exact Density Functionals (3)

Hardcore interaction and external potential:

$$\beta F = \sum_{i=1}^{L} \left\{ p_i \ln p_i + \Big(1 - \sum_{j=i-\sigma+1}^{i} p_j\Big) \ln\Big(1 - \sum_{j=i-\sigma+1}^{i} p_j\Big) - \Big(1 - \sum_{j=i-\sigma+1}^{i-1} p_j\Big) \ln\Big(1 - \sum_{j=i-\sigma+1}^{i-1} p_j\Big) \right\}$$

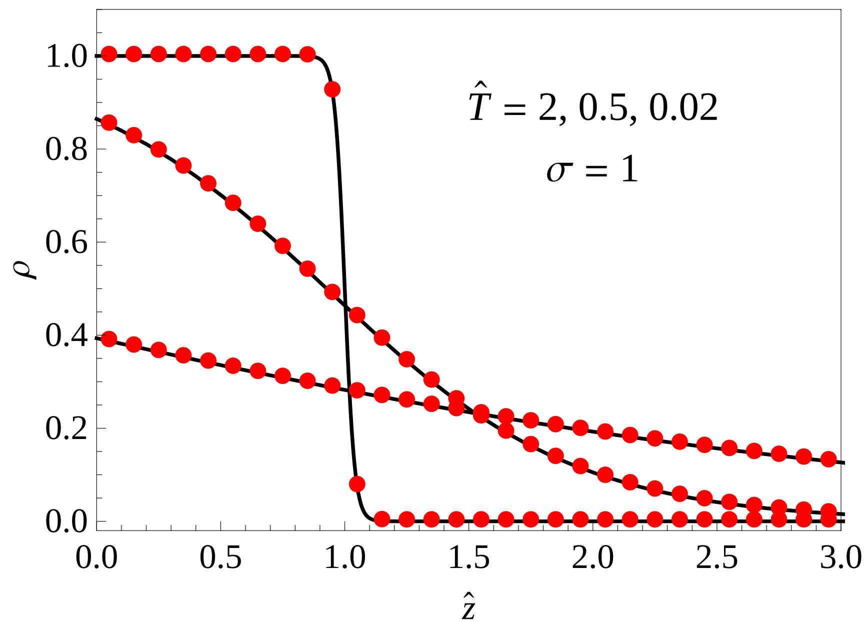
$$e^{-\beta(\mathcal{U}_i - \mu)} = p_i \prod_{k=i}^{i+\sigma-2} \left[1 - \sum_{j=k-\sigma+2}^{k} p_j\right] \prod_{k=i}^{i+\sigma-1} \left[1 - \sum_{j=k-\sigma+1}^{k} p_j\right]^{-1} ; \quad \zeta \doteq e^{\beta\mu}, \quad \lambda_i \doteq e^{-\beta\mathcal{U}_i}$$

Cases $\sigma = 1, 2, 3$:

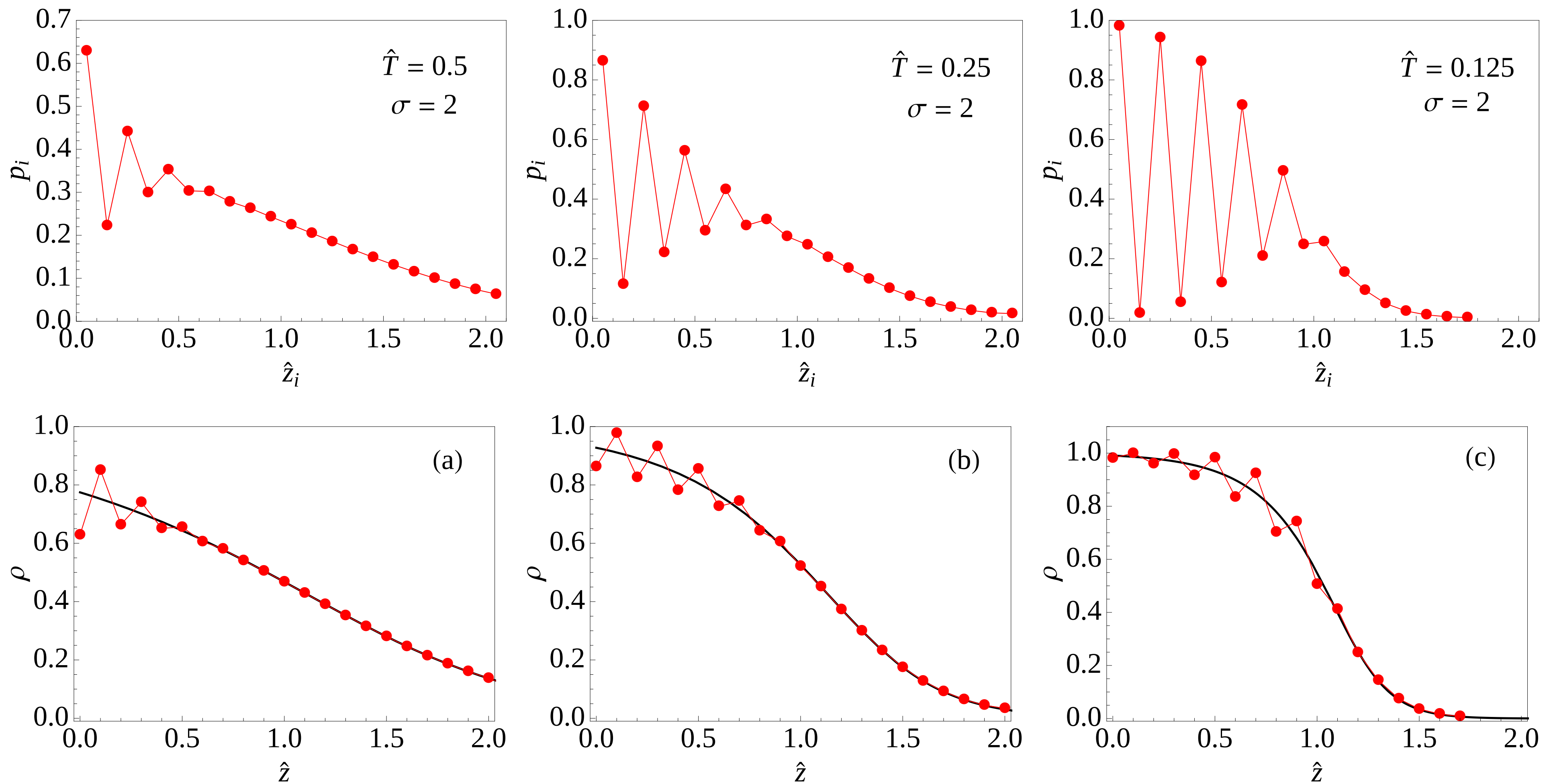
- $\zeta\lambda_i = \dfrac{p_i}{1 - p_i} \quad \Rightarrow \; p_i = 1 - \dfrac{1}{1 + \zeta\lambda_i}$
- $\zeta\lambda_i = \dfrac{p_i(1 - p_i)}{(1 - p_{i-1} - p_i)(1 - p_i - p_{i+1})} \simeq \dfrac{p_i^{\mathrm{mes}}(1 - p_i^{\mathrm{mes}})}{(1 - 2p_i^{\mathrm{mes}})^2} \quad \Rightarrow \; p_i^{\mathrm{mes}} = \dfrac{1}{2}\left[1 - \dfrac{1}{\sqrt{1 + \zeta\lambda_i}}\right]$
- $\zeta\lambda_i = \dfrac{p_i(1 - p_{i-1} - p_i)(1 - p_i - p_{i+1})}{(1 - p_{i-2} - p_{i-1} - p_i)(1 - p_{i-1} - p_i - p_{i+1})(1 - p_i - p_{i+1} - p_{i+2})} \simeq \dfrac{p_i^{\mathrm{mes}}(1 - 2p_i^{\mathrm{mes}})^2}{(1 - 3p_i^{\mathrm{mes}})^3}$

