Fermion hypernetted chain equations for the three-body distribution

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The fermion hypernetted chain equations for the three-body distribution function are derived in this paper. These equations are relatively complicated and some care is required for their derivation. The formulas are presented explicitly and an outline for their practical implementation discussed.

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I. INTRODUCTION

The fermion hypernetted chain (FHNC) equations were originally derived[1,2] for the study of uniform-density, nuclear matter. However, the formalism is just as easily applied to other many-fermion systems such as the electron gas,[3,4] and the equations can be further generalized for nonuniform systems.[5,6] The starting point for the formalism is the assumption of a many-fermion wave function in the form of a Slater determinant of one-fermion orbital functions times a correlation factor of the Jastrow form.[7–9] Optimization of this wave function is associated with the evaluation of the expectation value of the Hamiltonian and this is where the FHNC equations come in.

If the fermions interact in a pairwise fashion—the typical case—and only one- and two-body correlations are included in the Jastrow factor, one formulation expresses this expectation value in terms of the one-, two-, and three-body distribution functions.[10] The FHNC equations have been derived to evaluate the one- and two-body distribution functions from the assumed form for the many-fermion wave function. To evaluate the expectation value of the Hamiltonian, an approximation is normally introduced for the three-body distribution. The superposition approximation,[11] for instance, is a common choice. This allows the three-body distribution to be evaluated directly from the solutions of the two-body equations. A similar approach is taken in the solution of the classical HNC (hypernetted chain) equations. Within this formulation, then, it would be advantageous to have an exact formalism for the three-body distribution in order to investigate corrections to such approximations.

An alternate formulation eliminates the need for a three-body distribution by effecting a transformation of the kinetic energy that leads to the so-called Jackson-Feenberg[12] form for the energy. In place of the three-body distribution, there is a term which contains the off-diagonal elements of a one-body function. The Jackson-Feenberg form is clearly superior for the homogeneous system, since this one-body quantity can be evaluated directly from the solutions of the two-body FHNC equations.[13] The inhomogeneous system is more complex and many of the approximations possible for the homogeneous system no longer apply. It seems reasonable to suppose that such a direct evaluation of the one-body quantity is still possible, but the derivation of the appropriate relationships does not seem to have been investigated yet. Nevertheless, the three-body distribution need not be considered for the evaluation of the expectation value of the hamiltonian in a homogeneous many-fermion system and could potentially be unnecessary for the inhomogeneous system as well.

Where the three-body distribution would be important is in the study of many-fermion systems when three-body correlations are included in the Jastrow factor. The inclusion of three-body correlations appears to be important for certain systems, such as liquid helium.[15] A significant effort to introduce these correlations was made by Krotscheck and Saarela[14] and a call for the derivation of the three-body FHNC equations was made in that paper. It is the goal of this paper to present such a derivation.

An analogous derivation has been presented for the classical HNC equations by Wertheim[16] and much of that development can be tailored for the many-fermion system considered here. However, there are some important distinctions associated with the exchange structure of the corresponding diagrams in the FHNC case and some extra care is required in performing the necessary topological analysis. Further, the development of Wertheim ignored the contribution of what are known as elementary diagrams. Incorporation of these quantities requires some additional analysis.

II. SOME DEFINITIONS AND THE TWO-BODY FHNC EQUATIONS

It is useful to begin by summarizing the two-body equations. They will not be derived, but the quantities and concepts involved will be presented and the notation used will be carefully defined. This will provide a convenient base from which the three-body equations can be derived. It is of interest to present the equations that apply to an inhomogeneous system and not specialize to the more commonly treated homogeneous system. For that reason, the equations will correspond more closely with the formalism of Ripka,[5] who specifically treated this case. The interested reader may consult that reference for more details.

Unfortunately, Ripka[5] employed a set of notation that differs from that commonly used in the literature. The treatise of Clark[17] presents an alternative set of notation that seems to have become the *de facto* standard and the equations will be presented here with that notation. It should be noted, however, that Clark's work focuses on the homogeneous system and so, some minor changes are needed in the definitions when extending the notation to the inhomogeneous system.

The system of interest consists of a very large number of identical fermions interacting by a pairwise additive force

law and subject to an externally applied one-body potential. The number of fermions is assumed to be large enough that extending the system to infinite size would still provide a reasonable approximation for the system of interest. As an example, the electrons in a solid-state system of macroscopic size would fall into this category. It should be emphasized that the external potential is not assumed here to be uniform.

The coordinates of a single fermion consist of a set of three spatial coordinates plus a spin coordinate. These four coordinates will be collected under the single symbol x. A subscript will be used to distinguish between the coordinates of different fermions. The wave function for the system will be assumed to be the product

$$\Psi = DF, \tag{1}$$

where D is a Slater determinant of orthonormal one-fermion orbitals $\{\phi_j(x)\}$ and F is a correlation factor of the form

$$F = \exp\left\{ \frac{1}{2} \sum_j u^{(1)}(x_j) + \frac{1}{2} \sum_{j<k} u^{(2)}(x_j, x_k) + \cdots \right\}. \tag{2}$$

The sums in the exponent are over all fermions in the system and the functions are referred to as correlation potentials, $u^{(1)}(x)$ is the one-body correlation potential, $u^{(2)}(x,x')$ is the two-body correlation potential, and so on. By specifying the set of occupied orbitals and the correlation potentials, the wave function for the system is fully determined.

The focus of interest is the one-, two-, and three-body distribution functions, defined here as follows:

$$\rho(x) \equiv \Gamma^{(1)}(x) = \int \Psi^\dagger \left\{ \sum_j \delta(x - x_j) \right\} \Psi \, d\tau,$$

$$\Gamma^{(2)}(x,x') = \int \Psi^\dagger \left\{ \sum_{j,k} \delta(x - x_j)\, \delta(x' - x_k) \right\} \Psi \, d\tau, \tag{3}$$

$$\Gamma^{(3)}(x,x',x'') = \int \Psi^\dagger \left\{ \sum_{j,k,l} \delta(x - x_j)\, \delta(x' - x_k) \times \delta(x'' - x_l) \right\} \Psi \, d\tau.$$

The integrations are over all fermion coordinates and each Dirac delta function is applied to all four single-particle coordinates simultaneously. The special notation for the one-body distribution function $\rho(x)$ is customary. If the many-fermion wave function is given simply by a Slater determinant of orthonormal orbitals, evaluation of the distribution functions is straightforward. When the correlation factor is added, however, the expressions become much more complicated and it is necessary to derive alternate means of evaluating them.

The standard approach, at this point, is to expand the two-body portion of the correlation factor to obtain cluster expansions[18–21] for the distribution functions. The terms of the expansion can be more easily organized if they are represented by diagrams. It is this diagrammatic expansion that is used to derive the FHNC equations.

It is important to be clear on certain features of these diagrams and so, they will be described in some detail. A given diagram consists of a number of points and connections between them. Each point has a set of fermion coordinates associated with it and there are two basic types, depending on how the coordinates are used. Internal points have their coordinates integrated over and the external points do not. As a result, the diagram represents a function only of the coordinates of the external points and the number of external points can serve as an initial categorization. One-body diagrams contain one external point, two-body diagrams contain two external points, and so on. As might be surmized, the one-body distribution function can be expressed solely in terms of one-body diagrams, the two-body distribution function can be expressed solely in terms of one- and two-body diagrams, and so on.

Connections between points represent both exchange interactions and correlation interactions. The two-body FHNC equations derived in the literature[1,2] started from a formalism in which only two-body correlations were taken into account. If three-body correlations are to be included, some modification of the traditional formalism is required. Fortunately, this modification is more of a technical issue than a fundamental one. The FHNC equations are derived based on a topological analysis of the diagrams. This topological analysis is valid whether the diagrams contain elements representing three-body correlations or not. Introducing three-body correlations will leave the overall equations unchanged, but will change only some of the specifics regarding their ingredients. The associated three-point diagrammatic elements can be simply superimposed on the diagrams of the traditional cluster expansion and will have no effect on the basic nature of the diagrams themselves. So, in order to avoid the complications associated with adding further diagrammatic elements, the following develop will assume only one- and two-body correlations. This will allow the important points regarding the behavior of the diagrams to be made. Some comments on the modifications associated with adding three-body correlations will be made at the end of this section.

Hence, connections occur between pairs of points and there are two basic types. The first type is called an h-direct line and represents a factor of

$$h(x_1, x_2) = e^{u^{(2)}(x_1,x_2)} - 1, \tag{4}$$

where the sets of coordinates are those of the points being connected. This designation (as opposed to just calling it a direct line) is intended to distinguish this type of line from the direct-type line that will arise in the three-body diagrams. The second type is called a σ-exchange line, the function for which will be labeled $\sigma(x_1,x_2)$. This is, in general, a relatively complex function, but can be simplified with a specific choice for the one-body correlation potential. This will be described in more detail later. The σ-exchange line is a directed function, so that the order of the arguments is meaningful. It is possible to refer to a σ-exchange line coming into or out of a point. As with the h-direct lines, this designation is designed to distinguish it from the exchange-type lines that will arise in the three-body diagrams.

The diagrams appearing in the expansions can be generated by brute force and a topological analysis leads to a formalism in which only certain types of diagrams are dealt with directly. In particular, the various distribution functions are separated into quantities in which all the diagrams are linked and irreducible. These terms will now be defined.

A linked diagram is one in which all the points are linked to each other. Put another way, a linked diagram is one where it is always possible to travel, by way of h-direct and σ-exchange lines, from any one point in the diagram to any other. As it turns out, the one-body distribution function $\rho(x)$ is expanded solely in terms of linked, one-body diagrams. The two-body distribution contains unlinked contributions, but can be decomposed as

$$\Gamma^{(2)}(x_1,x_2)=\rho(x_1)\rho(x_2)+\Gamma_l^{(2)}(x_1,x_2), \tag{5}$$

where $\Gamma_l^{(2)}(x_1,x_2)$ contains only linked two-body diagrams. For reference purposes, $\Gamma_l^{(2)}(x_1,x_2)$ will be called the linked two-body distribution function. Likewise, the three-body distribution function is decomposed as

$$\begin{aligned}\Gamma^{(3)}(x_1,x_2,x_3)=&\rho(x_1)\rho(x_2)\rho(x_3)+\rho(x_1)\Gamma_l^{(2)}(x_2,x_3)\\&+\rho(x_2)\Gamma_l^{(2)}(x_1,x_3)+\rho(x_3)\Gamma_l^{(2)}(x_1,x_2)\\&+\Gamma_l^{(3)}(x_1,x_2,x_3),\end{aligned} \tag{6}$$

where $\Gamma_l^{(3)}(x_1,x_2,x_3)$ contains only linked three-body diagrams and will be called the linked three-body distribution function.

Irreducible diagrams are associated with what are known as articulation points. An articulation point is one whose removal from the diagram would cause it to be separated into two or more unconnected parts, at least one of which contains only internal points. If the separated parts of the diagram all contain at least one external point, this is not considered an articulation point. An irreducible diagram is one that does not contain any articulation points. There may still be points in an irreducible diagram whose removal would separate it into more than one part, but each part contains at least one external point. When such points occur in an irreducible diagram, they will be referred to as cutting points, using the nomenclature of Stell.[22] If an irreducible diagram does not have any cutting points, it will be referred to as fully irreducible.

With these definitions in place, it is now possible to state the rules governing the generation of the diagrammatic expansions for the distribution functions. It is important to realize that these rules are associated with the diagrammatic development of Ripka,[5] who tailored the rules towards the general inhomogeneous system. At issue is the fact that, in the traditional cluster expansion, diagrams with articulation points automatically cancel each other for homogeneous system but not for inhomogeneous systems. With Ripka's modified development, diagrams with articulation points can be eliminated for the inhomogeneous system as well. The linked, N-body distribution function is equal to the sum of all topologically distinct, linked, and irreducible N-body diagrams such that (a) each internal point has at least one h-direct line connected to it, (b) at most one h-direct line connects a give pair of points, and (c) if a point has a σ-exchange line coming into it, a σ-exchange line must also exit from it; there may be no more than one σ-exchange line coming into a point.

It is also useful to list the rules for converting the diagrams into quantities which can be evaluated.

(a) Give each external point a label corresponding to one of the arguments of the linked distribution function.

(b) Label each internal point.

(c) Introduce a factor of $h(x_j,x_k)$ for an h-direct line between points j and k. These points may be internal or external points.

(d) Introduce a factor of $\sigma(x_j,x_k)$ for a σ-exchange line from point k to point j.

(e) Introduce a factor of $\rho(x_j)$ if point j is connected to the rest of the diagram only with h-direct lines.

(f) Multiply by $(-)^{(n_\rho+n_L)}/S$, where n_ρ equals the total number of σ-exchange lines, n_L equals the number of closed σ-exchange line loops, and S is a symmetry number equal to the number of permutation operations that leave the topology of the connections unchanged.

(g) Integrate over all sets of internal coordinates.

In deriving the two-body FHNC equations, it turns out to be necessary to introduce a set of diagram elements that are not proper diagrams according to the rules above. Specifically, these elements have only one σ-exchange line connected to each of the external points. Otherwise, they satisfy all the rules. These diagrams will be referred to as *exchange line diagrams*.

The FHNC equations are obtained by considering the ways in which subdiagrams may be connected to each other. This requires some care in the treatment of external points. Two subdiagrams are connected by fusing external points from one to the other. What were originally two points become one, and it is important not to overcount the factors of the density that may appear due to rule *e* above. For this reason, subdiagrams will be represented without the external points explicitly shown. When the subdiagrams are connected and the fused external points become one, then the appropriate rules are applied to the fused point. When a diagram needs to be evaluated fully, as with the evaluation of the two-body distribution function, the external points will be shown explicitly, in which case the appropriate factors of $\rho(x)$ are added for the external points as well.

