

# The Sixth-Moment Sum Rule for the Pair Correlations of the Two-Dimensional One-Component Plasma: Exact Result

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The system under consideration is a two-dimensional one-component plasma in the fluid regime, at density  $n$  and arbitrary coupling  $\Gamma = \beta e^2$  ( $e =$  unit charge,  $\beta =$  inverse temperature). The Helmholtz free energy of the model, as the generating functional for the direct pair correlation  $c$ , is treated in terms of a convergent renormalized Mayer diagrammatic expansion in density. Using specific topological transformations within the bond-renormalized Mayer expansion, we prove that the nonzero contributions to the regular part of the Fourier component of  $c$  up to the  $k^2$ -term originate exclusively from the ring diagrams (unable to undertake the bond-renormalization procedure) of the Helmholtz free energy. In particular,  $\hat{c}(\mathbf{k}) = -\Gamma/k^2 + \Gamma/(8\pi n) - k^2/[96(\pi n)^2] + O(k^4)$ . This result fixes via the Ornstein–Zernike relation, besides the well-known zeroth-, second-, and fourth-moment sum rules, the new sixth-moment condition for the truncated pair correlation  $h$ ,  $n(\pi\Gamma n/2)^3 \int r^6 h(\mathbf{r}) d\mathbf{r} = 3(\Gamma - 6)(8 - 3\Gamma)/4$ .

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**KEY WORDS:** One-component plasma; logarithmic interaction; pair correlation; diagrammatic expansion; sum rule.

## 1. INTRODUCTION

Coulomb plasmas are the model systems for studying the effect of long-range interparticle interactions on statistics of classical lattice and continuous fluids. It was observed that, in arbitrary dimension, the long-range tail of the Coulomb potential gives rise to exact constraints, sum rules, for truncated particle correlations (for an exhausting review, see ref. 1), namely the zeroth- and second-moment conditions.<sup>(2, 3)</sup>

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The concentration on two dimensions (2d) with logarithmic interparticle interactions and on the one-component plasma (OCP), i.e., the continuous system of charged particles embedded in a spatially uniform background, brings some physical peculiarities and relevant mathematical simplifications providing additional exact information about the system, like:

- A formal relationship to the fractional quantum Hall effect;<sup>(4)</sup>
- An experimental evidence for the Wigner crystallization at low temperatures;<sup>(5)</sup>
- The dependence of the statistics on the only parameter-coupling constant  $\Gamma \sim 1/\text{temperature}$  (the charge density scales appropriately the distance);
- The availability of the equation of state<sup>(6)</sup>;
- The mapping to free fermions at special coupling  $\Gamma = 2$ <sup>(7)</sup> (for various sample's geometries, see review 8) characterized by a pure Gaussian decay of the truncated pair correlation  $h$ ; the evaluation of the leading term of the  $(\Gamma - 2)$ -expansion of  $h$ , indicating the change from monotonic to oscillatory behavior just at  $\Gamma = 2$ <sup>(7)</sup>;
- The rigorous derivation of the weak-coupling  $\Gamma \rightarrow 0$  Debye-Hückel limit<sup>(9)</sup>, and the systematic  $\Gamma$ -expansion of  $h$  in terms of a renormalized Mayer diagrammatic expansion;<sup>(10, 11)</sup>
- The shift of the compressibility equation to the fourth-moment condition<sup>(12–14)</sup> under the assumption of cluster conditions;
- A symmetry of thermodynamic quantities with respect to a complex transformation of particle coordinates<sup>(15)</sup> for arbitrary coupling  $\Gamma$ , implying a functional relation among the pair correlations. The last is equivalent to an infinite sequence of sum rules relating the coefficient of the short-distance expansion of two-particle correlations (the lowest level of the sequence was derived by Jancovici<sup>(16)</sup>). The generalization of the symmetry to multi-particle densities, possessing specific invariant structure, was given in ref. 17.
- The suggestion that, at arbitrary  $\Gamma$ , the 2d OCP is in the critical state<sup>(18, 19)</sup> in terms of the induced electrical-field correlations (but not the particle correlations). The free energy is therefore supposed to exhibit finite-size correction predicted by the conformal-invariance theory, as was verified by the rigorous finite-size treatment of the  $\Gamma = 2$  case and also numerically,<sup>(20)</sup> by using exact finite-size techniques,<sup>(4, 21–23)</sup> for coupling strengths  $\Gamma = 4$  and  $\Gamma = 6$ .

The present paper is devoted to a rigorous derivation of the new sixth-moment sum rule for the truncated pair correlation  $h$  of the 2d OCP. The mathematical basis comes from the convergent bond-renormalized Mayer expansion in density.<sup>(11)</sup> Within a specific classification of the diagrams in the renormalized format for the Helmholtz free energy, the functional generator for the direct pair correlation  $c$ , we prove that the regular part of the Fourier component of  $c$  is determined up to the  $k^2$ -term solely by the (unrenormalized) ring diagrams of the generating free energy. This result implies via the Ornstein–Zernike (OZ) relation, besides the known zeroth-, second-,<sup>(2,3)</sup> and fourth-moment<sup>(12–14)</sup> sum rules, the explicit formula for the sixth moment of  $h$ .

The paper is outlined as follows:

In Section 2, we recapitulate briefly the ordinary Mayer diagrammatic representation in density for  $h$  and  $c$  pair correlations and the (excess) Helmholtz free energy as the generating functional for both of them.

Section 3 deals with exactly solvable cases or limits of the 2d OCP, expressed in terms of  $h$ -moments. These involve the momentum sum rules, the  $\Gamma=2$  coupling together with the leading  $(\Gamma-2)$  correction term and the Debye–Hückel  $\Gamma \rightarrow 0$  limit. Here, we have registered a very important fact. The three known (appropriately rescaled) zeroth, second and fourth moments turn out to be  $\Gamma$ -polynomials of (successively increasing) *finite* order. By using the renormalized Mayer expansion<sup>(11)</sup> we were able to compute for the as-yet-unknown sixth  $h$ -moment the coefficients to a few lower orders of the  $\Gamma$ -expansion terms around the Debye–Hückel limit and observed, within the range of these low orders, the finite  $\Gamma$ -truncation also for this case. To our surprise, this finite truncation represented an exact interpolation between the  $\Gamma \rightarrow 0$  and  $\Gamma=2$  couplings and, moreover, reproduced correctly the leading  $(\Gamma-2)$  correction term.<sup>(7)</sup> Since the coupling  $\Gamma=2$  and its neighborhood do not play any special role in view of the  $\Gamma$ -expansion, the above fact was a strong indication and motivation for us.

Section 4 describes the formalism of the renormalized Mayer expansion.<sup>(11)</sup> The renormalization of bond factors consists in a multiple-bond expansion of Mayer functions and a consequent series elimination of field circles, resulting in the modified Bessel functions of second kind. The novelty lies in the classification of diagrams representing the Helmholtz free energy—the functional generator of  $c$ —according to the possibility of performing the series-elimination transformation: (1) simple unrenormalized bond generates the characteristic singular term of  $c$ ; (2) all unrenormalized ring diagrams (which cannot undertake the series-elimination procedure) generate the renormalized “watermelon” Meeron graph contribution to the regular part of  $c$ ; (3) every other diagram is expressible with all bonds

renormalized and as generator gives rise to a family of  $c$ -diagrams: the families do not overlap with one another and, as units, they exhibit remarkable “cancellation properties”.

The “cancellation” phenomena is the subject of the crucial Section 5 where we prove that, regardless of the topology of a separate graph belonging to class (3), the zeroth and second real-space moments of the  $c$ -diagrams family, generated from the underlying graph, vanish. The proof of the nullity of the zeroth moment follows from a trivial scaling property of the Bessel functions with respect to density. The proof of the second-moment condition is much more complicated. Besides the above scaling property it requires to introduce an elimination procedure for two-coordinated root points generated on renormalized bonds and to reveal “hidden zeros” due to the translational and rotational invariance of the infinite system, realized through per-partes integration of field-point coordinates.

In Conclusion, after evaluating the only contribution to the Fourier component of  $c$  up to the  $k^2$ -term, namely that of the renormalized Meeron graph, we write down by using the OZ relation the explicit formula for the sixth moment of  $h$ . The structure of higher-order moments of  $h$  is also discussed.

## 2. A SKETCH OF THE MAYER EXPANSION IN DENSITY<sup>(24)</sup>

We consider a system of identical pointlike particles in volume  $V$  of a  $d$ -dimensional space, interacting through pair potential  $v$ ;  $v$  will occur in combination called the Mayer function

$$f(i, j) = \exp[-\beta v(i, j)] - 1 \quad (1)$$

where  $\beta$  is the inverse temperature and, for notational convenience, a position vector  $\mathbf{r}_i$  is represented simply by  $i$ . In the inverse (density) format, i.e., with the density  $n(\mathbf{r}) = \langle \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \rangle$  as controlling variable, the (minus) excess free energy  $\bar{F}^{ex}$  is the relevant thermodynamic potential. Its Mayer diagrammatic representation reads

$$\beta \bar{F}^{ex} = \{ \text{all connected diagrams which consist of } N \geq 2 \text{ field (black)} \\ n\text{-circles and } f\text{-bonds, and are free of connecting circles} \} \quad (2)$$

(the removal of a connecting circle disconnects the diagram). The excess free energy is the generating functional for the truncated pair correlation

$$h(1, 2) = \frac{n_2(1, 2) - n(1)n(2)}{n(1)n(2)} \quad (3)$$

with the two-body density  $n_2(\mathbf{r}, \mathbf{r}') = \langle \sum_{i \neq j} \delta(\mathbf{r} - \mathbf{r}_i) \delta(\mathbf{r}' - \mathbf{r}_j) \rangle$  and for the direct correlation function  $c$ , in the sense that

$$h(1, 2) = -1 + [1 + f(1, 2)] \frac{1}{n(1) n(2)} \frac{\delta \beta \bar{F}^{ex}}{\delta f(1, 2)} \quad (4)$$

$$c(1, 2) = \frac{\delta^2 \beta \bar{F}^{ex}}{\delta n(1) \delta n(2)} \quad (5)$$

