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Multiple Scattering in Random Media.[1] III. Coherent Potential Propagators and Fluctuations

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An earlier microscopic approach to the theory of the averaged resolvent operator for an electron interacting with impurities is formulated in terms of coherent propagators. We study the corrections to the coherent potential approximation arising from fluctuations. For uncorrelated positions of the impurities, the linear, restricted, and general two-body additive approximations to the treatments of fluctuations are studied. For general correlations, the linear and restricted two-body additive approximations are studied. For both coherent and bare propagators, corresponding treatments of fluctuations involve the same correlation functions for impurities.

KEY WORDS: Coherent potential; fluctuations; multiple scattering.

1. INTRODUCTION

In I and II we presented[1] a "microscopic" approach to the theory of the propagation of electron waves in a system of randomly placed scatterers. Specifically, we were concerned with the determination of the average of the resolvent operator $G(E)$ for a prescribed probability distribution for the scatterers. The theory used the multiple-scattering formation and was developed with the bare-electron resolvent operators. The basic microscopic equations involve the site-dependent amplitudes

$$\langle 1|A_\alpha|2\rangle = \langle 1|T_\alpha|2\rangle \exp\left[i(1-2)R_\alpha\right]$$

This quantity is split into a mean value and a fluctuation. The fluctuation equations can be subjected to exact manipulations that exhibit collective

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contributions. Study of a linear approximation for the fluctuations yielded corrections to the quasicrystalline approximation.[2] The corrections involve the triplet as well as the pair static correlation functions. We also introduced the restricted and general two-body additive approximations for the functional dependence of the A_α on the scatterer positions. These, and more general microscopic assumptions, lead to truncations for a modified hierarchy of correlation functions for the scattering amplitudes.

In the present paper we rework these ideas, using a coherent potential resolvent operator in place of the bare-electron resolvent. The new resolvent is defined in terms of the exact self-energy operator $\Sigma(k \mid E)$ as the diagonal operator,

$$G_1(k \mid E) = \left\langle k \middle| \left[E - k^2/2 - \Sigma(k|E) \right]^{-1} \middle| k \right\rangle$$

The adaptation to the coherent potential propagator follows the prescriptions of Faulkner,[3] Gyorffy,[4] and Korringa and Mills.[5] Different developments of the coherent potential idea are given by Schwartz and Ehrenreich[6] and by Roth.[7] Our concern is to go beyond the coherent potential approximation (C.P.A.) to include fluctuation effects. It turns out to be easy to take over the results of I and II, and there is a one-to-one correspondence between the formulas for coherent and bare propagators. In particular, the treatment of fluctuations to the same accuracy (i.e., microscopic functional form) involves the same static correlation functions. We show that linear fluctuation theory gives no change in the coherent potential result for the uncorrelated case. This shows explicitly that the self-consistent C.P.A. incorporates some fluctuation effects of a theory based on bare propagators, and that it has a certain "stability." There are, however, changes for the system with general correlations, even when fluctuations are treated in the linear approximation or restricted two-body approximation (2BA). For the uncorrelated case, these changes appear in the general 2BA and higher accuracy approximations.

The use of exact propagators is physically appealing and is the general procedure in quantum field theory and many-body theory. In the present problem it was first introduced by Klauder[8] in a study of the uncorrelated case. To have convincing results one needs a systematic and controlled treatment of fluctuations. Since we use the multiple scattering formalism, the fluctuation analysis is directly in terms of the t matrix for single-atom scattering, rather than in terms of the potential. The way that the coherent potential is treated here is close in spirit to the general theory of the complex wave number and energy-dependent optical potential as developed in nuclear physics by Watson[9] and by Feshbach.[10] Here, the site-averaged scattering matrix is calculated with modified atomic-scattering matrices, with exact propagators, and with a suitable treatment of fluctuations. Then it is set equal to zero to determine the optical or coherent potential self-consistently.

2. INTRODUCTION OF THE COHERENT POTENTIAL

We adapt the results in I and II to the coherent potential propagator. The starting point is

$$\begin{aligned} G &= G_0 + G_0 V G \\ &= G_0 + G_0 T G_0 \end{aligned} \tag{1}$$

$$\begin{aligned} T &= V + V G_0 T, \qquad V = \Sigma_\alpha v_\alpha \\ G_0 &= (E - H_0)^{-1}, \qquad G = (E - H)^{-1} \end{aligned} \tag{2}$$

We introduce a potential $\Sigma(2 \mid E)$ and use a propagator

$$G_1(2) = \left[E - \Sigma(2 \mid E) - H_0 \right]^{-1} \tag{3}$$

The exact G also obeys

$$G = G_1 + G_1(V - \Sigma)G = G_1 + G_1 T^1 G_1 \tag{4}$$

We introduced the multiple-scattering description

$$\begin{aligned} T_\alpha &= t_\alpha\left(1 + G_0 \Sigma_{\beta \neq \alpha} T_\beta\right), \qquad T = \Sigma_\alpha T_\alpha \\ t_\alpha &= v_\alpha(1 + G_0 t_\alpha) \end{aligned} \tag{5}$$

We now introduce

$$T_\alpha^1 = t_\alpha^1\left(1 + G_1 \Sigma_{\beta \neq \alpha} T_\beta^1\right), \qquad T^1 = \Sigma_\alpha T_\alpha^1 \tag{6}$$