Uniform Gravitational Field (3): Density Functionals

- Gravitational potential: $\mathcal{U}_i = m_\mathrm{r} g z_i, \quad z_i = iV_\mathrm{c}$
- Mesoscopic resolution: $p_{i-\sigma+1} = \ldots = p_{i+\sigma-1} \doteq p_i^\mathrm{mes}$
- Two methods agree on mesoscopic length scale:
  - $\rho_i^\mathrm{vp} = \dfrac{\exp\left(\frac{\hat{p}}{\sigma\hat{T}}\right) - 1}{\exp\left(\frac{\hat{p}}{\sigma\hat{T}}\right) - 1 + \frac{1}{\sigma}}, \quad \exp\left(\dfrac{(\sigma-1)(\hat{p}-1)}{\sigma\hat{T}}\right)\dfrac{e^{\hat{p}/\sigma\hat{T}} - 1}{e^{1/\sigma\hat{T}} - 1} = e^{-\hat{z}_i/\hat{T}}$
  - $\zeta e^{-\hat{z}_i/\hat{T}} = p_i^\mathrm{mes}\dfrac{\left[1-(\sigma-1)p_i^\mathrm{mes}\right]^{\sigma-1}}{\left[1-\sigma p_i^\mathrm{mes}\right]^{\sigma}}, \quad \rho_i^\mathrm{mes} = \sigma p_i^\mathrm{mes}$
  - $\rho_i^\mathrm{vp} = \rho_i^\mathrm{mes}$ if $\zeta = e^{(\sigma-1)/\sigma\hat{T}}\left(e^{1/\sigma\hat{T}} - 1\right)$
- Microscopic resolution for $\sigma = 1$:
  no additional structures,
  solid lines: $\langle N_\mathrm{r}\rangle \gg 1$,
  circles: $\langle N_\mathrm{r}\rangle = 10$

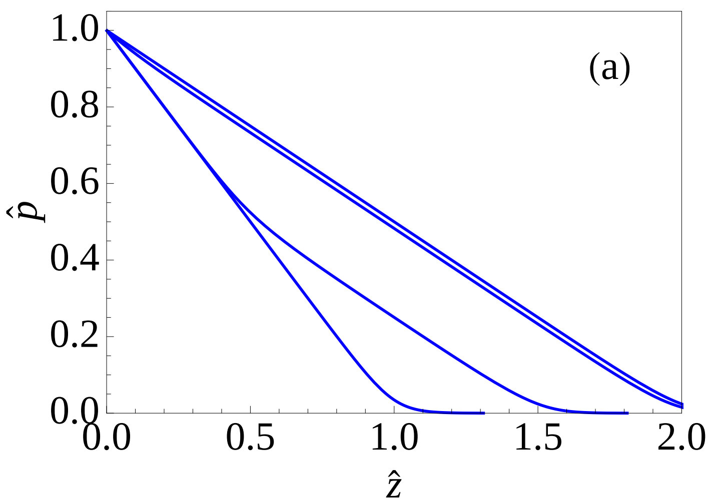


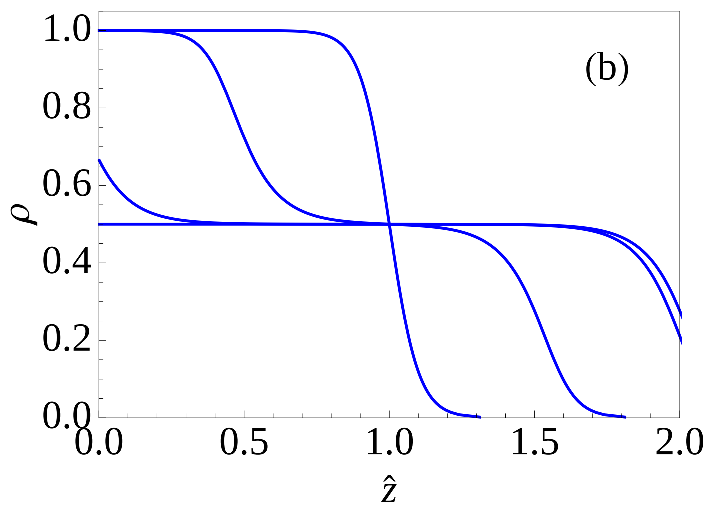
- Microscopic resolution for $\sigma = 2$:
- Recursion relation: $p_{i+1} = 1 - p_i - \dfrac{p_i(1-p_i)}{\zeta e^{-\hat{z}_i/\hat{T}}(1-p_i-p_{i-1})}, \quad i = 2, 3, \ldots$



Contact Interaction (1)

- Vacancy particles: $\epsilon_m(p) = pV_c + u, \quad u > 0$ (attractive), $\quad u < 0$ (repulsive)
- Density of vacant cells: $\bar{N}_v = \dfrac{e^{\hat{p}/\sigma\hat{T}}}{\left(e^{\hat{p}/\sigma\hat{T}} - 1\right)\left[e^{\hat{u}/\hat{T}}\left(e^{\hat{p}/\sigma\hat{T}} - 1\right) + 1\right]}, \quad \hat{u} \doteq \dfrac{u}{p_s V_c}$
- Density of occupied cells: $\rho = \dfrac{\sigma\left(e^{\hat{p}/\sigma\hat{T}} - 1\right)\left[e^{\hat{u}/\hat{T}}\left(e^{\hat{p}/\sigma\hat{T}} - 1\right) + 1\right]}{\sigma\left(e^{\hat{p}/\sigma\hat{T}} - 1\right)\left[e^{\hat{u}/\hat{T}}\left(e^{\hat{p}/\sigma\hat{T}} - 1\right) + 1\right] + e^{\hat{p}/\sigma\hat{T}}}$
- Pressure profile: $\exp\left(\dfrac{\hat{p}-1}{\hat{T}}\right) \dfrac{1 + e^{\hat{u}/\hat{T}}\left(e^{1/\sigma\hat{T}} - 1\right)}{1 + e^{\hat{u}/\hat{T}}\left(e^{\hat{p}/\sigma\hat{T}} - 1\right)} \dfrac{e^{\hat{p}/\sigma\hat{T}} - 1}{e^{1/\sigma\hat{T}} - 1} = e^{-\hat{z}/\hat{T}}$
- Results for $\hat{u} = 0, \ -0.5, \ 1, \ -5$





