Supporting information for "On the connections and differences among three mean-field approximations: a stringent test"

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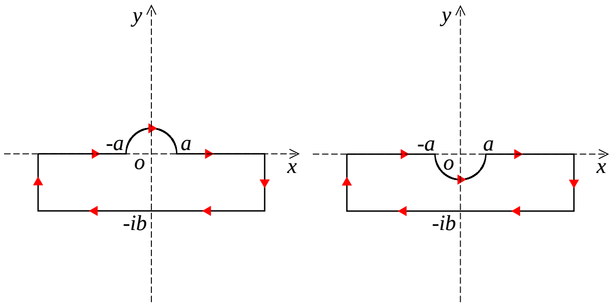

FIG. S1: Illustration of the path for the contour integration when the integrand $f(z)$ has only one pole at the origin $z = 0$. The contour in the complex plane is an almost full square passing through four points: $-\infty$, $+\infty$, $+\infty - ib$, and $-\infty - ib$ but avoiding the origin around which the path goes along a small semicircle of radius a either above (left) or below (right) the real axis. When taking $a \to 0$, the integration over the semicircle contributes $-i\pi\mathrm{Res}[f(z), z = 0]$ (left) or $i\pi\mathrm{Res}[f(z), z = 0]$ (right). Using either of the pathes and the residue theorem, the principal value of the integral defined as the sum of the two integrals: $f(x)$ over the interval $[-\infty, a]$ and $f(x)$ over the interval $[a, \infty]$ at the limit of $a \to 0$ is given by $-i\pi\mathrm{Res}[f(z), z = 0]$.

This supporting information provides an alternative way to derive the exact solutions to the one-dimensional nearest-neighbor model explained in the main text. For a nearest neighbor interaction $w(x) = w(x)\epsilon(2\sigma - x)$ where $\epsilon(x)$ is the step function, the usual configuration energy can be simplified as

$$\mathcal{U}(\bar{x}) = \sum_{i<j}^{N} w(x_i - x_j) = \sum_{i=1}^{N} w(x_i - x_{i+1}), \tag{S1}$$

where $\bar{x}$ denotes the collective variable $\bar{x} = x_1, x_2, \cdots, x_N$. This simplification allows us to work out the partition function of the isothermal-isobaric ensemble (NPT) [1]

$$\mathcal{Q}_{\mathrm{NPT}} = \int \cdots \int_{x_0<\cdots<x_N} d\bar{x}\, e^{-\beta\mathcal{U}(\bar{x})} e^{-\beta w(x_1-x_0)} e^{-PV} = \left\{ \int_0^{\infty} dx\, \exp\left[-\beta(w(x) + Px)\right] \right\}^N \tag{S2}$$

where $V = x_N - x_0$ is the volume (length), $\beta = 1/k_b T$ is the usual inverse temperature and P is the pressure with unit of force in one dimension. Consequently, the derivative of the free energy, $-\beta \ln \mathcal{Q}_{\mathrm{NPT}}$ with respect to the pressure yields the usual equation of state

$$\rho^B = -\left.\frac{L(s)}{L'(s)}\right|_{s=\beta P}, \tag{S3}$$

where $L(s)$ is the Laplace transform of the boltzmann factor $\exp(-\beta u)$ defined in the main text

$$L(s) = \int_0^{\infty} dx\, e^{-\beta w(x)} e^{-sx}. \tag{S4}$$

Although the derivation of the exact thermodynamics for the nearest neighbor model is straightforward, it is much more involved to obtain the structural properties in ordinary closed forms. Exact solution for the fourier transform of the pair direct correlation function defined as

$$\hat{c}(k) = \int_{-\infty}^{\infty} dx\, c(x) e^{-ikx} \leftrightarrow c(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, c(k) e^{ikx}, \tag{S5}$$

was obtained by Percus[2]. Using the physical meaning of the pair correlation function, we here provide an alternative derivation which leads to a transparent understanding of the structure properties in both real and reciprocal spaces.

