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Multiple Scattering in Random Media I. Restricted Two-Body Additive Approximation

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We present a microscopic theory of the problem of finding the properties of a particle interacting with potentials located at random sites. The sites are governed by a general probability distribution. The starting point is the multiple scattering equations for the amplitude $\langle k_1|T_\alpha|k_2\rangle$ in terms of the individual scattering amplitudes $\langle k_1|t_\alpha|k_2\rangle$. We work with quantities A_α defined by $\langle k_1|A_\alpha|k_2\rangle = \langle k_1|T_\alpha|k_2\rangle \exp[i(k_1 - k_2)R_\alpha]$. The theory is based on a splitting of the fundamental equation for A into equations for the mean $\overline{A}_\alpha \equiv A$ and the fluctuations δA_α. Neglect of the fluctuations yields the quasicrystalline approximation. We rearrange the equation for δA_α to isolate the collective part of the fluctuations. We then make the simplest microscopic truncation which is that δA_α is a restricted two-body additive function of the site positions. With the contribution of the collective fluctuations, this yields results for A that are accurate to order t^4.

KEY WORDS: Multiple scattering; random media.

1. INTRODUCTION

In the present series of papers we propose an approach to the theory of the propagation of waves in a medium with randomly placed scatterers.[1] For concreteness we focus on the electronic properties of systems with structural disorder. This is a much-studied problem of great practical interest, with a wealth of experimental data to be explained. It thus poses difficult challenges to a general theory.[2]

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The approach followed here diverges at a relatively early stage from standard treatments. We call it a "microscopic" theory of multiple scattering. The total scattering operator T is some function of the positions of the scattering centers, i.e., as a random variable obeying a random operator equation. For a prescribed probability distribution, there is an averaged T operator, which is one of the quantities to be determined. One can formally divide the equations for T into an equation for the average, $\overline{T}$, with a part that is driven by a suitable average involving the fluctuation δT. δT obeys a closely related random operator equation. A natural procedure is to set up a hierarchy of equations involving successively higher-order averaged correlation functions.[3] One is then faced with one problem of defining a truncation scheme. Standard theories operate directly with this "original" hierarchy, defining self-energy functions, vertex functions, etc.

The microscopic approach introduces a number of different viewpoints. First, one can do some rearrangements of the random operator equations. For example, in Section 4 of the present paper we eliminate the collective part of the fluctuations. This leads to a modified hierarchy for the correlation functions. Other manipulations of the microscopic equations are possible. In later papers we introduce a microscopic resolvent operator for the operator equations for the fluctuations. The resolvent, in turn, can be subjected to an analysis in terms of its average and its fluctuation. This allows one to define different hierarchies and truncations.

Second, new types of truncations are suggested by the microscopic theory. The iteration of the random operator equation in powers of the individual scatterer amplitude brings in successively more complex functional dependences of the fluctuations. The idea is to constrain the functional form of the random fluctuation. For example, it may be taken to be a two-body additive function of the site positions. This fixes all of the average correlation functions. It defines a truncation of higher-order correlation functions as linear functionals of lower-order functions. It is used in conjunction with suitable hierarchy equations. There is guaranteed accuracy to a given order in the individual scattering operators.

This same naive idea was the basis of our earlier work on the classical kinetic theory of fluids.[4] There it was used to provide truncation schemes for the Liouville equation. The truncations inevitably involve static correlation functions of higher order than the pair distribution. The point of view is that these static functions are given. Approximations such as the Kirkwood superposition approximation are made at a later stage, with reference to the particular system.

In the present work on multiple scattering theory, the first two papers correspond to the most primitive approach to kinetic theory. We use two

elementary truncations, namely, the restricted two-body approximation (2BA) and the general 2BA. In the first (present) paper, we introduce definitions and the basic governing equations in Section 2. In Section 3 we set down the equations for the diagonal and off-diagonal matrix elements of the mean value of a quantity associated with the average T matrix and the self-correlation function. The formal solution is given in terms of integral kernels depending on the fluctuations. Complete neglect of the fluctuations corresponds to Lax's quasicrystalline approximation.

Section 4 contains an analysis and manipulation of the microscopic fluctuation equation. We eliminate the collective part and study a linearized fluctuation theory. We also formulate the first equation of the associated hierarchy of correlation functions. Section 5 treats the restricted 2BA both for the case of totally uncorrelated scatterers and for general correlations. The equations are very simple, and in the case of separable scattering potentials one can find the exact solutions for an arbitrary probability distribution for the scattering centers. The total average-scattering amplitude and self-energy depend on the pair and triplet static distribution. We also superimpose collective contributions on the restricted 2BA and obtain results for the self-energy accurate to order t^4. Section 6 compares the results with two well-known theories. The first is the SCA (self-consistent approximation) of L. Schwartz and H. Ehrenreich.[2] The second is the EMA (effective medium approximation) of L. Roth.[2]

The second paper gives the corresponding analysis for the general 2BA, which is more accurate but more complicated. In later papers we develop a systematic general scheme.

2. GENERAL FORMULATION

Consider the Hamiltonian for an electron of unit mass moving in a potential due to impurities with site positions $\mathbf{R}_1, \ldots, \mathbf{R}_N$ ($\hbar = 1$):

$$H = \frac{p^2}{2} + V, \qquad V = \sum_{\alpha}^{N} v_\alpha \equiv \sum_{\alpha=1}^{N} v(\mathbf{x} - \mathbf{R}_\alpha) \tag{1}$$

The impurities have a probability distribution $W(\mathbf{R}_1, \ldots, \mathbf{R}_N)$. In each configuration there is a microscopic Green's operator in energy space:

$$\begin{aligned} G(E) &= (E + i\epsilon - H)^{-1} \\ G_0(E) &= (E + i\epsilon - p^2/2)^{-1} \end{aligned} \tag{2}$$

We are interested in computing the ensemble averaged Green's operator, in order to calculate the momentum spectral density and density of states.

In standard notation

$$G = G_0 + G_0VG = G_0 + G_0TG_0$$
$$T = V + VG_0T = \Sigma(1 + G_0T) \tag{3}$$

The multiple scattering formalism is introduced via the definitions[5]

$$t_\alpha = v_\alpha + v_\alpha G_0 t_\alpha$$
$$T_\alpha = t_\alpha\Big(1 + G_0 \sum_{\beta\neq\alpha} T_\beta\Big), \qquad T = \sum_{\alpha=1}^{N} T_\alpha \tag{4}$$

The momentum space matrix elements of T_α are

$$\langle \mathbf{k}_1|t_\alpha|\mathbf{k}_2\rangle = \langle \mathbf{k}_1|t|\mathbf{k}_2\rangle \exp\big[\, i(\mathbf{k}_2 - \mathbf{k}_1)\mathbf{R}_\alpha\big] \tag{5}$$

and we use the notation

$$\langle 1|t_\alpha|2\rangle = \langle 1|t|2\rangle \exp\big[\, i(2-1)R_\alpha\big] \tag{6}$$

Now introduce quantities A_α by the definition

$$\langle 1|T_\alpha|2\rangle = \langle 1|A_\alpha|2\rangle \exp\big[\, i(2-1)R_\alpha\big] \tag{7}$$

The basic microscopic equation is

$$\langle 1|A_\alpha|2\rangle = \langle 1|t|2\rangle + \langle 1|tG_0|\underline{3}\rangle \sum_{\beta\neq\alpha} \langle \underline{3}|A_\beta|2\rangle E_{\alpha\beta}(2-\underline{3}) \tag{8}$$

where

$$E_{\alpha\beta}(\lambda) = \exp\big[\, i\lambda(R_\beta - R_\alpha)\big] \tag{9}$$

Wave vectors that are underlined are to be summed.

