able for defect calculations. The lattice-statics method is often referred to as exact without an appropriate qualifier for the harmonic approximation. The present comparison (and indeed earlier comparisons) does not bear this out. This is admittedly a subjective judgement—Flocken and Hardy consider a 5–10% disagreement in displacements to be unsatisfactory, while the present author considers this to be a good agreement.

At the present time, it would seem that the most reliable method of calculation would be to use a real-space lattice approach near the defect but to replace the elastic continuum component of the calculation with a lattice-statics calculations. The flexibility to investigate nonsymmetric configurations would be impaired by such a program, however, and the computer time to carry out such a calculation would be much greater than with other methods. The reliability of interatomic potentials is not sufficiently good at the present time to warrant such an approach except as an occasional check on more approximate methods.

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Pair Effects in Disordered Alloys*

P. L. Leath
Physics Department, Rutgers University, New Brunswick, New Jersey 08903

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An error in keeping track of diagrams in the paper by Aiyer, Elliott, Krumhansl, and Leath is reported and corrected and a general rule for avoiding this kind of problem for larger clusters is presented. The recent work of Nickel and Krumhansl is shown to be in agreement with the corrected formula.

In a paper[1] (hereafter referred to as A) of a few years ago a general diagrammatic procedure for calculating configuration-averaged properties in disordered alloys was presented. In a recent paper Nickel and Krumhansl[2] have calculated the effects of the self-consistent scattering by pairs of defects in a generalization of the coherent-potential approximation which was in disagreement with the pair formula calculated in the last section of A. The purpose of this paper is to point out the omission in diagram counting that was made in that section, to show that, when corrected, there is full agreement with Ref. 2, and to emphasize that the diagrammatic technique presented in A, although at times tedious, is in fact correct and straightforward in its prescription for getting the proper generalization of the coherent-potential approximations.

We assume the reader's knowledge of the methods and notation of A and first point out the errors in Sec. VI of that paper. Then we show how this result could have been more simply obtained. Finally, we point out the equivalence of this work with that of Ref. 2.

The scattering by a pair of defects, which are a distance $\vec{R}$ apart, is calculated with the restriction $\vec{R} \neq 0$ strictly maintained so that there are no pair corrections to the single-site terms $\Sigma_S^1 = \tau'$ in Eq. (47) of A. [This statement is in contrast to the statement above Eq. (53).] We note that Eq. (47) can be written in the form

$$c\tau[\langle G(0)\rangle] = \tau'[G''(0)]/\{1 - \tau'[G''(0)]\langle G(0)\rangle\} , \qquad (1)$$

where

$$G''(0) = \langle G(0)\rangle/\{1 - \tau'[\langle G''(0)\rangle]\langle G(0)\rangle\} .$$

The pair terms summed in A were just those diagrams shown below in the first column of Fig. 1 where the double horizontal line represents the full *off-diagonal* propagator $\langle G(\vec{R})\rangle$, the wide solid horizontal line represents the full *diagonal* propagator $\langle G(\vec{0})\rangle$, and the open-circle vertex represents the bare vertex, uncorrected for multiple occupancy. The higher columns contain the multiple-occupancy corrections (the solid circle represents the fully corrected vertex).

We now come to the basic omission in Sec. VI of A. In Eq. (58), which should have been the sum of all the columns of Fig. 1, the correction terms

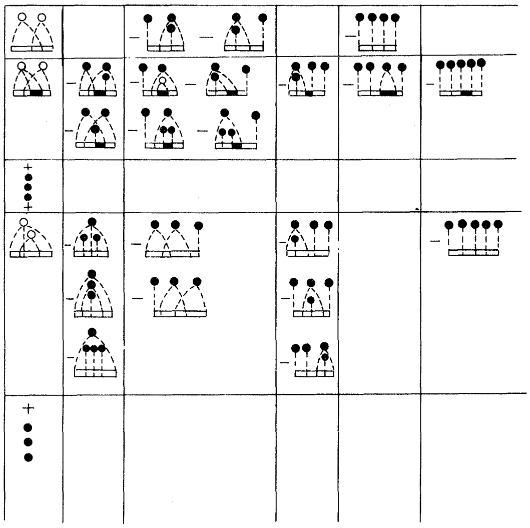

FIG. 1. Bare self-consistent self-energy diagrams (open vertices) containing scattering by a pair of sites (column 1) and their multiple-occupancy corrections (the black vertices indicate fully corrected values) with n irreducible parts [$(n+1)$st column]. The double horizontal line indicates $\langle G(\vec{R})\rangle$, whereas the wide single line represents $\langle G(0)\rangle$. The sum of all columns gives Eq. (6).