It is as a result of this issue that the notation of Clark must be slightly modified. For the homogeneous system, these factors of the density can be eliminated through a suitable redefinition of the diagrammatic elements, since the density is everywhere the same. This cannot be done with the inhomogeneous system, so the quantities appearing in Clark's review must be appropriately modified here.

Under this formulation, the one-body distribution function is equal to a single diagram consisting of just the external point; any other one-body diagram would not be irreducible. On the other hand, the linked, two-body distribution is equal to an infinite sum of two-body diagrams. These two-body diagrams are conveniently classified by how they connect to the external points. The connection can be with only h-direct

lines or, in addition to any *h*-direct lines, there may be two σ-exchange lines, one coming into the external point and one leaving. The sum of two-body diagrams of a particular type will be given a symbol, say *A*. Such a sum will not have the external points explicitly evaluated, and so factors of the density must be introduced later, if needed. Two subscripts will be given to represent the types of connections to the external points. A subscript "*d*" indicates a connection by only *h*-direct lines and a subscript "*e*" indicates that two σ-exchange lines connect to that external point. An "*e*" point may or may not have *h*-direct lines connected to it. There are four possible combinations of connections and the four sums are arranged in a 2×2 matrix

$$\underset{\sim}{A}(x_1,x_2)=\begin{pmatrix} A_{dd}(x_1,x_2) & A_{de}(x_1,x_2) \\ A_{ed}(x_1,x_2) & A_{ee}(x_1,x_2) \end{pmatrix}. \tag{7}$$

The first subscript indicates the type of connection at x_1 and the second at x_2. It may be noted that the quantities A_{de} and A_{ed} are rarely distinguished in the literature; they are generally equal to each other. However, the matrices formed above make subsequent analysis much easier and so this distinction will be made here. Further, it may be possible to formulate a special case of the theory in which these quantities actually differ, and it would be useful to have the more general form described here.

The sum of all two-body diagrams is given the symbol Γ and the four combinations of connections are collected in the matrix $\underset{\sim}{\Gamma}$. The sums of just those diagrams that do not contain any cutting points are given in the matrix $\underset{\sim}{X}(x_1,x_2)$. These are referred to as *non-nodal diagrams*. The sums of all the diagrams that contain at least one cutting point, the so-called nodal diagrams, are given in $\underset{\sim}{N}(x_1,x_2)$. It should be obvious that

$$\underset{\sim}{N}(x_1,x_2)+\underset{\sim}{X}(x_1,x_2)=\underset{\sim}{\Gamma}(x_1,x_2). \tag{8}$$

A further type of diagram is the composite diagram. Such diagrams can be decomposed as two or more two-body subdiagrams connected to each other only at the two external points. The sums of all diagrams that are not composite are given in $\underset{\sim}{S}(x_1,x_2)$. Diagrams that are not composite and which further contain no cutting points are referred to as elementary diagrams. The simplest two-body elementary diagrams is just the *h*-direct line and is evaluated as $h(x_1,x_2)$. The sums of all *other* elementary diagrams are given in $\underset{\sim}{E}(x_1,x_2)$.

The sum of all two-body exchange line diagrams is represented by $\Gamma_{cc}(x_1,x_2)$. It is also possible to distinguish those diagrams that do not have any cutting points, the sum of which is represented by $X_{cc}(x_1,x_2)$. The sum of all other diagrams is represented by $N_{cc}(x_1,x_2)$. In analogy with Eq. (8),

$$N_{cc}(x_1,x_2)+X_{cc}(x_1,x_2)=\Gamma_{cc}(x_1,x_2). \tag{9}$$

The sum of noncomposite exchange line diagrams is represented by $S_{cc}(x_1,x_2)$ and the sum of elementary exchange line diagrams is represented by $E_{cc}(x_1,x_2)$.

Now that these definitions have all been made, it is possible to state the two-body FHNC equations.

$$\underset{\sim}{N}(x_1,x_2)=\int \underset{\sim}{X}(x_1,x_3)\underset{\sim}{J}^d(x_3)\{\underset{\sim}{X}(x_3,x_2)+\underset{\sim}{N}(x_3,x_2)\}dx_3, \tag{10}$$

$$\begin{aligned} N_{cc}(x_1,x_2)=&-\int \sigma(x_1,x_3)N_{cc}(x_3,x_2)dx_3-\int N_{cc}(x_1,x_3) \\ &\times[N_{cc}(x_3,x_2)+X_{cc}(x_3,x_2)+\sigma(x_3,x_2)]dx_3 \\ &+\int \sigma(x_1,x_3)X_{cc}(x_3,x_4)[N_{cc}(x_4,x_2) \\ &+X_{cc}(x_4,x_2)+\sigma(x_4,x_2)]dx_3dx_4, \end{aligned} \tag{11}$$

$$X_{dd}(x_1,x_2)=g_B(x_1,x_2)-N_{dd}(x_1,x_2)-1, \tag{12}$$

$$\begin{aligned} X_{de}(x_1,x_2)=&\{E_{de}(x_1,x_2)+N_{de}(x_1,x_2)\}g_B(x_1,x_2) \\ &-N_{de}(x_1,x_2), \end{aligned} \tag{13}$$

$$\begin{aligned} X_{ed}(x_1,x_2)=&\{E_{ed}(x,x_2)+N_{ed}(x_1,x_2)\}g_B(x_1,x_2) \\ &-N_{ed}(x_1,x_2), \end{aligned} \tag{14}$$

$$\begin{aligned} X_{ee}(x_1,x_2)=&\{E_{ee}(x_1,x_2)+N_{ee}(x_1,x_2)+[E_{de}(x_1,x_2) \\ &+N_{de}(x_1,x_2)][E_{ed}(x_1,x_2)+N_{ed}(x_1,x_2)] \\ &-[E_{cc}(x_1,x_2)+N_{cc}(x_1,x_2)+\sigma(x_1,x_2)] \\ &\times[E_{cc}(x_2,x_1)+N_{cc}(x_2,x_1)+\sigma(x_2,x_1)]\} \\ &\times g_B(x_1,x_2)-N_{ee}(x_1,x_2), \end{aligned} \tag{15}$$

$$\begin{aligned} X_{cc}(x_1,x_2)=&\{E_{cc}(x_1,x_2)+N_{cc}(x_1,x_2) \\ &+\sigma(x_1,x_2)\}g_B(x_1,x_2)-N_{cc}(x_1,x_2) \\ &-\sigma(x_1,x_2), \end{aligned} \tag{16}$$

where

$$g_B(x_1,x_2)=[1+h(x_1,x_2)]\exp[E_{dd}(x_1,x_2)+N_{dd}(x_1,x_2)] \tag{17}$$

and

$$\underset{\sim}{J}^d(x)=\begin{pmatrix} \rho(x) & 1 \\ 1 & 0 \end{pmatrix}. \tag{18}$$

Equations (10)–(16) are ten in number and can be used to solve for the ten quantities $\underset{\sim}{N}(x_1,x_2)$, $\underset{\sim}{X}(x_1,x_2)$, $N_{cc}(x_1,x_2)$, and $X_{cc}(x_1,x_2)$. This would require the input of the quantities $\underset{\sim}{E}(x_1,x_2)$, $E_{cc}(x_1,x_2)$, $\sigma(x_1,x_2)$, and $h(x_1,x_2)$.

The quantity $h(x_1,x_2)$ is known if it is assumed that the two-body correlation potential has been given. Even if the two-body correlation potential is being sought, it may initially be guessed in order to solve the FHNC equations and then iteratively optimized. The quantity $\sigma(x_1,x_2)$ depends

on the choice of the one-body correlation potential (as well as the one-fermion orbital functions). A convenient choice that is commonly made is

$$u^{(1)}(x) = -\int [N_{dd}(x,x')\rho(x') + N_{de}(x,x')]dx'. \quad (19)$$

When this is done,

$$\sigma(x_1,x_2) = \sum_j \phi_j^\dagger(x_1)\phi_j(x_2) \quad (20)$$

is just the one-body density matrix for the Slater determinant wave function alone. For the uniform system, Eq. (19) reduces to zero, which corresponds to the optimum choice in this case. For the inhomogeneous system, the optimum choice for the correlation potential is a more complicated matter[6] and Eq. (19) is not correct. Its use would be justified only as a matter of convenience. An accurate treatment of the inhomogeneous system would have to go beyond this simple choice and a specific procedure to do this has been presented in the literature.[6] The one-body distribution function can be shown to be equal to

$$\rho(x) = \sigma(x,x) - N_{cc}(x,x) - \int N_{cc}(x,x')\Gamma_{cc}(x',x)dx'. \quad (21)$$

The sums of elementary diagrams must be approximated. Generally, some truncations of the sums are assumed and the quantities evaluated. A common choice is the FHNC/0 approximation, in which these sums are all set equal to zero. Other truncations have also been tried in the literature.[23]

All the necessary equations have now been presented to determine the one- and two-body distribution functions, assuming that the one-fermion orbital functions and the correlation potentials have been given. The FHNC equations can be solved iteratively, and the solution can be used in Eq. (21) to evaluate the one-body distribution function. The two-body distribution function is then given by

$$\begin{aligned}\Gamma^{(2)}(x_1,x_2) &= \rho(x_1)\rho(x_2) + \rho(x_1)\Gamma_{dd}(x_1,x_2)\rho(x_2) \\ &\quad + \rho(x_1)\Gamma_{de}(x_1,x_2) + \Gamma_{ed}(x_1,x_2)\rho(x_2) \\ &\quad + \Gamma_{ee}(x_1,x_2) \\ &= \mathbf{R}^T(x_1)\underset{\sim}{G}(x_1,x_2)\mathbf{R}(x_2), \end{aligned} \quad (22)$$

where two new quantities have been introduced:

$$\mathbf{R}(x) = \begin{pmatrix} \rho(x) \\ 1 \end{pmatrix} \quad (23)$$

and

$$\underset{\sim}{G}(x_1,x_2) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \underset{\sim}{\Gamma}(x_1,x_2). \quad (24)$$

The foregoing development only considered one- and two-body correlations. However, the equations will be unchanged if the three-body correlation potential is introduced, the modification being solely in the specification of the elementary diagrams. The FHNC equations generate a cluster expansion by constructing all possible nodal and composite connections of two-body diagrams, starting from a single *h*-direct line plus the set of elementary diagrams chosen for the calculation. It is necessary only to include elementary diagrams that have three-point elements representing the three-body correlations to get the full expansion with three-body correlations.

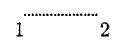
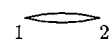
III. THE THREE-BODY DISTRIBUTION FUNCTION

The three-body FHNC equations can be derived in the same way as the two-body equations, but of course, the analysis is considerably more complicated. To simplify the procedure, the solution of the two-body equations can be incorporated into the equations. Instead of the basic *h*-direct lines and σ-exchange lines encountered in the previous section, Γ-direct lines, and Γ_{cc}-exchange lines will take their place. These line elements represent infinite sums of subdiagrams connecting two points of a larger diagram. This section lays the groundwork for the formalism by deriving an expression for the three-body distribution that can be used for the subsequent diagrammatic analysis. The three-body FHNC equations will be derived in the next section.

It is necessary to introduce some pictorial representations of the diagrammatic elements. Internal points will be represented by solid circles and external points will be represented by open circles. When an external point is included in a diagram, it is assumed that there is a factor of the density $\rho(x)$ if all the connections to that point are only with *h*-direct lines. This explicit inclusion of factors of the density can become a problem when diagrams are joined together. For instance, if an external point of one diagram with only direct connections is joined to another at an external point containing exchange line connections, the first diagram will carry along with it an extra, unnecessary factor of the density at that point. To avoid this situation, diagrams will be constructed in which the open circle external points are not shown explicitly. This implies that factors of the density, if ultimately needed, are not yet included at those points. When diagrams are joined together, an internal or external point will be generated and any needed factors of the density will be implicitly incorporated.

Consider a diagram which contains a two-body connection between two particular points. It is possible to construct an infinite set of diagrams which differ from this one only in the portion between the two particular points. The sum of all such diagrams then corresponds to adding all possible two-body connections between those points, which therefore results in a factor involving the components of $\underset{\sim}{\Gamma}(x_i,x_j)$ between the points. It is desirable to perform all such summations of diagrams implicitly and view all two-body connections as consisting of factors of $\Gamma_{\mu\nu}(x_i,x_j)$ rather than the more basic elements $h(x_i,x_j)$ and $\sigma(x_i,x_j)$. Another type of two-point connection can be constructed by considering a diagram in which an exchange line extends from one point to another. By summing all diagrams which differ only in the intermediate points and connections between them, the resulting diagram will have a contribution of

TABLE I. Two-point diagrams appearing in the three-body FHNC equations.

	appropriate sum of two-body terms, $\underset{\sim}{\Gamma}(x_1,x_2)$
	unity plus the appropriate sum of two-body terms
	the sum of two-point exchange line diagrams, $\Gamma_{cc}(x_1,x_2)$
	the sum of non-composite two-point exchange line diagrams, $S_{cc}(x_1,x_2)$

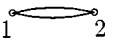
$\Gamma_{cc}(x,x')$ between the two points.

Diagrams are therefore to be constructed in which all two-point connections are of one of these two forms. It is necessary to define diagram elements to represent these connections and these are given in Table I. A dotted line represents a factor of the form $\Gamma_{\mu\nu}(x,x')$ and will be referred to as a Γ-direct line. Because it comes up fairly often, it is convenient to have another diagrammatic element that represents a factor of $G_{\mu\nu}(x,x')$. This is given by a double solid line between the points and will be referred to as a *G*-direct line. This is simply equal to a Γ-direct line plus a diagram with no connection between those points. Another two-point element is a directed solid line. This represents a factor of $\Gamma_{cc}(x,x')$ and will be referred to as an Γ_{cc}-exchange line. The final element in the table $S_{cc}(x_1,x_2)$ will not arise until the next section and so will be described there. There will also be components of the diagrams which connect three points to each other and these are distinct from the two-body connections. They are referred to as three-body connections and will be defined later.