To characterize the sites we introduce the microscopic two-point function

$$E_2(\lambda| - \lambda) = \sum_{\alpha}^{N} \sum_{\beta\neq\alpha} E_{\alpha\beta}(\lambda) \equiv NF_2(\lambda) \tag{10}$$

with the associated equilibrium pair distribution $\bar{F}_2(\lambda)$. $\bar{F}_2(\lambda)$ is the average, taken with the probability distribution W. It is independent of N and starts as the first power of the density. Because of translation invariance, the average $\bar{A}_\alpha$ is independent of α. To order t^2, in iteration

$$\langle 1|\bar{A}_\alpha|2\rangle = \langle 1|t|2\rangle + \langle 1|tG_0|\underline{3}\rangle\langle \underline{3}|t|2\rangle \bar{F}_2(2-\underline{3}) \tag{11}$$

Note that t is of order Ω^{-1}, where Ω is the volume of the system. Note also that $\bar{F}_2(0) = N$. We also encounter higher-order site correlation functions. The microscopic three-particle distribution is

$$F_3(\lambda_1|\lambda) = \frac{1}{N} \sum_{\alpha\neq\beta\neq\gamma} E_{\gamma\beta}(\lambda_1)E_{\gamma\alpha}(\lambda) \tag{12}$$

The average with W enters as one of the t^3 terms in the expansion of $\bar{A}_\alpha$. $\bar{F}_3$ is also independent of N and starts proportional to the square of the density.

Note that $\bar{A}_\alpha$ has both diagonal and off-diagonal elements. For the diagonal elements we have simply

$$\langle 1|\bar{T}_\alpha|1\rangle = \langle 1|\bar{A}_\alpha|1\rangle \tag{13}$$

For the off-diagonal elements

$$\langle 1|\bar{A}_\alpha|2\rangle = \overline{\langle 1|T_\alpha|2\rangle \exp\left[i(1-2)R_\alpha\right]} \tag{14}$$

Thus these elements represent "self-correlation" functions.

A number of static correlation functions will be encountered throughout the text. Let

$$\begin{aligned} \delta C &= C - \bar{C} \\ E_\alpha^1(\lambda) &= \sum_{\gamma \neq \alpha} E_{\gamma\alpha}(\lambda) \\ E_\alpha^0(\lambda) &= \sum_{\beta \neq \alpha} E_{\alpha\beta}(\lambda) \end{aligned} \tag{15}$$

The simplest static average is

$$\sum_\beta \overline{\delta E_\beta^0(\lambda)\delta E_\beta^1}(\lambda_1) = N\left\{\bar{F}_3(\lambda_1|-\lambda) + \bar{F}_2(\lambda-\lambda_1) - \bar{F}_2(\lambda)\bar{F}_2(\lambda_1)\right\} \tag{16}$$

3. EQUATIONS FOR THE AVERAGE

The first step is to split the basic equation for the A_α into equations for the average $\bar{A}_\alpha$ and the fluctuation δA_α. The average value $\bar{A}_\alpha$ is independent of α ($\bar{A}_\alpha = A$). We introduce a kernel

$$\langle 1|\bar{K}_0(2)|3\rangle = \langle 1|tG_0|3\rangle \bar{F}_2(2-3) \tag{17}$$

It is useful to separate terms involving the wave vector $3 = 2$. The equation for the average A is

$$\begin{aligned} \langle 1|A|2\rangle = {} & \langle 1|t|2\rangle + N\langle 1|tG^0|2\rangle\langle 2|A|2\rangle \\ & + \Delta(\underline{3}|2)\langle 1|\bar{K}_0(2)|\underline{3}\rangle\langle \underline{3}|A|2\rangle \\ & + \langle 1|tG_0|\underline{3}\rangle \sum_{\beta \neq \alpha} \overline{\delta E_{\alpha\beta}(2-\underline{3})\langle \underline{3}|\delta A_\beta|2\rangle}\,\Delta(\underline{3}|2) \end{aligned} \tag{18}$$

The last term expresses the effect of fluctuations and has no contribution from the intermediate state $3 = 2$. The symbol $\Delta(3|2)$ means exclusion of $3 = 2$. It is possible to express δA_α in the form

$$\langle 1|\delta A_\alpha|2\rangle = \langle 1|\Gamma_\alpha(2)|\underline{3}\rangle\langle \underline{3}|A|2\rangle\Delta(\underline{3}|2) \tag{19}$$

This involves only the off-diagonal elements $\langle 3|A|2\rangle$. The effects of fluctuations are contained in a new kernel

$$\langle 1|\bar{K}_1(2)|3\rangle = (1/N)\langle 1|tG_0|\underline{5}\rangle\Delta(\underline{5}\,|\,2)\sum_{\beta}\overline{\delta E^1_\beta(2-\underline{5})\langle \underline{5}|\Gamma_\beta(2)|3\rangle} \tag{20}$$

Now let $\bar{K} = \bar{K}_0 + \bar{K}_1$ and separate the equations for A into diagonal and off-diagonal parts.

$$\begin{aligned}\langle 1|A|2\rangle - \langle 1|\bar{K}(2)|\underline{3}\rangle\langle \underline{3}|A|2\rangle\Delta(\underline{3}|2) &= \langle 1|t|2\rangle\{1 + NG_0(2)\langle 2|A|2\rangle\}\\ \langle 2|A|2\rangle\{1 - N\langle 2|tG_0|2\rangle\} &= \langle 2|t|2\rangle + \langle 2|\bar{K}(2)|\underline{3}\rangle\Delta(\underline{3}|2)\langle \underline{3}|A|2\rangle\end{aligned} \tag{21}$$

In the future all intermediate wave vector sums exclude the value 2 unless indicated otherwise. It will be understood that everything depends parametrically on 2. We introduce a matrix notation and a resolvent matrix $R^* = (1 - \bar{K})^{-1}$, i.e.,

$$\langle 1|R^*|3\rangle - \langle 1|\bar{K}|\underline{4}\rangle\langle \underline{4}|R^*|3\rangle = \delta(1\,|\,3) \tag{22}$$

Then

$$\langle 1|A|2\rangle = \langle 1|R^*t|2\rangle\{1 + NG_0(2)\langle 2|A|2\rangle\} \tag{23}$$

For the diagonal element, we have

$$\begin{aligned}\langle 2|A|2\rangle\{1 - NG_0(2)Q(2)\} &= Q(2)\\ Q(2) &= \langle 2|R^*t|2\rangle\end{aligned} \tag{24}$$

The self-energy $\Sigma(2)$ is related to $\langle 2|A|2\rangle$ by

$$\Sigma(2) = \frac{N\langle 2|A|2\rangle}{1 + NG_0(2)\langle 2|A|2\rangle} = NQ(2) \tag{25}$$

The tasks of the theory are first to evaluate the kernel $\bar{K}_1$, and then to solve the resolvent equation to find R^*. Neglect of fluctuations entirely means setting $\bar{K} = \bar{K}_0$. The resolvent R^* is then obtained by solving the integral equations of the quasicrystalline approximation. Note that by one iteration

$$Q(2) = \langle 2|t|2\rangle + \langle 2|\bar{K}_0R^*t|2\rangle + \langle 2|\bar{K}_1R^*t|2\rangle \tag{26}$$

$\bar{K}_0$ is first order in t and the fluctuation kernel $\bar{K}_1$ is second order in t. Of course, it is easy to achieve accuracy to any desired power of t by iteration. This, however, does not dress propagators properly.