With regard to (2), this implies

$$h(1, 2) = \{ \text{all connected 1, 2-rooted diagrams which consist of field } n\text{-circles and } f\text{-bonds, and are free of articulation circles} \} \quad (6)$$

[the removal of an articulation circle disconnects the diagram into two or more components, of which at least one contains no root (white) circle];

$$c(1, 2) = \{ \text{all connected 1, 2-rooted diagrams which consist of field } n\text{-circles and } f\text{-bonds, and are free of connecting circles} \} \quad (7)$$

The link between  $h$  and  $c$  is established in terms of the OZ relation

$$h(1, 2) = c(1, 2) + \int c(1, 3) n(3) h(3, 2) d3 \quad (8)$$

If the system is infinite ( $V \rightarrow \infty$ ), homogeneous,  $n(1) = n$ , and both isotropic and translationally invariant,  $h(1, 2) = h(|1 - 2|)$ ,  $c(1, 2) = c(|1 - 2|)$ , it is useful to introduce the Fourier components

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{d/2}} \int \exp(i\mathbf{k} \cdot \mathbf{r}) \hat{f}(\mathbf{k}) d\mathbf{k} \quad (9a)$$

$$\hat{f}(\mathbf{k}) = \frac{1}{(2\pi)^{d/2}} \int \exp(-i\mathbf{k} \cdot \mathbf{r}) f(\mathbf{r}) d\mathbf{r} \quad (9b)$$

Especially, in  $d=2$  dimensions,

$$\begin{aligned} \hat{f}(\mathbf{k}) &= \int_0^\infty r f(r) J_0(kr) dr \\ &= \sum_{j=0}^\infty \frac{(-1)^j}{(j!)^2} \left(\frac{k^2}{4}\right)^j \frac{1}{2\pi} \int_0^\infty r^{2j} f(r) dr \end{aligned} \quad (10)$$

with  $J_0$  being the ordinary Bessel function. In the Fourier space, the OZ relation (8) takes the form

$$\hat{h}(k) = \hat{c}(k) + (2\pi)^{d/2} n \hat{c}(k) \hat{h}(k) \quad (8')$$

where  $k = |\mathbf{k}|$ .

### 3. MOTIVATION

The classical OCP is a system of particles of charge  $e$  embedded in a spatially uniform neutralizing background. In  $d=2$  dimensions, the Coulomb interaction energy is given by

$$-\beta v(1, 2) = \Gamma \ln |1 - 2| \quad (11a)$$

$$-\beta \hat{v}(\mathbf{k}) = -\Gamma/k^2 \quad (11b)$$

with  $\Gamma = \beta e^2$  being the coupling constant. We will concentrate on the thermodynamic limit of the fluid regime with constant density  $n(i) = n$  and use the notation

$$I_{2j} = \int r^{2j} h(\mathbf{r}) d\mathbf{r} \quad (12)$$

for the moments of the truncated pair correlation.

Let us first summarize exactly solvable cases of the model. In the weak coupling  $\Gamma \rightarrow 0$  limit,  $h$  displays the Debye–Hückel screening<sup>(9)</sup>

$$h(r; \Gamma \rightarrow 0) \simeq -\Gamma K_0(r \sqrt{2\pi\Gamma n}) \quad (13)$$

with  $K_0$  the modified Bessel function of second kind. Consequently,

$$\lim_{\Gamma \rightarrow 0} n \left( \frac{\pi\Gamma n}{2} \right)^j I_{2j}(\Gamma) = -(j!)^2 \quad (14)$$

At  $\Gamma=2$ , the mapping onto free fermions provides a pure Gaussian form of  $h$ ,<sup>(7)</sup>

$$h(r; \Gamma=2) = -\exp(-\pi n r^2) \quad (15)$$

implying

$$n(\pi n)^j I_{2j}(\Gamma=2) = -j! \quad (16)$$

The leading-order of the series expansion around  $\Gamma = 2$  results in<sup>(7)</sup>

$$h(r; \Gamma) = h(r; \Gamma = 2) + (\Gamma - 2) \delta h(r) + \dots \tag{17a}$$

$$\begin{aligned} \delta h(r) = & \text{Ei}(-\pi n r^2) - \frac{1}{2} \text{Ei}(-\pi n r^2/2) \\ & + \exp(-\pi n r^2) \left\{ \frac{1}{2} \text{Ei}(\pi n r^2/2) - [\ln(\pi n r^2) + C] \right\} \end{aligned} \tag{17b}$$

where  $C$  is Euler’s constant and  $\text{Ei}$  the exponential-integral function. From (17) one gets after some algebra

$$n \left( \frac{\pi \Gamma n}{2} \right)^j I_{2j}(\Gamma) = -j! + (\Gamma - 2) j! \left( \sum_{k=0}^j \frac{2^k - 1}{k + 1} - \frac{j}{2} \right) + O[(\Gamma - 2)^2] \tag{18}$$

The long-range tail of the Coulomb potential gives rise to exact constraints (sum rules) for the moments of the truncated two-body correlation, like the zeroth-moment (perfect screening) condition

$$n I_0 = -1 \tag{19a}$$

the second-moment (Stillinger–Lovett) condition<sup>(2, 3)</sup>

$$n \left( \frac{\pi \Gamma n}{2} \right) I_2 = -1 \tag{19b}$$

the fourth-moment (compressibility) condition<sup>(12–14)</sup>

$$n \left( \frac{\pi \Gamma n}{2} \right)^2 I_4 = -4 + \Gamma \tag{19c}$$

Note that the sum rules are consistent with exact formulae (14), (18).

The expressions for the rescaled moments (19) correspond to finite truncations of their  $\Gamma$ -expansion around  $\Gamma = 0$ . The  $\Gamma$ -expansion technique of  $h$ ,<sup>(11)</sup> explained and extended in the next section, enables one to evaluate systematically the coefficients of the  $\Gamma$ -expansion also for higher moments. For the sixth moment of  $h$ , we were able to attain with a little effort the third order of  $\Gamma$ , with the result

$$n \left( \frac{\pi \Gamma n}{2} \right)^3 I_6 = -36 + \frac{39}{2} \Gamma - \frac{9}{4} \Gamma^2 + 0 \times \Gamma^3 + O(\Gamma^4) \tag{20}$$

The appearance of the zero coefficient to the  $\Gamma^3$  power indicates the possibility of a finite  $\Gamma$ -truncation for  $I_6$ , too. This hypothesis is strongly supported by the fact that the truncation of (20) at the  $\Gamma^2$ -term interpolates correctly from the  $\Gamma \rightarrow 0$  limit [relation (14)] to the  $\Gamma = 2$  coupling in the sense that the rescaled moment  $I_6$  satisfies (18), i.e., the rhs of (20) acquires the exact value  $(-6)$  at  $\Gamma = 2$  and exhibits the exact prefactor  $21/2$  to the leading  $(\Gamma - 2)$  correction term. These facts were our primary motivation for proving rigorously the conjecture of the finite  $\Gamma$ -series-truncation of  $I_6$ .

It turns out to be more convenient to formulate the above sum rules in terms of the small- $\mathbf{k}$  expansion of the Fourier component of the direct correlation,  $\hat{c}(\mathbf{k})$ . Inserting (19) together with the suggested truncation of the sixth moment at the  $\Gamma^2$ -term (20) into the representation (10) for  $\hat{h}(\mathbf{k})$ , the OZ relation (8') implies the expected form

$$\hat{c}(\mathbf{k}) = -\frac{\Gamma}{k^2} + \frac{\Gamma}{8\pi n} - \frac{k^2}{96(\pi n)^2} + O(k^4) \quad (21)$$

Note the characteristic singular leading term of  $\hat{c}(\mathbf{k})$ ,  $-\beta\hat{v}(\mathbf{k}) = -\Gamma/k^2$ , succeeded by the regular  $k^2$ -series expansion part: its knowledge up to the  $k^{2j}$  term determines  $\hat{h}(\mathbf{k})$  up to the  $k^{2(j+2)}$  term, or equivalently, the real-space  $h$ -moments (12) up to  $I_{2(j+2)}$ .

#### 4. RENORMALIZED MAYER EXPANSION

The Mayer function  $f$  can be expanded in the inverse temperature  $\beta$  as follows

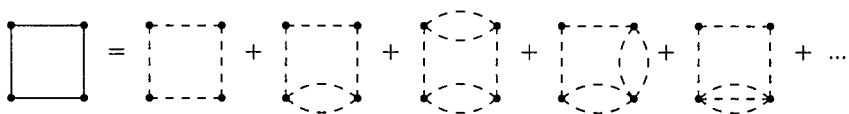
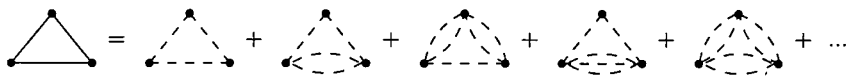
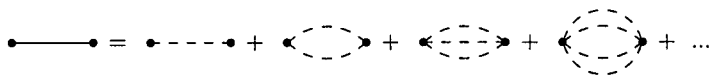
$$f(1, 2) = -\beta v(1, 2) + \frac{1}{2!} [-\beta v(1, 2)]^2 + \frac{1}{3!} [-\beta v(1, 2)]^3 + \dots \quad (22)$$