In order to have

$$T^1 = (V - \Sigma) + (V - \Sigma) G_1 T^1 \tag{7}$$

we take t_α^1 to satisfy

$$t_\alpha^1 = \left(v_\alpha - \frac{\Sigma}{N}\right) + \left(v_\alpha - \frac{\Sigma}{N}\right) G_1 t_\alpha^1 \tag{8}$$

In fact, keeping track of $1/N$ effects, the matrix amplitudes that satisfy

$$t' = \left(v - \frac{\Sigma}{N}\right) + \left(v - \frac{\Sigma}{N}\right) G_1 t^1 \tag{9}$$

can be replaced for the off-diagonal elements by

$$t_1 = v + v G_1 t_1 \tag{10}$$

i.e.,

$$\langle 1 | t_1 | 2 \rangle = \langle 1 | t^1 | 2 \rangle \qquad \text{for } 1 \neq 2 \tag{11}$$

But for the diagonal elements we have

$$\langle 1|t^1|1\rangle + \frac{\Sigma(1)}{N} = \langle 1|t_1|1\rangle \tag{12}$$

Thus there is a discontinuity in $\langle 1|t^1|2\rangle$ as $2 \to 1$. This is necessary since the total scattering in the strictly forward direction is different from that at any finite angle.

The object of introducing the Σ is to describe the coherent wave. After suitable approximations to treat fluctuations, and after averaging over site variables, we set

$$\langle 1|\overline{T}^1|1\rangle = 0 \tag{13}$$

as a condition to fix Σ. Hence

$$\overline{G}_1(1) = G_1(1) = G_0(1) + G_0(1)\overline{T}(1)G_0(1) \tag{14}$$

In sum, the conditions (12) and (13) determine Σ and $\langle 1|t^1|1\rangle$. The relation between t_1 and t is

$$t_1 = t + t(G_1 - G_0)t_1 \tag{15}$$

If we wish, we can eliminate t_1 in favor of t. For the delta function potential, t is the same for all matrix elements, diagonal as well as off-diagonal. The same thing is true for t_1 and

$$t_1 = \frac{t}{1 + t\left[G_0(\underline{3}) - G_1(\underline{3})\right]} \tag{16}$$

This relation involves Σ, which is independent of the wave vector for the delta function case.

The basic equation for $\langle 1|T_\alpha^1|2\rangle$ is now set up in terms of $\langle 1|t^1|2\rangle$. For the off-diagonal elements

$$\begin{aligned}\langle 1|A_\alpha^1|2\rangle &= \langle 1|t^1|2\rangle\left[1 + G_1(2)\Sigma_{\beta\neq\alpha}\langle 2|A_\beta^1|2\rangle\right] \\ &\quad + \langle 1|t^1G_1|\underline{3}\rangle\Delta(\underline{3}\,|\,2)\Sigma_{\beta\neq\alpha}E_{\alpha\beta}(2-\underline{3})\langle \underline{3}|A_\beta^1|2\rangle\end{aligned} \tag{17}$$

The equation for the diagonal elements has the same form with $1 \to 2$. Of course, we have to treat the diagonal t^1 terms carefully.

The formulation is now on the same footing as the earlier theory based on the free-electron propagator G_0. Even for the delta function potential, there are now two scattering amplitudes, viz., t_1 for the off-diagonal elements and $\langle 2|t^1|2\rangle = t_1 - \Sigma(2)/N$ for the diagonal elements. We fix attention on an initial wave vector 2, which will be a parameter throughout the discussion.

Let $\hat{K}_0^1$ be a matrix in particle space

$$\left\langle 1\left|\left(K_0^1\right)_{\alpha\beta}\right|3\right\rangle = N\langle 1|t^1G_1|3\rangle\Delta(3\,|\,2)E_{\alpha\beta}(2-3) \tag{18}$$

Let A^1 be the vector A_α and let ϕ be the vector $\phi_\alpha = 1$. Then

$$\left\langle 1\middle|\left(\overline{K}_0^1\right)_{\alpha\beta}\middle|3\right\rangle = \langle 1|t^1G_1|3\rangle \overline{F}_2(2-3)\Delta(3\,|\,2)(1-\delta_{\alpha,\beta})$$
$$= \left\langle 1\middle|\overline{K}_0^1\middle|3\right\rangle(1-\delta_{\alpha,\beta}) \tag{19}$$

is the same for every pair α, β when $\alpha \neq \beta$. This definition of $\overline{K}_0^1$ differs from that of $\overline{K}_0$ in I and II in that we now have a factor $\Delta(3\,|\,2)$. We will separate the terms involving $G_1(2)$ explicitly.

Our new starting point is

$$\langle 1|\mathbf{A}^1|2\rangle = \langle 1|t^1|2\rangle\boldsymbol{\phi} + \boldsymbol{\phi}\langle 1|t^1G_1|2\rangle\langle 2|\boldsymbol{\phi}\cdot\mathbf{A}^1|2\rangle$$
$$+\boldsymbol{\phi}\left\langle 1\middle|\frac{\overline{K}_0^1}{N}\boldsymbol{\phi}\cdot\mathbf{A}^1\middle|2\right\rangle + \left\langle 1\middle|\frac{\delta\hat{K}_0^1}{N}\mathbf{A}^1\middle|2\right\rangle \tag{20}$$

This holds for the diagonal element as well, i.e., $1\to 2$. Note that the wave vector 2 does not appear in the sums over wave vectors that arise in matrix multiplications.