The problem of solving the integral equation for R^* for a given kernel $\bar{K}$ may be attacked by numerical or variational methods. For general theoretical arguments it is appropriate to use Fredholm theory. The books of Smithies[6] and of Watson and Nuttall[7] may be consulted for discussions of cases where the theory must be modified. The resolvent operator is

expressed in terms of the iterated kernels of $\bar{K}$. Let

$$\sigma_n = \mathrm{Tr}(\bar{K})^n \qquad R^* = 1 + D/d \tag{27}$$

The Fredholm formulas are

$$d = \sum_0^\infty d_n, \qquad D = \sum_0^\infty D_n$$
$$d_0 = 1, \qquad d_1 = -\sigma_1, \qquad d_2 = \tfrac{1}{2}(\sigma_1^2 - \sigma_2) \tag{28}$$
$$D_0 = \bar{K}, \qquad D_1 = \bar{K}^2 - \bar{K}\sigma_1$$

The higher-order terms are computed from the recurrence relations

$$d_n = -(1/n)\mathrm{Tr}\, D_{n-1} \qquad D_n = d_n\bar{K} + \bar{K}D_{n-1} \tag{29}$$

If the kernel $\langle 1|\bar{K}(2)|3\rangle = \bar{K}(2;3)$ is independent of the first wave vector, we have $\bar{K}^2 = \bar{K}\sigma_1$, so that $D_1 = d_2 = 0$. The Fredholm expansion then terminates. This is the case for the one-dimensional delta function potential. Then

$$\Sigma(2) = Nt\langle 2|R^*|2\rangle = Nt/D(2) \qquad D(2) = 1 - \bar{K}(2;\underline{3}) \tag{30}$$

The QCA result uses $\bar{K}_0(2;3) = tG_0(3)\bar{F}_2(2-3)$, $\bar{K}_1 = 0$.

In the rest of this section we indicate the values of $\bar{K}_1$ that result from the analysis of the fluctuations by simple truncations.

The simplest noniteration truncation is the restricted 2BA. It is

$$\langle 1|\Gamma_\alpha(2)|3\rangle = \langle 1|H(2)|3\rangle\delta E_\alpha^0(2-3) \tag{31}$$

The function $\langle 1|H(2)|3\rangle \to \langle 1|tG_0|3\rangle$ as $t \to 0$. This two-body additive term agrees with the leading source term that drives the fluctuations. It guarantees at least t^3 accuracy for $Q(2)$. $\langle 1|H(2)|3\rangle$ will be determined by satisfying a hierarchy equation.

In the restricted 2BA, the kernel $\bar{K}_1$ may be written as

$$\begin{aligned}\langle 1|\bar{K}_1(2)|3\rangle = {} & \langle 1|tG_0|3\rangle\bar{F}_2(2-3) + N\langle 1|tG_0|3\rangle\langle 3|H|3\rangle \\ & + \langle 1|tG_0|\underline{5}\rangle\langle \underline{5}|H|3\rangle\bar{F}_2(3-\underline{5})\Delta(\underline{5}\,|\,3) \\ & + N\langle 1|tG_0|3\rangle\langle 3|H|3\rangle\bar{F}_2(2-3) \\ & + \langle 1|tG_0|\underline{5}\rangle\langle \underline{5}|H|3\rangle\{\bar{F}_3(3-\underline{5}\,|\,\underline{5}-2) \\ & - \bar{F}(2-\underline{5})F_2(2-3)\}\Delta(\underline{5}\,|\,3)\end{aligned} \tag{32}$$

In the first step in iteration for Γ_α, when $H \to tG_0$, the term on the first line (viz., $\bar{K}_0$) is $\sim nt$, where n is the density of scatterers. Note that the correlation functions $\bar{F}_2$ and $\bar{F}_3$ go as n and n^2, respectively, at low densities. The terms on the second line are of order nt^2. The third and fourth terms are of order n^2t^2.

It is to be noted that even the lowest approximation involves the three-particle static correlation function. This is necessary if one is to achieve t^3 accuracy for $Q(2)$.

In the completely random system, in this restricted 2BA, the off-diagonal elements $\langle 5|H|3\rangle$ do not contribute to K_1 because of the trivial nature of the static correlation functions. In addition $\bar{K}_0$ is zero. Then

$$\langle 1|\bar{K}_1(2)|3\rangle = N\langle 1|tG_0|3\rangle\langle 3|H|3\rangle \tag{33}$$

Anticipating our results, we find for the fully random system

$$\begin{aligned} \langle 3|H|3\rangle &= \langle 3|t|3\rangle G_0^*(3) \\ G_0^*(3) &= G_0(3)\big[1 - N\langle 3|tG_0|3\rangle\big]^{-1} \end{aligned} \tag{34}$$

For the special case of a one-dimensional delta function the scattering matrix $\langle 1|t|2\rangle$ is independent of the wave sectors. Then $\langle 1|\bar{K}_1(2)|3\rangle = Nt^2G_0(3)G_0^*(3)$. The resolvent R^* obeys

$$\langle 1|R^*|3\rangle - Nt^2G_0(\underline{4})G_0^*(\underline{4})\langle \underline{4}|R^*|3\rangle = \delta(1|3) \tag{35}$$

with the solution

$$\langle 1|R^*|3\rangle = \delta(1|3) + \frac{Nt^2G_0(3)G_0^*(3)}{1 - Nt^2G_0(\underline{4})G_0^*(\underline{4})} \tag{36}$$

The self-energy is

$$\Sigma(2) = Nt\langle 2|R^*|\underline{3}\rangle = Nt\big[1 - Nt^2G_0(\underline{4})G_0^*(\underline{4})\big]^{-1} \tag{37}$$

This is independent of the wave vector 2. The addition of collective effects leads to a dependence in the next order in t. This is shown in Section 5.

For this one-dimensional delta function (and also for separable three-dimensional t matrices) it is also possible to derive explicit results for $\Sigma(2)$ for the case of general randomness. The results are contained in Section 5.