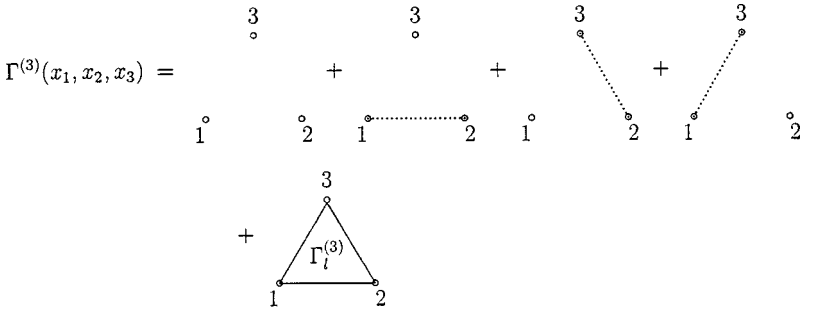
As a simple example, the two-body distribution function can be represented diagrammatically as

$\Gamma^{(2)}(x_1,x_2) =$  (25)

or, more concisely, as

$\Gamma^{(2)}(x_1,x_2) =$  (26)

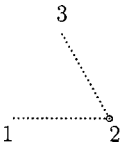
The three-body distribution function is given by

$\Gamma^{(3)}(x_1,x_2,x_3) =$  (27)

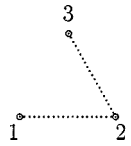
where the last term represents the linked, three-body distribution function.

In the diagrammatic development for the two-body FHNC equations,[5] the types of connections to the external points are made explicit. This can be done for the three-body equations as well, but the expressions can get cluttered when this is done. For this reason, the types of connections at the end points of subdiagrams will not usually be specified. When two diagrams are connected at a point, however, all allowed connections at that point are to be summed over. From the rules for constructing the basic diagrams, the ways in which two subdiagrams can be connected at a point are limited. At most, two exchange lines can connect to a point, so two *e*-type connections cannot be made to the same point. For instance, the combination $\Gamma_{de}(x,x')\Gamma_{ee}(x',x'')$ is not allowed. Further, from the way the two-body diagrams were constructed, a factor of the density must be added if only *d*-type connections are made to a point. For instance, a combination like $\Gamma_{dd}(x,x')\rho(x')\Gamma_{de}(x',x'')$ might be encountered and would require the intermediate factor of $\rho(x')$.

These restrictions are conveniently handled with the matrix $\underset{\sim}{J}^d(x)$ defined in Eq. (18). For example, consider the three-body diagram where two Γ-direct connections are made from external points 1 and 3 to the intermediate point 2. Including only the connecting point explicitly, the three-body diagram is evaluated as

 $= \underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)$ (28)

The result is in the form of a 2×2 matrix, indicating all the possible ways the connections can be made to the end points x_1 and x_3. If the other two external points are included explicitly in the diagram, all allowed connections to these points must be added in evaluating the diagram. This is readily achieved by using the vector $\mathbf{R}(x)$ defined in Eq. (23). Thus,



$$= \mathbf{R}^T(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\mathbf{R}(x_3) \tag{29}$$

A useful reduction can be made for expressions such as this. For an arbitrary 2×2 matrix $\underset{\sim}{A}$,

$$\mathbf{R^T}(x_1)\underset{\sim}{A}\mathbf{R}(x_2) = \mathrm{Tr}\left[\underset{\sim}{A}\begin{pmatrix}\rho(x_1)\rho(x_2) & \rho(x_2)\\ \rho(x_1) & 0\end{pmatrix}\right]$$

$$= \mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{A}\underset{\sim}{J}^d(x_2)\underset{\sim}{J}^e], \tag{30}$$

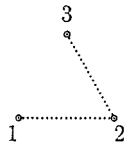
where

$$\underset{\sim}{J}^e = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}. \tag{31}$$

It can also be shown that

$$\rho(x_1)\mathbf{R^T}(x_2)\underset{\sim}{A}\mathbf{R}(x_3) = \mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{J}^e\underset{\sim}{J}^d(x_2)\underset{\sim}{A}\underset{\sim}{J}^d(x_3)\underset{\sim}{J}^e]. \tag{32}$$

Equation (29) can be rewritten as

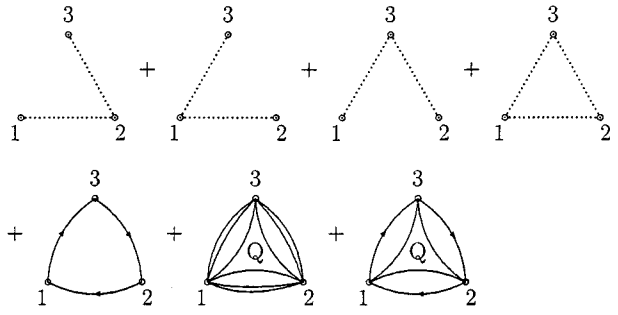


$$= \mathrm{Tr}\left[\underset{\sim}{J}^d(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\underset{\sim}{J}^d(x_3)\underset{\sim}{J}^e\right] \tag{33}$$

The rules for constructing and evaluating diagrams need only minor changes from those given in the previous section. For constructing all acceptable diagrams, all the rules remain with h-direct lines replaced by Γ-direct lines and σ-exchange lines replaced by Γ_{cc}-exchange lines. In addition, two points can be directly connected only through a single Γ-direct or Γ_{cc}-exchange line. In evaluating the diagrams, the same replacement of lines must be made. In addition, all allowed connections of diagrammatic elements at a point must be added.

Consider, now, the three-body distribution function. Once the two-body equations are solved, only the linked part is undetermined. Hence, focus attention on the linked three-body distribution function for now. It is possible to break this function up into several types of terms, depending on how the external points are connected to each other. It is first possible to separate out terms in which the external points are connected to each other only through two-point connections. The first type of diagram is one in which one point has two-point connections with each of the other points and that is all. The common point may be any one of the three so that there are three different diagrams of this type. The next type of diagram is where all three points are directly connected to each other. This is readily achieved with Γ-direct lines, but it can also be achieved with Γ_{cc}-exchange lines. The remaining terms must have true three-body connections between the external points. If there are two-point connections between external points, these portions can be extracted from the diagrams. Specifically, there can be no direct connections between any two points, a Γ-direct connection can exist between pairs of points, or all the points can be connected by Γ_{cc}-exchange line connections. Diagrammatically, the linked, three-body distribution function is given by

$\Gamma_l^{(3)}(x_1,x_2,x_3) =$

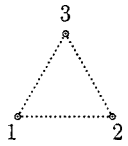


(34)

where the triangular element designated by Q represents the sum of all three-body terms that contain no direct two-point connections between any external points.

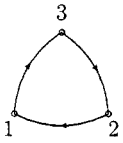
Interestingly, an algebraic expression can be extracted from this that is relatively simple. Start with the first three terms of Eq. (34). The first term has already been considered and is evaluated in Eq. (29). The other two differ only in the identity of the intermediate point and are evaluated in a similar way.

The fourth diagram of Eq. (34) is a bit more complicated in that the two-point chain closes in on itself. Adding all allowed connections at the external points, it can be reduced to the trace



$$= \mathrm{Tr}\left[\underset{\sim}{J}^d(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\underset{\sim}{J}^d(x_3)\underset{\sim}{\Gamma}(x_3,x_1)\right] \tag{35}$$

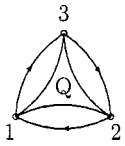
The fifth diagram is easily worked out as



$$= \Gamma_{cc}(x_1,x_2)\Gamma_{cc}(x_2,x_3)\Gamma_{cc}(x_3,x_1) \tag{36}$$

For the final diagrams, it should be noted that the three-point portions labeled by Q depend on how they connect to the external points, either with exchange lines or just direct lines. As with the two-point diagrams, these diagrams can be labeled with three indices that indicate the types of connections. Thus, $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ represents the sum of three-point diagrams where the connections to (x_1,x_2,x_3) are of the types $(\lambda\mu\nu)$, each index being either d or e. Depending on the specific indices for a given term, there will be restrictions on the allowed two-point diagrams between the external points.

For the very last term of Eq. (34), the connections of the three-point portion can only be with direct lines, so that this becomes



$$= Q^{ddd}(x_1,x_2,x_3)\Gamma_{cc}(x_1,x_2)\Gamma_{cc}(x_2,x_3)\Gamma_{cc}(x_3,x_1) \tag{37}$$

For the remaining term, there will be contributions from each possible set of indices for $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ and each will be considered in turn. Label each composite term by $T^{\lambda\mu\nu}(x_1,x_2,x_3)$, the superscripts corresponding to the superscripts that appear on $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$. With all direct connections for the three-point portion, adding all the possible two-point connections between external points leads to

$$\begin{aligned}
T^{ddd}(x_1,x_2,x_3) &= Q^{ddd}(x_1,x_2,x_3)\{\rho(x_1)\rho(x_2)\rho(x_3)+\rho(x_1)\mathbf{R}^{\mathbf{T}}(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\mathbf{R}(x_3)+\rho(x_2)\mathbf{R}^{\mathbf{T}}(x_3)\underset{\sim}{\Gamma}(x_3,x_1)\mathbf{R}(x_1)\\
&\quad+\rho(x_3)\mathbf{R}^{\mathbf{T}}(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\mathbf{R}(x_2)+\mathbf{R}^{\mathbf{T}}(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\mathbf{R}(x_3)\\
&\quad+\mathbf{R}^{\mathbf{T}}(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\underset{\sim}{J}^d(x_3)\underset{\sim}{\Gamma}(x_3,x_1)\mathbf{R}(x_1)+\mathbf{R}^{\mathbf{T}}(x_3)\underset{\sim}{\Gamma}(x_3,x_1)\underset{\sim}{J}^d(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\mathbf{R}(x_2)\\
&\quad+\mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\underset{\sim}{J}^d(x_3)\underset{\sim}{\Gamma}(x_3,x_1)]\}\\
&= Q^{ddd}(x_1,x_2,x_3)\mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{G}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{G}(x_2,x_3)\underset{\sim}{J}^d(x_3)\underset{\sim}{G}(x_3,x_1)].
\end{aligned} \tag{38}$$

If the three-point diagram has a single exchange line connection, say at point x_3, there results

$$\begin{aligned}
T^{dde}(x_1,x_2,x_3) &= Q^{dde}(x_1,x_2,x_3)\{\rho(x_1)\rho(x_2)+\mathbf{R}^{\mathbf{T}}(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\mathbf{R}(x_2)+\rho(x_1)\mathbf{R}^{\mathbf{T}}(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\mathbf{S}+\rho(x_2)\mathbf{S}^{\mathbf{T}}\underset{\sim}{\Gamma}(x_3,x_1)\mathbf{R}(x_1)\\
&\quad+\mathbf{R}^{\mathbf{T}}(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\mathbf{S}+\mathbf{R}^{\mathbf{T}}(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\underset{\sim}{J}^e\underset{\sim}{\Gamma}(x_3,x_1)\mathbf{R}(x_1)\\
&\quad+\mathbf{S}^{\mathbf{T}}\underset{\sim}{\Gamma}(x_3,x_1)\underset{\sim}{J}^d(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\mathbf{R}(x_2)+\mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{\Gamma}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{\Gamma}(x_2,x_3)\underset{\sim}{J}^e\underset{\sim}{\Gamma}(x_3,x_1)]\},
\end{aligned} \tag{39}$$

where

$$\mathbf{S}=\begin{pmatrix}1\\0\end{pmatrix}. \tag{40}$$

As with the previous term, the vector-matrix products can be replaced by traces, this time replacing $\underset{\sim}{J}^d(x)$ by $\underset{\sim}{J}^e$ at the exchange point. Equation (39) becomes

$$\begin{aligned}
&T^{dde}(x_1,x_2,x_3)\\
&\quad= Q^{dde}(x_1,x_2,x_3)\mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{G}(x_1,x_2)\underset{\sim}{J}^d(x_2)\\
&\qquad\times\underset{\sim}{G}(x_2,x_3)\underset{\sim}{J}^e\underset{\sim}{G}(x_3,x_1)].
\end{aligned} \tag{41}$$

Analogous expressions are obtained for T^{ded} and T^{edd}.

As might be expected, similar expressions are obtained for the terms where the three-point diagram has two or three exchange line connections. Thus,

$$\begin{aligned}
&T^{dee}(x_1,x_2,x_3)\\
&\quad= Q^{dee}(x_1,x_2,x_3)\mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{G}(x_1,x_2)\\
&\qquad\times\underset{\sim}{J}^e\underset{\sim}{G}(x_2,x_3)\underset{\sim}{J}^e\underset{\sim}{G}(x_3,x_1)]
\end{aligned} \tag{42}$$

and

$$\begin{aligned}
&T^{eee}(x_1,x_2,x_3)\\
&\quad= Q^{eee}(x_1,x_2,x_3)\mathrm{Tr}[\underset{\sim}{J}^e\underset{\sim}{G}(x_1,x_2)\underset{\sim}{J}^e\underset{\sim}{G}(x_2,x_3)\\
&\qquad\times\underset{\sim}{J}^e\underset{\sim}{G}(x_3,x_1)].
\end{aligned} \tag{43}$$

Going back to Eq. (34) and inserting the various terms that have been evaluated, a compact expression results. It is in fact easier to express the full three-body distribution, as follows:

$$\begin{aligned}\Gamma^{(3)}(x_1,x_2,x_3) &= \mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{G}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{G}(x_2,x_3)\underset{\sim}{J}^d(x_3)\\ &\quad\times\underset{\sim}{G}(x_3,x_1)]+\Gamma_{cc}(x_1,x_2)\Gamma_{cc}(x_2,x_3)\\ &\quad\times\Gamma_{cc}(x_3,x_1)\{1+Q^{ddd}(x_1,x_2,x_3)\}\\ &\quad+\sum_{\lambda\mu\nu}Q^{\lambda\mu\nu}(x_1,x_2,x_3)\mathrm{Tr}[\underset{\sim}{J}^\lambda(x_1)\underset{\sim}{G}(x_1,x_2)\underset{\sim}{J}^\mu(x_2)\\ &\quad\times\underset{\sim}{G}(x_2,x_3)\underset{\sim}{J}^\nu(x_3)\underset{\sim}{G}(x_3,x_1)]. \qquad (44)\end{aligned}$$

As a technical point, although $\underset{\sim}{J}^e$ does not depend on any coordinates, there is no mathematical impropriety if an argument is attached to it. Allowing such a generalization of the notation makes the expression above easier to present.