The first step is to find exact expressions for the mean values in terms of fluctuations. The fluctuation contribution to the mean value $\langle 1|\overline{A}_\alpha^1|2\rangle$ is

$$\overline{\Sigma_{\beta\neq\alpha}\left\langle 1\middle|\frac{(\delta k_0^1)_{\alpha\beta}}{n}\middle|\underline{3}\right\rangle\langle\underline{3}|\delta\mathbf{A}_\beta^1|2\rangle}$$

We will see that we can write

$$\begin{aligned}\left\langle 3|\delta A_\beta^1|2\right\rangle &= \left\langle 3|\Gamma_\beta^1|\underline{4}\right\rangle\left\langle\underline{4}|\overline{A}^1|2\right\rangle\\ \left\langle 3|\Gamma_\beta^1|2\right\rangle &= 0\end{aligned} \tag{21}$$

Using $\boldsymbol{\Gamma}^1$ to describe the fluctuations, we define a fluctuation kernel

$$\left\langle 1\middle|\left(\overline{K}_F\right)_{\alpha\beta}\middle|3\right\rangle = \left\langle 1\middle|\overline{\left(\delta K_0^1\right)_{\alpha\beta}\Gamma_\beta^1}\middle|3\right\rangle$$
$$= (1/N^2)\left\langle 1\middle|\boldsymbol{\phi}\,\overline{\delta\hat{K}_0^1\boldsymbol{\Gamma}}\middle|3\right\rangle\Delta(3\,|\,2)(1-\delta_{\alpha,\beta})$$
$$\equiv\langle 1|\overline{K}_F|3\rangle(1-\delta_{\alpha,\beta}) \tag{22}$$

This relies on the fact that $(\overline{K}_F)_{\alpha\beta}$ is again independent of the pair α, β.

The equation for the mean value $\overline{A}_\alpha^1 \equiv \overline{A}^1$ is

$$\langle 1|\overline{A}^1|2\rangle = \langle 1|t^1|2\rangle\left[1 + NG_1(2)\langle 2|\overline{A}^1|2\rangle\right] + \langle 1|\overline{K}^1\overline{A}^1|2\rangle \tag{23}$$

where

$$\overline{K}^1 = \overline{K}_0^1 + \overline{K}_F \tag{24}$$

The term containing $\overline{K}^1$ only involves the off-diagonal $\langle 3|\overline{A}^1|2\rangle$. A separate equation should be written for $1 = 2$.

The coherent potential approach is to define the potential by the condition that the diagonal element $\langle 2|\bar{A}^1|2\rangle = 0$. This yields the off-diagonal element

$$\langle 1|\bar{A}^1|2\rangle = \left\langle 1\left|(1-\bar{K}^1)^{-1}t^1\right|2\right\rangle, \qquad 1 \neq 2 \tag{25}$$

The equation for the diagonal element yields the result

$$\langle 2|t^1|2\rangle = -\left\langle 2\left|\bar{K}^1(1-\bar{K}^1)^{-1}t^1\right|2\right\rangle \tag{26}$$

We thus have the exact formal result for the optical potential

$$\Sigma(2) = N\langle 2|t_1|2\rangle + \left\langle 2\left|\bar{K}^1(1-\bar{K}^1)^{-1}t^1\right|2\right\rangle \tag{27}$$

In the second term we can put $t^1 \to t_1$, since the properties of $\bar{K}$ ensure that the diagonal $\langle 2|t^1|2\rangle$ does not occur. Finally we have the more compact form

$$\Sigma(2) = N\left\langle 2\left|(1-\bar{K})^{-1}t_1\right|2\right\rangle \tag{28}$$

The standard coherent potential approximation involves the complete neglect of the fluctuation kernel $\bar{K}_F$. For the case of a delta function potential we have the explicit result:

$$\left\langle 1|\bar{K}_0^1|3\right\rangle = x_1(2) \tag{29}$$

$$x_1(2) = t_1 G_1(\underline{3})\bar{F}_2(2-\underline{3})\Delta(\underline{3}\,|\,2) \tag{30}$$

$$\Sigma(2) = \frac{Nt_1}{1-x_1(2)} \tag{31}$$

In terms of the strength v of the delta potential

$$\Sigma(2) = \frac{Nv}{1 - vG_1(\underline{4}) - vG_1(\underline{3})\bar{F}_2(2-\underline{3})\Delta(\underline{3}\,|\,2)} \tag{32}$$

3. EQUATION DESCRIBING FLUCTUATIONS

To include the effects of fluctuations, we note that the off-diagonal fluctuation obeys the equation

$$\begin{aligned}\langle 1|\delta\mathbf{A}^1|2\rangle - \phi\left\langle 1\left|\frac{\bar{K}_0^1}{N}\phi\,\delta\mathbf{A}^1\right|2\right\rangle &= \left\langle 1\left|\frac{\delta\hat{K}_0^1}{N}\phi\bar{A}^1\right|2\right\rangle + \phi\langle 1|t^1G_1|2\rangle\langle 2|\phi\,\delta\mathbf{A}^1|2\rangle \\ &\quad + \delta\left\langle 1\left|\frac{\delta\hat{K}_0^1}{N}\delta\mathbf{A}^1\right|2\right\rangle \end{aligned} \tag{33}$$