The general 2BA provides a more accurate treatment of the fluctuations. We assume

$$\langle 1|\Gamma_\alpha(2)|3\rangle = \langle 1|H(2 - \underline{\lambda}; 2)|3\rangle \delta E_\alpha^0(\underline{\lambda})\Delta(\underline{\lambda}|0) \tag{38}$$

There is a special role for the wave vector $\lambda = 2 - 3$, but now we have a more general function H which is dependent on λ. This functional form is suggested by performing one iteration on the microscopic equation for Γ_α. Again the function H will be determined by forming an appropriate

hierarchy equation. This truncation gives

$$\langle 1|\bar{K}_1(2)|3\rangle = \langle 1|tG_0|2-\underline{\lambda}_1\rangle\langle 2-\underline{\lambda}_1|H(2-\lambda;2)|3\rangle \sum_\beta \frac{\overline{\delta E^0_\beta(\lambda)\delta E^1_\beta(\lambda_1)}}{N} \tag{39}$$

For the fully random (uncorrelated) system

$$\langle 1|\bar{K}_1(2)|3\rangle = N\langle 1|tG_0|2-\underline{\lambda}\rangle\langle 2-\underline{\lambda}|H(2-\underline{\lambda};2)|3\rangle \tag{40}$$

Anticipating our later study of H, we quote for the delta function case

$$\langle 1|\bar{K}_1(2)|3\rangle = Nt^2G_0^*(3)\{G_0(3) + tG_0^*(2-\underline{\lambda})G_0(3-\underline{\lambda}) + \cdots\} \tag{41}$$

4. ANALYSIS OF FLUCTUATIONS

4.1. Manipulation of Fluctuation Equation

The basic fluctuation equation is

$$\begin{aligned}\langle 1|\delta A_\alpha|2\rangle = {} & \langle 1|tG_0|2-\underline{\lambda}\rangle\delta E^0_\alpha(\underline{\lambda})\langle 2-\underline{\lambda}|A|2\rangle \\ & + \langle 1|tG_0|2-\underline{\lambda}\rangle\big(\bar{F}_2(\lambda)/N\big)\Big\langle 2-\underline{1}\Big|\sum_{\beta\neq\alpha}\delta A_\beta\Big|2\Big\rangle \\ & + \langle 1|tG_0|2-\underline{\lambda}\rangle\delta\sum_{\beta\neq\alpha}\delta E_{\alpha\beta}(\underline{\lambda})\langle 2-\underline{\lambda}|\delta A_\beta|2\rangle\end{aligned} \tag{42}$$

This way of writing the equation exhibits a linear part in the fluctuation equation. The linear part is also "collective," i.e., a symmetric sum over particle amplitudes. In the limit $N\to\infty$ one can ignore the restriction $\beta\neq\alpha$ in the collective term.

In the interest of compactness, we define the kernel

$$\langle 1|(K_0)_{\alpha\beta}|3\rangle = N\langle 1|tG_0|3\rangle E_{\alpha\beta}(2-3)(1-\delta_{\alpha,\beta}) \tag{43}$$

The average is the same for every pair and is $(\alpha\neq\beta)$ $\langle 1|\bar{K}_0|3\rangle = \langle 1|tG_0|3\rangle\bar{F}_2(2-3)$.

We will also frequently encounter the sum over the right-hand and left-hand particle indices

$$K^0_\alpha = \sum_\beta (K_0)_{\alpha\beta}, \qquad K^1_\alpha = \sum_\beta (K_0)_{\beta\alpha} \tag{44}$$

and a collective amplitude $\mathcal{A} = \sum_\alpha A_\alpha$. We will use a matrix notation with reference to wave vectors. Then

$$\begin{aligned}\langle 1|\delta A_\alpha|2\rangle = {} & (1/N)\langle 1|\delta K^0_\alpha(2)A|2\rangle + (1/N)\langle 1|\bar{K}_0(2)\delta\mathcal{A}|2\rangle \\ & + (1/N)\delta\Big\langle 1\Big|\sum_{\beta\neq\alpha}(\delta K_0)_{\alpha\beta}\delta A_\beta\Big|2\Big\rangle\end{aligned} \tag{45}$$

The term involving $\bar{K}_0$ includes the wave vector 2 in the matrix sum over intermediate vectors. It does not occur in terms involving δK_0.

A standard approach is to form a hierarchy of equations for correlation functions, starting from this microscopic equation. We will, however, show that it is profitable to manipulate the microscopic equation before proceeding to hierarchy formation.

We form an equation for the collective part

$$\delta\mathcal{A} = (1/N)\sum_\alpha \delta K_\alpha^0 \bar{A} + \bar{K}_0 \delta\mathcal{A} + (1/N)\sum_\beta \delta K_\beta^1 \delta A_\beta \tag{46}$$

and solve for $\delta\mathcal{A}$ using the resolvent $(1-\bar{K}_0)^{-1}$

$$\delta\mathcal{A} = \left(1-\bar{K}_0\right)^{-1}\left\{\sum_\alpha \delta K_\alpha^0 \frac{\bar{A}}{N} + \delta\sum_\beta \delta K_\beta^1 \delta\frac{A_\beta}{N}\right\} \tag{47}$$

Inserting this into the equation for δA_α, we have the revised starting equation

$$\delta A_\alpha = \left\{\delta K_\alpha^0 + \bar{K}_0 \frac{1}{1-\bar{K}_0}\sum_\gamma \frac{\delta K_\gamma^0}{N}\right\}\frac{A}{N}$$
$$+ \delta\sum_\beta (\delta K_0)_{\alpha\beta}\frac{\delta A_\beta}{N} + \bar{K}_0\frac{1}{1-\bar{K}_0}\delta\sum_\beta \frac{\delta K_\beta^1 \delta A_\beta}{N^2} \tag{48}$$

It contains higher-order collective terms of type $\sum_\beta \delta K_\beta^1 \delta A_\beta$. In the present elementary version we do no further manipulations to handle these terms.

We now free the equations of the overall matrix factor $\bar{A}$ by writing

$$\langle 1|\delta A_\alpha|2\rangle = \langle 1|\Gamma_\alpha(2)|\underline{3}\rangle\langle \underline{3}|A|2\rangle\Delta(\underline{3}\,|\,2) \tag{49}$$

Note that because $(\delta K_0)_{\alpha\beta}$ is a fluctuation, we do not encounter the value $3 = 2$ in the sum. Then

$$\langle 1|\Gamma_\alpha(2)|3\rangle = \langle 1|\delta J_\alpha(2)|3\rangle + \delta\sum_{\beta\neq\alpha}\langle 1|\delta L_{\alpha\beta}\Gamma_\beta|3\rangle \tag{50}$$

where

$$\delta J_\alpha(2) = \frac{1}{N}\delta K_\alpha^0 + \frac{1}{N^2}\bar{K}_0\frac{1}{1-\bar{K}_0}\sum_\gamma \delta K_\gamma^0 \tag{51}$$

$$\delta L_{\alpha\beta} = \frac{1}{N}(\delta K_0)_{\alpha\beta} + \frac{\phi_\alpha}{N^2}\bar{K}_0\frac{1}{1-\bar{K}_0}\delta K_\beta^1 \tag{52}$$

Here $\phi_\alpha = 1$ for every α.

We see that this is a nontrivial rearrangement. We can consider the results obtained when one neglects the nonlinear fluctuations. Then Γ_α is given by the source term δJ_α. The first part is a direct two-body additive

term involving $\sum_{\beta\neq\alpha}\delta E_{\alpha\beta}$. The second part is a collective term. For each α it involves $\sum_{\beta}\sum_{\gamma\neq\alpha}\delta E_{\beta\gamma} = \delta E_2$, i.e., pairs of particles not involving the α particle. This consideration suggests natural microscopic truncations when we include the nonlinear terms.

