

Analyticity in liquid metals

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(Received 4 February 1980)

The analytic properties are examined for several multiple-scattering theories of liquid metals. A condition is obtained for a positive density of states in terms of the properties of the kernel of an integral equation obeyed by the self-energy path operator. It is found that this condition is obeyed by the Gyorffy-Korringa-Mills theory as well as the quasicrystalline approximation. The theories are reformulated in terms of relative coordinates and the implications of these results on the conductivity problem are discussed.

I. INTRODUCTION

In recent years a number of multiple scattering results¹⁻¹⁰ have been obtained for the problem of the electronic structure of liquid and amorphous metals. A question arises as to the analytic structure of the theory and in particular whether a given result will yield a positive density of states (DOS). Some impetus was given to such a question when it was found that the modified quasicrystalline approximation¹⁰ (MQCA) gave a negative DOS for muffin-tin models of liquid Cu,¹¹ and Ni,¹² in the region of the d resonance. In addition, nonanalytic behavior was reported for the Ishida-Yonezawa (IY) theory.¹² Schwartz and Bansil have examined the problem,^{11,13,14} and they showed that the quasicrystalline approximation¹ (QCA) of Lax gives the proper analytic structure of the one-electron Green's function as do the coherent potential approximation (CPA) and the average T -matrix approximation (ATA) for the case of the crystalline alloy. In response to analyticity problems which arose for several alloy cluster CPA extensions,¹⁵ Mills and Ratanavararaksa¹⁶ have examined the alloy case and, in addition to giving a proof of analyticity for CPA and ATA, they have found an analytic cluster CPA, which they call the traveling cluster approximation. Their very interesting methods are unfortunately not directly applicable to the liquid-metal problem because the latter involves short-range order.

The work of Schwartz and Bansil has been based on a term-by-term approach to the multiple-scattering sequence, and Schwartz¹⁴ has obtained a formal result which is guaranteed to give a positive spectral weight function. Unfortunately these results are rather complicated. In the present work we shall take a simpler and less ambitious approach. Since most of the multiple-scattering theories can be formulated in terms of an integral equation for the scattering path operator¹⁷ and a related self-energy path operator,¹⁸ we will develop a criterion for analyticity based on

the properties of the kernels of these integral equations and discuss the several theories on this basis.

Actually the MQCA does not fit into the integral equation scheme. We have already addressed the MQCA problem in terms of several simple models—one involving a resonant atomic level,¹⁹ and the other a one-phase-shift muffin-tin model.²⁰⁻²² We have concluded on the basis of these studies that the MQCA fails because of an incomplete summation of site-diagonal terms in the scattering path operator. In fact we found that properly constructed muffin-tin versions of the QCA and IY theories,^{1,7} as well as the effective medium approximation (EMA)⁸ gave no difficulty with analyticity for the one-phase-shift model.

In Sec. II of this paper we will formulate the problem, and summarize the several theories in terms of integral equations for the scattering path operator and self-energy path operator. In Sec. III we develop the criterion for analyticity and discuss the various theories in relation to the criterion. Section IV gives a new formulation of the multiple-scattering series which separates the ionic and relative electronic coordinates, and we discuss here the relation of the present results with the vertex function which is useful for calculating transport properties. We next recall in Sec. V some results we had previously obtained for the one-orbital tight-binding model,²³⁻²⁵ and present our conclusions in a final section.

II. MULTIPLE-SCATTERING THEORY RESULTS

The problem we treat is that of an electron scattered by an array of ionic potentials $V_i = V(\vec{r} - \vec{R}_i)$ at positions \vec{R}_i , arranged in a distribution characteristic of a liquid or amorphous metal. The Hamiltonian we assume is

$$\mathcal{H} = \frac{p^2}{2m} + \sum_i v_i = \mathcal{H}_0 + V, \quad (2.1)$$

where we assume that the potentials are real and energy independent. The electronic structure is characterized by the one-electron Green's function²⁶

$$G = \langle (\omega - \mathcal{H})^{-1} \rangle_c, \quad (2.2)$$

where the average is over ionic configurations. The usual multiple-scattering approach^{6,8} is based on calculating the total scattering operator or T matrix, which obeys