Contact Interaction (2)

- Free energy functional with $v_c \doteq -\hat{u}/\hat{T}$:

$$\beta F[p_1,\ldots,p_L] = \sum_{i=1}^{L}\Bigg\{\Bigg(1-\sum_{j=i-\sigma}^{i}p_j\Bigg)\ln\Bigg(1-\sum_{j=i-\sigma}^{i}p_j + C_{i-\sigma,i}\Bigg) + p_i\ln\left(p_i - C_{i-\sigma,i}\right) + p_{i-\sigma}\ln\left(p_{i-\sigma} - C_{i-\sigma,i}\right) - p_{i-\sigma}\ln p_{i-\sigma} - \Bigg(1-\sum_{j=i-\sigma}^{i-1}p_j\Bigg)\ln\Bigg(1-\sum_{j=i-\sigma}^{i-1}p_j\Bigg)\Bigg\} \quad (1)$$

$$C_{i-\sigma,i} = \frac{A_i - \sqrt{A_i^2 - 4e^{-v_c}(e^{-v_c}-1)p_{i-\sigma}p_i}}{2(e^{-v_c}-1)}, \quad A_i = 1 + e^{-v_c}(p_{i-\sigma}+p_i) - \sum_{k=i}^{i-\sigma}p_k$$

- Grand potential: $\Omega[p_1,\ldots,p_L] = F[p_1,\ldots,p_L] + \sum_{i=1}^{L}(\mathcal{U}_i-\mu)p_i$

- Extremum condition: $\frac{\delta}{\delta p_i}\Omega[p_1,\ldots,p_L] = 0, \quad i=1,\ldots,L$

Contact Interaction (3)

- Take $\sigma = 1$ and consider limits $v_\mathrm{c} = 0$ and $v_\mathrm{c} = +\infty$
- Implementing extremum condition yelds

$$\zeta e^{-\beta \mathcal{U}_i} = \frac{[1-p_i][p_i - C_{i-1,i}][p_i - C_{i,i+1}]}{p_i[1-p_{i-1}-p_i+C_{i-1,i}][1-p_i-p_{i+1}+C_{i,i+1}]}$$

$$C_{i-1,i} = \frac{A_i - \sqrt{A_i^2 - 4\eta(\eta+1)p_{i-1}p_i}}{2\eta}, \quad A_i = 1 + \eta(p_{i-1}+p_i), \quad \eta = e^{-v_c} - 1$$

- $v_\mathrm{c} = 0$: Rods of size $\sigma = 1$ with hardcore repulsion only

$$C_{i,i+1} = p_i p_{i+1}, \quad \zeta e^{-\beta \mathcal{U}_i} = \frac{p_i}{1-p_i}$$

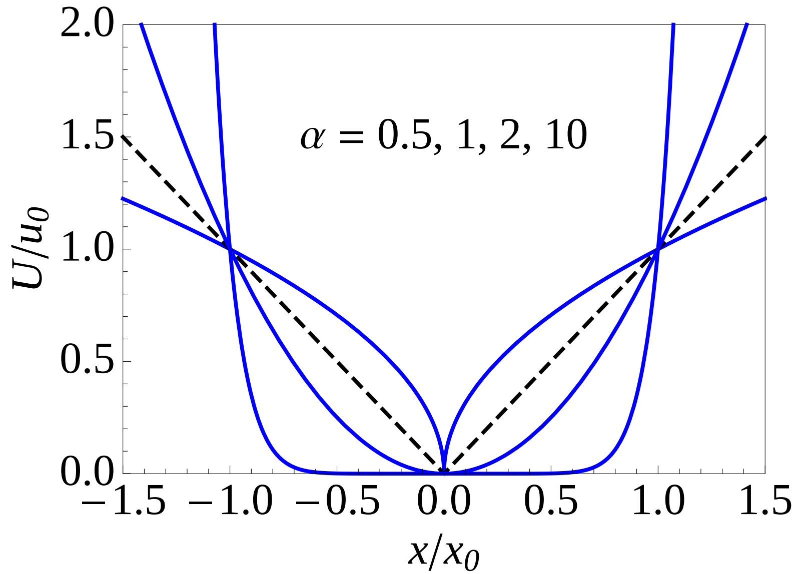
- $v_\mathrm{c} = +\infty$: Rods of size $\sigma = 2$ with hardcore repulsion only

$$C_{i,i+1} = 0, \quad \zeta e^{-\beta \mathcal{U}_i} = \frac{p_i(1-p_i)}{(1-p_{i-1}-p_i)(1-p_i-p_{i+1})}$$

Power-Law Trap (1): Vacancy Particles

- Trap potential: $\mathcal{U}(x) = \left|\frac{x}{x_0}\right|^\alpha, \quad \alpha > 0$

- Mass density: $\rho = \dfrac{\exp\left(\frac{\hat{p}}{\sigma\hat{T}}\right) - 1}{\exp\left(\frac{\hat{p}}{\sigma\hat{T}}\right) - 1 + \frac{1}{\sigma}}$



- Pressure profile: $\exp\left(\frac{(\sigma-1)(\hat{p}-\hat{p}_T)}{\sigma\hat{T}}\right)\frac{e^{\hat{p}/\sigma\hat{T}}-1}{e^{\hat{p}_T/\sigma\hat{T}}-1} = e^{-|\hat{x}|^\alpha/\hat{T}}$

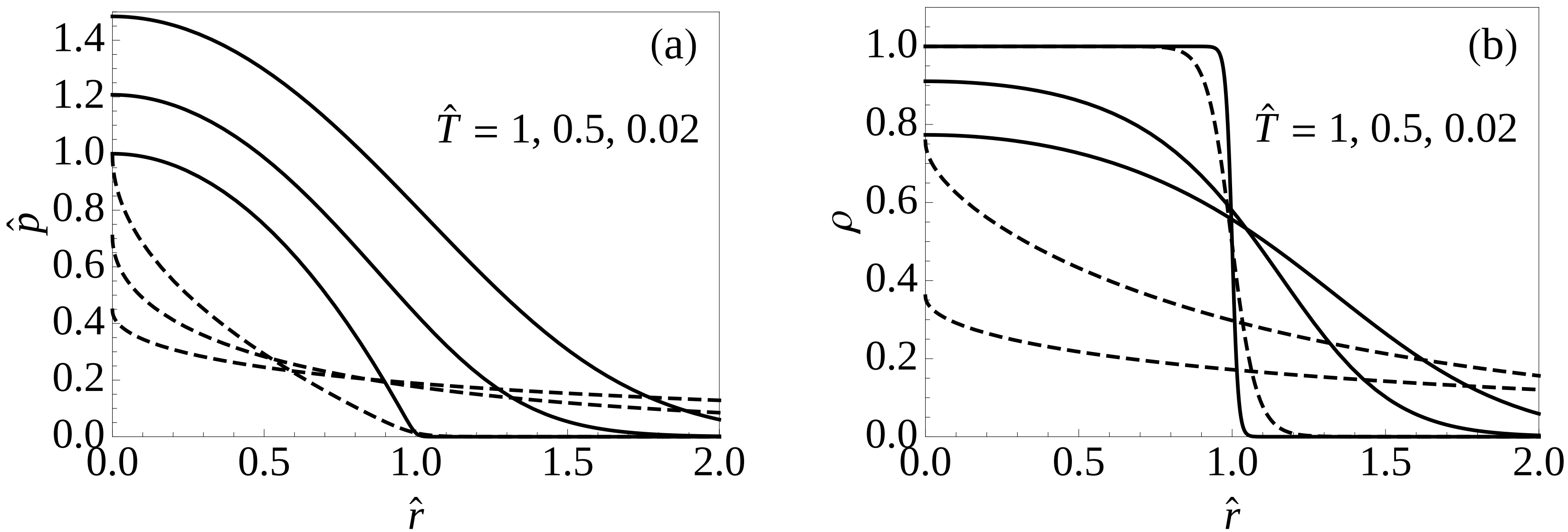
- Scaled variables: $\hat{x} \doteq \frac{x}{x_\mathrm{s}}, \qquad \hat{p}_T \doteq \frac{p_T}{p_\mathrm{s}}$