In the linear fluctuation theory the kernel $\bar{K}_1$ is

$$\begin{aligned}\langle 1|\bar{K}_1(2)|3\rangle &= \frac{1}{N^2}\left\langle 1\left|\sum_{\beta}\overline{\delta K_\beta^1\Gamma_\beta(2)}\right|3\right\rangle \\ &= \frac{1}{N}\langle 1|tG_0|\underline{4}\rangle\langle\underline{4}|tG_0|3\rangle\sum_{\alpha}\overline{\delta E_\alpha^1(2-\underline{4})\delta E_\alpha^0}(2-3) \\ &\quad + \langle 1|tG_0|\underline{5}\rangle\left\langle\underline{5}\left|\bar{K}_0\frac{1}{1-\bar{K}_0}tG_0\right|3\right\rangle\overline{\delta F_2(2-\underline{5})\delta F_2}(2-3)\end{aligned} \tag{53}$$

The second, collective contribution vanishes for the uncorrelated system and we have the results of a restricted 2BA with $\langle 1|H|3\rangle = \langle 1|tG_0|3\rangle$. For the case of general correlations there is a collective addition $\langle 1|\Delta_c\bar{K}_1(2)|3\rangle$. For the delta function case the sum over the three variables yields a t^3 correction

$$\Delta_c\bar{K}_1(2;\underline{3}) = \frac{NtG_0(2)+x}{1-x-NtG_0(2)}t^2G_0(\underline{3})G_0(\underline{5})\overline{\delta F_2(2-\underline{5})\delta F_2}(2-\underline{3}) \tag{54}$$

where

$$x = tG_0(\underline{4})\Delta(\underline{4}\,|\,2)\bar{F}_2(2-\underline{4}) \tag{55}$$

This is a t^4 correction to the self-energy.

4.2. Hierarchy Equation

We introduce correlation functions that have a nonzero average. The sum of the wave vectors occurring is zero. This is also the case for microscopic approximations to Γ_α. The simplest correlation functions are

$$\begin{aligned}U_2(\lambda) &= \sum_{\alpha}E_\alpha^1(\lambda)\Gamma_\alpha \\ U_3(\lambda_1\,\|\,\lambda) &= \sum_{\gamma\neq\beta\neq\alpha}E_{\gamma\beta}(\lambda_1)E_{\gamma\alpha}(\lambda)\Gamma_\alpha\end{aligned} \tag{56}$$

These are particle irreducible. We also work with wave-vector-irreducible quantities, i.e., none of the wave vectors is zero. A typical wave-vector-reducible quantity is $U_3(-\lambda\,\|\,\lambda) = NU_2(\lambda)$.

The first hierarchy equation is formed by taking the equation for Γ_α, multiplying by $E_{\gamma\alpha}(\lambda)$ for fixed $\gamma\neq\alpha$, and averaging. Since $E_{\gamma\alpha}(\lambda)\langle 1|\Gamma_\alpha|3\rangle$

is the same for each pair γ, α, we may taken $(1/N)\Sigma_\gamma \Sigma_\alpha \overline{E_{\gamma\alpha}(\lambda)\langle 1|\Gamma_\alpha|3\rangle}$, instead. This is the motivation for defining the collective quantity $U_2(\lambda)$.

The kernel $\bar{K}_1$ is given in terms of U_2 as

$$\langle 1|\bar{K}_1(2)|3\rangle = \langle 1|tG_0|2-\underline{\lambda}\rangle\langle 2-\underline{\lambda}|\bar{U}_2(\underline{\lambda})|3\rangle\Delta(\underline{\lambda}|0) \tag{57}$$

The hierarchy equation for $\bar{U}_2(\lambda)$ is

$$\langle 1|\bar{U}_2(\lambda)|3\rangle = \left\langle 1\left|\sum_\alpha \overline{\delta E_\alpha^1(\lambda)\delta J_\alpha}\right|3\right\rangle + \sum_\alpha \sum_{\beta\neq\alpha} \langle 1|\overline{\delta E_\alpha^1(\lambda)\delta L_{\alpha\beta}\Gamma_\beta}|3\rangle \tag{58}$$

To get a more explicit expression we first isolate the average parts of $\delta E_\alpha^1(\lambda)$ and of $\delta L_{\alpha\beta}$. This leads to

$$\begin{aligned}\langle 1|\bar{U}_2(\lambda)|3\rangle = {} & \left\langle 1\left|\sum_\alpha \overline{\delta E_\alpha^1(\lambda)\delta J_\alpha}\right|3\right\rangle - \bar{F}_2(\lambda)\left\langle 1\left|\frac{1}{1-\bar{K}_0}tG_0\right|2-\underline{\lambda}_1\right\rangle \\ & \langle 2-\underline{\lambda}_1|\bar{U}_2(\lambda)|3\rangle\Delta(\underline{\lambda}_1|0) - \left\langle 1\left|\frac{1}{1-\bar{K}_0}tG_0\right|2-\underline{\lambda}_1\right\rangle \\ & \frac{\bar{F}_2(\underline{\lambda}_1)}{N}\left\langle 2-\underline{\lambda}_1\left|\overline{E_2(\lambda|-\lambda)\sum_\beta \Gamma_\beta}\right|3\right\rangle \\ & + \sum_\alpha \sum_{\beta\neq\alpha} \langle 1|\overline{E_\alpha^1 L_{\alpha\beta}\Gamma_\beta}|3\rangle \end{aligned} \tag{59}$$

Next apply particle and wave vector reducibility to obtain

$$\begin{aligned}\sum_\alpha \sum_{\beta\neq\alpha} \langle 1|E_\alpha^1(\lambda)L_{\alpha\beta}\Gamma_\beta|3\rangle = {} & \langle 1|tG_0|2-\underline{\lambda}_1\rangle\Delta(\underline{\lambda}_1|\lambda)\langle 2-\underline{\lambda}_1|\bar{U}_3(-\lambda\,\|\,\underline{\lambda}_1)|3\rangle \\ & + N\langle 1|tG_0|2-\lambda\rangle\langle 2-\lambda|\bar{U}_2(\lambda)|3\rangle \\ & + \langle 1|tG_0|2-\underline{\lambda}_1\rangle\langle 2-\underline{\lambda}_1|\bar{U}_2(\underline{\lambda}_1-\lambda)|3\rangle\Delta(\underline{\lambda}_1|\lambda) \\ & + \left\langle 1\left|\frac{\bar{K}_0}{1-\bar{K}_0}tG_0\right|2-\underline{\lambda}_1\right\rangle \\ & \times\left\langle 2-\underline{\lambda}_1\left|\overline{\frac{E_2(\lambda|-\lambda)}{N}\sum_\beta E_\beta^1(\lambda_1)\Gamma_\beta}\right|3\right\rangle \end{aligned} \tag{60}$$