The terms on the left-hand side involve the off-diagonal fluctuations. On the right-hand side we only require the collective part of the diagonal fluctuation. We have

$$\left\{1 - N\langle 2|t^1G_1|2\rangle\right\}\langle 2|\boldsymbol{\phi}\cdot\delta\mathbf{A}^1|2\rangle = \left\langle 2\left|\frac{\delta K_2^1}{N}\bar{A}^1\right|2\right\rangle + \langle 2|\bar{K}_0^1\boldsymbol{\phi}\cdot\delta\mathbf{A}^1|2\rangle$$
$$+\,\delta\left\langle 2\left|\boldsymbol{\phi}\frac{\delta\hat{K}_0^1}{N}\,\delta\mathbf{A}^1\right|2\right\rangle \tag{34}$$

As in I and II, we eliminate the diagonal part of the fluctuations. We do this in a slightly different way so as to have a form with an explicit separation of the wave vector 2.

Define

$$N\langle 1|(P_0)_{\alpha\beta}|3\rangle = \left\langle 1\left|(K_0^1)_{\alpha\beta}\right|3\right\rangle + \phi_\alpha\langle 1|t^1G_1^*|2\rangle\left\langle 2\left|(\boldsymbol{\phi}\cdot\hat{K}_0^1)_\beta\right|3\right\rangle \tag{35}$$

$$G_1^*(2) = \frac{G_1(2)}{1 - N\langle 2|t^1G_1|2\rangle} \tag{36}$$

On eliminating the diagonal part of the fluctuations, we obtain

$$\langle 1|\delta\mathbf{A}^1|2\rangle - \boldsymbol{\phi}\langle 1|\bar{P}_0\boldsymbol{\phi}\cdot\delta\mathbf{A}^1|2\rangle = \langle 1|\delta\hat{P}_0\boldsymbol{\phi}\bar{A}^1|2\rangle + \delta\langle 1|\delta\hat{P}_0\delta\mathbf{A}^1|2\rangle \tag{37}$$

The collective part of the off-diagonal fluctuation obeys

$$\langle 1|\boldsymbol{\phi}\cdot\delta\mathbf{A}^1|2\rangle = \left\langle 1\left|(1 - N\bar{P}_0)^{-1}\delta P_2\bar{A}^1\right|2\right\rangle$$
$$+\,\delta\left\langle 1\left|(1 - N\bar{P}_0)^{-1}\boldsymbol{\phi}\,\delta\hat{P}_0\cdot\delta\mathbf{A}^1\right|2\right\rangle \tag{38}$$

$$\langle 1|P_2|3\rangle = \Sigma_\alpha\Sigma_{\beta\neq\alpha}\langle 1|(P_0)_{\alpha\beta}|3\rangle \tag{39}$$

Eliminating this as well, and setting

$$\langle 1|\delta A_\alpha|2\rangle = \langle 1|\Gamma_2^1|\underline{3}\rangle\langle\underline{3}|\bar{A}^1|2\rangle \tag{40}$$

we have

$$\langle 1|\boldsymbol{\Gamma}^1|3\rangle = \langle 1|\delta\hat{M}_0\boldsymbol{\phi}|3\rangle + \delta\langle 1|\delta\hat{M}_0\boldsymbol{\Gamma}^1|3\rangle \tag{41}$$

$$\langle 1|(\delta M_0)_{\alpha\beta}|3\rangle = \frac{1}{N}\left\langle 1\left|(\delta K_0^1)_{\alpha\beta}\right|3\right\rangle$$
$$+\,\phi_\alpha\left\langle 1\left|(1 - N\bar{P}_0)^{-1}t^1G_1^*\right|2\right\rangle\left\langle 2\left|(\boldsymbol{\phi}\,\delta\hat{K}_0^1)_\beta\right|3\right\rangle$$
$$+\,\frac{\phi_\alpha}{N}\left\langle 1\left|(1 - N\bar{P}_0)^{-1}\hat{P}_0(\boldsymbol{\phi}\cdot\delta\hat{K}_0^1)_\beta\right|3\right\rangle \tag{42}$$

with

$$\left\langle 1|\bar{P}_0|3\right\rangle = \frac{1}{N}\left\langle 1|\bar{K}_0^1|3\right\rangle + \left\langle 1|t^1G_1^*|2\right\rangle\left\langle 2|\bar{K}_0^1|3\right\rangle$$
$$\left\langle 1|\bar{P}_0|2\right\rangle = 0 \tag{43}$$