- Reference values: $x_\mathrm{s} = \frac{1}{2}N_\mathrm{r}\sigma V_\mathrm{c}, \quad p_\mathrm{s}V_\mathrm{c} = u_0\left|\frac{x_\mathrm{s}}{x_0}\right|^\alpha$

- Pressure p_T at $x = 0$ from $\frac{1}{V_\mathrm{c}}\int_{-\infty}^{+\infty} dx\rho(x) = N_\mathrm{r}$

Power-Law Trap (2): Vacancy Particles

- Simplified expressions for $\sigma = 1$: $\rho = 1 - e^{-\hat{p}/\hat{T}}$, $\dfrac{e^{\hat{p}/\hat{T}} - 1}{e^{\hat{p}_T/\hat{T}} - 1} = e^{-|\hat{x}|^\alpha/\hat{T}}$
- Results for $\alpha = 1/2$ (dashed curves) and $\alpha = 2$ (solid curves)



- Pressure at $x = 0$ from $\Gamma(1/\alpha + 1) f_{1/\alpha}\left(e^{\hat{p}_T/\hat{T}} - 1\right) \hat{T}^{1/\alpha} = 1$
- Fermi-Dirac function: $f_n(z) \doteq \dfrac{1}{\Gamma(n)} \displaystyle\int_0^\infty \frac{dx\, x^{n-1}}{z^{-1}e^x + 1}$

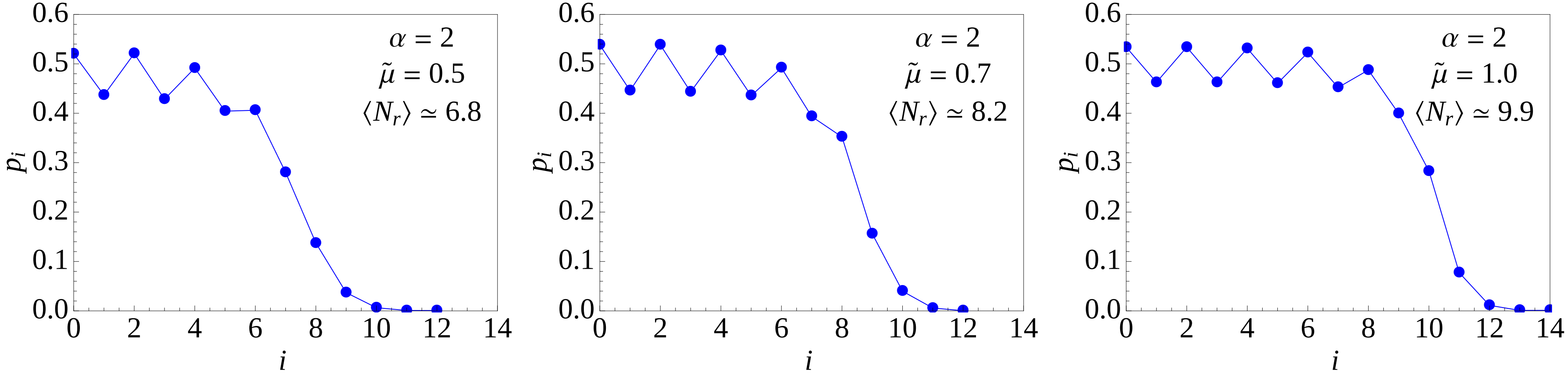
Power-Law Trap (3): Density Functionals

- $\tilde{T} \doteq \dfrac{k_\mathrm{B}T}{u_0}, \quad \tilde{\mu} \doteq \dfrac{\mu}{u_0}, \quad \zeta = e^{\tilde{\mu}/\tilde{T}}, \quad \lambda_i \doteq e^{-(i/I)^\alpha/\tilde{T}}, \quad I \doteq \dfrac{x_0}{V_\mathrm{c}} = 10$

- One-parameter recursion relation:

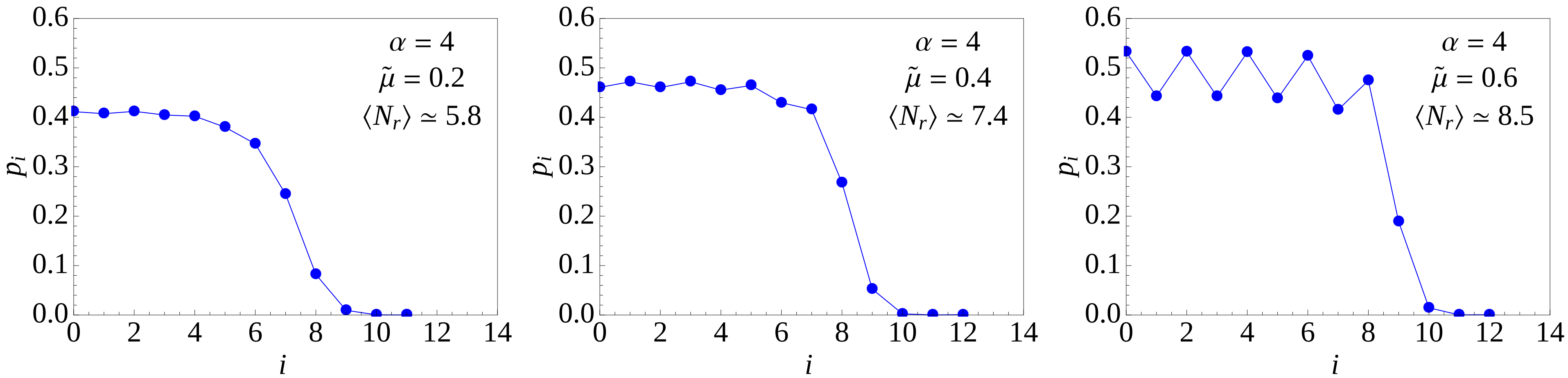
$$p_1 = 1 - p_0 - \sqrt{\frac{p_0(1-p_0)}{\zeta\lambda_0}}, \quad p_{i+1} = 1 - p_i - \frac{p_i(1-p_i)}{\zeta\lambda_i(1-p_i-p_{i-1})}, \quad i = 2, 3, \ldots$$

