Coherent potentials and self-energies for disordered solids

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The coherent-potential approximation and a self-consistent self-energy approximation are shown to produce identical results for a class of problems involving solids with disorder in both diagonal and off-diagonal tight-binding matrix elements. The two methods should give similar results for a great many physically interesting problems.

I. INTRODUCTION

In the study of amorphous or disordered systems a widely useful concept is that of an "effective medium," a homogeneous medium with its properties chosen so that the average behavior of an ensemble of disordered samples is reproduced in the behavior of one homogeneous sample. More specifically, the average eigenvalue distribution for Hamiltonians H with random matrix elements can be approximated by finding a nonrandom Hamiltonian H_e for which the resolvent operator or Green's function

$$G_e(z)=(z-H_e)^{-1} \tag{1.1}$$

approximates the average of the resolvents for an ensemble of realizations of the random H,

$$\langle G(z)\rangle=\langle (z-H)^{-1}\rangle \ . \tag{1.2}$$

Here and henceforth the angular brackets denote an ensemble average. The parameters of the effective Hamiltonian are usually found by examining formal perturbation expansions for $\langle G(z)\rangle$ in powers of fluctuating matrix elements of H, collecting and combining (exactly or approximately) important sets of terms, and identifying the result with the resolvent of a single H_e.

One popular and successful example of this approach is the coherent-potential approximation, which has been generalized to the homomorphic-cluster coherent-potential approximation (HCPA) by Yonezawa and Odagaki.[1] The original system being studied is broken up into a set of homomorphic clusters, within each of which there occur a few of the matrix-element fluctuations describing the disorder. The effective Hamiltonian is then specified by the requirement that the ensemble average of the t matrix representing scattering by a single cluster immersed in the effective medium must vanish. It has been well established that this approximation provides excellent results for a wide variety of disorder problems.

An alternative is the self-consistent self-energy approximation (SEA), which has been discussed by the present author in a recent paper[2] henceforth denoted by I. This approach introduces an approximation to the self-energy, Σ, defined by

$$\langle (z-H)^{-1}\rangle=(z-H_0-\Sigma)^{-1} \ . \tag{1.3}$$

Here H_0 is the ensemble average of the random H—i.e., the "virtual-crystal" Hamiltonian. Σ is chosen self-consistently as the average second-order expression in an expansion of the matrix-element fluctuations,

$$V=H-H_0 \ , \tag{1.4}$$

but using the resolvent of H_e as a propagator,

$$\Sigma=\langle V(z-H_0-\Sigma)^{-1}V\rangle \ . \tag{1.5}$$

Whereas the HCPA explicitly incorporates the effects of multiple scattering by fluctuations in a single cluster, the SEA collects effects of double scatterings by all pairs of correlated fluctuations. In simple cases, Σ and H_0 have the same form, so that the effective Hamiltonian is similar to the virtual-crystal Hamiltonian, but with an energy-dependent renormalization of both its diagonal and off-diagonal matrix elements. Such a renormalized form for H_e, of course, also results from the HCPA.

It is the purpose of this Brief Report to demonstrate a class of problems for which the HCPA and the SEA produce identical results, and further to discuss their relationship in situations where results from the two approximations differ.

II. IDENTICAL HCPA AND SEA RESULTS

The model Hamiltonian, representing a tight-binding solid with only nearest-neighbor interactions, is

$$H=\sum_i a_i|i\rangle\langle i|+\sum_{(i,j)} b_{ij}|i\rangle\langle j| \ . \tag{2.1}$$

The indices i and j label sites; a_i is the energy at site i; and b_{ij} is the transfer matrix element for a bond between neighboring sites i and j. We assume a lat-

tice structure such that each site is associated with n neighboring sites. In the HCPA, this is rewritten as

$$H = H_e + \sum_{(i,j)} V_{ij} \ . \tag{2.2}$$

H_e is an "effective-medium" Hamiltonian, which has each of its diagonal elements equal to a' and each nearest-neighbor element equal to b'. For each nearest-neighbor bond, V_{ij} is a 2×2 matrix (in the subspace spanned by $|i\rangle$ and $|j\rangle$), with the form

$$V = \begin{pmatrix} (a_{ij}-a')/n & b_{ij}-b' \\ b_{ij}-b' & (a_{ji}-a')/n \end{pmatrix} \ . \tag{2.3}$$

This describes the perturbation due to a homomorphic unit composed of a single bond and a portion $1/n$ of each of the two associated sites. The decomposition is an identity provided that for each site i the quantities a_{ij} are chosen so that

$$a_i = \sum_j a_{ij}/n \ . \tag{2.4}$$

Consistent with the coherent-potential approach is the additional assumption that the random a_{ij} can be chosen to be symmetric in i and j.