For the delta function potential, using the fact that

$$G_1^*(2) = G_0(2)\left[1 - Nt_1G_0(2)\right]^{-1} \tag{44}$$

$$\left\langle 1\middle|(\delta M_0)_{\alpha\beta}\middle|3\right\rangle = \frac{1}{N}\left\langle 1\middle|(\delta K_0^1)_{\alpha\beta}\middle|3\right\rangle + \frac{\phi_\alpha}{N^2}\left\langle 1\middle|(\phi\cdot\delta\hat{K}_0^1)_\beta\middle|3\right\rangle\frac{y_1(2)}{1-y_1(2)} \tag{45}$$

$$y_1(2) = Nt_1G_0(2) + x_1(2) \tag{46}$$

4. THE UNCORRELATED CASE

Here the averages $\bar{K}_0^1$ and $\bar{P}_0$ are zero, and $\delta\hat{M}_0 = \hat{M}_0$. We are interested in computing

$$\left\langle 1|\bar{K}_F|3\right\rangle = \frac{1}{N}\left\langle 1|t^1G_1|2-\underline{\lambda}\right\rangle\Delta(\underline{\lambda}\,|\,0)\left\langle 2-\underline{\lambda}\middle|\bar{U}_2^1(\lambda)\middle|3\right\rangle \tag{47}$$

$$\left\langle 1\middle|\bar{U}_2^1(\lambda)\middle|3\right\rangle = \phi\,\overline{\hat{E}(\lambda)\langle 1|\Gamma^1|3\rangle} \tag{48}$$

4.1. Linear Fluctuation Theory and the Restricted 2BA

In the linear fluctuation theory we simply approximate Γ^1 by the source term: Since, following II, we can check that the contribution of the collective part vanishes as $N \to \infty$,

$$\langle 1|\Gamma^1|3\rangle = (1/N)\langle 1|\hat{K}_0\phi|3\rangle \tag{49}$$

Then we have

$$\left\langle 1\middle|\bar{U}_2^1(\lambda)\middle|3\right\rangle = N^2\delta(\lambda\,|\,2-3)\langle 1|t^1G_1|3\rangle \tag{50}$$

We see that only $\langle 3\,|\,\bar{U}_2^1(2-3)\,|\,3\rangle$, i.e., $\langle 3\,|\,\Gamma^1\,|\,3\rangle$ contributes to $\bar{K}_F$. As a result we have a single diagonal element factor $\langle 3\,|\,t^1\,|\,3\rangle$:

$$\left\langle 1|\bar{K}_F|3\right\rangle = N\langle 1|t_1|3\rangle\langle 3|t^1|3\rangle G_1^2(3) \tag{51}$$

Let us first examine the results for a delta function potential. Then we have

$$\left\langle 1|\overline{K}_F|3\right\rangle = Nt_1\left\{t_1 - \frac{\Sigma(3)}{N}\right\}G_1^2(3) \tag{52}$$

$$\Sigma = \frac{Nt_1}{1 - t_1 G_1^2(\underline{3})\left[Nt_1 - \Sigma\right]}$$

The case $1 = 3$ contributes an effect that vanishes as $N \to \infty$. Of course $\Sigma(2)$ is independent of 2. This result is interesting since the solution for Σ that tends to zero as $t_1 \to 0$ is exactly $\Sigma = Nt_1$. Thus, with the coherent potential propagator the linearized fluctuations contribute nothing. The linear fluctuation effects that appeared in the theory based on the bare propagator are included in the self-consistent potential. This is also true for the general scattering matrix $\langle 1|t|2\rangle$.

For the delta function, the linear fluctuation theory based on the bare propagator gave

$$\Sigma = \frac{Nt_1}{1 - Nt^2 G_0^2(\underline{3})} \tag{53}$$

With the coherent potential

$$\Sigma = \frac{Nt}{1 + t\left[G_0(\underline{\lambda}) - G_1(\underline{\lambda})\right]} \tag{54}$$

But

$$G_0(\lambda) - G_1(\lambda) = -G_0(\lambda)G_1(\lambda)\Sigma \tag{55}$$

and in lowest order this tends to

$$-NtG_0(\lambda)G_0(\lambda) \tag{56}$$

In the restricted 2BA, we have the ansatz

$$\langle 1|\boldsymbol{\Gamma}^1|3\rangle = \langle 1|H^1|3\rangle \hat{E}(2-3)\phi \tag{57}$$

with

$$\left\langle 1\middle|\overline{U}_2^1(\lambda)\middle|3\right\rangle = N^2\delta(\lambda\,|\,2-3)\langle 1|H^1|3\rangle \tag{58}$$

$\langle 1|H^1|3\rangle$ is determined by forming an equation for $\overline{U}_2^1(2-3)$ by multiplying the $\boldsymbol{\Gamma}^1$ equation by $\mathbf{E}^1(2-3)$ and averaging. This leads to

$$\langle 1|H^1|3\rangle = \langle 1|t^1 G_1^*|3\rangle \tag{59}$$

With coherent propagators G_1^* is practically equal to G_1 since the denominator differs from unity by only a term of order t_1^4. For the bare propagator G_0^* differed from G_0 by a term of order t.

4.2. Iterations and the General 2BA

A single iteration, again noting that collective contributions vanish, yields

$$\langle 1|\Gamma^1|3\rangle = \frac{1}{N}\langle 1|\hat{K}_0^1\phi|3\rangle + \frac{1}{N^2}\delta\langle 1|\hat{K}_0^2\phi|3\rangle \tag{60}$$

$\hat{K}_0^2\phi$ contains 3BA terms. However, they do not contribute to $\overline{K}_F$ for the uncorrelated system. Thus 3BA terms do not affect the accuracy of Σ through terms of order t_1^4. We find

$$\begin{aligned}\left\langle 3\middle|\overline{U}_2^1(2-3)\middle|3\right\rangle &= N^2\langle 3|t^1G_1|3\rangle\left\{1 + N\langle 3|t^1G_1|3\rangle\right\}\\ \left\langle 4\middle|\overline{U}_2^1(2-4)\middle|3\right\rangle &= N\langle 4|t_1G_1|2+4-3\rangle\langle 2+4-3|t_1G_1|3\rangle\Delta(4\,|\,3)\end{aligned} \tag{61}$$