- $\tilde{T} = 0.1, \quad \alpha = 2$ (harmonic trap)

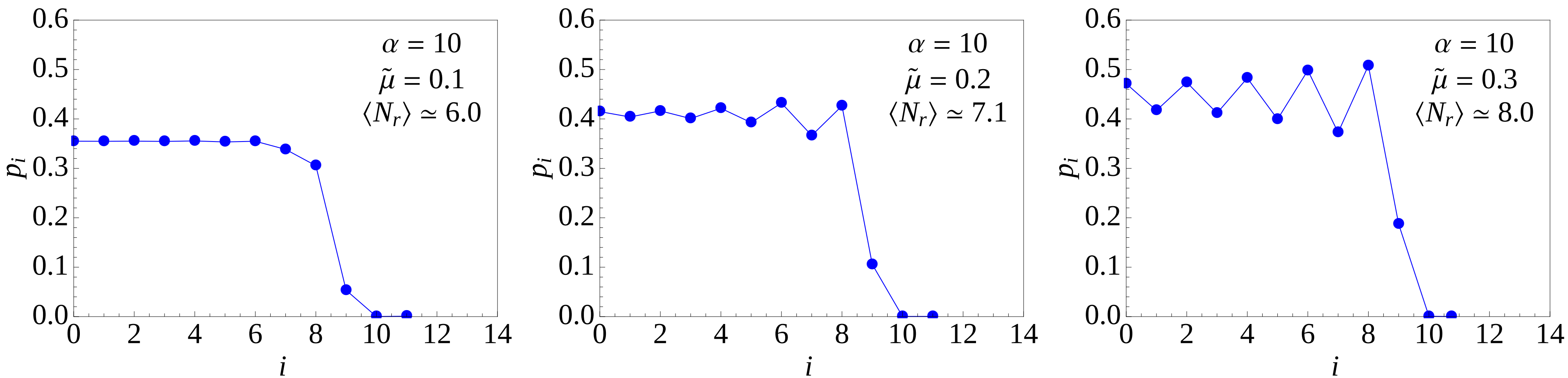


Power-Law Trap (4): Density Functionals

- $\tilde{T} = 0.1, \quad \alpha = 4$



- $\tilde{T} = 0.1, \quad \alpha = 10$

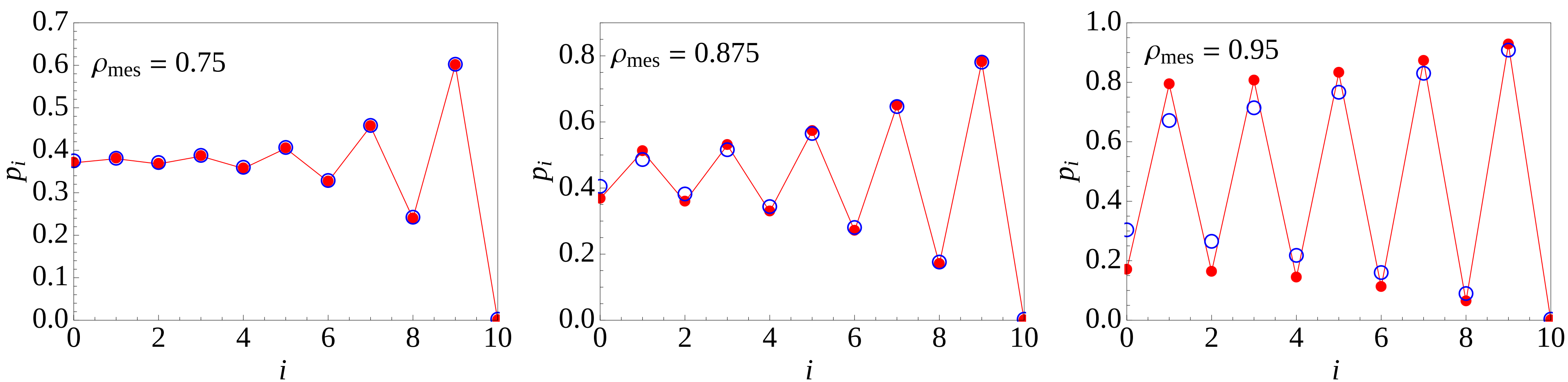


Box with Rigid Walls (1): $\sigma = 2$

- Narrow box: effects of two walls $\longrightarrow$ numerical analysis ($\bullet$)
- Wide box: effects of one wall $\longrightarrow$ exact analysis ($\circ$)

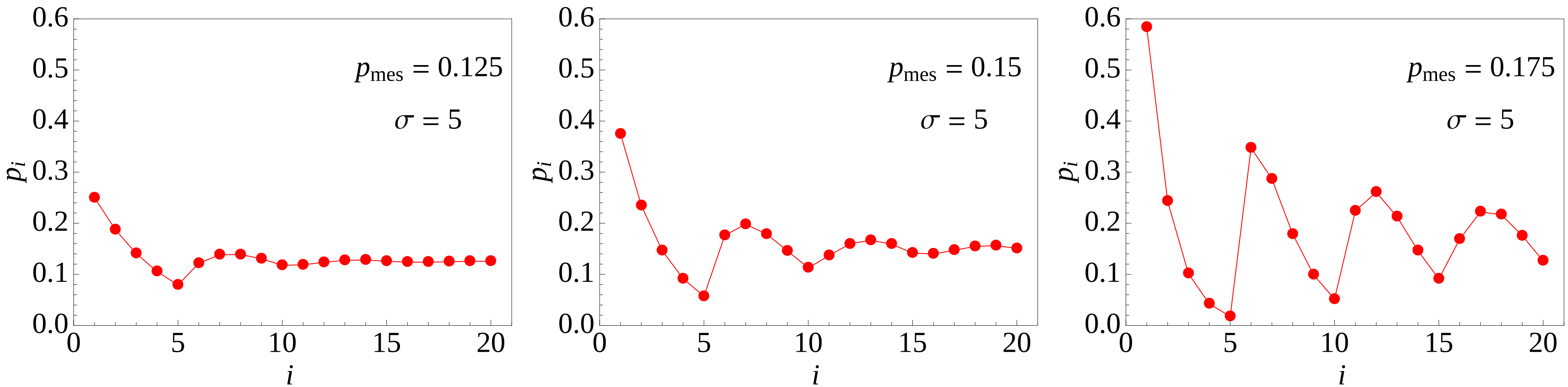
$$p_j = \frac{1}{2}\rho_{\rm mes}\left[1 - \left(\frac{\rho_{\rm mes}}{\rho_{\rm mes}-2}\right)^j\right], \quad j = 0,1,2,\ldots, \quad i = 10 - j$$