Graphically,

$$\begin{array}{c} f \\ \circ_1 \text{---} \circ_2 \end{array} = \begin{array}{c} -\beta v \\ \circ_1 \text{---} \circ_2 \end{array} + \alpha \begin{array}{c} \text{---} \text{---} \text{---} \\ \circ_1 \text{---} \text{---} \text{---} \circ_2 \end{array} + \alpha \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \\ \circ_1 \text{---} \text{---} \text{---} \text{---} \circ_2 \end{array} + \dots \quad (22')$$

where the factor  $1/(\text{number of interaction lines})!$  is automatically involved in each diagram. Let us perform the above  $f$ -decomposition within the diagrammatic representation (2) of  $\beta\bar{F}^{ex}$ :





etc. If there are only one- or two-coordinated field circles in a graph (by coordination of a vertex we mean its bond-coordination), we do nothing. If there are some three- or more-coordinated field circles in a graph, we can eliminate all two-coordinated field circles by a series transformation and arrive at a connected graph of field circles of coordination  $\geq 3$ , called skeleton. Grouping the diagrams which are reduced to the same skeleton after series elimination, the bonds connecting skeleton field circles become dressed according to

$$\begin{aligned}
 K(1,2) &= \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \dots \\
 &= \text{dressed bond} \quad (23)
 \end{aligned}$$

Equivalently,

$$K(1,2) = [-\beta u(1,2)] + \int [-\beta u(1,3)] n(3) K(3,2) d3 \quad (23')$$

or, in the case of an infinite homogeneous fluid,

$$\hat{K}(\mathbf{k}) = [-\beta \hat{u}(\mathbf{k})] + (2\pi)^{d/2} n[-\beta \hat{u}(\mathbf{k})] \hat{K}(\mathbf{k}) \quad (23'')$$

The procedure of bond renormalization thus implies

$$\beta \bar{F}^{ex}[n] = \text{diagram 1} + D_0[n] + \sum_{s=1}^{\infty} D_s[n] \quad (24a)$$

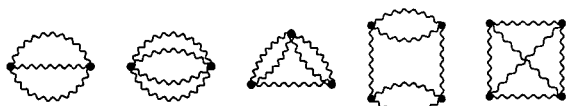
where  $D_0$  is the sum of all unrenormalized ring diagrams (which cannot undertake the renormalization procedure)

$$D_0 = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \dots \quad (24b)$$

and

$$\sum_{s=1}^{\infty} D_s = \left\{ \begin{array}{l} \text{all connected diagrams which consist of } N \geq 2 \text{ field} \\ n\text{-circles of coordination } \geq 3 \text{ and multiple } K\text{-bonds,} \\ \text{and are free of connecting circles} \end{array} \right\} \quad (24c)$$

represents the set all remaining completely renormalized graphs. Under multiple  $K$ -bonds we mean the possibility of an arbitrary number of  $K$ -bonds between a couple of field circles. The order of numeration of  $D$ -diagrams in (24c) is irrelevant, let us say



$$D_1 \quad D_2 \quad D_3 \quad D_4 \quad D_5 \quad (25)$$

and so on. The symbol  $D_s$  will reflect the notation of a given diagram and simultaneously its integral representation.

Having classified the renormalized graphs of  $\beta\bar{F}^{ex}$ , we proceed by considering the direct correlation  $c$ , defined by equation (5). From (24) one derives

$$c(1, 2) = \text{---} \text{---} + c_0(1, 2) + \sum_{s=1}^{\infty} c_s(1, 2) \quad (26a)$$

where  $c_0(1, 2) = \delta^2 D_0 / \delta n(1) \delta n(2)$  can be easily shown to correspond to the renormalized “watermelon” Meeron graph

$$c_0(1, 2) = \text{---} \text{---} = \frac{1}{2!} K^2(1, 2) \quad (26b)$$

and  $c_s(1, 2)$  with  $s = 1, 2, \dots$  denotes the whole family of 1,2-rooted diagrams generated from  $D_s$ ,

$$c_s(1, 2) = \frac{\delta^2 D_s}{\delta n(1) \delta n(2)} \quad (26c)$$

To get explicitly a given family  $c_s$ , one has to take into account the functional dependence of the dressed  $K$ -bonds (23) on the density as well. Since with regard to (23') it holds

$$\frac{\delta K(1, 2)}{\delta n(3)} = K(1, 3) K(3, 2) \tag{27}$$

the functional derivative of  $D_s$  with respect to the density field generates the root circle not only at field-circle positions, but also on  $K$ -bonds, causing their ‘‘correct K-K division’’. For example, in the case of generator  $D_1$  drawn in (25), we obtain

$$c_1(1, 2) = \begin{array}{ccc} \text{Diagram 1} & + & \text{Diagram 2} & + & \text{Diagram 3} \\ \text{Diagram 4} & + & \text{Diagram 5} & + & \text{Diagram 6} \end{array} \tag{28}$$

The diagrams in (28) represent six different configurations of a field circle with two root circles (1 and 2) attached to it. The configurations are: 1) root circles at the left and right vertices; 2) root circles at the top and bottom vertices; 3) root circles at the top and right vertices; 4) root circles at the top and left vertices; 5) root circles at the top and bottom vertices with a wavy line connecting them; 6) root circles at the top and right vertices with a wavy line connecting them.

It stands to reason that the coordination of field circles remains to be  $\geq 3$  after the functional derivation, while the root 1, 2-circles can be two-coordinated (just when being generated on a  $K$ -bond). The  $\{c_s\}_{s=1}^\infty$  diagram families evidently do not overlap with each other.

The specialization to the infinite 2d OCP, with dimensionless interaction energy (11), leads to the dressed  $K$ -bond (23) of the form

$$\hat{K}(\mathbf{k}) = -\frac{\Gamma}{k^2 + 2\pi\Gamma n} \tag{29a}$$

$$\begin{aligned} K(\mathbf{r}) &= -\frac{\Gamma}{2\pi} \int \frac{1}{k^2 + 2\pi\Gamma n} \exp(i\mathbf{k} \cdot \mathbf{r}) d\mathbf{k} \\ &= -\Gamma K_0(r \sqrt{2\pi\Gamma n}) \end{aligned} \tag{29b}$$

The series renormalization of the logarithmic interaction thus leads to the modified Bessel function of second kind: its decay to zero at asymptotically large distance makes the renormalized Mayer diagrams properly convergent.<sup>(11)</sup> Note the specific  $r \sqrt{n}$  dependence of  $K$  which has a fundamental impact on the  $n$ -classification of renormalized diagrams. As concerns the  $\Gamma$ -order of a given diagram  $D$  with  $N$  field circles and  $L$  bonds, every dressed bond (29) brings the factor  $\Gamma$  and enforces the substitution

$r' = r \sqrt{\Gamma}$  which manifests itself as the  $\Gamma^{-1}$  factor for each field-circle integration  $\sim \int r dr$ , so that the  $\Gamma$ -order =  $L - N$ . For example, in (25),  $D_1 \sim \Gamma$  and  $D_2, D_3, D_4, D_5$  constitute the complete set of  $\beta \bar{F}^{ex}$ -diagrams  $\sim \Gamma^2$ .

## 5. SUM RULES

Let the given completely renormalized diagram  $D_s$  ( $s = 1, \dots$ ) of the excess Helmholtz free energy be composed of  $N$  skeleton vertices  $i = 1, \dots, N$  and  $L$  bonds  $\alpha = 1, \dots, L$ .  $D_s$  can be formally expressed as

$$D_s[n] = \int \prod_{i=1}^N [di n(i)] \prod_{\alpha=1}^L K(\alpha_1, \alpha_2) \quad (30)$$

where  $\alpha_1, \alpha_2 \in \{1, \dots, N\}$ ,  $\alpha_1 < \alpha_2$  denotes the ordered pair of vertices joint by the  $\alpha$ -bond and we have omitted topological factors. Whenever not confusing, we will use the symbol  $K_\alpha \equiv K(\alpha_1, \alpha_2)$  and omit the ranges  $\{1, N\}$  and  $\{1, L\}$  for a sum or product over skeleton vertices  $i$  and bonds  $\alpha$ , respectively. The family of direct correlations  $c_s(\mathbf{r}, \mathbf{r}')$ , generated according to  $c_s(\mathbf{r}, \mathbf{r}') = \delta^2 D_s[n] / \delta n(\mathbf{r}) \delta n(\mathbf{r}')$ , can be straightforwardly expressed in the uniform-density regime  $n(i) = n$  as follows:

$$\begin{aligned} c_s(\mathbf{r}, \mathbf{r}') &= n^{N-2} \int \prod_i di \sum_{\substack{i, j \\ (i \neq j)}} \delta(\mathbf{r} - i) \delta(\mathbf{r}' - j) \prod_{\alpha} K_{\alpha} & (a) \\ &+ n^{N-1} \int \prod_i di \sum_i \delta(\mathbf{r} - i) \sum_{\alpha} K(\alpha_1, \mathbf{r}') K(\mathbf{r}', \alpha_2) \prod_{\beta \neq \alpha} K_{\beta} & (b) \\ &+ n^{N-1} \int \prod_i di \sum_i \delta(\mathbf{r}' - i) \sum_{\alpha} K(\alpha_1, \mathbf{r}) K(\mathbf{r}, \alpha_2) \prod_{\beta \neq \alpha} K_{\beta} & (c) \\ &+ n^N \int \prod_i di \sum_{\alpha} K(\alpha_1, \mathbf{r}') K(\mathbf{r}', \mathbf{r}) K(\mathbf{r}, \alpha_2) \prod_{\beta \neq \alpha} K_{\beta} & (d) \\ &+ n^N \int \prod_i di \sum_{\alpha} K(\alpha_1, \mathbf{r}) K(\mathbf{r}, \mathbf{r}') K(\mathbf{r}', \alpha_2) \prod_{\beta \neq \alpha} K_{\beta} & (e) \\ &+ n^N \int \prod_i di \sum_{\substack{\alpha, \beta \\ (\alpha \neq \beta)}} K(\alpha_1, \mathbf{r}) K(\mathbf{r}, \alpha_2) K(\beta_1, \mathbf{r}') K(\mathbf{r}', \beta_2) \prod_{\gamma \neq \alpha, \beta} K_{\gamma} & (f) \end{aligned} \quad (31)$$

where we have applied the functional relation (27). The (a) term on the rhs of (31) corresponds to the creation of root points at two skeleton vertices, the next two (b, c) terms to one root circle generated at the skeleton and the other one at a bond, the (d, e) terms to two root points at the same bond and the last (f) term represents two root points generated at different renormalized bonds  $\alpha \neq \beta$ . It stands to reason that now  $K(\mathbf{r}, \mathbf{r}') = K(|\mathbf{r} - \mathbf{r}'|)$  satisfying (A1), (A2a, b) and, consequently,  $c_s(\mathbf{r}, \mathbf{r}') = c_s(|\mathbf{r} - \mathbf{r}'|)$ .