We regroup this to write

$$\begin{aligned} & \langle 1|\bar{U}_2(\lambda)|3\rangle - N\langle 1|tG_0|2-\lambda\rangle\langle 2-\lambda|\bar{U}_2(\lambda)|3\rangle \\ & \quad - \langle 1|tG_0|2-\underline{\lambda}_1\rangle\langle 2-\underline{\lambda}_1|\bar{U}_2(\underline{\lambda}_1-\lambda)|3\rangle\Delta(\underline{\lambda}_1|\lambda) \\ & \quad + \bar{F}_2(\lambda)\left\langle 1\left|\frac{1}{1-\bar{K}_0}tG_0\right|2-\underline{\lambda}_1\right\rangle\langle 2-\underline{\lambda}_1|\bar{U}_2(\underline{\lambda}_1)|3\rangle\Delta(\underline{\lambda}_1|0) \\ & = \left\langle 1\left|\sum_\alpha \overline{\delta E_\alpha^1(\lambda)\delta J_\alpha}\right|3\right\rangle + \langle 1|\bar{B}_2(\lambda)+\bar{C}_2(\lambda)|3\rangle \end{aligned} \tag{61}$$

$$\langle 1|\bar{B}_2(\lambda)|3\rangle = \langle 1|tG_0|2-\underline{\lambda}_1\rangle\langle 2-\underline{\lambda}_1|\bar{U}_3(-\lambda\,\|\,\lambda_1)|3\rangle\Delta(\underline{\lambda}_1\,|\,\lambda) \tag{62}$$

$$\begin{aligned}\langle 1|\bar{C}_2(\lambda)|3\rangle &= -\left\langle 1\left|\frac{1}{1-\bar{K}_0}tG_0\right|2-\underline{\lambda}_1\right\rangle\frac{\bar{F}_2(\underline{\lambda}_1)}{N}\left\langle 2-\underline{\lambda}_1\left|\overline{E_2(\lambda\,|\,-\lambda)\sum_\beta\Gamma_\beta}\right|3\right\rangle \\ &\quad+\left\langle 1\left|\frac{\bar{K}_0}{1-\bar{K}_0}tG_0\right|2-\underline{\lambda}_1\right\rangle\left\langle 2-\underline{\lambda}_1\left|\overline{\frac{E_2(\lambda\,|\,-\lambda)}{N}\sum_\beta E^1_\beta(\underline{\lambda}_1)\Gamma_\beta}\right|3\right\rangle\end{aligned} \tag{63}$$

The explicit value of the source term is

$$\begin{aligned}\left\langle 1\left|\sum_\alpha\overline{\delta E^1_\alpha(\lambda)\delta J_\alpha}\right|3\right\rangle &= \langle 1|tG_0|3\rangle\sum_\alpha\overline{\delta E^1_\alpha(\lambda)\delta E^0_\alpha}(2-3) \\ &\quad+\frac{1}{N}\left\langle 1\left|\frac{\bar{K}_0}{1-\bar{K}_0}tG_0\right|3\right\rangle\overline{\delta E_2(\lambda|\,-\lambda)\delta E_2}(2-3\,|\,3-2)\end{aligned} \tag{64}$$

The first term is of order $N(Nt)$ if $\lambda = 2-3$, and of order Nt if $\lambda \neq 2-3$.

If $\lambda = 2-3$, or $\lambda \neq 2-3$, the second term is of order Nt.

In the restricted 2BA where we only consider $\lambda = 2-3$, the collective part of the source does not come into play in the $N\to\infty$ limit. But it does appear in the general 2BA. It also had a finite effect in the linear theory where the form of Γ_α had a term $\sim\delta F_2(2-3)$. We will show that it is easy to enrich the restricted 2BA to include the collective source term. In so doing one achieves t^4 accuracy in the expression for the self-energy.

5. THE RESTRICTED 2BA

5.1. Integral Equation

In the present section we study the microscopic truncation

$$\langle 1|\Gamma_\alpha(2)|3\rangle = \langle 1|H(2)|3\rangle\delta E^0_\alpha(2-3) \tag{31}$$

The object is to find the matrix elements $\langle 1|H(2)|3\rangle$ to construct the kernel $\langle 1|\bar{K}_1(2)|3\rangle$ of Section 2. To fix H we use the hierarchy equation for $\bar{U}_2(\lambda)$ for the special value $\lambda = 2-3$.

We set down the surviving part of the averages in the limit $N\to\infty$. The direct source term becomes

$$\langle 1|\bar{J}_2(2-3)|3\rangle = N^2\langle 1|tG_0|3\rangle\{1+\bar{F}_2(2-3)\} \tag{65}$$

The two-particle correlation functions are

$$\langle 1|\bar{U}_2(2-3)|3\rangle = N^2\langle 1|H|3\rangle\{1+\bar{F}_2(2-3)\} \tag{66}$$

$$\langle 1|\bar{U}_2(\lambda)|3\rangle = N\{1+\bar{F}_2(2-3)\}\bar{I}_0(2-3|\lambda)\langle 1|H|3\rangle, \qquad \lambda \neq 2-3 \tag{67}$$

$$\bar{I}_0(2-3|\lambda) = \frac{\bar{F}_3(2-3|-\lambda)+\bar{F}_2(2-3-\lambda)-\bar{F}_2(\lambda)\bar{F}_2(2-3)}{1+\bar{F}_2(2-3)} \tag{68}$$

The three-particle correlation function is determined by the same H:

$$\langle 1|\bar{U}_2(3-2\,\|\,\lambda_1)|3\rangle = N^2\langle 1|H|3\rangle\bar{F}_2(\lambda_1+3-2) \tag{69}$$

which is the only contribution that survives the $N\to\infty$ limit. Eliminating $\langle 1|H(2)|3\rangle$, we see that the restricted 2BA is equivalent to the truncation

$$\langle 1|\bar{U}_3(3-2\,\|\,\lambda_1)|3\rangle = \frac{\bar{F}_2(\lambda_1+3-2)}{1+\bar{F}_2(2-3)}\langle 1|\bar{U}_2(2-3)|3\rangle \tag{70}$$

$$\langle 1|\bar{U}_2(\lambda)|3\rangle = \langle 1|\bar{U}_2(2-3)|3\rangle\frac{\bar{I}_0(2-3|\lambda)}{N}(2-3|\lambda) \tag{71}$$

One finds that the terms in $\bar{U}_2(\lambda_1)$ involving sums over λ_1 vanish in the $N\to\infty$ limit. $\bar{C}_2(\lambda)$ vanishes while $\bar{B}_2$ contributes.