- Boundary coherence length: $\xi = \dfrac{1}{\ln(2/\rho_{\rm mes}-1)}$



Box with Rigid Walls (2): $\sigma = 1, 2, \ldots$

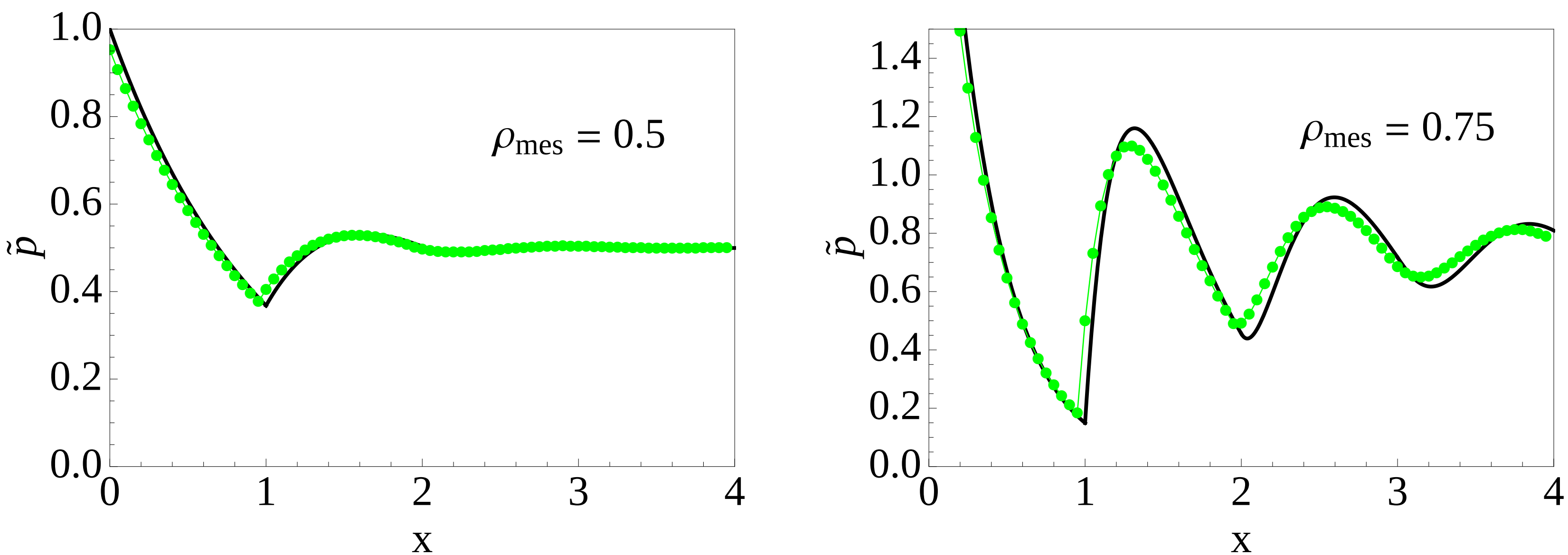
- $p_i = p_{\text{mes}} \dfrac{\left[1 - \sigma p_{\text{mes}}\right]^{i-1}}{\left[1 - (\sigma - 1) p_{\text{mes}}\right]^{i}}, \quad i = 1, \ldots, \sigma - 1$
- $p_{i+1} = 1 - \displaystyle\sum_{j=i-\sigma+2}^{i} p_j - \frac{p_{i-\sigma+2}}{\zeta} \prod_{k=i-\sigma+2}^{i} \left[\left(1 - \sum_{j=k-\sigma+2}^{k} p_j \right) \Big/ \left(1 - \sum_{j=k-\sigma+1}^{k} p_j \right) \right]$
- Fugacity: $\zeta = \dfrac{p_{\text{mes}} \left[1 - (\sigma - 1) p_{\text{mes}}\right]^{\sigma-1}}{\left[1 - \sigma p_{\text{mes}}\right]^{\sigma}} \quad : \; 0 < p_{\text{mes}} < \dfrac{1}{\sigma}$
- Boundary conditions: $p_i = 0$ and $\displaystyle\lim_{i \to \infty} p_i = p_{\text{mes}} = \frac{\rho_{\text{mes}}}{\sigma}$



Box with Rigid Walls (3): $\sigma \to \infty$

Continuum limit: $V_c \to 0,\ \sigma \to \infty; \quad 0 < x_i \doteq \dfrac{i-1}{\sigma} < 1,\ i = 1, \ldots, \sigma - 1; \quad \sigma p_i \to \tilde{p}(x)$

- $0 < x < 1: \quad \tilde{p}(x) = se^{-sx}, \quad s \doteq \dfrac{\rho_{\mathrm{mes}}}{1-\rho_{\mathrm{mes}}}, \quad \zeta = se^{s}$
- $x > 1: \quad h(x) = \zeta \exp\left(-\int_{x-1}^{x} dx' h(x')\right), \quad h(x) \doteq \dfrac{\tilde{p}(x)}{1 - \int_x^{x+1} dx' \tilde{p}(x')}$ [Percus 1976]
- Solution: $\tilde{p}(x) = \tilde{p}(x-m) \sum_{k=0}^{m} \dfrac{s^k}{k!} (x-k)^k e^{-(m-k)s}, \quad m \leq x \leq m+1$



Box with Rigid Walls (4): Solution of Percus Equation

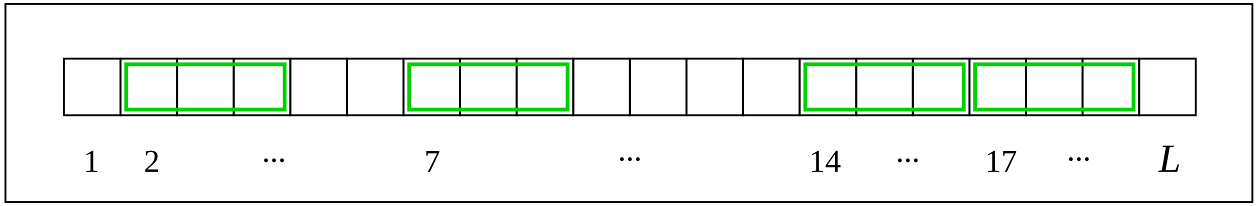
Transformation proposed by Vanderlick, Scriven, and Davis 1986:

- $h(x) = \zeta \exp\left(-\int_{x-1}^{x} dx' h(x')\right), \quad h(x) = \dfrac{\tilde{p}(x)}{1 - \int_x^{x+1} dx' \tilde{p}(x')}, \quad x > 1$
- $h'(x) = h(x)\big[h(x-1) - h(x)\big], \quad \tilde{p}(x+1) = \tilde{p}(x) - \dfrac{d}{dx}\left(\dfrac{\tilde{p}(x)}{h(x)}\right)$
- $0 \leq x \leq 1: \quad h(x-1) = 0 \;\Rightarrow\; h(x) = \dfrac{1}{x + \zeta^{-1}}, \quad \tilde{p}(x) = s e^{-sx}, \quad \zeta = s e^{s}$
- $\Rightarrow \; \dfrac{\tilde{p}(x+m)}{\tilde{p}(x)} = \sum_{k=0}^{m} \dfrac{s^k}{k!}(x+m-k)^k e^{-(m-k)s}, \quad 0 \leq x \leq 1$
- $\Rightarrow \; \tilde{p}(x) = \tilde{p}(x-m) \sum_{k=0}^{m} \dfrac{s^k}{k!}(x-k)^k e^{-(m-k)s}, \quad m \leq x \leq m+1$