indicated by the examples in Fig. 2 should have been included. These terms contain just two $\langle G(\vec{R})\rangle$ factors, both of which lie inside a single irreducible part (let us call it τ_R). Since the irreducible part τ_R is enclosed between all possible single-particle scatterings, the sum of these diagrams is

$$\tau_R\{1-\tau'[G''(0)]\langle G(0)\rangle\}^{-2}. \qquad (2)$$

The irreducible part τ_R can be evaluated by considering it to be made up of $\tau'[G''(0)]$, the single-particle self-energy with all insertions, but where one of the $\langle G(0)\rangle$ lines in $\tau'[G''(0)]$ is replaced by all parts containing two $\langle G(\vec{R})\rangle$ propagators; namely, replaced by

$$\langle G(\vec{R})\rangle^2\tau'[G''(0)]/\{1-\tau'[G''(0)]\langle G(0)\rangle\}$$
$$=c\tau[\langle G(0)\rangle]\langle G(\vec{R})\rangle^2, \qquad (3)$$

where the equality follows from Eq. (1). Thus, we find

$$\tau_R=\left(\frac{\partial\tau'[G''(0)]}{\partial\langle G(0)\rangle}\right)c\tau[\langle G(0)\rangle]\langle G(\vec{R})\rangle^2$$
$$=\frac{(1-c)}{c}\,\tau'[G''(0)]^2\tau[\langle G(0)\rangle]\langle G(\vec{R})\rangle^2, \qquad (4)$$

since

$$\tau'[G''(0)]=cV/[1-(1-c)V\langle G(0)\rangle].$$

The insertion of τ_R into Eq. (2) leads immediately, with simplifications from Eq. (1), to the simple result

$$c^2(1-c)\tau[\langle G(0)\rangle]^3\langle G(\vec{R})\rangle^2 \qquad (5)$$

for the contribution of the diagrams shown in Fig. 2. The value of these correction diagrams, since they *do not* appear anywhere in Fig. 1 but were included in Eq. (58) of A, should be subtracted with the corrected result

$$\zeta'[\langle G(0)\rangle,\ \langle G(\vec{R})\rangle]=c^2\zeta-\left(\frac{\Sigma_S^2[\Gamma(0),\ \Gamma(R)]}{1-\{\langle G(0)\rangle+\langle G(\vec{R})\rangle\}\Sigma_S^2[\Gamma(0),\ \Gamma(\vec{R})]}-\zeta'[\langle G(0)\rangle,\ \langle G(\vec{R})\rangle]-c\tau[\langle G(0)\rangle]\right.$$
$$\left.-c^2\tau[\langle G(0)\rangle]^2\langle G(\vec{R})\rangle-c^3\tau[\langle G(0)\rangle]^3\langle G(\vec{R})\rangle^2-c^2(1-c)\tau[\langle G(0)\rangle]^3\langle G(\vec{R})\rangle^2\right), \qquad (6)$$

where

$$\Sigma_S^2[\Gamma(0),\ \Gamma(\vec{R})]=\tau'[\Gamma(0)]+\zeta'[\Gamma(0),\ \Gamma(\vec{R})]$$

as in A, and Eq. (1) has been used to simplify the last four terms. [$\Gamma(0)$ rather than $G''(0)$ appearing in Eq. (58) of A in these terms was also in error, although this didn't affect the final answer.] This immediately leads to the result

$$\Sigma_S^2=\frac{\tau_2[\Gamma'(0),\ \Gamma'(\vec{R})]}{1-[\Gamma'(0)+\Gamma'(R)]\tau_2[\Gamma'(0),\ \Gamma'(\vec{R})]}, \qquad (7)$$

where

$$\tau_2[\Gamma'(0),\ \Gamma'(\vec{R})]=c\tau[\Gamma'(0)]+\frac{c^2\tau[\Gamma'(0)]^2\Gamma'(\vec{R})}{1-\tau[\Gamma'(0)]\Gamma'(\vec{R})}, \qquad (8)$$

which, by multiplying numerator and denominator of Eq. (7) by $1-c\tau[\Gamma'(0)]\Gamma'(\vec{R})$, can be put into the form [Eq. (63) of A]

$$\Sigma_S^2(\vec{R})=\frac{c\tau+c^2(1-c)\eta_2}{1+c\tau\Gamma'(0)+c^2(1-c)\eta_2[\Gamma'(0)+\Gamma'(\vec{R})]}, \qquad (9)$$

where $\tau=\tau[\Gamma'(0)]$, but where η_2 now has the value

$$\eta_2=\tau^3\Gamma'(\vec{R})^2/[1-\tau\Gamma'(\vec{R})], \qquad (10)$$

in contrast to Eq. (64) of A. This is precisely the

FIG. 2. Those diagrams containing two $\langle G(\vec{R})\rangle$ factors both of which are within a single irreducible part.