The fluctuation kernel is

$$\begin{aligned}\langle 1|\overline{K}_F|3\rangle &= \frac{\langle 1|t_1G_1|3\rangle}{N}\left\langle 3\middle|\overline{U}_2^1(2-3)\middle|3\right\rangle\\ &\quad + \frac{\langle 1|t_1G_1|4\rangle}{N}\left\langle 4\middle|\overline{U}_2^1(2-4)\middle|3\right\rangle\Delta(\underline{4}\,|\,3)\end{aligned} \tag{62}$$

The first term is contained in the restricted 2BA. The second term is new and contains no diagonal t^1 elements. For a delta function potential

$$\begin{aligned}\langle 1|\overline{K}_F|3\rangle &= t_1G_1^2(3)\left\{1 + G_1(3)\left[Nt_1 - \Sigma(3)\right]\right\}\left\{Nt_1 - \Sigma(3)\right\}\\ &\quad + Nt_1^3G_1(\underline{4})G_1(\underline{4}-2+3)G_1(3)\Delta(\underline{4}\,|\,3)\end{aligned} \tag{63}$$

To order t_1^4 (we can neglect the first term in K_F which is of order t_1^5),

$$\Sigma(2) = Nt_1\left[1 - Nt_1^3G_1(\underline{4})G_1(\underline{4}-2+3)G_1(3)\right]^{-1} \tag{64}$$

This provides a correction to the coherent potential approximation.

We now turn to the general 2BA. The ansatz is

$$\begin{aligned}\langle 1|\Gamma^1(2)|3\rangle &= \left\langle 1\middle|H^1(2)\middle|3\right\rangle\hat{E}(2-3)\phi\\ &\quad + \left\langle 1\middle|H^1(2-\underline{\lambda})\middle|3\right\rangle\hat{E}(\lambda)\phi\Delta(\underline{\lambda}\,|\,2-3)\end{aligned} \tag{65}$$

We can repeat the analysis of II, changing G_0 to G_1 and t to t^1. In the general 2BA, the three-body correlation function $\overline{U}_3^1$ is zero for the uncorrelated case. A special role is played by $\overline{U}_2^1(2-3)$. In the $N\to\infty$ limit we have

$$\left\langle 1\middle|\overline{U}_2^1(2-3)\middle|3\right\rangle = N^2\langle 1|t^1G_1^*|3\rangle \tag{66}$$

In $1=3$ we encounter $\langle 3|t^1|3\rangle = \langle 3|t_1 - \Sigma(3)/N|3\rangle$.

In $\lambda \neq 2-3$ we have the analog of II, Eq. (29):

$$\left\langle 1\middle|\overline{U}_2^1(\lambda)\middle|3\right\rangle - N\langle 1|t^1G_1|2-\lambda\rangle\left\langle 2-\lambda\middle|\overline{U}_2^1(\lambda)\middle|3\right\rangle$$
$$-\langle 1|t_1G_1|2-\lambda-\underline{\lambda}_1\rangle\left\langle 2-\lambda-\underline{\lambda}_1\middle|\overline{U}_2^1(\underline{\lambda}_1)\middle|3\right\rangle$$
$$= N^2\langle 1|t^1G_1|3-\lambda\rangle\langle 3-\lambda|t^1G_1^*|3\rangle \tag{67}$$

This is a nontrivial integral equation. If it is treated by iteration we find a result for the fluctuation kernel in lowest order that is similar to Eq. (63). Several of the G_1 propagators are replaced by G_1^*. The first iteration of (67) involves the integral $\overline{U}_2(\lambda_1)$ term. Since the leading term in $\overline{U}_2^1(\lambda)$ is already of order t_1^2 this is of order t_1^3 and leads to a t_1^5 correction to the self-energy.

A more detailed analysis is possible for separable potentials. For the delta function potential we use the function $S^1(\lambda\,|\,\lambda_1)$, which is the solution of

$$S^1(\lambda\,|\,\lambda_1)\left\{1-\left[Nt_1-\Sigma(2-\lambda)\right]G_1(2-\lambda)\right\}$$
$$-\frac{Lt_1}{2\pi}\int G_1(2-\lambda-\lambda_2)S^1(\lambda_2\,|\,\lambda_1)\,d\lambda_2 = \delta(\lambda-\lambda_1) \tag{68}$$

Then

$$\left\langle 1\middle|\overline{U}_2^1(\lambda)\middle|3\right\rangle = N^2t_1^2\int S^1(\lambda\,|\,\lambda_1)G_1(3-\lambda_1)\,d\lambda_1\,G_1^*(3) \tag{69}$$

$$\left\langle 1\middle|\overline{K}_F(2)\middle|3\right\rangle = Nt_1\frac{L}{2\pi}\int G_1(\lambda)G_1^*(\lambda)\left[Nt_1-\Sigma(\lambda)\right]d\lambda$$
$$+Nt_1^3\left(\frac{L}{2\pi}\right)^2\int\int\int G_1(2-\lambda)S'(\lambda\,|\,\lambda_1)$$
$$\times G_1(\lambda_2-\lambda_1)G_1^*(\lambda_2)\,d\lambda\,d\lambda_1\,d\lambda_2 \tag{70}$$

The first term is of order t_1^5 and will be dropped (although it is easy to compute it to lowest order).