In this section, we aim at proving the validity of the moment equalities

$$\int c_s(\mathbf{r}) d\mathbf{r} = 0 \quad (32a)$$

$$\int r^2 c_s(\mathbf{r}) d\mathbf{r} = 0 \quad (32b)$$

for every family  $s=1, 2, \dots$ , regardless of the topology of the generating diagram  $D_s$ . To keep the interchange-particle symmetry and the translational-invariance property of the problem, we will use instead of (32a, b) the following equivalent definitions of the moments:

$$J_0^{(s)} = \frac{1}{V} \int c_s(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (33a)$$

$$J_2^{(s)} = \frac{1}{V} \int |\mathbf{r} - \mathbf{r}'|^2 c_s(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (33b)$$

The introduction of volume  $V$  into the formulation of the infinite-volume limit does not mean any loss of rigour. Definitions (33a, b) have to be understood in the sense that an arbitrary one of integration coordinates  $\mathbf{r}, \mathbf{r}', \{i\}$  can be taken, due to the invariance of the integrated function with respect to a uniform shift in all variables, as a reference and put at the origin  $\mathbf{0}$ , with the simultaneous cancellation of  $V$ . The right choice of the reference can simplify otherwise tedious algebra.

### 5.1. Proof of the Zeroth-Moment Condition (32a)

By using the definition (33a), the zeroth moment of  $c_s$  (31) can be expressed as

$$J_0^{(s)} = N(N-1) n^{N-2} \frac{1}{V} \int \prod_i di \prod_\alpha K_\alpha \quad (a)$$

$$+ 2Nn^{N-1} \frac{1}{V} \int \prod_i di \sum_\alpha \frac{\partial K_\alpha}{\partial n} \prod_{\beta \neq \alpha} K_\beta \quad (b+c)$$

$$+ n^N \frac{1}{V} \int d\mathbf{r} \int \prod_i di \sum_\alpha \frac{\partial K(\alpha_1, \mathbf{r})}{\partial n} K(\mathbf{r}, \alpha_2) \prod_{\beta \neq \alpha} K_\beta \quad (d)$$

$$+ n^N \frac{1}{V} \int d\mathbf{r} \int \prod_i di \sum_\alpha K(\alpha_1, \mathbf{r}) \frac{\partial K(\mathbf{r}, \alpha_2)}{\partial n} \prod_{\beta \neq \alpha} K_\beta \quad (e)$$

$$+ n^N \frac{1}{V} \int \prod_i di \sum_{\substack{\alpha, \beta \\ (\alpha \neq \beta)}} \frac{\partial K_\alpha}{\partial n} \frac{\partial K_\beta}{\partial n} \prod_{\gamma \neq \alpha, \beta} K_\gamma \quad (f)$$

$$(34)$$

where we have taken into account relation (A2a). Since

$$\int d\mathbf{r} \left[ \frac{\partial K(\alpha_1, \mathbf{r})}{\partial n} K(\mathbf{r}, \alpha_2) + K(\alpha_1, \mathbf{r}) \frac{\partial K(\mathbf{r}, \alpha_2)}{\partial n} \right] = \frac{\partial^2 K(\alpha_1, \alpha_2)}{\partial n^2}$$

we find

$$J_0^{(s)} = \frac{\partial^2}{\partial n^2} \left[ \frac{n^N}{V} \int \prod_{i=1}^N di \prod_{\alpha=1}^L K_\alpha \right] \quad (35)$$

Let us put say  $i = 1$  at the origin  $\mathbf{0}$ , and “cancel” the integration over 1 with volume  $V$ . As  $K(\alpha_1, \alpha_2) = -\Gamma K_0(\sqrt{2\pi\Gamma n} |\alpha_1 - \alpha_2|)$  for the 2d OCP, the evoked substitution  $i' = i\sqrt{2\pi\Gamma n}$  for  $(N-1)$  remaining coordinates  $i = 2, \dots, N$  results in the factor  $1/n^{(N-1)}$ . Therefore,

$$J_0^{(s)} \sim \frac{\partial^2}{\partial n^2} \frac{n^N}{n^{(N-1)}} = 0 \quad (36)$$

in agreement with (32a).

## 5.2. Proof of the Second-Moment Condition (32b)

By using the definition (33b), the second moment of  $c_x$  (31) is written as

$$J_2^{(s)} = \frac{n^{N-2}}{V} \int \prod_i di \sum_{\substack{i,j \\ (i \neq j)}} |i-j|^2 \prod_{\alpha} K_{\alpha} \quad (a)$$

$$+ \frac{2n^{N-1}}{V} \int \prod_i di \sum_{i,\alpha} \int |\mathbf{r}-i|^2 K(\alpha_1, \mathbf{r}) K(\mathbf{r}, \alpha_2) d\mathbf{r} \prod_{\beta \neq \alpha} K_{\beta} \quad (b+c)$$

$$+ \frac{2n^N}{V} \int \prod_i di \sum_{\alpha} \int |\mathbf{r}-\mathbf{r}'|^2 K(\alpha_1, \mathbf{r}) K(\mathbf{r}, \mathbf{r}') K(\mathbf{r}', \alpha_2) d\mathbf{r} d\mathbf{r}' \prod_{\beta \neq \alpha} K_{\beta} \quad (d+e)$$

$$+ \frac{n^N}{V} \int \prod_i di \sum_{\substack{\alpha,\beta \\ (\alpha \neq \beta)}} \int |\mathbf{r}-\mathbf{r}'|^2 K(\alpha_1, \mathbf{r}) K(\mathbf{r}, \alpha_2) \\ \times K(\beta_1, \mathbf{r}') K(\mathbf{r}', \beta_2) d\mathbf{r} d\mathbf{r}' \prod_{\gamma \neq \alpha, \beta} K_{\gamma} \quad (f)$$

(37)

The integrations over  $\mathbf{r}$  and  $\mathbf{r}'$  in (37) correspond to root points generated on renormalized  $K$ -bonds, and interacting with another root point at the skeleton or with one another. In Appendix A we show how to transform these integrals to the form with exclusively skeleton  $|i-j|^2$ ,  $\Phi(|i-j|)$  and  $\Psi(|i-j|)$  interactions [for definitions of  $\Phi$  and  $\Psi$  see (A7) and (A10), respectively] and appropriately “decorated” bonds [under decoration, we mean the derivation with respect to density, equation (A2a)]. The successive application of formulae (A8), (A10) and (A9) to the respective terms (b+c), (d+e) and (f) of (37) yields

$$J_2^{(s)} = \frac{n^{N-2}}{V} \int \prod_i di \sum_{\substack{i,j \\ (i \neq j)}} |i-j|^2 \prod_{\alpha} K_{\alpha} \quad (a)$$

$$+ \frac{2n^{N-1}}{V} \int \prod_i di \sum_{\alpha} \left[ \sum_i \frac{1}{2} (|\alpha_1 - i|^2 + |\alpha_2 - i|^2) \frac{\partial K_{\alpha}}{\partial n} + N\Phi_{\alpha} \right] \prod_{\beta \neq \alpha} K_{\beta} \quad (b+c)$$

$$+ \frac{2n^N}{V} \int \prod_i di \sum_{\alpha} \Psi_{\alpha} \prod_{\beta \neq \alpha} K_{\beta} \quad (d+e)$$

$$+ \frac{n^N}{V} \int \prod_i di \sum_{\substack{\alpha,\beta \\ (\alpha \neq \beta)}} \left[ \frac{1}{4} (|\alpha_1 - \beta_1|^2 + |\alpha_1 - \beta_2|^2 \right. \\ \left. + |\alpha_2 - \beta_1|^2 + |\alpha_2 - \beta_2|^2) \right. \\ \left. \times \frac{\partial K_{\alpha}}{\partial n} \frac{\partial K_{\beta}}{\partial n} + \frac{\partial K_{\alpha}}{\partial n} \Phi_{\beta} + \frac{\partial K_{\beta}}{\partial n} \Phi_{\alpha} \right] \prod_{\gamma \neq \alpha, \beta} K_{\gamma} \quad (f)$$

(38)

Let us now define the auxiliary function

$$\begin{aligned}
 G^{(s)}(n) &= \frac{2n^{N+1}}{V} \int \prod_i di \sum_{\alpha} \Phi_{\alpha} \prod_{\beta \neq \alpha} K_{\beta} \\
 &\equiv \frac{n^{N+1}}{V} \int \prod_i di \left( \sum_{\alpha} \Phi_{\alpha} \prod_{\beta \neq \alpha} K_{\beta} + \sum_{\beta} \Phi_{\beta} \prod_{\alpha \neq \beta} K_{\alpha} \right) \quad (39)
 \end{aligned}$$

Up to the prefactor  $2/V$ , it originates from  $D_s(n)$  (30) by picking out successively bonds one after the other and interchanging the bond factor  $K \rightarrow n\Phi$ .  $\Phi_{\alpha}$  is expressible from (A7) and (29a) in the form

$$\Phi_{\alpha} = \frac{4\Gamma^2}{(2\pi\Gamma n)^2} \int \frac{p^2}{(p^2+1)^4} \exp[i\mathbf{p} \cdot (\alpha_1 - \alpha_2) \sqrt{2\pi\Gamma n}] d\mathbf{p} \quad (40)$$

