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Coherent-Potential Approximation for Random Systems with Short-Range Correlations

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The multiple-scattering equations for a particle in a finite random system of discrete identical scatterers with short-range correlation, which were the subject of a recent paper by Gyorffy, are cast into a form in which the limit for an infinite homogeneous system is easily obtained.

Gyorffy[1] has shown how pair correlation effects can be incorporated in the coherent-potential approximation. For lattice-based systems such as random substitutional alloys this generalization is straightforward, but for, e.g., liquid metals, the nonlocal character of the coherent potential introduces a difficulty which Gyorffy did not quite resolve. This is seen from his final equations (56)–(59), in which the volume Ω and the number of scatterers N remain explicit and the terms are not grouped in such a way that the limit $\Omega \to \infty$, $N \to \infty$, $N/\Omega = n$ is easily taken. What is needed is a limiting procedure for obtaining the mean behavior of a wave traveling in a homogeneous medium from the multiple-scattering equations for a system of N scatterers. An *ab initio* distinction between local and nonlocal parts of scattering operators makes this easy. A reader familiar with Gyorffy's paper will find the following almost self-explanatory.

Let the single-particle Hamiltonian, resolvent and mean resolvent, respectively, be

$$H = H_0 + \sum_1^N V_i\,, \tag{1}$$

$$G(z) = (z - H)^{-1}\,, \tag{2}$$

$$G_c(z) = [z - H_0 - W(z)]^{-1}\,. \tag{3}$$

The coherent potential $W(z)$ is defined by [cf. Gyorffy's Eq. (47)]

$$\langle G \rangle = G_c, \tag{4}$$

where $\langle\ \rangle$ means the average over all configurations of the scatterers, and thus W is independent of the coordinates of the scatterers. It is in general nonlocal and in the limit of an infinite homogeneous system it is (apart from z) a function of p only.

With the modified interaction H_1 defined by

$$H_1 = \sum V_i - W, \tag{5}$$

we obtain an equation for G in terms of G_c, namely,

$$G = G_c + G_c H_1 G, \tag{6}$$

which in turn permits G to be expressed in terms of a T matrix, defined by

$$TG_c = H_1 G; \tag{7}$$

thus [Gyorffy's Eq. (10)],

$$G = G_c + G_c T G_c\,. \tag{8}$$

Equation (4) now takes the form

$$\langle T \rangle = 0. \tag{9}$$

From Eqs. (7, 8), one has

$$T = H_1 + H_1 G_c T\,. \tag{10}$$

We now deviate from Gyorffy's approach (although it is possible to follow his method somewhat further) and divide T into local and nonlocal parts, corresponding in Eq. (10) to the different terms in H_1 [Eq. (5)]. Thus we let

$$T = \hat{T} - q\,, \tag{11}$$

where $-q$ is the nonlocal part, corresponding to the terms in Eq. (10) involving W,

$$q = W + W G_c T\,, \tag{12}$$

while $\hat{T}$ is a sum of local parts [notation analogous to Gyorffy's (11)ff.],

$$\hat{T}=\sum Q_i\,, \tag{13}$$

corresponding to the terms in Eq. (10) involving V_i,

$$Q_i = V_i + V_i G_c T\,. \tag{14}$$

In terms of the single-scattering operator t_i defined by

$$t_i = V_i + V_i G_c t_i \equiv t(R_i)\,, \tag{15}$$

one finally has [cf. Gyorffy's (12)]

$$Q_i = t_i + t_i G_c (\textstyle\sum' Q_j - q), \tag{16}$$

(the summation $\sum'$ excludes $j=i$), and from Eqs. (9), (11), and (12),

$$\langle q\rangle = W\,, \tag{17}$$

$$\langle \hat{T}\rangle = \sum\langle Q_i\rangle = W\,. \tag{18}$$

Let $f(R_1\cdots R_N)$ be the normalized distribution function, and let the symbol $\langle\ \rangle$ be defined by [cf. Gyorffy's (21)ff.]