The superposition approximation[11] arises by assuming that the major contribution to the three-body distribution is in the form of a product of two-body distributions between the three pairs of points. This corresponds to eliminating all but the first term on the right-hand side of Eq. (44)

$$\begin{aligned}\Gamma^{(3)}_{SA}(x_1,x_2,x_3) &= \mathrm{Tr}[\underset{\sim}{J}^d(x_1)\underset{\sim}{G}(x_1,x_2)\underset{\sim}{J}^d(x_2)\underset{\sim}{G}(x_2,x_3)\underset{\sim}{J}^d(x_3)\underset{\sim}{G}(x_3,x_1)]. \qquad (45)\end{aligned}$$

Note that the second term of Eq. (44) also consists of two-point connections only between external points, but this is not properly associated with the superposition approximation, since these Γ_{cc}-exchange line connections do not contribute directly to the two-body distribution function.

IV. THE THREE-BODY FHNC EQUATIONS

The three-body FHNC equations are designed to evaluate the quantities $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$. The approach taken is a modification of that of Wertheim[16] for the classical HNC case. Many of the quantities to be introduced are analogous to those found in the classical case. A number of the details, especially those associated with the exchange structure of the diagrams, are different.

The set of diagrams that appears in $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ consists of all the irreducible three-point diagrams that have no two-point connections between the external points. This set of diagrams can be further decomposed in terms of the cutting points that are present. To prepare for this development, note that the removal of any cutting point will result in at least one diagrammatic fragment that contains only one external point. The cutting point will be considered to be associated with that external point. It is possible for a cutting point to be associated with all three external points at the same time, but otherwise, a cutting point can be associated with only one external point. Now, there may be a sequence of cutting points associated with a given external point. These would correspond to nodes along a two-point connection. One of these cutting points will result in the largest possible fragment containing that external point alone, and this will be referred to as the *maximal cutting point*. An external point can have associated with it at most one maximal cutting point. The diagrams in $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ will be classified according to how many maximal cutting points they contain 0, 1, 2, or 3.

Consider, first, the set of diagrams that contain three maximal cutting points. There is one special case in which all the cutting points are the same one. The contribution to $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ is readily worked out to be

$$\begin{aligned}Q^{\lambda\mu\nu}_{3a}(x_1,x_2,x_3) &= \int dx_4\{\Gamma_{\lambda d}(x_1,x_4)\Gamma_{\mu d}(x_2,x_4)\Gamma_{\nu d}(x_3,x_4)\rho(x_4)\\ &\quad+\Gamma_{\lambda d}(x_1,x_4)\Gamma_{\mu d}(x_2,x_4)\Gamma_{\nu e}(x_3,x_4)\\ &\quad+\Gamma_{\lambda d}(x_1,x_4)\Gamma_{\mu e}(x_2,x_4)\Gamma_{\nu d}(x_3,x_4)\\ &\quad+\Gamma_{\lambda e}(x_1,x_4)\Gamma_{\mu d}(x_2,x_4)\Gamma_{\nu d}(x_3,x_4)\}. \qquad (46)\end{aligned}$$

The only other way a diagram can have three cutting points is when the external points are all connected to different external points of an internal three-point subdiagram. This three-point subdiagram is necessarily irreducible and cannot contain any cutting points (else at least one of the designated maximal cutting points would not actually be maximal). They are therefore fully irreducible. There are no other restrictions on these diagrams; for instance, there may be two-point connections between their external points. Label the sum of such fully irreducible, three-point diagrams by $C^{\lambda\mu\nu}(x_1,x_2,x_3)$. Working out all the allowed connections, the contribution to $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ is given by

$$\begin{aligned}Q^{\lambda\mu\nu}_{3b}(x_1,x_2,x_3) &= \int dx_4dx_5dx_6\sum_{\lambda'\lambda''}\Gamma_{\lambda\lambda'}(x_1,x_4)J^d_{\lambda'\lambda''}(x_4)\\ &\quad\times\sum_{\mu'\mu''}\Gamma_{\mu\mu'}(x_2,x_5)J^d_{\mu'\mu''}(x_5)\\ &\quad\times\sum_{\nu'\nu''}\Gamma_{\nu\nu'}(x_3,x_6)J^d_{\nu'\nu''}(x_6)C^{\lambda''\mu''\nu''}(x_4,x_5,x_6). \qquad (47)\end{aligned}$$

The diagrams with two maximal cutting points must have a three-point subdiagram which contains the unique external point that does not have an associated cutting point. The other two external points have two-point connections to the other points of the three-point subdiagram. This subdiagram is fully irreducible and has no further restrictions. Therefore, the contribution to $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ is given by

$$\begin{aligned}Q^{\lambda\mu\nu}_2(x_1,x_2;x_3) &= \int dx_4dx_5\sum_{\lambda'\lambda''}\Gamma_{\lambda\lambda'}(x_1,x_4)J^d_{\lambda'\lambda''}(x_4)\\ &\quad\times\sum_{\mu'\mu''}\Gamma_{\mu\mu'}(x_2,x_5)J^d_{\mu'\mu''}(x_5)\\ &\quad\times C^{\lambda''\mu''\nu}(x_4,x_5,x_3). \qquad (48)\end{aligned}$$

The point x_3 is distinguished from the other two in this function. There are clearly two other quantities which differ only in the choice of the unique external point.

The diagrams with only one maximal cutting point must contain a three-point subdiagram which connects to the two external points that do not have cutting points. The third external point must have a two-point connection with the third point of that three-point subdiagram. These three-point subdiagrams are fully irreducible, but because of the construction of $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$, there can be no two-point connections between the two external points that are contained in it. No such restrictions are placed on connections between the other pairs of external points of the subdiagram. If points x_2 and x_3 are designated as the points between which two-point connections are not allowed, label the associated sum of diagrams by $X^{\lambda\mu\nu}(x_1,x_2,x_3)$. The associated contribution to $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ is given by

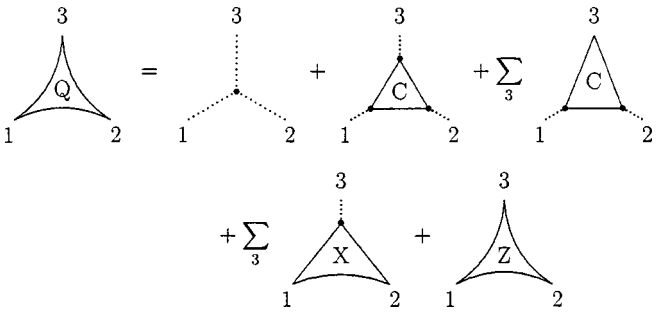
$$Q_1^{\lambda\mu\nu}(x_1;x_2,x_3) = \int dx_4 \sum_{\lambda'\lambda''} \Gamma_{\lambda\lambda'}(x_1,x_4) J^d_{\lambda'\lambda''}(x_4) X^{\lambda''\mu\nu}(x_4;x_2,x_3). \tag{49}$$

There are clearly two more sums which differ only in the choice of external point to be treated specially.

The final contribution contains those three-point diagrams which are fully irreducible but allow no two-point connections between any of the external points. Label the sum of these diagrams by $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$. The contribution to $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ is given by

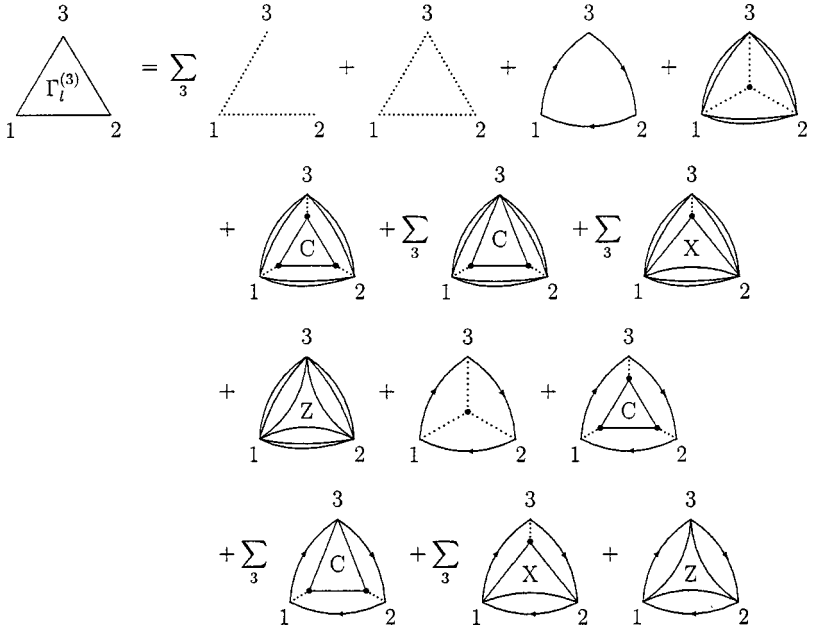
$$Q_0^{\lambda\mu\nu}(x_1,x_2,x_3) = Z^{\lambda\mu\nu}(x_1,x_2,x_3). \tag{50}$$

There are five sums of three-point diagrams that have been defined, and they are summarized in Table II. Further development is extremely tedious without going to a diagrammatic shorthand. In addition to the two-point elements already presented, diagrammatic elements can be introduced for the three-point quantities defined so far. The symbols to be used are included in Table II. When generating an expansion of diagrams, it often happens that one point of a diagram is treated differently from the other two, but there are other, equivalent diagrams included in the sum that differ only in permutations of the external points. Rather than include each permutation explicitly, such combinations will be represented by a summation sign with the number of equivalent terms indicated under the sign. Which terms are to be included should be clear from the construction. Following this prescription, the following diagrammatical representation for $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ is obtained:



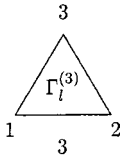
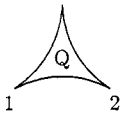
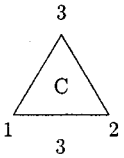
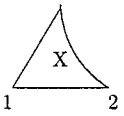
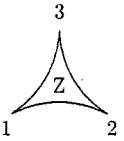
(51)

Using this, Equation (34) becomes



(52)

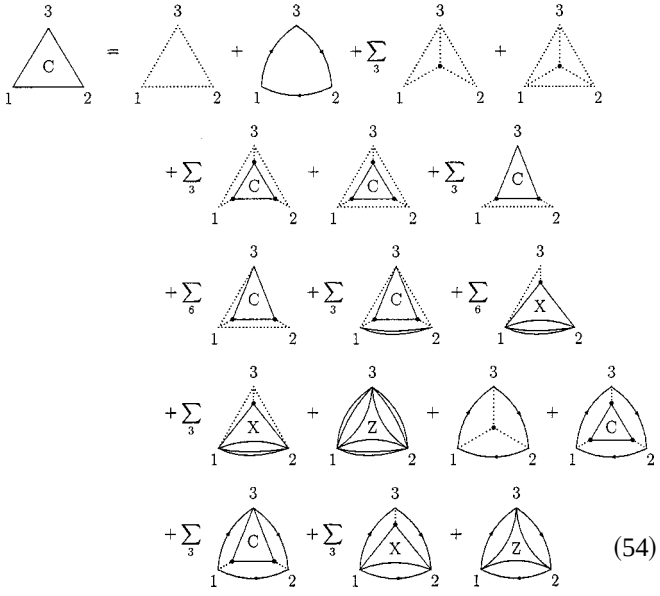
TABLE II. Three-point sums appearing in the equations.

sum	description	symbol
$\Gamma_l^{(3)\lambda\mu\nu}(x_1,x_2,x_3)$	all linked, irreducible three-point diagrams	
$Q^{\lambda\mu\nu}(x_1,x_2,x_3)$	all linked, irreducible three-point diagrams without two-point connections between external points	
$C^{\lambda\mu\nu}(x_1,x_2,x_3)$	all linked, fully irreducible three-point diagrams	
$X^{\lambda\mu\nu}(x_1;x_2,x_3)$	all linked, fully irreducible three-point diagrams without two-point connections between points x_2 and x_3	
$Z^{\lambda\mu\nu}(x_1,x_2,x_3)$	all linked, fully irreducible three-point diagrams without two-point connections between external points	

As noted earlier, the lack of explicit circles for the external points implies that the connections to these points are left unspecified. The quantity on the left is equal to $\Gamma_l^{(3)\lambda\mu\nu}(x_1,x_2,x_3)$, which is not the same thing as $\Gamma_l^{(3)}(x_1,x_2,x_3)$, even though the same symbol is being used. To be clear on this issue, the two are related by