$$T = \sum_i v_i (1 + G_0 T), \quad (2.3)$$

where $G_0(\omega - \mathcal{H}_0)^{-1}$ is the free-electron Green's function. In terms of the configuration average $T = \langle \mathcal{T} \rangle$ of the T matrix, we have

$$G = G_0 + G_0 T G_0 \quad (2.4)$$

The well-known expansion^{1,6} for the T matrix can be given in terms of the scattering path operator¹⁷ \mathcal{T}_{ij} , by

$$\mathcal{T} = \sum_{ij} \mathcal{T}_{ij}, \quad (2.5)$$

$$\mathcal{T}_{ij} = t_i \delta_{ij} + t_i G_0 t_j (1 - \delta_{ij}) + \sum_{i'j'} t_i G_0 t_{i'} G_0 t_{j'} + \dots,$$

where the prime indicates that no two successive indices are equal. Here the single-site T matrix obeys the equation

$$t_i = v_i (1 + G_0 t_i). \quad (2.6)$$

The next quantity which we construct is the medium path operator.⁸

$$Q(\bar{R}, \bar{R}') = \left\langle \sum_{ij} \rho_i(\bar{R}) \mathcal{T}_{ij} \rho_j(\bar{R}') \right\rangle_c, \quad (2.7)$$

where $\rho_i(\bar{R}) = \delta(\bar{R} - \bar{R}_i)$ is the density of the i th ion at R . $T(\bar{R}, \bar{R}')$ can be expanded⁸ using Eq. (2.5) into a series of terms involving n -particle distribution

functions. Furthermore we have for the total scattering matrix

$$T = \int Q(\bar{R}, \bar{R}') d\bar{R} d\bar{R}'. \quad (2.8)$$

Various decouplings of these distribution functions yield different approximation schemes^{5-9,27} for most of which $Q(R, R')$ obeys an integral equation of the form

$$Q(\bar{R}, \bar{R}') = n t_c(\bar{R}) \left[\delta(\bar{R} - \bar{R}') + \int \tilde{G}(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}') d\bar{R}'' \right], \quad (2.9)$$

in terms of a medium locator t_c and a medium propagator \tilde{G} . We emphasize that Q and \tilde{G} are operators on the electron coordinates \bar{r}, \bar{r}' as well as the ionic coordinates [i.e., we have $Q(\bar{r}, \bar{r}', \bar{R}, \bar{R}')$ and $t_c(\bar{r}, \bar{r}', \bar{R})$]. An alternative form for these operators in terms of relative coordinates $\bar{r} - \bar{R}, \bar{r}' - \bar{R}'$, and $\bar{R} - \bar{R}'$, will be given in Sec. IV. We can relate Q to quantities used in the work of Schwartz and Ehrenreich^{6,10}

$$Q(\bar{R}_\alpha, \bar{R}_\beta) = n \delta(\bar{R}_\alpha - \bar{R}_\beta) \langle Q_{\alpha\alpha} \rangle_c^\alpha + n^2 g(\bar{R}_\alpha - \bar{R}_\beta) \langle Q_{\alpha\beta} \rangle_c^{\alpha\beta}, \quad (2.10)$$

where, e.g., $\langle Q_{\alpha\alpha} \rangle_c^\alpha$ is a conditional average over all particles except the α th. Actually we find the use of " R_α " rather confusing as it looks discrete but is continuous. The difference in notation may have caused errors.²⁰

We summarize in Table I the medium locator and propagator for several theories. It is convenient to write these results in terms of two operators $G_1(\bar{R})$ and $G_2(\bar{R}, \bar{R}')$ defined as follows. The medium locator obeys an integral equation of the form

$$t_c(\bar{R}) = v_{\bar{R}} + v_{\bar{R}} G_1(\bar{R}) t_c(\bar{R}), \quad (2.11)$$

TABLE I. Green's function operators for Eqs. (2.11), (2.12), and (2.19) for various theories.