Through terms of order $(Nt_1)^3$ we can replace $S^1(\lambda\,|\,\lambda_1)$ by $W^1(\lambda\,|\,\lambda_1)$, which is the solution of

$$W^1(\lambda\,|\,\lambda_1)-\frac{Lt_1}{2\pi}\int G_1(2-\lambda-\lambda_2)W^1(\lambda_2\,|\,\lambda_1)\,d\lambda_2 = \delta(\lambda-\lambda_1) \tag{71}$$

This leads to an improved result in the low-density case. The Fourier transform solution is

$$W^1(\lambda\,|\,\lambda_1) = \frac{1}{2\pi}\int\left[e^{i(\lambda_1-\lambda)x}+\frac{Lt_1}{2\pi}\tilde{G}_1(x)e^{i(\lambda+\lambda_1-2)x}\right]B(x)\,dx$$
$$B^{-1}(x) = 1-\left[\frac{Lt_1}{2\pi}\tilde{G}_1(x)\right]^2 \tag{72}$$

This leads to

$$\bar{K}_F(2;\underline{3}) = \frac{Nt_1^3}{2\pi}\left(\frac{L}{2\pi}\right)^2 \int \tilde{G}_1^3(x)\left[e^{i2x} + \frac{Lt_1}{2\pi}\tilde{G}_1(x)\right]B(x)\,dx \qquad (73)$$

where

$$\tilde{G}_1(x\,|\,E) = \tilde{G}_0(x\,|\,E-\Sigma) = \int d\lambda\, e^{i\lambda x}\left[E - \Sigma - \frac{\lambda^2}{2} + i\epsilon\right]^{-1} \qquad (74)$$

Here we have neglected contributions to $\bar{K}_F(2;3)$ that involve $\langle 3|t^1|3\rangle$ through propagators G_1^*. These contribute t_1^7 corrections.

It is a straightforward matter to carry the theory a stage further, so as to include effects of the three-point correlation functions $\bar{U}_3$, along the lines detailed in II.

5. GENERAL CORRELATIONS

We will only make a detailed analysis for the linear fluctuation theory and for the restricted 2BA (including collective effects). The theory then involves at most triplet static correlation functions. The general 2BA involves four-point static functions.

In the linear fluctuation theory

$$\langle 1|\Gamma^1|3\rangle = \langle 1|\delta\hat{M}_0\phi|3\rangle \qquad (75)$$

with $\delta\hat{M}_0$ given by Eq. (42). For simplicity we work with the delta function case. We have

$$\begin{aligned}\left\langle i\middle|\bar{U}_2^1(\lambda)\middle|3\right\rangle &= \langle 1|t^1G_1|3\rangle\Sigma_\lambda\, \overline{\delta E_\alpha^1(\lambda)\,\delta E_\alpha^1(2-3)} \\ &\quad - N\left\langle 1|t^1G_1|3\right\rangle\bar{F}_2(\lambda)\bar{F}_2(2-3)y_1/(1-y_1) \qquad (76)\end{aligned}$$

In particular, as $N\to\infty$

$$\left\langle 3\middle|\bar{U}_2^1(2-3)\middle|3\right\rangle = N^2\langle 3|t^1G_1|3\rangle\left[1 + \bar{F}_2(2-3)\right] \qquad (77)$$

The fluctuation kernel may be written as a sum of three terms:

$$\begin{aligned}\bar{K}_F &= \bar{K}_{F^1} + \bar{K}_{F^2} + \bar{K}_c \\ \left\langle 1|\bar{K}_{F^1}|\underline{3}\right\rangle &= Nt_1G_1^2(\underline{3})\langle\underline{3}|t^1|3\rangle\left[1 + \bar{F}_2(2-\underline{3})\right]\Delta(\underline{3}\,|\,2) \qquad (78)\\ \left\langle 1|\bar{K}_{F^2}|\underline{3}\right\rangle &= Nt_1^2G_1(2-\underline{\lambda})G_1(\underline{3})\left\{\bar{F}_3(\lambda\,|\,2-3) - \bar{F}_2(\underline{\lambda}+3-2)\right. \\ &\qquad \left. - \bar{F}_2(\lambda)\bar{F}_2(2-3)\right\}\end{aligned}$$

The collective part is

$$\langle 1|\bar{K}_c|\underline{3}\rangle = -x_1^2(2)y_1(2)/[1-y_1(2)] \tag{79}$$

and

$$\Sigma(2) = Nt_1/\left[1 - x_1(2) - \bar{K}_F(2\,|\,\underline{3})\right] \tag{80}$$

In the coherent potential approximation

$$\langle 3|t^1|3\rangle = t_1 - \Sigma(3)/N = -t_1x_1(3)/[1-x_1(3)] \tag{81}$$

and is of order t_1^2. If this approximation is used to estimate $\bar{K}_{F^1}$ we find

$$\langle 1|\bar{K}_F|\underline{3}\rangle = -t_1^2G_1^2(\underline{3})\frac{x_1(\underline{3})}{1-x_1(\underline{3})}\left[1+\bar{F}_2(2-\underline{3})\right] \tag{82}$$

This contributes to order t_1^4 in the self energy. The collective part of the kernel also contributes terms of order t_1^4, but of a different type since it involves $y_1x_1^2$.