With the aid of the scaling argument leading to relation (36),  $G^{(s)}$  can be shown to scale with  $n$  like

$$G^{(s)}(n) \sim \frac{n^{N+1}}{n^{N-1}n^2} = n^0 \quad (41)$$

As a consequence,  $\partial G^{(s)}(n)/\partial n = 0$ . Explicitly,

$$\begin{aligned}
 0 &= \frac{2(N+1)n^N}{V} \int \prod_i di \sum_{\alpha} \Phi_{\alpha} \prod_{\beta \neq \alpha} K_{\beta} \\
 &\quad + \frac{2n^{N+1}}{V} \int \prod_i di \sum_{\alpha} \frac{\partial \Phi_{\alpha}}{\partial n} \prod_{\beta \neq \alpha} K_{\beta} \\
 &\quad + \frac{n^{N+1}}{V} \int \prod_i di \sum_{\substack{\alpha, \beta \\ (\alpha \neq \beta)}} \left( \Phi_{\alpha} \frac{\partial K_{\beta}}{\partial n} + \Phi_{\beta} \frac{\partial K_{\alpha}}{\partial n} \right) \prod_{\gamma \neq \alpha, \beta} K_{\gamma} \quad (42)
 \end{aligned}$$

Subtracting  $\{\text{Eq. (42)}\}/n$  from formula (38), the latter takes a simpler form

$$\begin{aligned}
 J_2^{(s)} &= \frac{n^{N-2}}{V} \int \prod_i di \sum_{\substack{i, j \\ (i \neq j)}} |i-j|^2 \prod_{\alpha} K_{\alpha} \\
 &\quad + \frac{n^{N-1}}{V} \int \prod_i di \sum_{i, \alpha} (|\alpha_1 - i|^2 + |\alpha_2 - i|^2) \frac{\partial K_{\alpha}}{\partial n} \prod_{\beta \neq \alpha} K_{\beta}
 \end{aligned}$$



$$\begin{aligned}
 & + \frac{2n^N}{V} \int \prod_i di \sum_{\alpha} \left[ \Psi_{\alpha} - \frac{1}{n} \frac{\partial(n\Phi_{\alpha})}{\partial n} \right] \prod_{\beta \neq \alpha} K_{\beta} \\
 & + \frac{n^N}{4V} \int \prod_i di \sum_{\substack{\alpha, \beta \\ (\alpha \neq \beta)}} (|\alpha_1 - \beta_1|^2 + |\alpha_1 - \beta_2|^2 + |\alpha_2 - \beta_1|^2 + |\alpha_2 - \beta_2|^2) \\
 & \times \frac{\partial K_{\alpha}}{\partial n} \frac{\partial K_{\beta}}{\partial n} \prod_{\gamma \neq \alpha, \beta} K_{\gamma}
 \end{aligned} \tag{43}$$

It is trivial to show that

$$\begin{aligned}
 & \Psi_{\alpha} - \frac{1}{n} \frac{\partial(n\Phi_{\alpha})}{\partial n} \\
 & = - \int e^{i\mathbf{p} \cdot (\alpha_1 - \alpha_2)} \Delta_{\mathbf{p}} \left[ \frac{\Gamma^2}{4n(p^2 + 2\pi\Gamma n)^2} - \frac{\pi\Gamma^3}{(p^2 + 2\pi\Gamma n)^3} \right] d\mathbf{p} \\
 & = |\alpha_1 - \alpha_2|^2 \int e^{i\mathbf{p} \cdot (\alpha_1 - \alpha_2)} \left[ \frac{\Gamma^2}{4n(p^2 + 2\pi\Gamma n)^2} - \frac{\pi\Gamma^3}{(p^2 + 2\pi\Gamma n)^3} \right] d\mathbf{p} \\
 & = \frac{|\alpha_1 - \alpha_2|^2}{4n^2} \left( n \frac{\partial}{\partial n} \right)^2 K_{\alpha}
 \end{aligned} \tag{43'}$$

Equation (43) together with the complementary one (43') represent the formulation of the second moment of  $\hat{c}_s$  in the renormalized format in terms of quadratic interactions exclusively between pairs of skeleton vertices.

For tactical reasons, we now specify the connectivity of diagram  $D_s$ , instead of enumerating present renormalized bonds  $\alpha = 1, \dots, L$ , by the set  $\{v_{ij}\}_{i, j=1}^N$  where  $v_{ij} = v_{ji}$  is the number of  $K$ -bonds between skeleton vertices  $i, j$  ( $v_{ij} = 0$  if there is no bond between  $i, j$ ). Let us choose a couple of skeleton vertices, say 1 and 2, and group all factors in (43), (43') associated with the  $|1 - 2|^2$  interaction:

$$\begin{aligned}
 & \frac{n^{N-2}}{V} \int \prod_i di |1 - 2|^2 \prod_{\substack{u, v=3 \\ (u < v)}}^N K^{v_{uv}}(u, v) \\
 & \times \left\{ 2K^{v_{12}}(1, 2) \prod_{i=3}^N K^{v_{1i}}(1, i) \prod_{j=3}^N K^{v_{2j}}(2, j) \right. \\
 & \left. + 2v_{12} K^{v_{12}-1}(1, 2) \left[ n \frac{\partial K(1, 2)}{\partial n} \right] \prod_{i=3}^N K^{v_{1i}}(1, i) \prod_{j=3}^N K^{v_{2j}}(2, j) \right.
 \end{aligned}$$

$$\begin{aligned}
& + K^{v_{12}}(1, 2) \left[ n \frac{\partial}{\partial n} \prod_{i=3}^N K^{v_{1i}}(1, i) \right] \prod_{j=3}^N K^{v_{2j}}(2, j) \\
& + K^{v_{12}}(1, 2) \prod_{i=3}^N K^{v_{1i}}(1, i) \left[ n \frac{\partial}{\partial n} \prod_{j=3}^N K^{v_{2j}}(2, j) \right] \\
& + \frac{1}{2} v_{12} K^{v_{12}-1}(1, 2) \left[ \left( n \frac{\partial}{\partial n} \right)^2 K(1, 2) \right] \prod_{i=3}^N K^{v_{1i}}(1, i) \prod_{j=3}^N K^{v_{2j}}(2, j) \\
& + \frac{1}{2} v_{12} (v_{12} - 1) K^{v_{12}-2}(1, 2) \left[ n \frac{\partial K(1, 2)}{\partial n} \right]^2 \prod_{i=3}^N K^{v_{1i}}(1, i) \prod_{j=3}^N K^{v_{2j}}(2, j) \\
& + \frac{1}{2} v_{12} K^{v_{12}-1}(1, 2) \left[ n \frac{\partial K(1, 2)}{\partial n} \right] \left[ n \frac{\partial}{\partial n} \prod_{i=3}^N K^{v_{1i}}(1, i) \right] \prod_{j=3}^N K^{v_{2j}}(2, j) \\
& + \frac{1}{2} v_{12} K^{v_{12}-1}(1, 2) \left[ n \frac{\partial K(1, 2)}{\partial n} \right] \prod_{i=3}^N K^{v_{1i}}(1, i) \left[ n \frac{\partial}{\partial n} \prod_{j=3}^N K^{v_{2j}}(2, j) \right] \\
& + \frac{1}{2} K^{v_{12}}(1, 2) \left[ n \frac{\partial}{\partial n} \prod_{i=3}^N K^{v_{1i}}(1, i) \right] \left[ n \frac{\partial}{\partial n} \prod_{j=3}^N K^{v_{2j}}(2, j) \right] \} \quad (44)
\end{aligned}$$

In the case of the considered Bessel functions (29), the operator  $n(\partial/\partial n)$  acting on  $K(i, j)$  can be substituted by a coordinate-operator as follows

$$\begin{aligned}
n \frac{\partial}{\partial n} K(i, j) &= \frac{1}{2} \left( r_{ij} \frac{\partial}{\partial r_{ij}} \right) K(|\mathbf{r}_i - \mathbf{r}_j|) \\
&\equiv \frac{1}{2} \mathbf{R}_{ij} K(|\mathbf{r}_i - \mathbf{r}_j|) \quad (45)
\end{aligned}$$

As one can derive directly from the definition (45), there exist more equivalent representations of operator  $\mathbf{R}_{ij}$ ,

$$\begin{aligned}
\mathbf{R}_{ij} &= r_{ij} \frac{\partial}{\partial r_{ij}} \\
&= (\mathbf{r}_i - \mathbf{r}_j) \cdot \nabla_i \\
&= (\mathbf{r}_j - \mathbf{r}_i) \cdot \nabla_j \\
&= \frac{1}{2} (\mathbf{r}_i - \mathbf{r}_j) \cdot (\nabla_i - \nabla_j) \quad (46)
\end{aligned}$$

Finally, denoting  $F_{ij} = K^{\alpha y}(|i-j|)$  and summing over all pairs of skeleton vertices, Eqs. (43), (44) and (45) imply

$$\begin{aligned}
J_2^{(s)}/n^{N-2} &= \frac{1}{V} \int \prod_i di \prod_{u < v} F_{uv} \sum_{i < j} |i-j|^2 \\
&\times \left\{ 2 + \frac{1}{F_{ij}} (\mathbf{R}_{ij} F_{ij}) + \frac{1}{8F_{ij}} (\mathbf{R}_{ij}^2 F_{ij}) \right. \\
&+ \frac{1}{2} \sum_{k \neq i, j} \left[ \frac{1}{F_{ik}} (\mathbf{R}_{ik} F_{ik}) + \frac{1}{F_{jk}} (\mathbf{R}_{jk} F_{jk}) \right] \\
&+ \frac{1}{8F_{ij}} (\mathbf{R}_{ij} F_{ij}) \sum_{k \neq i, j} \left[ \frac{1}{F_{ik}} (\mathbf{R}_{ik} F_{ik}) + \frac{1}{F_{jk}} (\mathbf{R}_{jk} F_{jk}) \right] \\
&\left. + \frac{1}{8} \sum_{k, l \neq i, j} \frac{1}{F_{ik} F_{jl}} (\mathbf{R}_{ik} F_{ik}) (\mathbf{R}_{jl} F_{jl}) \right\} \quad (47)
\end{aligned}$$