	$G_1(\bar{R})$	$G_2(\bar{R}, \bar{R}')$
QCA ^a	G_0	G_0
GKM ^b	G	G
SE ^c	$G_0 + \int \tilde{G}(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}') G_0 d\bar{R}'' d\bar{R}'$	$= G_1(\bar{R})$
IY ^d	$G_0 + \int \tilde{G}_0(\bar{R}, \bar{R}') n t_c(\bar{R}') \times \left[G_0 + \int \tilde{G}_0(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}''') \times \tilde{G}_0(\bar{R}''', \bar{R}') d\bar{R}'' d\bar{R}''' \right] d\bar{R}'$	G_0
EMA ^e	$G_M^R = G_0 + \int \tilde{G}(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}''') G_0 d\bar{R}'' d\bar{R}'''$	$G_M^{R'R'} = G_0 + \int \tilde{G}(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}''') \tilde{G}(\bar{R}''', \bar{R}') d\bar{R}'' d\bar{R}'''$

^aReference 1.

^bReference 5.

^cReference 6.

^dReference 7.

^eReference 8.

and the medium propagator has the form

$$\tilde{G}(\bar{R}, \bar{R}') = G_0 + h(\bar{R} - \bar{R}')G_2(\bar{R}, \bar{R}') \quad (2.12)$$

where $h(R) = g(R) - 1$ with g the pair distribution function (PDF). Results for G_1 and G_2 for the QCA, Gyorffy-Korringa-Mills (GKM), Schwartz-Ehrenreich (SE), IY, and EMA theories are given in Table I. For the IY we have $\tilde{G}_0(\bar{R}, \bar{R}') = G_0g(R - R')$ which is the \tilde{G} for QCA (and IY) results. For EMA and SE theories \tilde{G} is given by Eq. (2.12). As we shall discuss further below G_M^R in the EMA corresponds to the medium which is missing a medium ion at R , and $G_M^{R'}$ is the same quantity with ions missing at R and R' , both approximated in a modified Kirkwood approximation to be described below.

In addition to the medium path operator it is often convenient to define a self-energy path operator¹⁸ $\sigma(\bar{R}, \bar{R}')$, such that the self-energy is given by

$$\sigma = \int \sigma(\bar{R}, \bar{R}') d\bar{R} d\bar{R}' \quad (2.13)$$

Schwartz and Ehrenreich actually based their work on $\sigma_r = n \int \sigma(\bar{R}, \bar{R}') d\bar{R}'$. The self-energy obeys the equation $G = (\omega - H_0 - \Sigma)^{-1}$. We have $T = \Sigma + \Sigma G$ and $TG_0 = \Sigma G$. The corresponding results for the path operator are

$$Q(\bar{R}, \bar{R}') = \sigma(\bar{R}, \bar{R}') + \int \sigma(\bar{R}, \bar{R}'') G \sigma(\bar{R}'', \bar{R}') d\bar{R}'' d\bar{R}''' \quad (2.14)$$

and

$$\int Q(\bar{R}, \bar{R}') G_0 d\bar{R}' = \int \sigma(\bar{R}, \bar{R}') G d\bar{R}' \quad (2.15)$$

It is easy to show that σ obeys the integral equation

$$\sigma(\bar{R}, \bar{R}') = n t_c(\bar{R}) \left\{ \delta(\bar{R} - \bar{R}') + \int [\tilde{G}(\bar{R}, \bar{R}'') - G_0] \times \sigma(\bar{R}'', \bar{R}') d\bar{R}'' \right\} \quad (2.16)$$

That is, the kernel differs by the removal of the G_0 part.

Because of the integral equation for t_c , Eq. (2.11), the scattering path operator and self-energy path operator equations can be rewritten

$$Q(\bar{R}, \bar{R}') = n v_{\bar{R}} \left\{ \delta(\bar{R} - \bar{R}') + \int K_Q(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}') d\bar{R}'' \right\} \quad (2.17)$$

$$\sigma(\bar{R}, \bar{R}') = n v_{\bar{R}} \left\{ \delta(\bar{R} - \bar{R}') + \int K_\sigma(\bar{R}, \bar{R}'') \sigma(\bar{R}'', \bar{R}') d\bar{R}'' \right\} \quad (2.18)$$

The kernels are given by

$$K_\sigma(\bar{R}, \bar{R}') = \frac{1}{n} \delta(\bar{R} - \bar{R}') G_1(\bar{R}) + h(\bar{R} - \bar{R}') G_2(\bar{R}, \bar{R}') \quad (2.19)$$

$$K_Q(\bar{R}, \bar{R}') = K_\sigma(\bar{R}, \bar{R}') + G_0$$

These results are now in the form to discuss the analytic properties and generalized optical theorem. We note that the Q form is useful for muffin-tin calculations and the σ form for pseudopotentials.