Exploring Generalizations (1)

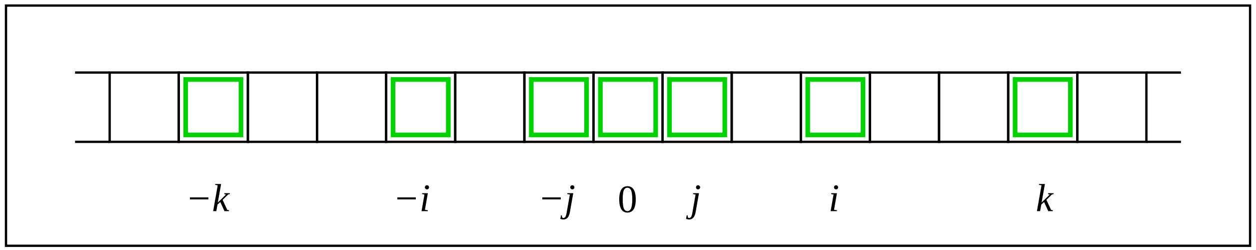
Long-range interactions

- Vacancy particles: $\mathcal{V}_{ij} \neq 0$ restricted to first-neighbor rods
- Density functionals: $\mathcal{V}_{ij} \neq 0$ restricted to $|i-j| < \sigma$



- Symmetric cluster with equivalent-neighbor interaction:

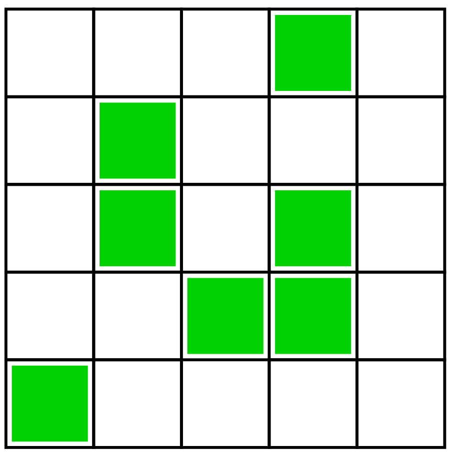
$$\mathcal{V}_{ij} = Gm_{\mathrm{r}}^2 x_{ij} \quad \to \quad \mathcal{U}_i = Gm_{\mathrm{r}}^2 \sum_{|j|\leq|i|} x_{ij}, \quad x_{ij} \doteq |i-j|V_{\mathrm{c}}$$

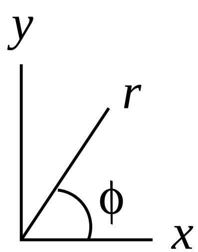


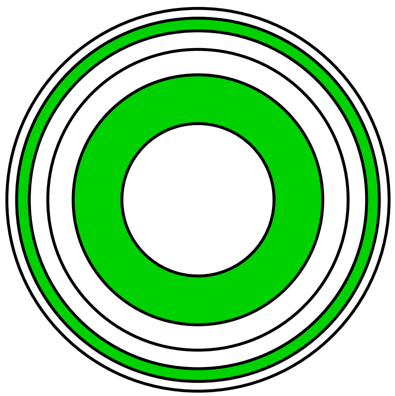
Exploring Generalizations (2)

Higher dimensions

- $\mathcal{D} = 2$ and $\sigma = 1$
- Cells of area V_c and different shapes
- Hardcore exclusion interaction only.
- Equivalent results for cells of any shape
- Select cells with special symmetry
- Add potential $U(y)$ or $U(r)$







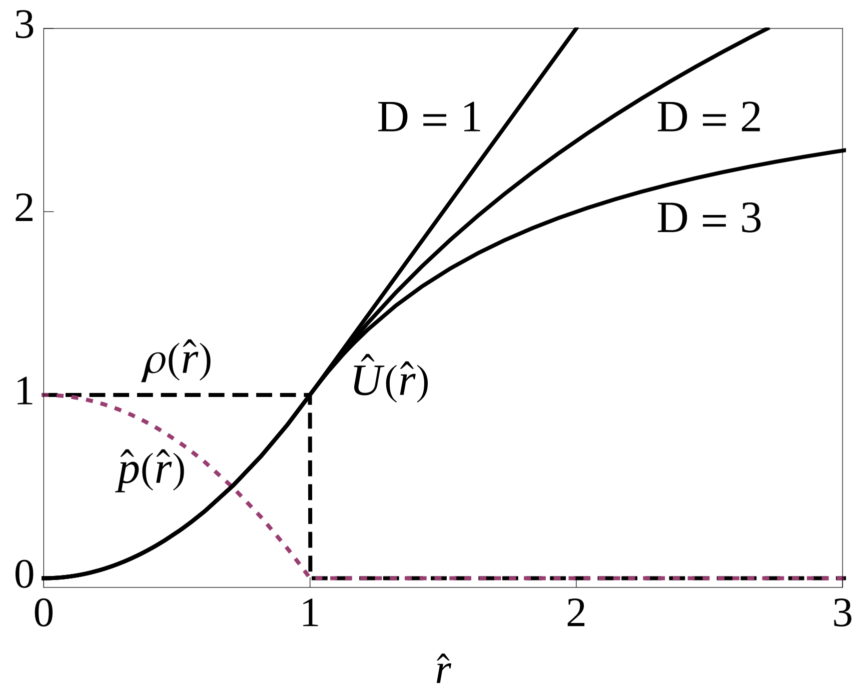
Self-Gravitating Lattice Gas (1): Potentials

$$\mathcal{V}_{ij} = \begin{cases} G_1 m_r^2 r_{ij} & : \mathcal{D} = 1, \\ G_2 m_r^2 \ln r_{ij} & : \mathcal{D} = 2, \\ -G_3 m_r^2 r_{ij}^{-1} & : \mathcal{D} = 3. \end{cases} \qquad g(r) \doteq -\frac{1}{m_r}\frac{d\mathcal{U}}{dr} = -\frac{G_\mathcal{D} m_{in}}{r^{\mathcal{D}-1}}$$

$T = 0$: solid cluster with $r_s^\mathcal{D} = \frac{N_r V_c \mathcal{D}}{\mathcal{A}_\mathcal{D}}$ and $p_s = \frac{\mathcal{A}_\mathcal{D} G_\mathcal{D}}{2\mathcal{D}} \frac{m_r^2}{V_c^2} r_s^2$

- $\rho(\hat{r}) = \theta(1 - \hat{r})$
- $\hat{p}(\hat{r}) = 1 - \hat{r}^2$
- $\hat{\mathcal{U}}(\hat{r}) = \hat{r}^2 \quad : 0 \leq \hat{r} \leq 1$

$$\hat{\mathcal{U}}(\hat{r}) = \left\{ \begin{array}{ll} 2\hat{r} - 1 & : \mathcal{D} = 1, \\ 2\ln \hat{r} + 1 & : \mathcal{D} = 2, \\ 3 - 2/\hat{r} & : \mathcal{D} = 3, \end{array} \right\} \quad \hat{r} \geq 1$$