In what follows we aim at proving the nullity of the rhs of (47), *irrespective of* the particular form of the bond-dependent functions  $F_{ij}(r_{ij})$  (provided that the integrals exist what certainly applies to our case of  $F$ -functions). As shown in Appendix B, due to a scaling transformation of coordinates in integrals of translationally-invariant functions over infinite  $2d$  space, Eq. (47) is reducible to a simpler relation

$$\begin{aligned}
8J_2^{(s)}/n^{N-2} &= \int \prod_i di \prod_{u < v} F_{uv} \sum_{i < j} |i-j|^2 \\
&\times \left\{ \sum_{k \neq i, j} \left[ \frac{1}{2F_{ik}} (\mathbf{r}_i - \mathbf{r}_j) \cdot \nabla_i F_{ik} + \frac{1}{2F_{jk}} (\mathbf{r}_j - \mathbf{r}_i) \cdot \nabla_j F_{jk} \right] \right. \\
&\left. + \sum_{k, l \neq i, j} \frac{1}{F_{ik} F_{jl}} [(\mathbf{r}_j - \mathbf{r}_k) \cdot \nabla_i F_{ik}] [(\mathbf{r}_i - \mathbf{r}_l) \cdot \nabla_j F_{jl}] \right\} \quad (48)
\end{aligned}$$

Let us consider  $\{F_{ij}\}$  to be the functions of  $r_{ij}^2$  rather than  $r_{ij}$ , without changing the symbol  $F$ . Thus

$$\nabla_i F_{ij}(r_{ij}^2) = \frac{dF_{ij}(r_{ij}^2)}{d(r_{ij}^2)} 2(\mathbf{r}_i - \mathbf{r}_j) \quad (49)$$

Using the notation

$$\tilde{F}_{ij} = \frac{1}{F_{ij}} \frac{dF_{ij}(r_{ij}^2)}{d(r_{ij}^2)} \quad (50)$$

Eq. (49) can be rewritten as follows

$$\nabla_i F_{ij} = 2(\mathbf{r}_i - \mathbf{r}_j) F_{ij} \tilde{F}_{ij} \quad (49')$$

Inserting (49') into (48) and grouping the  $\tilde{F}$  and  $\tilde{F}\tilde{F}$  terms we obtain

$$\begin{aligned} 8J_2^{(s)}/n^{N-2} = & \int \prod_i di \prod_{u < v} F_{uv} \left\{ \sum_{(i < j)} \tilde{F}_{ij} \sum_{k \neq i, j} \mathbf{r}_{ij} \cdot (r_{ik}^2 \mathbf{r}_{ik} - r_{jk}^2 \mathbf{r}_{jk}) \right. \\ & + 2 \sum_{(i < j)} \sum_{(k < l)} \tilde{F}_{ij} \tilde{F}_{kl} [r_{ik}^2 (\mathbf{r}_{ij} \cdot \mathbf{r}_{kj}) (\mathbf{r}_{il} \cdot \mathbf{r}_{kl}) + r_{il}^2 (\mathbf{r}_{ij} \cdot \mathbf{r}_{lj}) (\mathbf{r}_{ik} \cdot \mathbf{r}_{lk}) \\ & \left. + r_{jk}^2 (\mathbf{r}_{ji} \cdot \mathbf{r}_{ki}) (\mathbf{r}_{jl} \cdot \mathbf{r}_{kl}) + r_{jl}^2 (\mathbf{r}_{ji} \cdot \mathbf{r}_{li}) (\mathbf{r}_{jk} \cdot \mathbf{r}_{lk}) \right] \} \quad (51) \end{aligned}$$

with the obvious notation  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ .

Our further goal is to prove the nullity of the rhs of (51). We show that the per-partes integration of the bilinear  $\tilde{F}\tilde{F}$  term in (51) gives a linear  $\tilde{F}$  term which exactly eliminates the linear  $\tilde{F}$  term in (51). To do so, we express the bilinear  $\tilde{F}\tilde{F}$  term in integral (51) in an "ansatz" form

$$\begin{aligned} & \int \prod_i di \prod_{u < v} F_{uv} [(\mathbf{r}_{12} \tilde{F}_{12} + \mathbf{r}_{13} \tilde{F}_{13} + \dots + \mathbf{r}_{1N} \tilde{F}_{1N}) \cdot \mathbf{Q}_1 \\ & + (\mathbf{r}_{21} \tilde{F}_{12} + \mathbf{r}_{23} \tilde{F}_{23} + \dots + \mathbf{r}_{2N} \tilde{F}_{2N}) \cdot \mathbf{Q}_2 + \dots] \quad (52) \end{aligned}$$

The vector functions  $\mathbf{Q}_i$  must be linear combinations of  $\tilde{F}_{kl}$  with  $k, l \neq i$  since the terms  $\tilde{F}_{ij} \tilde{F}_{ij}$  vanish in (51);  $\mathbf{Q}_1 = \mathbf{Q}_1^{(2,3)} \tilde{F}_{23} + \mathbf{Q}_1^{(2,4)} \tilde{F}_{24} + \dots + \mathbf{Q}_1^{(N-1,N)} \tilde{F}_{N-1,N}$ , etc. In general,

$$\mathbf{Q}_i = \sum_{\substack{k, l \neq i \\ k < l}} \mathbf{Q}_i^{(k,l)} \tilde{F}_{kl} \quad (53)$$

where the three-point vector coefficients  $\mathbf{Q}_i^{(k,l)}$ ,

$$\mathbf{Q}_i^{(k,l)} \neq 0 \quad \text{iff} \quad i \neq k \neq l \quad (54a)$$

depend only on coordinates  $\{\mathbf{r}_i, \mathbf{r}_k, \mathbf{r}_l\}$ . It is natural to extend their definition as follows

$$\mathbf{Q}_i^{(k,l)} = \mathbf{Q}_i^{(l,k)} \quad (54b)$$

Comparing Eq.(52) with (51), the coefficients to the  $\tilde{F}_{ik}\tilde{F}_{il}$  ( $i \neq k \neq l$ ) and  $\tilde{F}_{ij}\tilde{F}_{kl}$  ( $i \neq j \neq k \neq l$ ) terms imply the respective restrictions on  $\mathbf{Q}$ -vectors:

$$\mathbf{r}_{ki} \cdot \mathbf{Q}_k^{(i,l)} + \mathbf{r}_{li} \cdot \mathbf{Q}_l^{(i,k)} = 4r_{kl}^2(\mathbf{r}_{ki} \cdot \mathbf{r}_{li})^2 \quad (55a)$$

$$\begin{aligned} & \mathbf{r}_{ij} \cdot \mathbf{Q}_i^{(k,l)} + \mathbf{r}_{ji} \cdot \mathbf{Q}_j^{(k,l)} + \mathbf{r}_{kl} \cdot \mathbf{Q}_k^{(i,j)} + \mathbf{r}_{lk} \cdot \mathbf{Q}_l^{(i,j)} \\ & = 4[r_{ik}^2(\mathbf{r}_{ij} \cdot \mathbf{r}_{kj})(\mathbf{r}_{il} \cdot \mathbf{r}_{kl}) + r_{il}^2(\mathbf{r}_{ij} \cdot \mathbf{r}_{lj})(\mathbf{r}_{ik} \cdot \mathbf{r}_{lk}) \\ & \quad + r_{jk}^2(\mathbf{r}_{ji} \cdot \mathbf{r}_{ki})(\mathbf{r}_{jl} \cdot \mathbf{r}_{kl}) + r_{jl}^2(\mathbf{r}_{ji} \cdot \mathbf{r}_{li})(\mathbf{r}_{jk} \cdot \mathbf{r}_{lk})] \end{aligned} \quad (55b)$$

with no order inequalities put on  $\{i, j, k, l\}$ . The important feature of the ansatz proposal (52) consists in the equality

$$\prod_{u < v} F_{uv}(\mathbf{r}_{i,1}\tilde{F}_{i1} + \dots + \mathbf{r}_{i,N}\tilde{F}_{iN}) = \frac{1}{2} \nabla_i \left( \prod_{u < v} F_{uv} \right) \quad (56)$$

[see relation (49')]. Using formula (56) for every term in (52), the consequent per-partes integrations lead to

$$(52) = -\frac{1}{2} \int \prod_i di \prod_{u < v} F_{uv} \sum_i \nabla_i \cdot \mathbf{Q}_i \quad (57)$$

The point is that the functions  $\{\tilde{F}_{kl}\}$  in  $\mathbf{Q}_i$  (53) do not depend on coordinate  $\mathbf{r}_i$ , and therefore the nabla operator acts only on coefficients  $\{\mathbf{Q}_i^{(k,l)}\}$ . This is why expression (52) becomes linear in  $\tilde{F}$ -functions. It compensates the linear term in (51) just when

$$\nabla_i \cdot \mathbf{Q}_i^{(k,l)} = 2\mathbf{r}_{kl} \cdot (r_{ki}^2 \mathbf{r}_{ki} - r_{li}^2 \mathbf{r}_{li}) \quad (58)$$

To summarize,  $J_2^{(s)}$ , given by (51), equals to zero provided there exists a three-point vector function  $\mathbf{Q}_i^{(k,l)}$  with properties (54a), (54b) and satisfying conditions (55a), (55b) and (58). One can readily verify on computer that such vector function exists: it is the homogeneous polynomial of the fifth order and its  $x$ -component reads

$$\begin{aligned} [\mathbf{Q}_i^{(k,l)}]_x &= \frac{2}{3}(-2u_x^4 v_x - 2u_x v_x^4 + 2u_x^3 v_x^2 + 2u_x^2 v_x^3 - 2u_x^3 v_y^2 - 2u_x^2 v_y^3 \\ & \quad - u_x v_y^4 - u_y^4 v_x - u_x^3 u_y v_y - u_y v_x^3 v_y - 3u_x v_x^2 v_y^2 - 3u_x^2 u_y^2 v_x \\ & \quad - u_x u_y^3 v_y - u_y v_x v_y^3 + 6u_x u_y^2 v_x^2 + 6u_x^2 v_x v_y^2 - 6u_x u_y^2 v_y^2 \\ & \quad - 6u_y^2 v_x v_y^2 + 8u_x u_y v_y^3 + 8u_y^3 v_x v_y) \end{aligned} \quad (59)$$

where  $\mathbf{u} = \mathbf{r}_k - \mathbf{r}_i$  and  $\mathbf{v} = \mathbf{r}_l - \mathbf{r}_i$ . The  $y$ -component  $[\mathbf{Q}_i^{(k,l)}]_y$  results from (59) under interchange transformation  $u_x \leftrightarrow u_y, v_x \leftrightarrow v_y$ . We conclude that  $J_2^{(s)} = 0$ , confirming relation (32b).