III. ANALYTIC PROPERTIES

The exact one-electron Green's function is analytic in the ω plane except on the real axis, and $\text{Im}G$ is negative definite for ω in the upper half plane. These properties are sometimes called the Herglotz property.¹⁶ We shall usually simply use the term analytically. The Herglotz property guarantees a positive density of states, since the DOS is given by $n(\omega) = -\pi^{-1} \text{Im tr}G$.

The unperturbed Green's function $(\omega - G_k^0)^{-1}$ in a momentum representation, has a pole on the real axis at $G_k^0 = \hbar^2 k^2 / 2m$. The exact Green's function Eq. (2.2) in a momentum representation is diagonal with

$$G_{\bar{k}} = [\omega - G_{\bar{k}}^0 - \Sigma_{\bar{k}}(\omega)]^{-1} \quad (3.1)$$

It is well known that $\Sigma_{\bar{k}}(\omega)$ and $G_{\bar{k}}$ are diagonal because of translational symmetry after configuration averaging. We see that in order for $G_{\bar{k}}$ to be analytic we must have $\text{Im} \Sigma_{\bar{k}} < 0$ for ω in the upper half plane. Thus a criterion for analyticity is that $\Sigma - \Sigma^\dagger$ be a negative definite operator for $\text{Im} \omega > 0$.

In terms of the T matrix, Schwartz and Bansil¹¹ argue that the free-electron pole in the Green's function cancels out between the two terms in Eq. (2.4) and that, therefore, analyticity is related to the negative definite character of $i^{-1}(T - T^\dagger)$. Specifically in momentum space the spectral weight function

$$S(\bar{k}, \omega) = -(\pi N)^{-1} \text{Im} G_{\bar{k}}(\omega)$$

is given by

$$S(\bar{k}, \omega) = -(\pi N)^{-1} \text{Im} T_{\bar{k}}(\omega) / (\omega - k^2)^2 \quad (3.2)$$

These authors point out that the optical theorem

$$\mathcal{T} - \mathcal{T}^\dagger = \mathcal{T}^\dagger (G_0 - G_0^\dagger) \mathcal{T} \quad (3.3)$$

guarantees the negative definite character of the exact unaveraged $\mathcal{T} - \mathcal{T}^\dagger$, since G_0 has the Herglotz property. We now proceed to generalize this result for the scattering and self-energy path operators. The form of both the integral equations, Eqs. (2.17) and (2.18), is

$$A = b(1 + KA) \quad (3.4)$$

where b is Hermitian and 1 is the unit operator.

It is quite easy to prove the theorem:

$$A - A^\dagger = A^\dagger(K - K^\dagger)A \quad (3.5)$$

Applying this result to the integral equations for $Q(R, R')$ and $\sigma(R, R')$, we have

$$Q(\bar{R}, \bar{R}') - Q^\dagger(\bar{R}', \bar{R}) = \int Q^\dagger(\bar{R}'', \bar{R}) [K_Q(\bar{R}'', \bar{R}''') - K_Q^\dagger(\bar{R}''', \bar{R}'')] Q(\bar{R}''', \bar{R}) d\bar{R}'' d\bar{R}''' \quad (3.6)$$

$$\sigma(\bar{R}, \bar{R}') - \sigma^\dagger(\bar{R}', \bar{R}) = \int \sigma^\dagger(\bar{R}'', \bar{R}) [K_\sigma(\bar{R}'', \bar{R}''') - K_\sigma^\dagger(\bar{R}''', \bar{R}'')] \sigma(\bar{R}''', \bar{R}') d\bar{R}'' d\bar{R}''' \quad (3.7)$$

We can integrate these equations over \bar{R}, \bar{R}' to obtain the condition on T and Σ . We see that the condition is now that K_σ and K_Q , Eq. (2.19), must have the Herglotz property. Since $K_Q = K_\sigma + G_0$, and G_0 is Herglotz, we must examine K_σ in particular for the several theories.