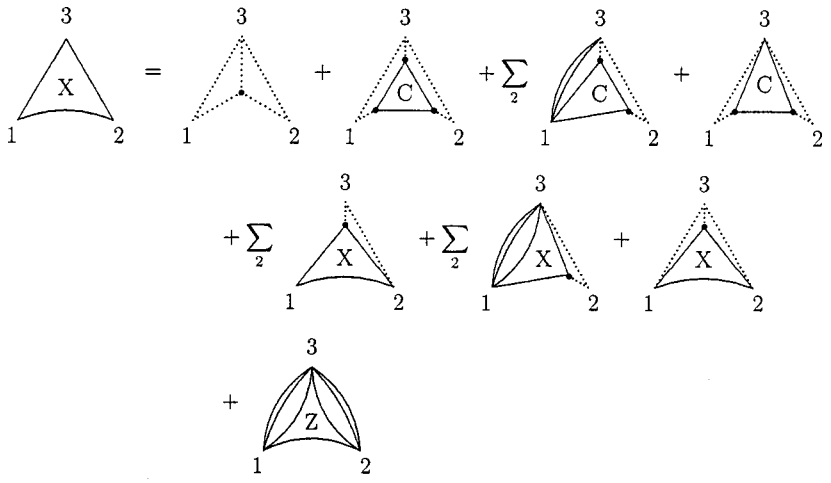
$$\Gamma_l^{(3)}(x_1,x_2,x_3) = \sum_{\lambda\mu\nu} R_\lambda(x_1)R_\mu(x_2)R_\nu(x_3)\Gamma_l^{(3)\lambda\mu\nu}(x_1,x_2,x_3). \tag{53}$$

The linked, three-body distribution function corresponds to a sum of all the linked, irreducible three-body diagrams. The quantity $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ represents a diagrammatic expansion that contains a subset of these: all those that are fully irreducible. A diagrammatic expansion for this quantity can therefore be obtained by removing those diagrams in Eq. (52) that are not fully irreducible. There results



(54)

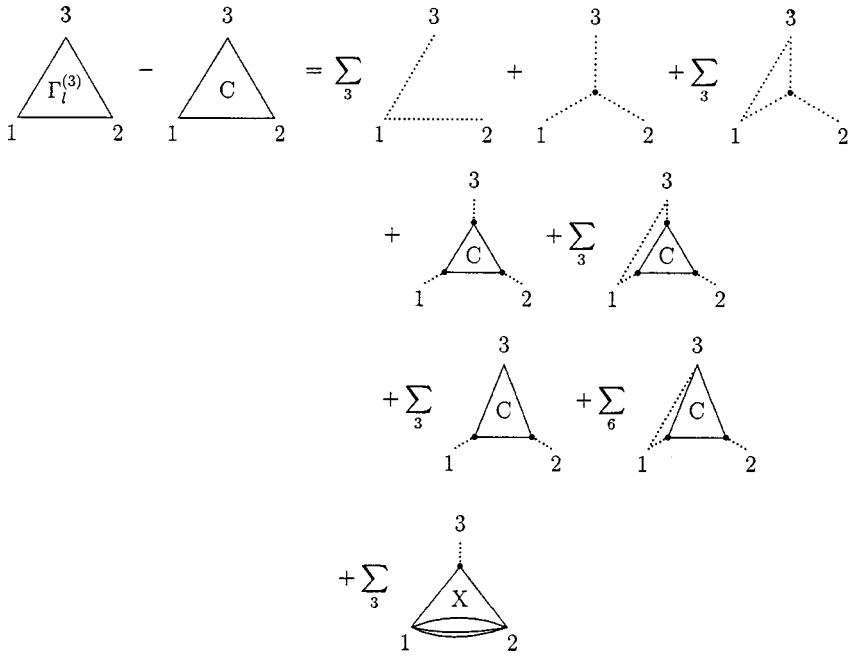
The diagrammatic expansion for $X^{\lambda\mu\nu}(x_3;x_1,x_2)$ contains all the diagrams of a subset of those in $C^{\lambda\mu\nu}(x_1,x_2,x_3)$: those that contain no two-point connections between x_1 and x_2. Removing all such diagrams from Eq. (54), there results



(55)

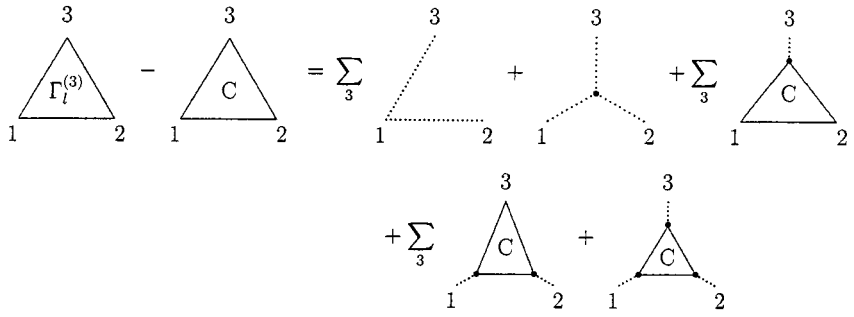
Note that if diagrams having two-point connections between any external points are removed, the only diagram that remains on the right hand side corresponds to $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$, as is required.

To derive some direct relationships between three-point sums, consider taking the difference of Eqs. (52) and (54)



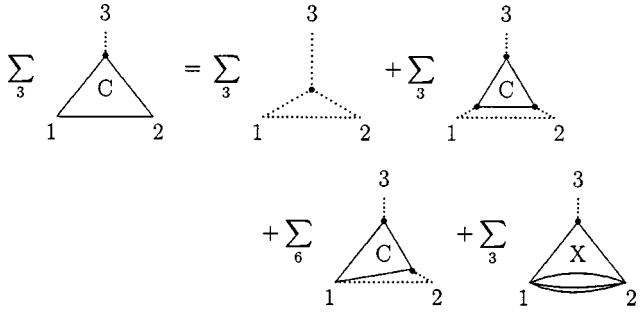
(56)

Next, consider this difference on topological grounds. By subtracting $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ from $\Gamma_l^{(3)\lambda\mu\nu}(x_1,x_2,x_3)$, all the fully irreducible diagrams are removed from the sum of linked, irreducible diagrams. What remains, therefore, are just those diagrams that have at least one cutting point. Focus first on the diagrams with one cutting point. There are two cases to consider. The first is to have that cutting point be one of the external points and joining it to the other two by two-point connections. The second is to have one external point joined by a two-point connection to a three-point diagram which contains the other two external points. This three- point diagram has no restrictions other than that it be fully irreducible. The sum of such three-point diagrams is therefore given by $C^{\lambda\mu\nu}(x_1,x_2,x_3)$. There are three such terms, depending on which external point is joined by the two-point connection. Diagrams with two cutting points are constructed by joining two external points by two-point connections to a three-point diagram that contains the third external point. The three-point diagrams must be fully irreducible and are otherwise unrestricted. The sum of them is therefore given by $C^{\lambda\mu\nu}(x_1,x_2,x_3)$. There are three topologically different such terms, depending on which external point is contained in the three-point diagram. Finally, there is the set of diagrams that have three cutting points. As in the decomposition of the linked, three-body distribution function, there are two cases: one where all three cutting points correspond to the same internal point and one where all three external points are connected directly to different points of a fully irreducible internal subdiagram. Diagrammatically, then, the difference can be expressed by



(57)

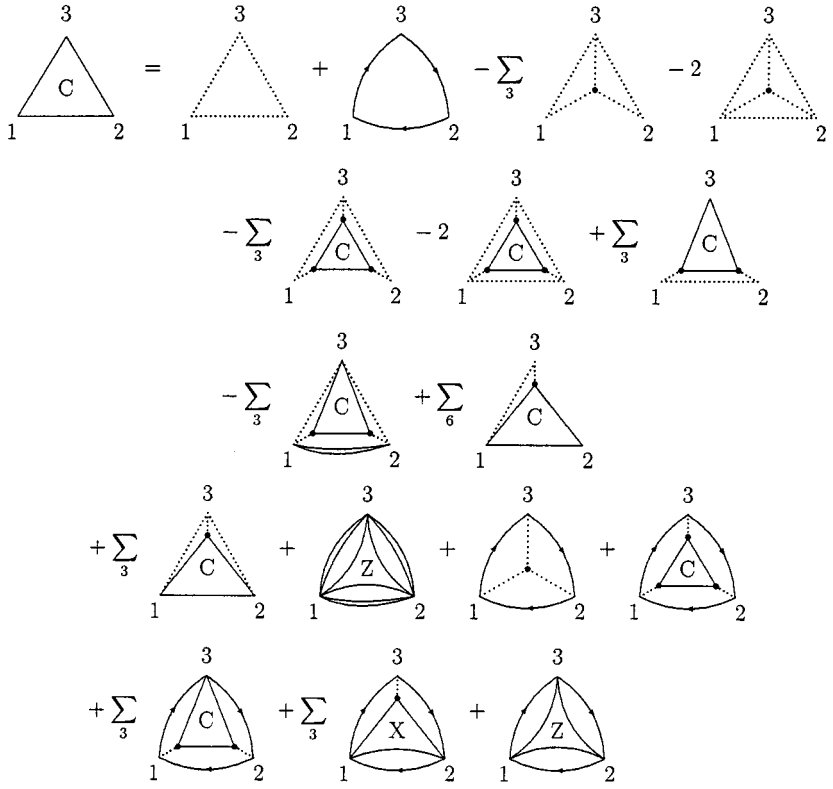
Equating (56) and (57) leads to a relation between $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ and $X^{\lambda\mu\nu}(x_1;x_2,x_3)$ (and its permutations). Rearranging a bit, this becomes



(58)

It may be noted that each term in this equation can be separated into three, each one distinguished by which external point has a cutting point. It is tempting to separate the entire equation into three, one for each external point. However, this separation is not necessarily valid, since there may be extra terms that should be included in the separate equations, but that happen to cancel in the combination and so are not present in Eq. (58). Fortunately, it is not necessary to separate the sum in the following development.

Equation (58) can be rearranged to solve for the single term containing the sum of permutations of $X^{\lambda\mu\nu}(x_1;x_2,x_3)$, which can then be used to replace two of the terms in Eq. (54) to yield

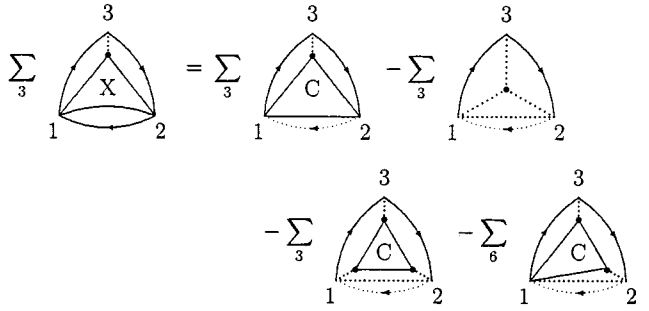


(59)

There remains only one term that contains a dependence on $X^{\lambda\mu\nu}(x_1;x_2,x_3)$. A little manipulation can generate a relationship that can be used to eliminate this dependence. First, note that only $X^{\lambda dd}(x_1;x_2,x_3)$ or one of its permutations contributes to this diagram. Second, the two-body FHNC equations yield

$$\Gamma_{cc}(x_1,x_2)=[1+\Gamma_{dd}(x_1,x_2)]S_{cc}(x_1,x_2) \tag{60}$$

so that the Γ_{cc}-exchange line can be replaced by a product of $S_{cc}(x_1,x_2)$ and a G- direct line. Introducing a new two-point diagrammatic element, a directed dotted line, to represent $S_{cc}(x_1,x_2)$ (see Table I), Eq. (58) can be introduced to give



(61)

By introducing this into Eq. (59), the resulting equation contains only two different types of three-body diagrams $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ and $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$. As might be expected, an algebraic representation of this equation would be rather unwieldy. The specific expressions are given in the appendix. The advantage of the diagrammatic development is clear. The evaluation of the three-body distribution function now revolves around a proper identification of $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$. The Percus-Yevick approximation is equivalent to setting this quantity to zero.[16] This would give an equation for $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ alone. The FHNC approximation requires a more involved analysis.

The function $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ contains all the fully irreducible three-point diagrams that do not contain any two-point connections between external points. These are analogous to the non-nodal diagrams encountered in the two-body FHNC equations. As with the two-body case, this sum can be separated into two terms: a sum of noncomposite diagrams and a sum of composite diagrams. The sum of noncomposite diagrams in $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ are referred to as elementary diagrams and the sum of these diagrams is represented by $E^{\lambda\mu\nu}(x_1,x_2,x_3)$. The function $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$, by construction, contains all linked, three-point diagrams that have no two-point connections between external points. This sum contains a sum of fully irreducible diagrams, which is precisely $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$, and a sum of diagrams that contain at least one cutting point. Define the difference

$$Y^{\lambda\mu\nu}(x_1,x_2,x_3)=Q^{\lambda\mu\nu}(x_1,x_2,x_3)-Z^{\lambda\mu\nu}(x_1,x_2,x_3) \tag{62}$$

as this sum of all the three-point diagrams that have at least one cutting point. By construction, these diagrams are noncomposite, although not elementary. The sum of all noncomposite three-point diagrams without two-point connections between external points is therefore given by $Y^{\lambda\mu\nu}(x_1,x_2,x_3)+E^{\lambda\mu\nu}(x_1,x_2,x_3)$.

Now, all the composite three-point diagrams encountered in $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$ and $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ must be constructed from the joining of non-composite diagrams at all three external points. If two diagrams were joined at only two external points, there would result a two-point connection between the two external points. Such diagrams have been excluded from these sums by definition. Further, the sum of all composite diagrams in $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ is constructed by joining noncomposite diagrams in the sum $Y^{\lambda\mu\nu}(x_1,x_2,x_3)+E^{\lambda\mu\nu}(x_1,x_2,x_3)$. Using the information so far deduced, it is desired to derive relations for the functions $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ in terms of the elementary diagrams.