## 6. CONCLUSION

The Fourier transform of (26a) results in

$$\hat{c}(\mathbf{k}) = -\Gamma/k^2 + \hat{c}_0(\mathbf{k}) + \sum_{s=1}^{\infty} \hat{c}_s(\mathbf{k}) \quad (60)$$

With regard to the equalities (32a, b) proved in the previous section, we have

$$\hat{c}_s(\mathbf{k}) = O(k^4) \quad (s = 1, 2, \dots) \quad (61)$$

Using the formula<sup>(25)</sup>

$$\int_0^{\infty} x^{1+2s} K_0^2(x) dx = 2^{(2s-1)} \frac{(s!)^4}{(2s+1)!} \quad (s \geq 0) \quad (62)$$

the contribution of the renormalized Meeron-graph (26b) to the Fourier component of the direct correlation reads

$$\hat{c}_0(\mathbf{k}) = \frac{\Gamma}{8\pi n} - \frac{k^2}{96(\pi n)^2} + O(k^4) \quad (63)$$

Consequently, the expansion of  $\hat{c}(\mathbf{k})$  up to the  $k^2$ -term coincides with the suggested formula (21) and, via the OZ relation, the (rescaled) sixth moment of  $h$  is indeed a finite  $\Gamma$ -truncation

$$n \left( \frac{\pi \Gamma n}{2} \right)^3 \int r^6 h(\mathbf{r}) d\mathbf{r} = \frac{3}{4} (\Gamma - 6)(8 - 3\Gamma) \quad (64)$$

as indicated in (20).

In conclusion, we would like to stress that the derivation of the sixth moment of  $h$  was possible due to the property (61), valid separately for *each* family of direct-correlation diagrams generated from the corresponding, completely renormalized, graph of the Helmholtz free energy. The

higher-order coefficients of the  $\mathbf{k}$ -expansion of  $\hat{c}_s(\mathbf{k})$  ( $s = 1, 2, \dots$ ) we were able to attain do not longer vanish, e.g.,

$$\hat{c}_1(\mathbf{k}) = -\frac{k^4}{(2\pi n)^3} \frac{2}{(4!)^2 5!} \int_0^\infty K_0^3(x) [176x + 108x^3 + 9x^5] dx + O(k^6) \quad (65)$$

where the numerical value of the integral  $\approx 116.68\dots$ . This fact indicates that the eight- and higher-order (appropriately rescaled) moments of  $h$  are probably infinite series in  $\Gamma$ . However, there might exist another mechanism for the exact solvability of higher-order moments as well. We believe that the present method will answer this interesting question.

### APPENDIX A

Here, we derive an algebraic procedure removing a two-coordinated root point, generated by the functional derivation with respect to density at a renormalized  $K$ -bond and interacting quadratically with another root point (generated either at a skeleton more-than-two-coordinated vertex or at a bond), in the representation of the second moment of a  $c_s$ -family (sub-Section 5.2). We consider the uniform regime with constant density  $n$  and translationally + rotationally invariant interactions

$$K(\mathbf{r}_1, \mathbf{r}_2) = \int \exp[i\mathbf{p} \cdot (\mathbf{r}_1 - \mathbf{r}_2)] \hat{K}(\mathbf{p}) \frac{d\mathbf{p}}{2\pi} \quad (A1)$$

$K$  as the function of  $n$  is given by the uniform analogue of functional relation (27),

$$\frac{\partial K(|\mathbf{r}_1 - \mathbf{r}_2|)}{\partial n} = \int K(|\mathbf{r}_1 - \mathbf{r}|) K(|\mathbf{r} - \mathbf{r}_2|) d\mathbf{r} \quad (A2a)$$

or, in the 2d Fourier picture,

$$\frac{\partial \hat{K}(\mathbf{p})}{\partial n} = 2\pi \hat{K}^2(\mathbf{p}) \quad (A2b)$$

Let us first consider the case represented schematically as follows

$$f(\mathbf{u}_1, \mathbf{u}_2) = \begin{array}{c} \mathbf{u}_1 \quad \mathbf{r} \quad \mathbf{u}_2 \\ \text{---} \bullet \text{---} \\ | \\ \text{---} \bullet \text{---} \\ \text{---} \end{array} = \int r^2 K(|\mathbf{u}_1 - \mathbf{r}|) K(|\mathbf{r} - \mathbf{u}_2|) d\mathbf{r} \quad (A3)$$

where  $\mathbf{u}_1$  and  $\mathbf{u}_2$  skeleton vectors define the bond decorated via (27) by the two-coordinated root point  $\mathbf{r}$ , integrated out and interacting via  $r^2$ -interaction with another root point (whose coordination is irrelevant at this stage), put for simplicity at the origin  $\mathbf{0}$ . Using the Fourier representation of  $K$ , (A3) can be rewritten in the form

$$f(\mathbf{u}_1, \mathbf{u}_2) = -\frac{1}{2} \int d\mathbf{r} \int \frac{d\mathbf{p}}{2\pi} \int \frac{d\mathbf{q}}{2\pi} \hat{K}(\mathbf{p}) \hat{K}(\mathbf{q}) \times \{e^{i\mathbf{p} \cdot \mathbf{u}_1} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{u}_2)} \Delta_p [e^{-i\mathbf{p} \cdot \mathbf{r}}] + e^{i\mathbf{p} \cdot (\mathbf{u}_1 - \mathbf{r})} e^{-i\mathbf{q} \cdot \mathbf{u}_2} \Delta_q [e^{i\mathbf{q} \cdot \mathbf{r}}]\} \quad (\text{A4})$$

Integrating twice per partes in (A4) over  $p(q)$  [what can be certainly done for our  $\hat{K}$  (29a) with vanishing boundary contributions] and then integrating over  $\mathbf{r}$ , implying  $\delta(\mathbf{p} - \mathbf{q})$ , we get

$$f(\mathbf{u}_1, \mathbf{u}_2) = - \int d\mathbf{p} \{e^{i\mathbf{p} \cdot (\mathbf{u}_1 - \mathbf{u}_2)} \hat{K}(\mathbf{p}) \Delta \hat{K}(\mathbf{p}) + \frac{1}{2} \hat{K}^2(\mathbf{p}) (e^{-i\mathbf{p} \cdot \mathbf{u}_2} \Delta_p [e^{i\mathbf{p} \cdot \mathbf{u}_1}] + e^{i\mathbf{p} \cdot \mathbf{u}_1} \Delta_p [e^{-i\mathbf{p} \cdot \mathbf{u}_2}]) + \hat{K}(\mathbf{p}) \nabla \hat{K}(\mathbf{p}) \cdot \nabla_p e^{i\mathbf{p} \cdot (\mathbf{u}_1 - \mathbf{u}_2)}\} \quad (\text{A5})$$

Integrating per partes once more the last term in (A5), we finally arrive at

$$f(\mathbf{u}_1, \mathbf{u}_2) = \frac{1}{2} (u_1^2 + u_2^2) \int e^{i\mathbf{p} \cdot (\mathbf{u}_1 - \mathbf{u}_2)} \hat{K}^2(\mathbf{p}) d\mathbf{p} + \int e^{i\mathbf{p} \cdot (\mathbf{u}_1 - \mathbf{u}_2)} |\nabla \hat{K}(\mathbf{p})|^2 d\mathbf{p} \quad (\text{A6})$$

With regard to the “decoration” relation (A2b), (A6) can be written in a more consistent form

$$f(\mathbf{u}_1, \mathbf{u}_2) = \frac{1}{2} (u_1^2 + u_2^2) \frac{\partial K(|\mathbf{u}_1 - \mathbf{u}_2|)}{\partial n} + \Phi(|\mathbf{u}_1 - \mathbf{u}_2|) \quad (\text{A7})$$

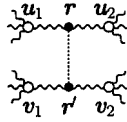
$$\Phi(\mathbf{u}) = \int e^{i\mathbf{p} \cdot \mathbf{u}} |\nabla \hat{K}(\mathbf{p})|^2 d\mathbf{p}$$

This equation admits a trivial generalization

$$\int |\mathbf{r} - \mathbf{u}|^2 K(|\mathbf{u}_1 - \mathbf{r}|) K(|\mathbf{r} - \mathbf{u}_2|) d\mathbf{r} = \frac{1}{2} (|\mathbf{u}_1 - \mathbf{u}|^2 + |\mathbf{u}_2 - \mathbf{u}|^2) \frac{\partial K(|\mathbf{u}_1 - \mathbf{u}_2|)}{\partial n} + \Phi(|\mathbf{u}_1 - \mathbf{u}_2|) \quad (\text{A8})$$