Consider first the QCA. We have

$$K_\sigma^{\text{QCA}}(\bar{R}, \bar{R}') = \left[\frac{1}{n} \delta(\bar{R} - \bar{R}') + h(\bar{R} - \bar{R}') \right] G_0 \quad (3.8)$$

The free-electron Green's function is of course Herglotz; furthermore the coefficient is proportional to the liquid structure factor

$$S(\bar{R} - \bar{R}') = \delta(\bar{R} - \bar{R}') + nh(\bar{R} - \bar{R}') \quad (3.9)$$

which is a positive definite matrix. The eigenvalues are just the Fourier transform $S_k = 1 + nh_k$, which is the x-ray interference function. Thus the QCA is analytic.¹¹

For the GKM we have

$$K_\sigma^{\text{GKM}}(\bar{R}, \bar{R}') = \frac{1}{n} S(\bar{R} - \bar{R}') G \quad (3.10)$$

Thus if we assume that G has the Herglotz property, then we find self-consistently that T and G are analytic.

The remaining self-consistent theories are equivalent to GKM for the random liquid.² For the correlated liquid, the structure of K_σ is more complex, so that it is difficult to say anything precise about the analytic properties. Thus for the IY theory we have

$$K_\sigma^{\text{IY}}(\bar{R}, \bar{R}') = n^{-1} S(\bar{R} - \bar{R}') G_0 + n^{-1} \delta(\bar{R} - \bar{R}') [G_1^{\text{IY}}(\bar{R}) - G_0] \quad (3.11)$$

Here the first term is Herglotz but while the second term involves the positive definite quantity $\delta(\bar{R} - \bar{R}')$, the analytic structure of its factor is unknown. For the SE theory we have

$$K_\sigma^{\text{SE}}(\bar{R}, \bar{R}') = n^{-1} S(\bar{R} - \bar{R}') G_1^{\text{SE}}(\bar{R}) \quad (3.12)$$

which is proportional to the positive definite structure factor. As in the case of the EMA (see below) it is possible to argue that $G_1^{\text{SE}}(\bar{R})$ is an approximation²⁸ to the Green's function for the medium consisting of

all ions except one at R , and thus in principle at least is Herglotz. However $K_\sigma(\bar{R}, \bar{R}')$ is not symmetric and

$$i^{-1} [K_\sigma(\bar{R}, \bar{R}') - K_\sigma^\dagger(\bar{R}', \bar{R})]$$

involves

$$i^{-1} [G_1^{\text{SE}}(\bar{R}) - G_1^{\text{SE}\dagger}(\bar{R}')] \quad ,$$

which may not be negative definite, unless \bar{R} and \bar{R}' are equal.

For the EMA we have

$$K_\sigma^{\text{EMA}}(\bar{R}, \bar{R}') = n^{-1} \delta(\bar{R} - \bar{R}') G_M^{\bar{R}} + h(\bar{R} - \bar{R}') G_M^{\bar{R}\bar{R}'} \quad (3.13)$$

It can be shown⁸ that $G_M^{\bar{R}}$ corresponds to the medium excluding an ion at \bar{R} , in the sense of the single-site modified Kirkwood approximation¹⁸ which characterizes the EMA. The Kirkwood approximation replaces the n -body distribution function by a product of PDF's as in Eq. (3.20) below. In the EMA the n -body distribution function is approximated by a product of PDF's along the scattering chain (as in the QCA) but out of chain correlations, i.e., site equalities and h correlations ($h = g - 1$) are included only to the extent that they do not cross. A diagram analysis of this has been given.²³

For $G_M^{\bar{R}_0}$ this corresponds to using $Q^{\bar{R}_0}(\bar{R}, \bar{R}')$ in Eq. (2.8), which obeys Eq. (2.9) with the density n replaced by $ng(r - R_0)$, i.e.,

$$Q^{\bar{R}_0}(\bar{R}, \bar{R}') = nt_c(\bar{R})g(\bar{R} - \bar{R}_0) \times \left[\delta(\bar{R} - \bar{R}') + \int \tilde{G}(\bar{R}, \bar{R}'') Q^{\bar{R}_0}(\bar{R}'', \bar{R}') \right] \quad (3.14)$$

This obeys the identity⁸

$$\int \tilde{G}(\bar{R}, \bar{R}'') Q(\bar{R}'', \bar{R}') d\bar{R}'' = G_0 \int Q^{\bar{R}}(\bar{R}'', \bar{R}') d\bar{R}'' \quad (3.15)$$

from which our interpretation of $G_M^{\bar{R}_0}$ follows from Table I.