For all direct-type connections, the composite diagrams must all be made from three-point diagrams with all direct connections. This leads to the expression

$$\begin{aligned}Z^{ddd}(x_1,x_2,x_3)&=E^{ddd}(x_1,x_2,x_3)+\frac{1}{2!}[E^{ddd}(x_1,x_2,x_3)\\&\quad+Y^{ddd}(x_1,x_2,x_3)]^2+\frac{1}{3!}[E^{ddd}(x_1,x_2,x_3)\\&\quad+Y^{ddd}(x_1,x_2,x_3)]^3+\cdots\\&=E^{ddd}(x_1,x_2,x_3)+\exp[E^{ddd}(x_1,x_2,x_3)\\&\quad+Y^{ddd}(x_1,x_2,x_3)]-E^{ddd}(x_1,x_2,x_3)\\&\quad-Y^{ddd}(x_1,x_2,x_3)-1\\&=g_{3B}(x_1,x_2,x_3)-Y^{ddd}(x_1,x_2,x_3)-1,\end{aligned} \tag{63}$$

where

$$g_{3B}(x_1,x_2,x_3)=\exp[E^{ddd}(x_1,x_2,x_3)+Y^{ddd}(x_1,x_2,x_3)]. \tag{64}$$

In the case that there is one exchange-line connection, the composite diagrams can always be decomposed so that one part contains the exchange-line connection and all the rest contain only direct-line connections. In this case,

$$\begin{aligned}Z^{dde}(x_1,x_2,x_3)&=E^{dde}(x_1,x_2,x_3)+[E^{dde}(x_1,x_2,x_3)\\&\quad+Y^{dde}(x_1,x_2,x_4)]Q^{ddd}(x_1,x_2,x_3)\\&=E^{dde}(x_1,x_2,x_3)g_{3B}(x_1,x_2,x_3)\\&\quad+Y^{dde}(x_1,x_2,x_3)[g_{3B}(x_1,x_2,x_3)-1].\end{aligned} \tag{65}$$

Similar relations hold when the exchange connection is on a different external point.

The situation with two exchange-line connections is more complicated. The composite diagrams can be constructed so that only one part contains both exchange-line connections and the rest only direct-line connections, or the exchange-line connections can be on two different parts. This leads to

$$
\begin{aligned}
Z^{dee}(x_1,x_2,x_3) &= E^{dee}(x_1,x_2,x_3)+[E^{dee}(x_1,x_2,x_3)+Y^{dee}(x_1,x_2,x_3)]Q^{ddd}(x_1,x_2,x_3)\\
&\quad +[E^{dde}(x_1,x_2,x_3)+Y^{dde}(x_1,x_2,x_3)]Q^{ded}(x_1,x_2,x_3)\\
&= E^{dee}(x_1,x_2,x_3)g_{3B}(x_1,x_2,x_3)+Y^{dee}(x_1,x_2,x_3)[g_{3B}(x_1,x_2,x_3)-1]\\
&\quad +[E^{dde}(x_1,x_2,x_3)+Y^{dde}(x_1,x_2,x_3)][E^{ded}(x_1,x_2,x_3)+Y^{ded}(x_1,x_2,x_3)]g_{3B}(x_1,x_2,x_3). \qquad (66)
\end{aligned}
$$

Analogous equations hold for the other two cases.

The final equation is derived in the same way, although with a few more complications. It is possible to have all three exchange-line connections on one part of the composite or to have two on one part and one on another (there are three ways to do this) or to have one on three different parts. To ensure that each combination is included and not overcounted, we get

$$
\begin{aligned}
Z^{eee}(x_1,x_2,x_3) &= E^{eee}(x_1,x_2,x_3)+[E^{eee}(x_1,x_2,x_3)+Y^{eee}(x_1,x_2,x_3)]Q^{ddd}(x_1,x_2,x_3)+[E^{dee}(x_1,x_2,x_3)\\
&\quad +Y^{dee}(x_1,x_2,x_3)]Q^{edd}(x_1,x_2,x_3)+[E^{ede}(x_1,x_2,x_3)+Y^{ede}(x_1,x_2,x_3)]Q^{ded}(x_1,x_2,x_3)\\
&\quad +[E^{eed}(x_1,x_2,x_3)+Y^{eed}(x_1,x_2,x_3)]Q^{dde}(x_1,x_2,x_3)+[E^{edd}(x_1,x_2,x_3)+Y^{edd}(x_1,x_2,x_3)]\\
&\quad \times[E^{ded}(x_1,x_2,x_3)+Y^{ded}(x_1,x_2,x_3)]Q^{dde}(x_1,x_2,x_3),\\
&= E^{eee}(x_1,x_2,x_3)g_{3B}(x_1,x_2,x_3)+Y^{eee}(x_1,x_2,x_3)[g_{3B}(x_1,x_2,x_3)-1]+[E^{dee}(x_1,x_2,x_3)\\
&\quad +Y^{dee}(x_1,x_2,x_3)][E^{edd}(x_1,x_2,x_3)+Y^{edd}(x_1,x_2,x_3)]g_{3B}(x_1,x_2,x_3)+[E^{ede}(x_1,x_2,x_3)\\
&\quad +Y^{ede}(x_1,x_2,x_3)][E^{ded}(x_1,x_2,x_3)+Y^{ded}(x_1,x_2,x_3)]g_{3B}(x_1,x_2,x_3)+[E^{eed}(x_1,x_2,x_3)\\
&\quad +Y^{eed}(x_1,x_2,x_3)][E^{dde}(x_1,x_2,x_3)+Y^{dde}(x_1,x_2,x_3)]g_{3B}(x_1,x_2,x_3)+[E^{edd}(x_1,x_2,x_3)\\
&\quad +Y^{edd}(x_1,x_2,x_3)][E^{ded}(x_1,x_2,x_3)+Y^{ded}(x_1,x_2,x_3)][E^{dde}(x_1,x_2,x_3)\\
&\quad +Y^{dde}(x_1,x_2,x_3)]g_{3B}(x_1,x_2,x_3) \qquad (67)
\end{aligned}
$$

All the equations necessary for computing the three-body distribution are now derived. There are a large number of them and it is useful to see how they are related to each other. For this purpose, a general computational procedure is devised as follows.

(a) Choose a set of elementary diagrams $E^{\lambda\mu\nu}(x_1,x_2,x_3)$. This is not as simple an issue as might be surmised. In analogy with the FHNC/0 approximation for the two-body equations, one may choose the empty set for this. There is reason to suspect[23] that some useful results can be obtained in this way. However, if three-body correlations are to be investigated, it is necessary that a more careful choice be made. This issue will be discussed in the Conclusions section.

(b) Make an initial guess for the functions, $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$. This will be modified in an iterative fashion during this procedure. Presumably, setting all the functions initially to zero, as in the Percus-Yevick approximation, will be satisfactory.

(c) Using a combination of Eqs. (59) and (61), $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ can be computed self-consistently from the guessed values for $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ and the two-body functions.

(d) Equation (55) can be solved self-consistently from the guessed values for $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ and the computed values for $C^{\lambda\mu\nu}(x_1,x_2,x_3)$.

(e) Equation (51) can be rearranged to an expression for $Y^{\lambda\mu\nu}(x_1,x_2,x_3)$, which can then be solved directly using the computed values for $C^{\lambda\mu\nu}(x_1,x_2,x_3)$ and $X^{\lambda\mu\nu}(x_1;x_2,x_3)$.

(f) Equations (63)–(67) can be solved directly for the new values of $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$.

(g) The new and old values for $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$ are compared. If they are close enough, they can be used in the next step. Otherwise, the process starting from step (*c*) should be repeated.

(h) Equation (62) is used to compute $Q^{\lambda\mu\nu}(x_1,x_2,x_3)$.

(i) Equation (44) is used to compute the three-body distribution.

It may be noted that the common procedure nowadays for solving the FHNC equations involves a functional optimization of the correlation potentials and not a direct iterative solution as described above. Nevertheless, the equations derived in this paper can still be used as a starting point to construct the associated Euler equations for the correlation potentials.

V. CONCLUSIONS

The three-body FHNC equations have been derived and are reported here explicitly. A uniform system is not assumed; they are derived for the general inhomogeneous system. They are, as expected, very complicated and would be difficult to solve. Routine use would certainly not be expected to be worthwhile. Nevertheless, they would be valuable for directly testing the validity of the various approximations used and their explicit presentation here would help to that end. Further, there may be cases where a highly accurate solution is required and the expressions derived here may be useful for that. In particular, situations where three-body correlations should be taken into account would require an accurate treatment of the three-body distribution and the equations derived here would serve as a starting point in that direction.

One further issue is worth discussing here. The equations derived in this paper are more closely associated with the Fantoni-Rosati[1] (FR) formulation of FHNC theory than with the Krotscheck-Ristig[2] (KR) formulation. As a result, these equations suffer the same shortcomings (and strengths) as the FR two-body equations. The solution of these FHNC equations depends directly on the choice of elementary diagrams that is made. The common choice for the two-body equations involves a truncation of the cluster expansion of elementary diagrams up to a specific number of points, the so-called FHNC/n approximation. It has been noted[2] that the cluster expansion contains divergences that end up canceling each other in the full sum. However, the FHNC/n truncation of elementary diagrams results in an incomplete cancellation[17] that could be harmful for computed results. The KR formulation aims to ensure a proper cancellation of these divergent terms, even at a truncated level. However, it is useful to note that the three-body equations derived in this paper do not rely on the specifics of the two-body elements. They could just as easily come from solution of the KR-FHNC equations as from the FR-FHNC equations. Whether using two-body elements from the KR formulation would yield an improvement over the FR formulation is not clear, but would be worth investigating.

This cancellation phenomenon is expected to occur in the three-body equations as well and probably to a stronger degree. The KR formulation was developed by enforcing the correct small-k behavior of the structure factor, a property which is intimately tied to the sequential relation between the one- and two-body distributions. It is this property that the FR formulation does not handle satisfactorily. There are indications that calculations within the FR formulation yield satisfactory total energies. For instance, calculations on the electron gas[3,4] lead to energies in excellent agreement with quantum Monte Carlo[24] results. However, optimization of the three-body correlation potential is a more delicate matter. In this case, it seems crucial that the sequential relation between the three- and two-body distributions be satisfied. Hence, one might suspect that the three-body equations derived in this paper may be deficient in this respect. This is certainly worth future investigation. There are two obvious directions to go at this point. First, it may be possible to recast the formulas in this paper in a way that is consistent with the KR formulation of the two-body equations. Even though this would result in the elimination of certain diagrams (as it does in the two-body equations), there may be a profitable return due to the satisfaction of the sequential relations. Second, there may be alternative truncations of the elementary diagrams that lead to satisfaction or at least acceptably approximate satisfaction of the sequential relations. These truncations will depend on the two-body elements used and may work better within one formalism than the other. In any case, the results in this paper could serve as a suitable starting point.

APPENDIX: THE ALGEBRAIC FHNC THREE-BODY EQUATIONS

Although all the formulas for the three-body distribution are in principle given, they are mostly in diagrammatic form and must be translated to an algebraic form before they can be practically implemented. The resulting expressions are necessarily lengthy, but it is useful to have them written down for potential use. They are presented in this appendix in all their glory.

A direct translation is, of course, possible, but the expressions are very long. It is possible to streamline them a bit without sacrificing the explicit nature of the expressions by introducing a new three-component array $\mathcal{G}^{\alpha\beta\gamma}$, the indices being either d or e. It is defined by the following expressions:

$$\mathcal{G}^{d\beta\gamma}=\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \quad \mathcal{G}^{e\beta\gamma}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{A1}$$

This array $\mathcal{G}^{\alpha\beta\gamma}$ can be used when joining two diagrammatic portions with ends of type β and γ to each other. The overall type for the point of the joined diagram then corresponds to the index α. This array will be used in the following expressions. The procedure presented in the text will be repeated here with the diagrammatic equations replaced by algebraic expressions.

(a) Choose a set of elementary diagrams $E^{\lambda\mu\nu}(x_1,x_2,x_3)$.

(b) Make an initial guess for the functions $Z^{\lambda\mu\nu}(x_1,x_2,x_3)$.

(c) Use the following equations to solve for $C^{\lambda\mu\nu}(x_1,x_2,x_3)$.

$$
\begin{aligned}
C^{ddd}(x_1,x_2,x_3)=&\Gamma_{dd}(x_1,x_2)\Gamma_{dd}(x_2,x_3)\Gamma_{dd}(x_3,x_1)-\Big\{\int dx_4\{\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\rho(x_4)\\
&+\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{de}(x_3,x_4)+\Gamma_{dd}(x_1,x_4)\Gamma_{de}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\\
&+\Gamma_{de}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\}+\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)\Gamma_{d\nu}(x_3,x_6)\\
&\times J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Big\}\{\Gamma_{dd}(x_1,x_2)\Gamma_{dd}(x_2,x_3)+\Gamma_{dd}(x_2,x_3)\Gamma_{dd}(x_3,x_1)\\
&+\Gamma_{dd}(x_3,x_1)\Gamma_{dd}(x_1,x_2)+2\Gamma_{dd}(x_1,x_2)\Gamma_{dd}(x_2,x_3)\Gamma_{dd}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{d\lambda}(x_2,x_4)\Gamma_{d\mu}(x_3,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_1,x_4,x_5)\{\Gamma_{dd}(x_2,x_3)\\
&-\Gamma_{dd}(x_1,x_2)\Gamma_{dd}(x_1,x_3)G_{dd}(x_2,x_3)\}+\int dx_4dx_5\Gamma_{d\lambda}(x_3,x_4)\Gamma_{d\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)\\
&\times C^{d\lambda'\mu'}(x_2,x_4,x_5)\{\Gamma_{dd}(x_3,x_1)-\Gamma_{dd}(x_2,x_3)\Gamma_{dd}(x_2,x_1)G_{dd}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_3,x_4,x_5)\{\Gamma_{dd}(x_1,x_2)\\
&-\Gamma_{dd}(x_3,x_1)\Gamma_{dd}(x_3,x_2)G_{dd}(x_1,x_2)\}+\int dx_4\Gamma_{d\lambda}(x_1,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'dd}(x_4,x_2,x_3)\{\Gamma_{dd}(x_1,x_2)\\
&+\Gamma_{dd}(x_1,x_3)+\Gamma_{dd}(x_1,x_2)\Gamma_{dd}(x_1,x_3)\}+\int dx_4\Gamma_{d\lambda}(x_2,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'dd}(x_4,x_3,x_1)\{\Gamma_{dd}(x_2,x_3)\\
&+\Gamma_{dd}(x_2,x_1)+\Gamma_{dd}(x_2,x_3)\Gamma_{dd}(x_2,x_1)\}+\int dx_4\Gamma_{d\lambda}(x_3,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'dd}(x_4,x_1,x_2)\{\Gamma_{dd}(x_3,x_1)\\
&+\Gamma_{dd}(x_3,x_2)+\Gamma_{dd}(x_3,x_1)\Gamma_{dd}(x_3,x_2)\}+G_{dd}(x_1,x_2)G_{dd}(x_2,x_3)G_{dd}(x_3,x_1)Z^{ddd}(x_1,x_2,x_3),
\end{aligned}
\tag{A2}
$$