The probability of finding a nearest (1-st order) neighbor in the vicinity of x given that there is one particle located at the origin is simply found to be:

$$\rho^B g_1(x)\, dx = \frac{\exp(-\beta w(x) - s|x|)}{L(s)} \epsilon(|x| - \sigma)\, dx. \tag{S6}$$

$g_1(x)$ is an even function and the normalization condition requires $\int_{-\infty}^{\infty} dx\, \rho^B g_1(x) = 2$, which means that there are two nearest neighbors, one on the left of the given particle and the other on its right. Furthermore, the probability of finding its next-to-nearest (2-nd order) neighbor in one direction (e.g. the right) is given by the convolution of two $\rho^B g_1(x)$ functions

$$\rho^B g_2(x)\, dx = \int_{\sigma}^{x-\sigma} dy\, \rho^B g_1(y) \rho^B g_1(x-y) \cdot \epsilon(x - 2\sigma)\, dx \qquad \text{for } x > 0 \tag{S7}$$

Following this argument, we find that the usual pair correlation function $g(x)$ for which $\rho^B g(x) dx$ gives the conditional probability of finding any other particle in the vicinity of x is the sum of the probabilities of finding any n-th order neighbor

$$\rho^B g(x) = \sum_{n=1}^{\infty} \rho^B g_n(x) \tag{S8}$$

with $\rho^B g_n(x)$ given by the convolution between $\rho^B g_{n-1}(x)$ and $\rho^B g_1(x)$

$$\rho^B g_n(x)\, dx = \int_{(n-1)\sigma}^{x-\sigma} dy\, \rho^B g_{n-1}(y) \rho^B g_1(x-y) \cdot \epsilon(x - n\sigma)\, dx \qquad \text{for } x > 0 \tag{S9}$$

and $g_n(x)$ is always an even function. It is instructive to write the fourier transform of $g_1(x)$ as the sum of a ratio between two Laplace transform and its complex conjugates

$$\rho^B \hat{g}_1(k) = J(k, s) + \text{c.c.} = \frac{L(s + ik)}{L(s)} + \text{c.c.} \tag{S10}$$

The complex conjugate of the preceding terms is generally abbreviated as c.c., which specifically stands for $J^*(k, s) = J(-k, s)$ in the above eq. (S10). Using the convolution expression eq. (S9) for $\rho^B g_n(x)$ and repeatedly inserting the definition eq. (S10) for $J(k,s)$, one simply arrives at the fourier transform of $g_n(x)$

$$\rho^B \hat{g}_n(k) = J^n(k,s) + \text{c.c.}. \tag{S11}$$

Therefore, the fourier transform of the pair correlation function is given by

$$\rho^B \hat{g}(k) = \sum_{n=1}^{\infty} J^n(k,s) + \text{c.c.} = \frac{J(k,s)}{1-J(k,s)} + \lim_{N\to\infty} \frac{J^N(k,s)}{J(k,s)-1} + \text{c.c.} \tag{S12}$$

The second term is proportional to the dirac delta function that accounts for the divergence of $\hat{g}(k)$ at $k = 0$ because its fourier transform is a constant

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, \left(e^{-ikx} + e^{ikx}\right) \lim_{N\to\infty} \frac{J^N(k,s)}{J(k,s)-1} = -2\pi i \text{Res}[f(z), z=0] = 2\pi\rho^B. \tag{S13}$$

with the auxiliary function $f(z) = \lim_{N\to\infty} \frac{J^N(z,s)}{J(z,s)-1} e^{izx}$ and $f(z) = \lim_{N\to\infty} \frac{J^N(z,s)}{J(z,s)-1} e^{-izx}$ (see Fig S1 for an explanation of the contour integral). The nontrival portion of $\rho^B\hat{g}(k)$ thus corresponds to the fourier transform of $\rho^B h(x) = \rho^B[g(x) - 1]$

$$\rho^B \hat{h}(k) = \frac{J(k,s)}{1-J(k,s)} + \text{c.c.} \tag{S14}$$

The usual pair direct correlation function of a bulk system can be expressed in the Fourier space as

$$\rho^B \hat{c}(k) = \frac{\rho^B \hat{h}(k)}{1+\rho^B \hat{h}(k)} = \frac{J(k,s) + J(-k,s) - 2J(k,s)J(-k,s)}{1 - J(k,s)J(-k,s)} \tag{S15}$$

The expression for $\hat{c}(k)$ agrees with the Percus' solution[2].

[1] V. H. Takahasi, Proc. Phys. Math. Soc. Jpn. **24**, 60 (1942).

[2] J. K. Percus, Journal of Statistical Physics **28**, 67 (1982).