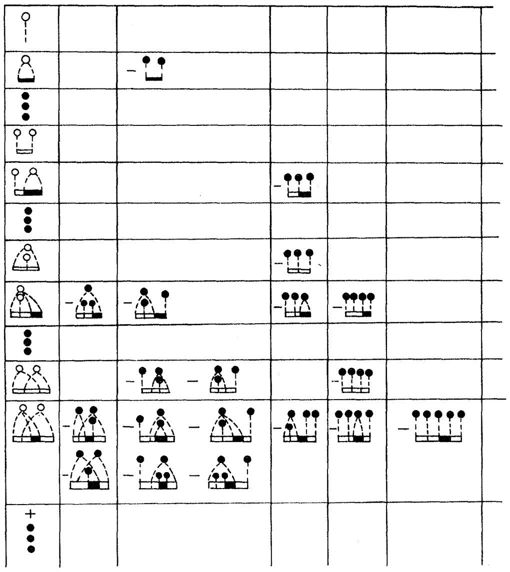

FIG. 3. Repeat of Fig. 1 for the case of those diagrams (column 1) which would appear in the t matrix for scattering by an *isolated* pair of defects. The sum of all columns gives Eq. (15).

form derived by Nickel and Krumhansl[2] using both a similar diagrammatic and the coherent-potential methods which, as they have pointed out, has the proper limit at low concentration.

At this point it is, perhaps, worth noting that by dividing the numerator and denominator by the factor

$$1+c(1-c)\tau^2\Gamma'(\vec{R})^2/[1-\tau\Gamma'(\vec{R})]\ , \tag{11}$$

Eq. (9) above can be put in the form

$$\Sigma_S^2(\vec{R})=c\tau\Big/\left(1+c\tau\Gamma'(0)-\frac{c(1-c)\tau^2\Gamma'(\vec{R})^2}{1-(1-c)\tau\Gamma'(\vec{R})}\right), \tag{12}$$

which is precisely the formula derived in Eq. (42) of A for the non-self-consistent pair scattering, but with the propagator replacement

$$\begin{aligned} &P(0)\rightarrow\Gamma'(0)\ ,\\ &p_2(\vec{R})\rightarrow\Gamma'(\vec{R})\ . \end{aligned} \tag{13}$$

Clearly this result is physically what one would have expected and is the simple generalization of that which happened in the single-site case; namely, in n-cluster scattering going over from the direct to the self-consistent expression, one does not replace P by the full $\langle G\rangle$ but by a $\Gamma'=\langle G\rangle/1+\Sigma\langle G\rangle$, where the terms are $n\times n$ matrices in the sense defined in A. Also it should be pointed out that Eq. (65) in A is simply wrong, although it did not affect any of the results, since $\Gamma'(0)$ as defined in Eq. (54) not only has scattering by site $\vec{0}$ excluded but also that by site $\vec{R}$.

The mistake in A is now clearly seen although it was rather subtle and not at all trivial to correct. Therefore, a simplified way of calculating the diagram which avoids these subtleties seems in order. Consider for the moment summing those diagrams D shown in the first column of Fig. 3. These diagrams are not only double counted in places, but a few of them are not even irreducible. Nevertheless, the sum of the first column, the bare contribution, is

$$D_{\text{bare}}=c\tau+\frac{c^2\tau^2\langle G(\vec{R})\rangle}{1-\tau\langle G(\vec{R})\rangle}\ . \tag{14}$$