Self-Gravitating Lattice Gas (2): Differential Equations

Analysis for $T > 0$:

- $g(r) = -\frac{G_{\mathcal{D}}}{r^{\mathcal{D}-1}} \frac{m_{\mathrm{r}}}{V_{\mathrm{c}}} \int_0^r dr' \big(\mathcal{A}_{\mathcal{D}} r'^{\mathcal{D}-1}\big) \rho(r')$
- $\frac{dp}{dr} = \frac{m_{\mathrm{r}}}{V_{\mathrm{c}}} g(r)\rho(r) = -\frac{G_{\mathcal{D}}\mathcal{A}_{\mathcal{D}}}{r^{\mathcal{D}-1}} \frac{m_{\mathrm{r}}^2}{V_{\mathrm{c}}^2} \rho(r) \int_0^r dr' r'^{\mathcal{D}-1} \rho(r')$
- density profile from $\rho'' + \frac{\mathcal{D}-1}{\hat{r}}\rho' - \frac{1-2\rho}{\rho(1-\rho)}(\rho')^2 + \frac{2\mathcal{D}}{\hat{T}}\rho^2(1-\rho) = 0, \quad \rho'(0) = 0$
- pressure profile from $\hat{p}'' + \frac{\mathcal{D}-1}{\hat{r}}\hat{p}' - \frac{(\hat{p}')^2}{\hat{T}\big(e^{\hat{p}/\hat{T}} - 1\big)} + 2\mathcal{D}\big(1 - e^{-\hat{p}/\hat{T}}\big)^2 = 0, \quad \hat{p}'(0) = 0$

Second boundary condition:

- $\mathcal{D} \int_0^\infty d\hat{r}\, \hat{r}^{\mathcal{D}-1} \rho(\hat{r}) = 1, \quad 2\mathcal{D}(\mathcal{D}-1) \int_0^\infty d\hat{r}\, \hat{r}^{2\mathcal{D}-3} \hat{p}(\hat{r}) = 1$
- $\mathcal{D} = 1$: $\rho(0) = 1 - e^{-1/\hat{T}}, \quad \hat{p}(0) = 1$

Self-Gravitating Lattice Gas (3): Asymptotics

For $\hat{r} \gg 1$ we assume $\rho(\hat{r}) \ll 1$: $\dfrac{\rho''}{\rho} + \dfrac{\mathcal{D}-1}{\hat{r}}\dfrac{\rho'}{\rho} - \left(\dfrac{\rho'}{\rho}\right)^2 + \dfrac{2}{\hat{T}}\rho = 0$

- $\mathcal{D} = 1$: $\rho(\hat{r})_{\rm as} = \dfrac{1}{\hat{T}}\,\mathrm{sech}^2\left(\dfrac{\hat{r}}{\hat{T}}\right)$
- $\mathcal{D} = 2$: $\rho(\hat{r}) \sim \hat{r}^{-2\left[1+\sqrt{1+2a/\hat{T}}\right]}$, $a = \dfrac{1}{2\hat{T}}$ (at low $\hat{T}$)

For $\hat{T} \gg 1$ we drop last term in asymptotic ODE:

- $\mathcal{D} = 1$: $\rho \sim a e^{-b\hat{r}}$
- $\mathcal{D} = 2$: $\rho \sim a\hat{r}^{-b}$

For $\hat{T} \ll 1$ we set $m_{\rm in} = m_{\rm t}$: $\displaystyle\int_{p_0}^{p} \frac{dp'}{1 - e^{-p'V_{\rm c}/k_{\rm B}T}} = -\frac{G_{\mathcal{D}} m_{\rm t} m_{\rm r}}{V_{\rm c}} \int_{r_{\rm s}}^{r} \frac{dr}{r^{\mathcal{D}-1}}$

- $\mathcal{D} = 1$: $\rho(\hat{r})_{\rm ap} \simeq e^{-2(\hat{r}-1)/\hat{T}}$
- $\mathcal{D} = 2$: $\rho(\hat{r})_{\rm ap} \simeq \hat{r}^{-2/\hat{T}}$
- $\mathcal{D} = 3$: $\rho(\hat{r})_{\rm ap} \simeq e^{-2(1-1/\hat{r})/\hat{T}}$

Work Completed, in Progress, and Planned

- *Interacting hard rods: distribution of microstates and density functional.*
  J. Chem. Phys. **139**, 054113 (2013).
- *Statistically interacting vacancy particles.*
  Phys. Rev. E **89**, 012157 (2014).
- *Interacting hard rods in heterogeneous environment.*
  (Manuscript in preparation).
- *Polydisperse hard rods in discrete and continuous media.*
  (Work in progress).
- *Bethe ansatz for driven hard rods.*
  (Work in progress).

Statistical Interaction

Generalized Pauli principle [Haldane 1991]

How is the number of states accessible to one particle of species m affected if particles (of any species m') are added?

$$\Delta d_m \doteq -\sum_{m'} g_{mm'} \Delta N_{m'} \qquad \Rightarrow \; d_m = A_m - \sum_{m'} g_{mm'} (N_{m'} - \delta_{mm'})$$

Energy and multiplicity of many-body states

$$E(\{N_m\}) = E_{\mathrm{pv}} + \sum_{m=1}^{M} N_m \epsilon_m, \qquad W(\{N_m\}) = \prod_{m=1}^{M} \underbrace{\begin{pmatrix} d_m + N_m - 1 \\ N_m \end{pmatrix}}_{\frac{\Gamma(d_m + N_m)}{\Gamma(N_m+1)\Gamma(d_m)}}$$

- E_{pv}: energy of reference state
- N_m: number of particles from species m
- ϵ_m: particle activation energies
- $g_{mm'}$: statistical interaction coefficients
- A_m: capacity constants
- d_m: number of open slots for a particle of species m

Thermodynamics with Statistical Interaction

System specifications:

- particle energies ϵ_m
- statistical interaction coefficients $g_{mm'}$
- capacity constants A_m

Two tasks:

- combinatorial problem: $W(\{N_m\})$
- extremum problem: $\delta(U - TS - \mu\mathcal{N}) = 0$

Partition function [Wu 1994]: $Z = \sum_{\{N_m\}} W(\{N_m\}) e^{-\beta E(\{N_m\})} = \prod_m \left(\frac{1+w_m}{w_m}\right)^{A_m}$

$$e^{\epsilon_m/k_\mathrm{B}T} = (1+w_m)\prod_{m'=1}^{M}\left(1+w_{m'}^{-1}\right)^{-g_{m'm}}, \quad m = 1,\ldots,M.$$

Average number of particles: $w_m\langle N_m\rangle + \sum_{m'} g_{mm'}\langle N_{m'}\rangle = A_m, \quad m = 1,\ldots,M$

Configurational entropy [Isakov 1994]:

$$S(\{N_m\}) = k_\mathrm{B}\sum_{m=1}^{M}\Big[\big(N_m+Y_m\big)\ln\big(N_m+Y_m\big) - N_m\ln N_m - Y_m\ln Y_m\Big]$$

$$Y_m \doteq A_m - \sum_{m'=1}^{M} g_{mm'}N_{m'}$$