We thus find the integral equation

$$\begin{aligned}&\langle 1|\bar{U}_2(2-3)|3\rangle - N\langle 1|tG_0|3\rangle\langle 3|\bar{U}_3(2-3)|3\rangle\\ &-\langle 1|tG_0|\underline{\lambda}\rangle\frac{\bar{F}_2(3-\underline{\lambda})}{1+\bar{F}_2(2-3)}\langle 2|\bar{U}_2(2-3)|3\rangle\\ &\quad = N^2\langle 1|tG_0|3\rangle\{1+\bar{F}_2(2-3)\}\end{aligned} \tag{72}$$

In terms of $\langle 1|H|3\rangle$, this is

$$\langle 1|H|3\rangle - N\langle 1|tG_0|3\rangle\langle 3|H|3\rangle - \langle 1|\psi|\underline{\lambda}\rangle\langle\underline{\lambda}|H|3\rangle = \langle 1|tG_0|3\rangle \tag{73}$$

where

$$\langle 1|\psi(2;3)|\lambda\rangle = \frac{\langle 1|tG_0|\lambda\rangle\bar{F}_2(3-\lambda)}{1+\bar{F}_2(2-3)} \tag{74}$$

For complete randomness we have the solution

$$\langle 3|H|3\rangle = \langle 3|tG_0^*|3\rangle \tag{75}$$

which is the result quoted in Section 3. For complete randomness $\langle 1|H|3\rangle$

is not needed for the kernel $\langle 1|\bar{K}_1(2)|3\rangle$, since for $\lambda \neq 2-3$ $\langle 2-\lambda|\bar{U}_2(\lambda)|3\rangle$ vanishes.

5.2. One-Dimensional Delta Function

We return to the general random system, treating the delta-function case when $\langle 1|t|2\rangle$ is independent of the wave vectors. All of the correlation functions are independent of the first wave vector. Then

$$H(3) = \frac{tG_0(3)}{1 - NtG_0(3) - \psi(2;3\,|\,\underline{\lambda})} \tag{76}$$

The kernel $\langle 1|\bar{K}_1(2)|3\rangle$ is

$$\bar{K}_1(2;3) = NtH(2;3)\big[1 + \bar{F}_2(2-3)\big]\left[G_0(3) + \frac{G_0(2-\underline{\lambda})}{N}\bar{I}_0(2-3\,|\,\underline{\lambda})\right] \tag{77}$$

Since both the kernels $\bar{K}_0$ and $\bar{K}_1$ are independent of the first wave vector, we can find the resolvent R^*. This leads to a self-energy

$$\Sigma(2) = Nt/\mathcal{D}(2) \tag{78}$$

$$\mathcal{D}(2) = 1 - tG_0(\underline{3})\bar{F}_2(2-\underline{3}) - NtH(2;\underline{3})\big(1 + \bar{F}_2(2-3)\big)\left[G_0(3) + G_0\frac{(2-\underline{\lambda})}{N}\bar{I}_0(2-3\,|\,\underline{\lambda})\right] \tag{79}$$

The expression for the self-energy has the form of a rational fraction in t. The complete expression in the enriched restricted 2BA is obtained by addition of the contribution of the collective terms. We now turn to this topic.

5.3. Addition of the Collective Contribution

In the restricted 2BA we lose most of the effects of the collective terms. The direct part of the source term for Γ_α is of order t. The treatment of nonlinear fluctuations leads to $tG_0(3) \to tG_0{}^*(3)$ for the zero correlation case. It only gives part of the t^2 term in Γ_α correctly in iteration. The collective part of the source term is also of order t^2. It was treated in the linear fluctuation theory, and gave a finite contribution when there are correlations.

It is a simple matter to include the collective effect along with the restricted 2BA. We demonstrate a procedure for the delta-function case.

Consider the ansatz

$$\Gamma_\alpha = H(3)\left[\delta E_\alpha^0(2-3) + \frac{1}{N}\frac{y}{1-y}\delta E_2(2-3\,|\,3-2)\right]$$
$$= \frac{H(3)}{tG_0(3)}\delta J_\alpha(2;3) \tag{80}$$

$$y = NtG_0(2) + x, \qquad x = tG_0(\underline{5})\bar{F}_2(2-\underline{5})\Delta(\underline{5}|2) \tag{81}$$

The ansatz for Γ_2 is now enhanced to include the collective part of the source term. Since $H(3)\to tG_0(3)$ as $t\to 0$ this will be accurate at least to lowest order. One can now determine H in the same way as before, i.e., multiply Γ_α by $\delta E_\alpha^1(2-3)$, sum over α, and take the average. One finds that in the $N\to\infty$ limit there is no change in $H(2;3)$. Thus there is simply an addition to $\bar{K}_1(2;3)$ due to collective terms. It is

$$\Delta_c^* \bar{K}_1(2;3) = \frac{y}{1-y}H(2;3)\delta\overline{F_2(2-\underline{5})\delta F_2}(2-3)tG_0(\underline{5}) \tag{82}$$

The total kernel is now accurate through order t^3, so that the self-energy is accurate to order t^4.

5.4. General Case

To handle the case of a general $\langle 1|t|2\rangle$ and arbitrary correlations, write

$$\langle 3|\bar{U}_2(2-3)|3\rangle = \frac{\varphi(3)}{1-N\langle 3|tG_0|3\rangle} + \frac{\langle 3|\psi|\underline{\lambda}\rangle\langle 2-\underline{\lambda}|\bar{U}_2(2-3)|3\rangle}{1-N\langle 3|tG_0|3\rangle} \tag{83}$$

$$\varphi(1) = N^2\langle 1|tG_0|3\rangle\{1+\bar{F}_2(2-3)\} \tag{84}$$

We have used the integral equation to express the diagonal elements in terms of the off diagonal $\langle 2-\lambda|\bar{U}_2(2-3)|3\rangle$ for $\lambda\neq 2-3$. The off diagonal $\langle 2-\lambda|\bar{U}_2(\lambda)|3\rangle$ may also be expressed in terms of these quantities. Elimination of the $\langle 3|\bar{U}_2(2-3)|3\rangle$ leads to a new equation

$$\langle 1|\bar{U}_2(2-3)|3\rangle - \langle 1|\psi_1|\underline{\lambda}\rangle\langle\underline{\lambda}|\bar{U}_2(2-3)|3\rangle = \varphi_1(1) \tag{85}$$

$$\varphi_1(1) = \varphi(1)\{1+N\langle 3|tG_0|3\rangle\} \tag{86}$$

$$\langle 1|\psi_1|\lambda\rangle = \langle 1|\psi|\lambda\rangle + N\langle 1|tG_0^*|3\rangle\langle 3|\psi|\lambda\rangle \tag{87}$$

We view everything as driven by $\langle 1|\bar{U}_2(2-3)|3\rangle$. It obeys a nonseparable integral equation. The Fredholm theory gives in lowest order

$$\langle 1|\bar{U}_2(2-3)|3\rangle = \varphi_1(1) + \frac{\langle 1|\psi_1|\underline{\lambda}_1\rangle\varphi_1(\underline{\lambda}_1)}{1-\mathrm{Tr}\psi_1} \tag{88}$$

The kernel $\bar{K}_1$ is

$$\langle 1|\bar{K}_1(2)|3\rangle = (1/N)\langle 1|tG_0|3\rangle\langle 3|\bar{U}_2(2-3)|3\rangle + (1/N)\langle 1|tG_0|2-\underline{\lambda}\rangle(\bar{I}_0/N)(2-3\,|\,\underline{\lambda})\langle 2-\underline{\lambda}|\bar{U}_2(2-3)|3\rangle \tag{89}$$

Eliminating the $\langle 3|\bar{U}_2(2-3)|3\rangle$ we obtain

$$\langle 1|\bar{K}_1(2)|3\rangle = (1/N)\langle 1|tG_0^*|3\rangle\varphi(3) + (1/N)\Big[\langle 1|tG_0^*|3\rangle + \langle 1|tG_0|(2-\underline{\lambda})/N\rangle\bar{I}_0(2-3\,|\,\underline{\lambda})\Big]\langle\underline{\lambda}|\bar{U}_2(2-3)|3\rangle \tag{90}$$

This exhibits explicitly the t^3 correction to $\bar{K}_1$ in the restricted 2BA. To get the complete kernel to order t^3 we have to add the collective contribution.