$$
\begin{aligned}
C^{dde}(x_1,x_2,x_3)=&\Gamma_{dd}(x_1,x_2)\Gamma_{d\alpha}(x_2,x_3)\mathcal{G}^{e\alpha\beta}\Gamma_{\beta d}(x_3,x_1)-\Big\{\int dx_4\{\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{\alpha d}(x_3,x_4)\rho(x_4)\\
&+\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{\alpha e}(x_3,x_4)+\Gamma_{dd}(x_1,x_4)\Gamma_{de}(x_2,x_4)\Gamma_{\alpha d}(x_3,x_4)\\
&+\Gamma_{de}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{\alpha d}(x_3,x_4)\}+\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)\Gamma_{\alpha\nu}(x_3,x_6)\\
&\times J^d_{\lambda\lambda'}(x_4)J^d_{\lambda\lambda'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Big\}\mathcal{G}^{e\alpha\beta}\{\Gamma_{dd}(x_1,x_2)\Gamma_{d\beta}(x_2,x_3)+\Gamma_{d\gamma}(x_2,x_3)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta d}(x_3,x_1)\\
&+\Gamma_{\beta d}(x_3,x_1)\Gamma_{dd}(x_1,x_2)+2\Gamma_{dd}(x_1,x_2)\Gamma_{d\gamma}(x_2,x_3)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta d}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{d\lambda}(x_2,x_4)\Gamma_{\alpha\mu}(x_3,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_1,x_4,x_5)\mathcal{G}^{e\alpha\beta}\{\Gamma_{d\beta}(x_2,x_3)\\
&-\Gamma_{dd}(x_1,x_2)\Gamma_{d\lambda}(x_1,x_3)\mathcal{G}^{\beta\gamma\delta}G_{d\delta}(x_2,x_3)\}+\int dx_4dx_5\Gamma_{\alpha\lambda}(x_3,x_4)\Gamma_{d\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)\\
&\times C^{d\lambda'\mu'}(x_2,x_4,x_5)\mathcal{G}^{e\alpha\beta}\{\Gamma_{\beta d}(x_3,x_1)-\Gamma_{d\gamma}(x_2,x_3)\Gamma_{dd}(x_2,x_1)\mathcal{G}^{\beta\gamma\delta}G_{\delta d}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{\alpha\lambda'\mu'}(x_3,x_4,x_5)\mathcal{G}^{e\alpha\beta}\{\mathcal{G}^{\beta dd}\Gamma_{dd}(x_1,x_2)\\
&-\Gamma_{\gamma d}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta d}(x_3,x_2)G_{dd}(x_1,x_2)\}+\int dx_4\Gamma_{d\lambda}(x_1,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'b\alpha}(x_4,x_2,x_3)\mathcal{G}^{e\alpha\beta}\\
&\times\{\mathcal{G}^{\beta dd}\Gamma_{dd}(x_1,x_2)+\Gamma_{d\beta}(x_1,x_3)+\Gamma_{dd}(x_1,x_2)\Gamma_{d\beta}(x_1,x_3)\}\\
&+\int dx_4\Gamma_{d\lambda}(x_2,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'b\alpha}(x_4,x_1,x_3)\mathcal{G}^{e\alpha\beta}\{\mathcal{G}^{\beta dd}\Gamma_{dd}(x_1,x_2)+\Gamma_{d\beta}(x_2,x_3)\\
&+\Gamma_{dd}(x_1,x_2)\Gamma_{d\beta}(x_2,x_3)\}+\int dx_4\Gamma_{\alpha\lambda}(x_3,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'dd}(x_4,x_1,x_2)\mathcal{G}^{e\alpha\beta}\{\Gamma_{\beta d}(x_3,x_1)+\Gamma_{\beta d}(x_3,x_2)\\
&+\Gamma_{\gamma d}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta d}(x_3,x_2)\}+Z^{dd\alpha}(x_1,x_2,x_3)\mathcal{G}^{e\alpha\beta}G_{dd}(x_1,x_2)G_{d\gamma}(x_2,x_3)\mathcal{G}^{\beta\gamma\delta}G_{\delta d}(x_3,x_1),
\end{aligned}
\tag{A3}
$$

$$
\begin{aligned}
C^{dee}(x_1,x_2,x_3)=&\,\Gamma_{d\alpha}(x_1,x_2)\mathcal{G}^{e\alpha\beta}\Gamma_{\beta\alpha'}(x_2,x_3)\mathcal{G}^{e\alpha'\beta'}\Gamma_{\beta'd}(x_3,x_1)-\Big\{\int dx_4\{\Gamma_{dd}(x_1,x_4)\Gamma_{\alpha d}(x_2,x_4)\Gamma_{\alpha' d}(x_3,x_4)\rho(x_4)\\
&+\Gamma_{dd}(x_1,x_4)\Gamma_{\alpha d}(x_2,x_4)\Gamma_{\alpha' e}(x_3,x_4)+\Gamma_{dd}(x_1,x_4)\Gamma_{\alpha e}(x_2,x_4)\Gamma_{\alpha' d}(x_3,x_4)\\
&+\Gamma_{de}(x_1,x_4)\Gamma_{\alpha d}(x_2,x_4)\Gamma_{\alpha' d}(x_3,x_4)\}+\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_1,x_4)\Gamma_{\alpha\mu}(x_2,x_5)\Gamma_{\alpha'\nu}(x_3,x_6)\\
&\times J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Big\}\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\{\Gamma_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\beta'}(x_2,x_3)\\
&+\Gamma_{\beta\gamma'}(x_2,x_3)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta' d}(x_3,x_1)+\Gamma_{\beta' d}(x_3,x_1)\Gamma_{d\beta}(x_1,x_2)\\
&+2\Gamma_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\gamma\gamma'}(x_2,x_3)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta' d}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{\alpha\lambda}(x_2,x_4)\Gamma_{\alpha'\mu}(x_3,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_1,x_4,x_5)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\{\Gamma_{\beta\beta'}(x_2,x_3)\\
&-\Gamma_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}G_{\delta\gamma'}(x_2,x_3)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta' d}(x_3,x_1)\}+\int dx_4dx_5\Gamma_{\alpha'\lambda}(x_3,x_4)\Gamma_{d\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)\\
&\times C^{\alpha\lambda'\mu'}(x_2,x_4,x_5)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\{\mathcal{G}^{\beta dd}\Gamma_{\beta' d}(x_3,x_1)-\Gamma_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\gamma'}(x_2,x_3)\mathcal{G}^{\beta'\gamma'\delta'}G_{\delta' d}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{d\lambda}(x_1,x_4)\Gamma_{\alpha\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{\alpha'\lambda'\mu'}(x_3,x_4,x_5)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\{\mathcal{G}^{\beta' dd}\Gamma_{d\beta}(x_1,x_2)\\
&-G_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\gamma'}(x_2,x_3)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta' d}(x_3,x_1)\}\\
&+\int dx_4\Gamma_{d\lambda}(x_1,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'\alpha\alpha'}(x_4,x_2,x_3)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\{\mathcal{G}^{\beta' dd}\Gamma_{d\beta}(x_1,x_2)+\mathcal{G}^{\beta dd}\Gamma_{d\beta'}(x_1,x_3)\\
&+\Gamma_{d\beta}(x_1,x_2)\Gamma_{d\beta'}(x_1,x_3)\}+\int dx_4\Gamma_{\alpha\lambda}(x_2,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda' b\alpha'}(x_4,x_1,x_3)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\{\mathcal{G}^{\beta' dd}\Gamma_{d\beta}(x_1,x_2)\\
&+\Gamma_{\beta\beta'}(x_2,x_3)+\Gamma_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\beta}(x_2,x_3)\}+\int dx_4\Gamma_{\alpha'\lambda}(x_3,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda' b\alpha}(x_4,x_1,x_2)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\\
&\times\{\mathcal{G}^{\beta dd'}\Gamma_{\beta' d}(x_3,x_1)+\Gamma_{\beta'\beta}(x_3,x_2)+\Gamma_{d\gamma'}(x_1,x_3)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta'\beta}(x_3,x_2)\}\\
&+Z^{d\alpha\alpha'}(x_1,x_2,x_3)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}G_{d\gamma}(x_1,x_2)\mathcal{G}^{\beta\gamma\delta}G_{\delta\gamma'}(x_2,x_3)\mathcal{G}^{\beta'\gamma'\delta'}G_{\delta' d}(x_3,x_1),
\end{aligned}
\tag{A4}
$$

$$
\begin{aligned}
C^{eee}(x_1,x_2,x_3)=&\,\Gamma_{\beta\alpha'}(x_1,x_2)\mathcal{G}^{e\alpha'\beta'}\Gamma_{\beta'\alpha''}(x_2,x_3)\mathcal{G}^{e\alpha''\beta''}\Gamma_{\beta''\alpha}(x_3,x_1)\mathcal{G}^{e\alpha\beta}\\
&-\Big\{\int dx_4\{\Gamma_{\alpha d}(x_1,x_4)\Gamma_{\alpha' d}(x_2,x_4)\Gamma_{\alpha'' d}(x_3,x_4)\rho(x_4)+\Gamma_{\alpha d}(x_1,x_4)\Gamma_{\alpha' d}(x_2,x_4)\Gamma_{\alpha'' e}(x_3,x_4)\\
&+\Gamma_{\alpha d}(x_1,x_4)\Gamma_{\alpha' e}(x_2,x_4)\Gamma_{\alpha'' d}(x_3,x_4)+\Gamma_{\alpha e}(x_1,x_4)\Gamma_{\alpha' d}(x_2,x_4)\Gamma_{\alpha'' d}(x_3,x_4)\}\\
&+\int dx_4dx_5dx_6\Gamma_{\alpha\lambda}(x_1,x_4)\Gamma_{\alpha'\mu}(x_2,x_5)\Gamma_{\alpha''\nu}(x_3,x_6)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Big\}\\
&\times\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}\{\Gamma_{\beta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta'\beta''}(x_2,x_3)+\Gamma_{\beta'\gamma''}(x_2,x_3)\mathcal{G}^{\beta''\gamma''\delta''}\Gamma_{\delta''\beta}(x_3,x_1)\\
&+\Gamma_{\beta''\gamma}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\beta'}(x_1,x_2)+2\Gamma_{\delta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta'\gamma''}(x_2,x_3)\mathcal{G}^{\beta''\gamma''\delta''}\Gamma_{\delta''\gamma}(x_3,x_1)\}\\
&+\int dx_4dx_5\Gamma_{\alpha'\lambda}(x_2,x_4)\Gamma_{\alpha''\mu}(x_3,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{\alpha\lambda'\mu'}(x_1,x_4,x_5)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}
\end{aligned}
$$

$$\times\{\mathcal{G}^{\beta dd}\Gamma_{\beta'\beta''}(x_2,x_3)-\Gamma_{\delta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}G_{\delta'\gamma''}(x_2,x_3)\mathcal{G}^{\beta''\gamma''\delta''}\Gamma_{\delta''\gamma}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}\}$$

$$+\int dx_4dx_5\Gamma_{\alpha''\lambda}(x_3,x_4)\Gamma_{\alpha\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{\alpha'\lambda'\mu'}(x_2,x_4,x_5)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}$$

$$\times\{\mathcal{G}^{\beta' dd}\Gamma_{\beta''\beta}(x_3,x_1)-\Gamma_{\delta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta'\gamma''}(x_2,x_3)\mathcal{G}^{\beta''\gamma''\delta''}G_{\delta''\gamma}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}\}$$

$$+\int dx_4dx_5\Gamma_{\alpha\lambda}(x_1,x_4)\Gamma_{\alpha'\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{\alpha''\lambda'\mu'}(x_3,x_4,x_5)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}$$

$$\times\{\mathcal{G}^{\beta'' dd}\Gamma_{\beta\beta'}(x_1,x_2)-G_{\delta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta'\gamma''}(x_2,x_3)\mathcal{G}^{\beta''\gamma''\delta''}\Gamma_{\gamma''\gamma}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}\}$$

$$+\int dx_4\Gamma_{\alpha\lambda}(x_1,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'\alpha'\alpha''}(x_4,x_2,x_3)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}\{\mathcal{G}^{\beta'' dd}\Gamma_{\beta\beta'}(x_1,x_2)+\mathcal{G}^{\beta' dd}\Gamma_{\beta\beta''}(x_1,x_3)$$

$$+\Gamma_{\beta'\gamma}(x_2,x_1)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\beta''}(x_1,x_3)\}$$

$$+\int dx_4\Gamma_{\alpha'\lambda}(x_2,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'\alpha\alpha''}(x_4,x_1,x_3)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}\{\mathcal{G}^{\beta'' dd}\Gamma_{\beta\beta'}(x_1,x_2)$$

$$+\mathcal{G}^{\beta dd}\Gamma_{\beta'\beta''}(x_2,x_3)+\Gamma_{\beta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}\Gamma_{\delta'\beta''}(x_2,x_3)\}$$

$$+\int dx_4\Gamma_{\alpha''\lambda}(x_3,x_4)J^d_{\lambda\lambda'}(x_4)C^{\lambda'\alpha\alpha'}(x_4,x_1,x_2)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}\{\mathcal{G}^{\beta' dd}\Gamma_{\beta''\beta}(x_3,x_1)$$