The coherent potential approximation no longer accounts for all of the terms of order t_1^3 in the optical Σ. The missing terms, arising in the linear fluctuations theory, are given by $\bar{K}_F$. Since $\bar{F}_3$ and $\bar{F}_2(\lambda)\bar{F}_2(2-3)$ are proportional to the square of the density, at low density

$$\langle 1|\bar{K}_F|3\rangle \rightarrow -t_1^2G_1(\underline{\lambda})G_1(\underline{3})\bar{F}_2(\underline{\lambda}+\underline{3}) \tag{83}$$

This term is independent of the wave vector 2.

We next study the treatment of fluctuations with the restricted 2BA and its obvious extensions. If one neglects collective terms, the ansatz is

$$\langle 1|\Gamma_\alpha^1|3\rangle = \langle 1|H^1|3\rangle\delta E_\alpha^0(2-3) \tag{84}$$

Then

$$\left\langle 3\middle|\bar{U}_2^1(2-3)\middle|3\right\rangle = N^2\langle 3|H^1|3\rangle\left\{1+\bar{F}_2(2-3)\right\} \qquad \text{as } N\rightarrow\infty \tag{85}$$

For $\lambda \neq 2-3$

$$\left\langle 2-\lambda\middle|\bar{U}_2^1(\lambda)\middle|3\right\rangle = N^2\langle 2-\lambda|H^1|3\rangle$$
$$\times\left\{\bar{F}_3(\lambda\,|\,2-3) - \bar{F}_2(\lambda+3-2) - \bar{F}_2(\lambda)\bar{F}_2(2-3)\right\} \tag{86}$$

The determination of H^1 follows the lines of I, but we must be careful to handle the diagonal elements of t^1 properly.

Let

$$\left\langle 1\middle|x^1(2;3)\middle|\lambda\right\rangle = \frac{\langle 1|t^1G_1|\lambda\rangle\,\bar{F}_2(3-\lambda)\Delta(\lambda\,|\,1)\Delta(\lambda\,|\,3)}{1+\bar{F}_2(2-3)} \tag{87}$$

This matrix has no diagonal elements and also $\lambda \neq 3$, with 2 and 3 playing the role of parameters. Then we find

$$\langle 3|H^1|3\rangle = \langle 3|C|3\rangle / [1 - N\langle 3|C|3\rangle] \tag{88}$$

with

$$\langle 3|C|3\rangle = \langle 3|t^1 G_1|3\rangle + \left\langle 3\left| x^1 \frac{1}{1-\psi^1} t_1 G_1 \right| 3\right\rangle \tag{89}$$

We also have

$$\langle 1|H^1|3\rangle = \left\langle 1\left| \frac{1}{1-\psi^1} t_1 G_1 \right| 3\right\rangle / [1 - N\langle 3|C|3\rangle] \tag{90}$$

If this is applied to the delta function case we have, after some algebra,

$$\langle 1|H^1|3\rangle = t_1^{**} \Big/ \left[E - N t_1^{**} - \frac{k_3^2}{2} \right], \qquad 1 \neq 3 \tag{91}$$

$$\langle 3|H^1|3\rangle = \left[t_1^{**} - \frac{\Sigma(3)}{N} \right] \Big/ \left[E - N t_1^{**} - \frac{k_3^2}{2} \right] \tag{92}$$

Here

$$t_1^{**} = t_1 / [1 - Q(2;3)] \tag{93}$$

$$Q(2;3) = \frac{t_1 G_1(\underline{\lambda}) \bar{F}_2(3 - \underline{\lambda}) \Delta(\underline{\lambda}\,|\,3)}{1 + \bar{F}_2(2-3)} \tag{94}$$

The fluctuation kernel is

$$\begin{aligned}\langle 1|\bar{K}_{F^1} + \bar{K}_{F^2}|3\rangle = {} & N t_1 G_1(3) \langle 3|H^1|3\rangle \{1 + \bar{F}_2(2-3)\} \\ & + N t_1 G_1(2 - \underline{\lambda}) \Delta(\underline{\lambda}\,|\,2-3) \langle 2 - \underline{\lambda}|H^1|3\rangle \\ & \times \{\bar{F}_3(\lambda\,|\,2-3) - \bar{F}_2(\lambda + 3 - 2) - \bar{F}_2(\lambda)\bar{F}_2(2-3)\}\end{aligned} \tag{95}$$

Of course, we must add the contribution of the collective part to the fluctuation kernel, viz., $-x_1^2 y_1 (1 - y_1)^{-1}$.

There are some obvious generalizations of the restricted 2BA. For example, the ansatz (75) can be generalized to

$$\langle 1|\Gamma^1|3\rangle = \langle 1|I|3\rangle \langle 1|\delta \hat{M}_0 \phi|3\rangle \tag{96}$$

and the amplitude $\langle 1|I|3\rangle$ determined by forming the moment

$$\langle 1|\delta \hat{M}_0 \phi|\underline{1}^1\rangle \langle \underline{1}^1|\Gamma|3\rangle$$

as applied to equation (41). This leads to higher-order collective contributions. However, this is best left to be done in a systematic theory, based on an analysis of the underlying function space.

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