6. RELATION TO OTHER WORK

We first compare the results of the restricted 2BA with the SCA of Schwartz and Ehrenreich (SE).[7] It will suffice to treat the one-dimensional delta-function case. We define a quantity

$$\langle 1|\sigma|2\rangle = \frac{\langle 1|A|2\rangle}{1 + NG_0(2)\langle 2|A|2\rangle} \tag{91}$$

The SE equations, in our notation, are for the uncorrelated case

$$\langle 1|\sigma|2\rangle = \langle 1|t|2\rangle + \langle 1|A|\underline{3}\rangle NG_0(\underline{3})\langle\underline{3}|\sigma|3\rangle G_0(\underline{3})\langle\underline{3}|t|2\rangle \tag{92}$$

where the bar under wave vectors means a sum. For the delta-function potential $\langle 1|\sigma|2\rangle$ is independent of 1:

$$\sigma(2) = t\big[1 + L\big] \tag{93}$$

In the SE theory L and $\sigma(2)$ are also independent of 2:

$$L = A(\underline{3})NG_0^2(\underline{3})\sigma(\underline{3}) \tag{94}$$

Write

$$1 + L = 1/(1-\xi) \tag{95}$$

Then ξ satisfies a continued fraction

$$\xi = \frac{Nt^2G_0^2(\underline{3})}{1-\xi-NtG_0(\underline{3})} = \frac{Nt^2G_0^2(\underline{3})}{1-NtG_0(\underline{3}) - \dfrac{Nt^2G_0^2(\underline{4})}{1-\xi-NtG_0(\underline{4})}} \tag{96}$$

In the restricted 2BA we found

$$\xi = Nt^2 G_0(\underline{3}) G_0^*(\underline{3}) \tag{97}$$

There is agreement to the first power of t in the denominator of ξ.

We can carry out a corresponding comparison for general randomness. For simplicity we study the delta-function problem. In the present theory we use the total kernel $\bar{K}$ in the restricted 2BA and obtain

$$\sigma(2) = t/\mathfrak{D}(2), \qquad \mathfrak{D}(2) = 1 - \xi(2) \tag{98}$$

as given in Section 5.

The Schwartz–Ehrenreich equations for this case may be written as

$$\sigma(2) = t(1 + M)/\left[1 - \Phi(2)\right] \tag{99}$$

where

$$\Phi(2) = A(\underline{3}) G_0(\underline{3}) \bar{F}_2(2 - \underline{3}) \tag{100}$$

Since

$$A(2) = \frac{\sigma(2)}{\left[1 - NG_0(2)\sigma(2)\right]} \tag{101}$$

$$A(2) = \frac{t(1 + M)}{\left[1 - \Phi(2) - NG_0(2)t(1 + M)\right]} \tag{102}$$

The quantity M is

$$M = A(\underline{3}) G_0(\underline{3}) \sigma(\underline{3}) \left[N + \bar{F}_2(\underline{4} - \underline{3}) G_0(\underline{4})\right] \tag{103}$$

We have to solve the difficult nonlinear integral equation for Φ,

$$\Phi(2) = t \frac{(1 + M) G_0(\underline{3}) \bar{F}_2(2 - \underline{3})}{1 - \Phi(\underline{3}) - NtG_0(\underline{3})(1 + M)} \tag{104}$$

together with a determination of M.

We may write the solution as

$$\sigma(2) = \frac{t}{1 - \xi^*(2)}, \qquad \xi^*(2) = \frac{\Phi(2) + M}{1 + M} \tag{105}$$

We note that M is of order t^2 and $\Phi(2)$ is of order t. To t^2 accuracy we may put $\xi^*(2) \to \Phi(2) + M$ in the SE equations. Here M can be evaluated to the first power in σ

$$M \to t^2 G_0(\underline{3}) \frac{\left[N + G_0(\underline{4}) \bar{F}_2(\underline{3} - \underline{4})\right]}{1 - NtG_0(\underline{3}) - \Phi(\underline{3})} \tag{106}$$

We iterate Φ once and set $M = 0$:

$$\Phi(2) \to tG_0(\underline{3})\bar{F}_2(2-\underline{3}) + \frac{\left[\Phi(\underline{3}) + NtG_0(\underline{3})\right]G_0(\underline{3})\bar{F}_2(2-\underline{3})t}{1 - NtG_0(\underline{3}) - \Phi(\underline{3})} \tag{107}$$

Comparison of this expression with the present theory verifies two obvious points. The first is that even without the collective contribution the restricted 2BA involves the three-point static correlation function and with it a dependence on the wave vector 2. Second, the collective contribution brings in the four-point function and with it a further 2 dependence. This is of course a consequence of the exactness to order t^3. Schwartz and Ehrenreich employ approximations in setting up their equations, so that only the pair distribution enters.

We will only make a comparison with the EMA of L. Roth [8] for the uncorrelated case. As noted by Roth, the theory is then equivalent to earlier theories of Faulkner[9] and Klauder.[10] In the case of general correlations, it is more natural to compare the EMA with the general 2BA.

In the uncorrelated case and a delta-function potential, the EMA is very simple. There is the relation between the exact $G(2)$ and $\Sigma(2)$

$$G(2) = G_0(2)\{1 - G_0(2)\Sigma(2)\}^{-1} \tag{108}$$

Then the self-energy is independent of 2 and approximated by

$$\Sigma(2) = Nt/\left[1 + t\left[I_0 - I\right]\right]$$
$$I_0 = G_0(\underline{3}), \qquad I = G(\underline{4}) \tag{109}$$

We combine the two equations to form the fraction

$$\Sigma = Nt \Big/ \left[1 - t\frac{G_0^2(\underline{3})}{1 - G_0(\underline{3})\Sigma}\right] \tag{110}$$

where we have used $I_0 - I = -G_0(\underline{3})G(\underline{3})\Sigma$. This is identical to the SCA.

Naturally, this comparison of the restricted 2BA with the SCA and the EMA only holds in the small-t region. It is a physically appealing feature of the SCA and EMA that they use exact medium propagators. Of course this leads to difficult computational problems in satisfying self-consistency. However, one can hope that they are reasonable approximations in a larger domain of Nt and t values. The uncertainty lies in the neglect of higher-order elementary scattering acts. The 2BA on the other hand constructs an explicit approximation to the propagator for all values of Nt and t. However, there is no reason to expect it to be accurate for large values of t. The domain of validity of all of these approaches can only be assessed within the framework of a systematic theory.

We have tried to show that the microscopic approach to multiple scattering is quite flexible. With simple rearrangements of the basic equations and with elementary truncations, one can obtain accurate results in the small-t domain. It is also possible to introduce self-consistent propagator theories with a different choice of the linear fluctuation terms. Finally expressions for the average of products of resolvent operators, of a type needed in the study of transport and localization, may be obtained directly.

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