Thus the full value D is determined by subtracting all the higher columns from D_{bare},

$$D=c\tau+\frac{c^2\tau\langle G(\vec{R})\rangle}{1-\tau\langle G(\vec{R})\rangle}-\left(\frac{\Sigma_S^2[\Gamma(0),\ \Gamma(\vec{R})]}{1-[\langle G(0)\rangle+\langle G(\vec{R})\rangle]\Sigma_S^2[\Gamma(0),\ \Gamma(\vec{R})]}-D\right), \tag{15}$$

where Σ_S^2 is precisely the set of diagrams identified as Σ_S^2 in Eq. (6) above and is just the full self-energy for scattering by single and pairs of defects. But, since D cancels out of (15) and since ξ' cancels out of (6), this is just a simple rederivation of Eq. (6) and leads to Eq. (9) as above. In fact, it is not necessary to put precisely the diagrams one wants to sum in the first column of bare diagrams (since the D always cancels out of the calculation) but only necessary to recognize the correct class of diagrams in the correction columns. As a general rule, it seems one should, for the most simplicity of calculations, always sum the diagrams which would appear in the t matrix for scattering by an *isolated* cluster of size n.

Finally, let us briefly discuss the various recent attempts to generalize the coherent-potential approximation to the case of scattering by pairs of defects. From the diagrammatic method one can see that the proper generalization of the coherent-potential approximation to pairs is that of Eq. (33) of Ref. 2 where the t matrix for the scattering by each pair of defects embedded in the effective medium was set equal to zero. Recently Cyrot-Lackmann and Ducastelle[3] have attempted a generalization of the coherent-potential approximation essentially by setting

$$\langle\tau_n+{\textstyle\sum_m'}\,(\tau_n\langle G\rangle\tau_m+\tau_n\langle G\rangle\tau_m\langle G\rangle\tau_n+\cdots)\rangle=0\ , \tag{16}$$

where τ_n is the single-site scattering at site n. This formula is not equivalent to the diagrammatic formula (12) above because of the summation over

m. If they had set the scattering by the two general sites n and m to zero,

$$T^{(2)}_{nm} = \langle \tau_n + \tau_n \langle G \rangle \tau_m + \tau_n \langle G \rangle \tau_m \langle G \rangle + \cdots \rangle = 0 \ , \qquad (17)$$

formula (12) above would have been obtained. This could, perhaps, be done by modifying their technique only slightly. The generalization of Freed and Cohen[4] also is improper because they also did not set the average scattering by a pair of defects in the medium to zero. In this case they do not even get the proper limit at low concentrations. The generalizations to larger n clusters than two now also seems to be that clearly the average t matrix for scattering each particular n cluster must be set to zero as suggested also in Ref. 2.

The way to perform the formal calculation of scattering by pairs and larger clusters of defects now seems clear, at least within this model containing only diagonal randomness. It would be very useful to see numerical calculations to check the properties of these formulas with regard to the physically expected qualitative features.

Finally, the effect of the disorder at high concentration is becoming quite well understood now, within the model of only diagonal randomness. This model can, however, only be of limited use in real systems,[5] so that more sophisticated physical models, including off-diagonal disorder, should be considered within the spirit of the configuration-averaging techniques now developed for the diagonal model. Some attempts have recently been made along these lines[6] which are useful in certain circumstances.

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Comment on Effective Ion-Ion Interactions in Metals

Robert W. Shaw, Jr. and Volker Heine*
Bell Laboratories, Murray Hill, New Jersey 07974

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It is found that the contributions of both nonlocality in the pseudopotential and exchange correlation in the screening reduce the cutoff radius of the strong screened Coulomb repulsion between ions in metals, thus revealing extra oscillations at short range in the effective interionic interaction. This analysis of the situation resolves some previous puzzles, and lends support to arguments about structural stability based on rearrangements of near neighbors.

Though the interatomic spacing in simple metallic systems is determined primarily by the volume-dependent contributions to the total energy,[1-3] it is the small structure-dependent contributions which govern many of the physically interesting properties of metals and their alloys, including phonon frequencies, elastic constants, and the relative energies of different crystal structures.[3,4] The structure-dependent part of the energy, U_s, can be expressed as a sum over reciprocal lattice vectors g involving the "energy-wave-number characteristic" $\Phi_{bs}(g)$, or alternatively, as a sum of effective screened interionic potentials $\Phi(r)$ in real space. While numerical calculations have almost invariably been done in terms of reciprocal space because the convergence is better, they have often been interpreted with semiquantitative arguments involving the real-space picture of the interaction potential $\Phi(r)$. The latter was found in early work to have a sharp minimum in the region of the nearest-neighbor position.[4] Naturally, this was an appealing result because it suggested correlations between crystal structure and the position of the minimum. Several such interpretations and arguments in terms of $\Phi(r)$ may be found in the recent review article by Heine and Weaire.[3]

Structural arguments based on real-space interatomic potentials are attractive because of their