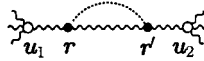
The double application of formula (A8) solves immediately the problem of two root points generated on two different bonds:



The final result reads

$$\begin{aligned}
 & \int |\mathbf{r} - \mathbf{r}'|^2 K(|\mathbf{u}_1 - \mathbf{r}|) K(|\mathbf{r} - \mathbf{u}_2|) K(|\mathbf{v}_1 - \mathbf{r}'|) K(|\mathbf{r}' - \mathbf{v}_2|) d\mathbf{r} d\mathbf{r}' \\
 &= \frac{1}{4} [|\mathbf{u}_1 - \mathbf{v}_1|^2 + |\mathbf{u}_1 - \mathbf{v}_2|^2 + |\mathbf{u}_2 - \mathbf{v}_1|^2 + |\mathbf{u}_2 - \mathbf{v}_2|^2] \\
 & \quad \times \frac{\partial K(|\mathbf{u}_1 - \mathbf{u}_2|)}{\partial n} \frac{\partial K(|\mathbf{v}_1 - \mathbf{v}_2|)}{\partial n} \\
 & \quad + \frac{\partial K(|\mathbf{u}_1 - \mathbf{u}_2|)}{\partial n} \Phi(|\mathbf{v}_1 - \mathbf{v}_2|) + \frac{\partial K(|\mathbf{v}_1 - \mathbf{v}_2|)}{\partial n} \Phi(|\mathbf{u}_1 - \mathbf{u}_2|) \quad (A9)
 \end{aligned}$$

When the two root points are generated on the same bond,



there holds

$$\begin{aligned}
 & \int K(|\mathbf{u}_1 - \mathbf{r}|) |\mathbf{r} - \mathbf{r}'|^2 K(|\mathbf{r} - \mathbf{r}'|) K(|\mathbf{r}' - \mathbf{u}_2|) \\
 &= -2\pi \int e^{i\mathbf{p} \cdot (\mathbf{u}_1 - \mathbf{u}_2)} \hat{K}^2(\mathbf{p}) \Delta \hat{K}(\mathbf{p}) d\mathbf{p} \\
 &\equiv \Psi(|\mathbf{u}_1 - \mathbf{u}_2|) \quad (A10)
 \end{aligned}$$

### APPENDIX B

In this part, we establish the transition from relation (47) to Eq. (48). The origin of bond-dependent  $F$ -factors is irrelevant with the only proviso that the integrals exist.

Let us first consider the integral over infinite 2d space

$$\frac{1}{V} \int |\mathbf{r}_1 - \mathbf{r}_2|^2 f(|\mathbf{r}_1 - \mathbf{r}_2|) d\mathbf{r}_1 d\mathbf{r}_2 = \int r^2 f(\mathbf{r}) d\mathbf{r} \quad (B1)$$

written in the center-of-mass inertia; the supposed translational invariance of function  $f_{12} \equiv f(r_{12})$  is important. The scaling transformation of coordinate  $\mathbf{r} \rightarrow (1 + \lambda)\mathbf{r}$  does not alter the infinite boundary, and hence

$$\int r^2 f(\mathbf{r}) d\mathbf{r} = (1 + \lambda)^4 \int r^2 f[(1 + \lambda)\mathbf{r}] d\mathbf{r} \quad (\text{B2})$$

Expanding  $(1 + \lambda)^4 = 1 + 4\lambda + 6\lambda^2 + O(\lambda^3)$  and

$$f(\mathbf{r} + \lambda\mathbf{r}) = f(\mathbf{r}) + \lambda(\mathbf{r} \cdot \nabla) f + \frac{1}{2}\lambda^2(\mathbf{r} \cdot \nabla)^2 f - \frac{1}{2}\lambda^2(\mathbf{r} \cdot \nabla) f + O(\lambda^3) \quad (\text{B3})$$

in Eq. (B2), the nullity of coefficients to the  $\lambda$  and  $\lambda^2$  powers implies, respectively,

$$0 = \frac{1}{V} \int |1 - 2|^2 [4f_{12} + (\mathbf{R}_{12} f_{12})] d1 d2 \quad (\text{B4a})$$

$$0 = \frac{1}{V} \int |1 - 2|^2 \left[ 6f_{12} + \frac{7}{2}(\mathbf{R}_{12} f_{12}) + \frac{1}{2}(\mathbf{R}_{12}^2 f_{12}) \right] d1 d2 \quad (\text{B4b})$$

where we have adopted the operator notation given in (46). Note that the sum of two zeros  $\{\text{Eq. (B4a)}\}/8 + \{\text{Eq. (B4b)}\}/4$ ,

$$0 = \frac{1}{V} \int |1 - 2|^2 \left[ 2f_{12} + (\mathbf{R}_{12} f_{12}) + \frac{1}{8}(\mathbf{R}_{12}^2 f_{12}) \right] d1 d2 \quad (\text{B5})$$

with substitution  $f_{12} = F_{12}$  corresponds to the rhs of (47) for the simplest  $N = 2$  case.

Let us introduce the functions  $g_{12}$  and  $\bar{g}_{12}$  as follows

$$F_{12} g_{12} = \int d3 \cdots dN \prod_{\substack{u, v=1 \\ (u < v)}}^N F_{uv} \quad (\text{B6})$$

$$F_{12} \bar{g}_{12} = \int d3 \cdots dN \prod_{\substack{u, v=1 \\ (u < v)}}^N F_{uv} \sum_{i=3}^N \left[ \frac{1}{F_{1i}} (\mathbf{R}_{1i} F_{1i}) + \frac{1}{F_{2i}} (\mathbf{R}_{2i} F_{2i}) \right] \quad (\text{B7})$$

Both functions evidently possess the translational-invariance property. The sequence of operations  $\{\text{Eq. (B5) for } f_{12} = F_{12}g_{12}\} - \{\text{Eq. (B4a) for } f_{12} = F_{12}(\mathbf{R}_{12}g_{12})\}/4 + \{\text{Eq. (B4a) for } f_{12} = F_{12}\bar{g}_{12}\}/8$  leads to

$$0 = \frac{1}{V} \int d1 d2 |1-2|^2 \left[ 2F_{12}g_{12} + (\mathbf{R}_{12}F_{12})g_{12} + \frac{1}{8}(\mathbf{R}_{12}^2F_{12})g_{12} + \frac{1}{2}F_{12}\bar{g}_{12} + \frac{1}{8}(\mathbf{R}_{12}F_{12})\bar{g}_{12} + \frac{1}{8}F_{12}(\mathbf{R}_{12}\bar{g}_{12}) - \frac{1}{8}F_{12}(\mathbf{R}_{12}^2g_{12}) \right] \quad (\text{B8})$$

We take advantage of the flexibility in choosing operator  $\mathbf{R}$  (46), and evaluate  $\mathbf{R}_{12}^2g_{12}$  first by applying  $\mathbf{R}_{12} = (\mathbf{r}_1 - \mathbf{r}_2) \cdot \nabla_1$  and then by applying  $\mathbf{R}_{12} = (\mathbf{r}_2 - \mathbf{r}_1) \cdot \nabla_2$ , with the result

$$F_{12}(\mathbf{R}_{12}^2g_{12}) = F_{12}(\mathbf{R}_{12}g_{12}) + F_{12}(\mathbf{R}_{12}\bar{g}_{12}) + \int d3 \dots dN \prod_{u < v} F_{uv} \sum_{i, j=3}^N \frac{1}{F_{1i}F_{2j}} \times \{ [(\mathbf{r}_2 - \mathbf{r}_i) \cdot \nabla_1 F_{1i}] [(\mathbf{r}_1 - \mathbf{r}_j) \cdot \nabla_2 F_{2j}] - (\mathbf{R}_{1i}F_{1i})(\mathbf{R}_{2j}F_{2j}) \} \quad (\text{B9})$$

The substitution of (B9) into (B8) gives

$$0 = \frac{1}{V} \int \prod_i di \prod_{u < v} F_{uv} |1-2|^2 \left\{ 2 + \frac{1}{F_{12}} (\mathbf{R}_{12}F_{12}) + \frac{1}{8F_{12}} (\mathbf{R}_{12}^2F_{12}) + \frac{1}{2} \sum_{i=3}^N \left[ \frac{1}{F_{1i}} (\mathbf{R}_{1i}F_{1i}) + \frac{1}{F_{2i}} (\mathbf{R}_{2i}F_{2i}) \right] + \frac{1}{8} \frac{1}{F_{12}} (\mathbf{R}_{12}F_{12}) \sum_{i=3}^N \left[ \frac{1}{F_{1i}} (\mathbf{R}_{1i}F_{1i}) + \frac{1}{F_{2i}} (\mathbf{R}_{2i}F_{2i}) \right] + \frac{1}{8} \sum_{i, j=3}^N \frac{1}{F_{1i}F_{2j}} (\mathbf{R}_{1i}F_{1i})(\mathbf{R}_{2j}F_{2j}) - \frac{1}{16} \sum_{i=3}^N \left[ \frac{1}{F_{1i}} (\mathbf{r}_1 - \mathbf{r}_2) \cdot \nabla_1 F_{1i} + \frac{1}{F_{2i}} (\mathbf{r}_2 - \mathbf{r}_1) \cdot \nabla_2 F_{2i} \right] - \frac{1}{8} \sum_{i, j=3}^N \frac{1}{F_{1i}F_{2j}} [(\mathbf{r}_2 - \mathbf{r}_i) \cdot \nabla_1 F_{1i}] [(\mathbf{r}_1 - \mathbf{r}_j) \cdot \nabla_2 F_{2j}] \right\} \quad (\text{B10})$$

Combining Eq.(B10) for each pair of skeleton vertices with Eq. (47), the latter reduces to relation (48).

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