The HCPA then takes as the values of a' and b' those for which, at any complex energy z, the single-cluster scattering matrix

$$T_{ij} = [1 - V_{ij}(z - H_e)^{-1})]^{-1} V_{ij} \tag{2.5}$$

has zero expectation value when averaged over the random values of a_{ij} and b_{ij}. Furthermore, contributions of products of t matrices of different bonds to the averaged resolvent are neglected, so that the Green's function for the system is simply taken to be

$$G_{\mathrm{CPA}} = (z - H_e)^{-1} \ , \tag{2.6}$$

and in particular the average density of states is

$$g(E) = -\pi^{-1}\,\mathrm{Im}[N^{-1}\,\mathrm{Tr}(E - H_e)^{-1}] \ , \tag{2.7}$$

with E taken to lie just above the real energy axis. The cluster t matrix involves only the diagonal elements of G_{CPA}, denoted by

$$\Gamma_d(z) = \langle i|(z - H_e)^{-1}|i\rangle \tag{2.8}$$

and the nearest-neighbor ones,

$$\Gamma_n(z) = \langle i|(z - H_e)^{-1}|j\rangle \tag{2.9}$$

with i,j neighbors. The evaluation of T_{ij} is most easily accomplished by the unitary transformation which diagonalizes all the 2×2 matrices. In the diagonal basis,

$$T_\pm = V_\pm/(1 - V_\pm \Gamma_\pm) \ , \tag{2.10}$$

where

$$X_\pm = X_d \pm X_n$$

with $X = \Gamma$, V, or T. The HCPA equations for the effective Hamiltonian parameters thus reduce to

$$\langle [V_\pm/(1 - V_\pm \Gamma_\pm)] \rangle = 0 = \Gamma_\pm^{-1}[\langle (1 - V_\pm \Gamma_\pm)^{-1}\rangle - 1] \ . \tag{2.11}$$

A special case of interest occurs when the random quantities a_{ij} and b_{ij} of each cluster are related to a single random number ϵ_{ij} for that cluster

$$a_{ij} = a + A\epsilon_{ij} \ , \quad b_{ij} = b + B\epsilon_{ij} \ . \tag{2.12}$$

The quantities A and B are constants, and the ϵ_{ij} are independent identically distributed random variables with mean value zero. The mean values of a_i and b_{ij} are thus a and b. A consequence of this form is that the quantities

$$V_\pm = (a - a')/n \pm (b - b') + (A/n \pm B)\epsilon_{ij} \tag{2.13}$$

are each distributed as ϵ except for a shifted mean and a scale factor.

Now further suppose that the probability distribution for ϵ has the semielliptic form

$$P(\epsilon) = (2/\pi)(1 - \epsilon^2)^{1/2} \ , \quad -1 \leq \epsilon \leq 1 \ . \tag{2.14}$$

Then the HCPA equation (2.11) reduces to

$$\langle V_\pm \rangle + (\mathrm{Var}\, V_\pm)\Gamma_\pm = 0 \ , \tag{2.15a}$$

where the mean values of $V_\pm$ are

$$\langle V_\pm \rangle = (a - a')/n \pm (b - b') \tag{2.15b}$$

and the variances are

$$\mathrm{Var}\, V_\pm = (A/n \pm B)^2/4 \ . \tag{2.15c}$$

Equations (2.15) give the effective Hamiltonian parameters, and the HCPA Green's function takes the form

$$\Gamma_d(z) = N^{-1}\,\mathrm{Tr}\left[z' \sum_i |i\rangle\langle i| - b' \sum_{(i,j)} |i\rangle\langle j|\right]^{-1} \tag{2.16a}$$

with

$$z' = z - a - \left(\frac{n}{A}\right)\left(\frac{A^2}{n^2} + B^2\right)\Gamma_d + \frac{AB}{2}\Gamma_n \tag{2.16b}$$

and

$$b' = b + \left(\frac{1}{4}\right)\left(\frac{A^2}{n^2} + B^2\right)\Gamma_n + \frac{AB}{2n}\Gamma_d \ . \tag{2.16c}$$

In this form the HCPA result can be compared directly with Eq. (7) of I:

$$\begin{aligned} z' &= z - a - (\beta_1 + n\alpha)\Gamma_d - 2n\gamma\Gamma_n \ , \\ b' &= b + (\beta_2 + \alpha)\Gamma_n + 2\gamma\Gamma_d \ . \end{aligned} \tag{2.17}$$

The coefficients of the Green's functions in Eq. (2.17) involve the expectation values of products of

matrix-element fluctuations. They are defined, using the notation of this paper, as follows:

$$\begin{aligned} \alpha &\equiv \langle (b_{ij}-b)^2 \rangle = B^2/4 \ , \\ \beta_1 &\equiv \langle (a_i-a)^2 \rangle = A^2/4n \ , \\ \beta_2 &\equiv \langle (a_i-a)(a_j-a) \rangle = A^2/4n^2 \ , \\ \gamma &\equiv \langle (a_i-a)(b_{ij}-b) \rangle = AB/4n \ . \end{aligned} \tag{2.18}$$

The SEA equations are thus identical with those from the HCPA for this particular distribution of variations in the Hamiltonian matrix elements.