$$+\mathcal{G}^{\beta dd}\Gamma_{\beta''\beta'}(x_3,x_2)+\Gamma_{\beta\gamma''}(x_1,x_3)\mathcal{G}^{\beta''\gamma'\delta''}\Gamma_{\delta''\beta'}(x_3,x_2)\}$$

$$+Z^{\alpha\alpha'\alpha''}(x_1,x_2,x_3)\mathcal{G}^{e\alpha\beta}\mathcal{G}^{e\alpha'\beta'}\mathcal{G}^{e\alpha''\beta''}G_{\delta\gamma'}(x_1,x_2)\mathcal{G}^{\beta'\gamma'\delta'}G_{\delta'\gamma''}(x_2,x_3)\mathcal{G}^{\beta''\gamma''\delta''}G_{\delta''\gamma}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}$$

$$+\Gamma_{cc}(x_3,x_2)\Gamma_{cc}(x_2,x_1)\Gamma_{cc}(x_1,x_3)$$

$$\times\Bigg\{1+\int dx_4[\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\rho(x_4)+\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{de}(x_3,x_4)$$

$$+\Gamma_{dd}(x_1,x_4)\Gamma_{de}(x_2,x_4)\Gamma_{dd}(x_3,x_4)+\Gamma_{de}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)]$$

$$+\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)\Gamma_{d\nu}(x_3,x_6)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)$$

$$+\int dx_4dx_5\Gamma_{d\lambda}(x_2,x_4)\Gamma_{d\mu}(x_3,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_1,x_4,x_5)$$

$$+\int dx_4dx_5\Gamma_{d\lambda}(x_3,x_4)\Gamma_{d\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_2,x_4,x_5)$$

$$+\int dx_4dx_5\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_3,x_4,x_5)+Z^{ddd}(x_1,x_2,x_3)\Bigg\}$$

$$+S_{cc}(x_2,x_1)\Gamma_{cc}(x_1,x_3)\Gamma_{cc}(x_3,x_2)\Bigg\{\int dx_4\Gamma_{d\lambda}(x_3,x_4)J^d_{\lambda\lambda'}(x_4)C^{dd\lambda'}(x_1,x_2,x_4)$$

$$-\int dx_4[\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\rho(x_4)+\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{de}(x_3,x_4)$$

$$+\Gamma_{dd}(x_1,x_4)\Gamma_{de}(x_2,x_4)\Gamma_{dd}(x_3,x_4)+\Gamma_{de}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)]\Gamma_{dd}(x_1,x_2)$$

$$-\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)\Gamma_{d\nu}(x_3,x_6)$$

$$\times J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Gamma_{dd}(x_1,x_2)$$

$$-\int dx_4dx_5\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_3,x_4)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_2,x_4,x_5)\Gamma_{dd}(x_1,x_2)$$

$$-\int dx_4dx_5\Gamma_{d\lambda}(x_2,x_4)\Gamma_{d\mu}(x_3,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_1,x_4,x_5)\Gamma_{dd}(x_1,x_2)\Bigg\}$$

$$
\begin{aligned}
&+S_{cc}(x_3,x_2)\Gamma_{cc}(x_2,x_1)\Gamma_{cc}(x_1,x_3)\Big\{\int dx_4\Gamma_{d\lambda}(x_1,x_4)J^d_{\lambda\lambda'}(x_4)C^{dd\lambda'}(x_2,x_3,x_4)\\
&-\int dx_4[\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\Gamma_{dd}(x_1,x_4)\rho(x_4)+\Gamma_{dd}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\Gamma_{de}(x_1,x_4)\\
&+\Gamma_{dd}(x_2,x_4)\Gamma_{de}(x_3,x_4)\Gamma_{dd}(x_1,x_4)+\Gamma_{de}(x_2,x_4)\Gamma_{dd}(x_3,x_4)\Gamma_{dd}(x_1,x_4)]\Gamma_{dd}(x_2,x_3)\\
&-\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_2,x_4)\Gamma_{d\mu}(x_3,x_5)\Gamma_{d\nu}(x_1,x_6)\\
&\times J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Gamma_{dd}(x_2,x_3)\\
&-\int dx_4dx_5\Gamma_{d\lambda}(x_2,x_4)\Gamma_{d\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_3,x_4,x_5)\Gamma_{dd}(x_2,x_3)\\
&-\int dx_4dx_5\Gamma_{d\lambda}(x_3,x_4)\Gamma_{d\mu}(x_1,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_2,x_4,x_5)\Gamma_{dd}(x_2,x_3)\Big\}\\
&+S_{cc}(x_1,x_3)\Gamma_{cc}(x_3,x_2)\Gamma_{cc}(x_2,x_1)\Big\{\int dx_4\Gamma_{d\lambda}(x_2,x_4)J^d_{\lambda\lambda'}(x_4)C^{dd\lambda'}(x_3,x_1,x_4)\\
&-\int dx_4[\Gamma_{dd}(x_3,x_4)\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)\rho(x_4)+\Gamma_{dd}(x_3,x_4)\Gamma_{dd}(x_1,x_4)\Gamma_{de}(x_2,x_4)\\
&+\Gamma_{dd}(x_3,x_4)\Gamma_{de}(x_1,x_4)\Gamma_{dd}(x_2,x_4)+\Gamma_{de}(x_3,x_4)\Gamma_{dd}(x_1,x_4)\Gamma_{dd}(x_2,x_4)]\Gamma_{dd}(x_3,x_1)\\
&-\int dx_4dx_5dx_6\Gamma_{d\lambda}(x_3,x_4)\Gamma_{d\mu}(x_1,x_5)\Gamma_{d\nu}(x_2,x_6)\\
&\times J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)J^d_{\nu\nu'}(x_6)C^{\lambda'\mu'\nu'}(x_4,x_5,x_6)\Gamma_{dd}(x_3,x_1)\\
&-\int dx_4dx_5\Gamma_{d\lambda}(x_3,x_4)\Gamma_{d\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\lambda\lambda'}(x_5)C^{d\lambda'\mu'}(x_1,x_4,x_5)\Gamma_{dd}(x_3,x_1)\\
&-\int dx_4dx_5\Gamma_{d\lambda}(x_1,x_4)\Gamma_{d\mu}(x_2,x_5)J^d_{\lambda\lambda'}(x_4)J^d_{\mu\mu'}(x_5)C^{d\lambda'\mu'}(x_3,x_4,x_5)\Gamma_{dd}(x_3,x_1)\Big\}
\end{aligned}
\tag{A5}
$$

Equations (A3) and (A4) can be permuted to give equivalent expressions in which the direct-line and exchange-line connections are on different external points. There are eight equations in all.

(d) Use the following equations to solve for $X^{\lambda\mu\nu}(x_1;x_2,x_3)$:

$$
\begin{aligned}
X^{\lambda\mu\nu}(x_1;x_2,x_3)=&\Big\{\int dx_4[\Gamma_{\alpha d}(x_1,x_4)\Gamma_{\alpha' d}(x_2,x_4)\Gamma_{\alpha'' d}(x_3,x_4)\rho(x_4)+\Gamma_{\alpha d}(x_1,x_4)\Gamma_{\alpha' d}(x_2,x_4)\Gamma_{\alpha'' e}(x_3,x_4)\\
&+\Gamma_{\alpha d}(x_1,x_4)\Gamma_{\alpha' e}(x_2,x_4)\Gamma_{\alpha'' d}(x_3,x_4)+\Gamma_{\alpha e}(x_1,x_4)\Gamma_{\alpha' d}(x_2,x_4)\Gamma_{\alpha'' d}(x_3,x_4)]\\
&+\int dx_4dx_5dx_6\Gamma_{\alpha\sigma}(x_1,x_4)\Gamma_{\alpha'\tau}(x_2,x_5)\Gamma_{\alpha''\upsilon}(x_3,x_6)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)J^d_{\upsilon\upsilon'}(x_6)C^{\sigma'\tau'\upsilon'}(x_4,x_5,x_6)\\
&+\int dx_4dx_5\Gamma_{\alpha'\sigma}(x_2,x_4)\Gamma_{\alpha''\tau}(x_3,x_5)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)C^{\alpha\sigma'\tau'}(x_1,x_4,x_5)\\
&+\int dx_4\Gamma_{\alpha\sigma}(x_1,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\alpha'\alpha''}(x_4;x_2,x_3)\Big\}\mathcal{G}^{\lambda\alpha\beta}\mathcal{G}^{\mu\alpha'\beta'}\mathcal{G}^{\nu\alpha''\beta''}\Gamma_{\beta'\gamma}(x_2,x_1)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\beta''}(x_1,x_3)\\
&+\Big\{\int dx_4dx_5\Gamma_{\alpha\sigma}(x_1,x_4)\Gamma_{\alpha'\tau}(x_2,x_5)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)C^{\alpha''\sigma'\tau'}(x_3,x_4,x_5)\\
&+\int dx_4\Gamma_{\alpha'\sigma}(x_1,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\alpha\alpha''}(x_4;x_2,x_3)\Big\}\mathcal{G}^{\lambda\alpha\beta}\mathcal{G}^{\mu\alpha'\beta'}\mathcal{G}^{\nu\alpha''\beta''}\Gamma_{\beta'\gamma}(x_2,x_1)\mathcal{G}^{\beta\gamma\delta}\Gamma_{\delta\beta''}(x_1,x_3)
\end{aligned}
$$

$$+\left\{\int dx_4 dx_5 \Gamma_{\alpha\sigma}(x_1,x_4)\Gamma_{\alpha''\tau}(x_3,x_5)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)C^{\alpha'\sigma'\tau'}(x_2,x_4,x_5)\right.$$
$$\left.+\int dx_4 \Gamma_{\alpha''\sigma}(x_3,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\alpha\alpha'}(x_4;x_1,x_2)\right\}\mathcal{G}^{\lambda\alpha\beta}\mathcal{G}^{\mu\alpha'\beta'}\mathcal{G}^{\nu\alpha''\beta''}\Gamma_{\beta''\gamma}(x_3,x_1)\mathcal{G}^{\beta\gamma\delta}G_{\delta\beta'}(x_1,x_2)$$
$$+\int dx_4 \Gamma_{\alpha\sigma}(x_1,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\alpha'\alpha''}(x_4;x_2,x_3)\mathcal{G}^{\lambda\alpha\beta}\mathcal{G}^{\mu\alpha'\beta'}\mathcal{G}^{\nu\alpha''\beta''}\{\mathcal{G}^{\beta''dd}\Gamma_{\beta\beta'}(x_1,x_2)$$
$$+\mathcal{G}^{\beta'dd}\Gamma_{\beta\beta''}(x_1,x_3)\}+Z^{\alpha\alpha'\alpha''}(x_1,x_3,x_3)\mathcal{G}^{\lambda\alpha\beta}\mathcal{G}^{\mu\alpha'}\mathcal{G}^{\nu\alpha''\beta''}G_{\beta'\gamma}(x_2,x_1)\mathcal{G}^{\beta\gamma\delta}G_{\delta\beta''}(x_1,x_3) \quad \text{(A6)}$$

(e) Use the following equations to solve for $Y^{\lambda\mu\nu}(x_1,x_2,x_3)$:

$$Y^{\lambda\mu\nu}(x_1,x_2,x_3)=\int dx_4[\Gamma_{\lambda d}(x_1,x_4)\Gamma_{\mu d}(x_2,x_4)\Gamma_{\nu d}(x_3,x_4)\rho(x_4)+\Gamma_{\lambda d}(x_1,x_4)\Gamma_{\mu d}(x_2,x_4)\Gamma_{\nu e}(x_3,x_4)$$
$$+\Gamma_{\lambda d}(x_1,x_4)\Gamma_{\mu e}(x_2,x_4)\Gamma_{\nu d}(x_3,x_4)+\Gamma_{\lambda e}(x_1,x_4)\Gamma_{\mu d}(x_2,x_4)\Gamma_{\nu d}(x_3,x_4)]$$
$$+\int dx_4 dx_5 dx_6 \Gamma_{\lambda\sigma}(x_1,x_4)\Gamma_{\mu\tau}(x_2,x_5)\Gamma_{\nu v}(x_3,x_6)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)J^d_{vv'}(x_6)C^{\sigma'\tau'v'}(x_4,x_5,x_6)$$
$$+\int dx_4 dx_5 \Gamma_{\lambda\sigma}(x_1,x_4)\Gamma_{\mu\tau}(x_2,x_5)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)C^{\sigma'\tau'\nu}(x_4,x_5,x_3)$$
$$+\int dx_4 dx_5 \Gamma_{\mu\sigma}(x_2,x_4)\Gamma_{\nu\tau}(x_3,x_5)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)C^{\sigma'\tau'\lambda}(x_4,x_5,x_1)$$
$$+\int dx_4 dx_5 \Gamma_{\nu\sigma}(x_3,x_4)\Gamma_{\lambda\tau}(x_1,x_5)J^d_{\sigma\sigma'}(x_4)J^d_{\tau\tau'}(x_5)C^{\sigma'\tau'\mu}(x_4,x_5,x_2)$$
$$+\int dx_4 \Gamma_{\lambda\sigma}(x_1,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\mu\nu}(x_4;x_2,x_3)$$
$$+\int dx_4 \Gamma_{\mu\sigma}(x_2,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\nu\lambda}(x_4;x_3,x_1)$$
$$+\int dx_4 \Gamma_{\nu\sigma}(x_3,x_4)J^d_{\sigma\sigma'}(x_4)X^{\sigma'\lambda\mu}(x_4;x_1,x_2). \quad \text{(A7)}$$

The rest of the equations needed for the procedure are already presented in algebraic form in the main part of the paper. They will not be repeated here. The formulas above, while rather complicated and long, are amenable to the generation of computer code to perform the calculations.

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