$$\langle F(R_1\cdots R_N)\rangle = \int F f\, d^N R. \tag{19}$$

The average density is

$$\rho(R) = \sum\langle\delta(R-R_i)\rangle\,, \tag{20}$$

while the conditional density $g(R,R')$ is defined as follows:

$$g(R,R')\,\rho(R) = \rho(R,R') \equiv \sum_{i\neq j}\langle\delta(R-R_i)\delta(R'-R_j)\rangle\,. \tag{21}$$

The "correlation hole" is given by $\bar{g}(R,R')$, defined as

$$\bar{g}(R,R') = g(R,R') - \rho(R'). \tag{22}$$

One has

$$\int\rho(R)\, dR = N, \quad \int\bar{g}(R,R')\, dR' = -1. \tag{23}$$

In terms of a mean local operator $Q(R)$, defined by

$$\rho(R)Q(R) = \sum\langle\delta(R-R_i)Q_i\rangle\,, \tag{24}$$

we can express $\langle\hat{T}\rangle$ as

$$\langle\hat{T}\rangle = \sum\langle Q_i\rangle = \int dR\,\rho(R)Q(R)\,, \tag{25}$$

so that the self-consistency condition (18) becomes

$$\int dR\,\rho(R)Q(R) = W\,. \tag{26}$$

From Eqs. (16) and (24) one finds

$$\begin{aligned}\rho(R)Q(R) &= \sum\langle\delta(R-R_i)t_i\rangle + \sum_{i\neq j}\langle\delta(R-R_i)t_i G_c Q_j\rangle \\ &\quad - \sum\langle\delta(R-R_i)t_i G_c q\rangle \\ &= t(R)\rho(R) + t(R)G_c\Big[\int dR' \sum_{i\neq j}\langle\delta(R-R_i) \\ &\quad \times\delta(R'-R_j)Q_j\rangle - \sum\langle\delta(R-R_i)q\rangle\Big]\,. \end{aligned} \tag{27}$$

The truncation proposed by Gyorffy [in his Eq. (23)] corresponds to making in Eq. (27) the approximations

$$\sum_{i\neq j}\langle\delta(R-R_i)\delta(R'-R_j)Q_j\rangle \approx \rho(R,R')Q(R')\,, \tag{28}$$

$$\sum\langle\delta(R-R_i)q\rangle \approx \rho(R)\langle q\rangle\,. \tag{29}$$

This gives

$$Q(R) = t(R) + t(R)G_c\int dR'\,\bar{g}(R,R')Q(R'), \tag{30}$$

which, together with Eqs. (26) and (15), defines the problem.

The limit for an infinite homogeneous system can now be taken. With

$$H_0 = \epsilon(p)\,, \tag{31}$$

$$\rho(R) = n\,, \tag{32}$$

$$\bar{g}(R,R') = \bar{g}(R-R')\,, \tag{33}$$

$$W = W(p)\,, \tag{34}$$

and the notation

$$\int\bar{g}(R-R')Q(R')\,dR' = \bar{g} * Q\,, \tag{35}$$

one finally obtains the following set of equations for $W(p,z)$:

$$G_c = (z-\epsilon-W)^{-1}\,, \tag{36}$$

$$Q = t + t\,G_c\bar{g} * Q\,, \tag{37}$$

$$t = V + V\,G_c t\,, \tag{38}$$

$$\int Q dR = W/n\,. \tag{39}$$

The uncorrelated case[2] corresponds to the neglect of $\bar{g}$. Equations (36) – (39) should be compared with Gyorffy's (56)-(59). Aside from the fact that we use configuration space while Gyorffy uses the momentum representation, the difference is that our result involves no separate reference to the volume Ω and particle number N and that the equations are somewhat simpler in appearance and contain the conventional correlation function $\bar{g}(R-R')$ instead of Gyorffy's function $\hat{g}(p''-p')$, in his Eq. (58).

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