III. DISCUSSION

The equivalence of the effective Hamiltonian parameters from the SEA and the HCPA holds only for the special case of semiellipticaly distributed random variables, but it should be noted that a rather wide range of types of disorder is included. When the parameter A is zero, the disorder is purely off-diagonal. When A is nonzero, there is also diagonal disorder, but with fluctuations in energies of neighboring sites which are *not* statistically independent. On the other hand, fluctuations in diagonal matrix elements which *are* independent can be treated by the usual CPA when there is no off-diagonal disorder. It is simple to show that, in this case as well, the CPA and SEA equations are equivalent provided the distribution of site energies is of the semielliptic form. Thus there are two quite different cases of pure diagonal disorder for which the two techniques give exactly the same results.

When A and B are equal in absolute value, the Hamiltonian has the form of a linearized spin-wave treatment of disordered magnetic systems,[3] which is also the form appropriate for treating lattice vibrations in harmonic solids with varying force constants.[4] In fact, for the two-dimensional spin-wave case, a SEA analysis was given by Krey.[5] Numerical evaluations of the density of states, using exchange integrals with a Gaussian distribution, have been made by Huber[6]: There is excellent agreement of the numerical with the SEA results. (It may be noted that corrections to the SEA from "cumulant diagrams" representing multiple scattering from a single fluctuation are similar to, but not identical with, the cumulants which would vanish identically for Gaussian distributions, which led Krey to claim the equivalence of the HCPA and SEA for that distribution, whereas the equivalence actually occurs for the semielliptic case.)

When the disorder in a random Hamiltonian does not have the semielliptic form, the effective Hamiltonian parameters from the HCPA and the SEA will not be the same. For distributions which are not unlike the semielliptic distributions, however, the cluster t matrix will have a small mean even though it is not zero. And many physical systems do involve distributions which *are* similar to the semiellipse: They are unimodal, have well-defined variances, and in fact are nonzero only over a finite range.[7]

In summary, then, the SEA yields effective Hamiltonians, and their associated resolvent operators or Green's functions, which are sometimes identical with those from the HCPA and which should be very similar to those from the HCPA in many other physically similar situations. The well-recognized success of coherent potential solutions to a wide range of problems thus encourages confidence in the results of SEA calculations. This conclusion is useful for three reasons. First, the HCPA equations explicitly involve the full structure of the probability distribution of random quantities, although one realizes that the results should not, in fact, be very sensitive to details of the distribution. In contrast, the SEA equations involve directly the means, variances, and correlations of random elements (which are also the most directly accessible parameters of the distributions from an experimental point of view). Second, the SEA formalism is substantially simpler from a computational standpoint (again, primarily because the analytical details of the probability distributions do not enter). One might mention also the ambiguity associated with the choice of clusters in the HCPA, which presumably calls for trying various alternative decompositions of the original problem.

Third, the HCPA is by its nature restricted to treating correlations among random elements within a single cluster. Any extension of the range of assumed correlations can be dealt with only, if at all, by the use of larger clusters, with drastic increases in complexity resulting. In the SEA, by contrast, longer-range correlations lead simply to an effective Hamiltonian with interactions among neighbors beyond the nearest.

It can be hoped that the SEA can provide useful results, with reasonable effort, for problems not readily amenable to treatment by the CPA.

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[1]F. Yonezawa and T. Odagaki, Solid State Commun. 27, 1199 (1978); 27, 1203 (1978); J. Phys. Soc. Jpn. 47, 379 (1979); 47, 388 (1979).

[2]C. G. Montgomery, Phys. Rev. B 25, 7773 (1983).

[3]C. G. Montgomery, J. I. Krugler, and R. M. Stubbs, Phys. Rev. Lett. 25, 669 (1970); D. L. Huber, Phys. B 8, 2124 (1973).

[4]C. G. Montgomery, J. Low Temp. Phys. 39, 13 (1980).

[5]U. Krey, Int. J. Magn. 5, 137 (1973).

[6]D. L. Huber, Solid State Commun. 14, 1153 (1974).

[7]The SEA in the form presented here should *not* be expected to give realistic results for alloy systems for example. The boundedness of fluctuations can be expected since an extremely large fluctuation in a real system would correspond to a structural instability, rather than a statistically rare occurrence.