In the same modified Kirkwood sense $G_M^{\bar{R}\bar{R}'}$ is an approximation to a Green's function excluding ions

at R and R' . Successive use of Eq. (3.15) and Table I gives

$$\begin{aligned} G_M^{\bar{R}\bar{R}'} &= G_0 + G_0 \int Q^{\bar{R}}(\bar{R}_1, \bar{R}_2) \tilde{G}(\bar{R}_2, \bar{R}') d\bar{R}_1 d\bar{R}_2 \\ &= G_M^{\bar{R}} + G_0 \int Q^{\bar{R}}(\bar{R}_1, \bar{R}_2) h(\bar{R}_2 - \bar{R}') \tilde{G}(\bar{R}_2, \bar{R}_3) Q^{\bar{R}'}(\bar{R}_3, \bar{R}_4) d\bar{R}_1, \dots, d\bar{R}_4 G_0 \end{aligned} \quad (3.16)$$

The first term involves only exclusions of an ion at \bar{R} , while the second term adds in all the exclusions of \bar{R}' which do not involve crossed correlations. A similar argument can be made reversing the roles of \bar{R} and \bar{R}' .

If $G^{\bar{R}}$ and $G^{\bar{R}'}$ exactly excluded the missing ions,

would Eq. (3.13) be Herglotz? We find that if a certain conjecture is valid and if the Kirkwood approximation is correct, the answer is yes. We have been able to prove the following theorem: if $g_s(\bar{R}_1, \dots, \bar{R}_s)$ is an s -body distribution function, then the operator on \bar{R} and \bar{R}' (for fixed $\bar{R}_1, \dots, \bar{R}_s$)

$$\begin{aligned} P_s(\bar{R}, \bar{R}', \bar{R}_1, \dots, \bar{R}_s) &= \frac{1}{n} \delta(\bar{R} - \bar{R}') \frac{g_{s+1}(\bar{R}, \bar{R}_1, \dots, \bar{R}_s)}{g_s(\bar{R}_1, \dots, \bar{R}_s)} + \frac{g_{s+2}(\bar{R}, \bar{R}', \bar{R}_1, \dots, \bar{R}_s)}{g_s(\bar{R}_1, \dots, \bar{R}_s)} \\ &\quad - \frac{g_{s+1}(\bar{R}, \bar{R}_1, \dots, \bar{R}_s) g_{s+1}(\bar{R}', \bar{R}_1, \dots, \bar{R}_s)}{g_s^2(\bar{R}_1, \dots, \bar{R}_s)} \end{aligned} \quad (3.17)$$

is positive semidefinite. Proof: by definition

$$n^s g_s(\bar{R}_1, \dots, \bar{R}_s) = \left\langle \sum_{i_1, \dots, i_s}'' \rho_{i_1}(\bar{R}_1) \dots \rho_{i_s}(\bar{R}_s) \right\rangle_c \quad (3.18)$$

where $\langle \rangle_c$ is an average over ionic configurations, $\rho_i(\bar{R}) = \delta(\bar{R} - \bar{R}_i)$, and the double prime means no two indices are equal. It follows that

$$\begin{aligned} P_s(\bar{R}, \bar{R}') &= \frac{n^{-s-2}}{g_s(\bar{R}_1, \dots, \bar{R}_s)} \left\langle \sum_{i_1, \dots, i_s}'' \left[\sum_{j \neq i_1, \dots, i_s} \rho_j(\bar{R}) - \frac{ng_{s+1}(\bar{R}, \bar{R}_1, \dots, \bar{R}_s)}{g_s(\bar{R}_1, \dots, \bar{R}_s)} \right] \right. \\ &\quad \times \left. \left[\sum_{j \neq i_1, \dots, i_s} \rho_j(\bar{R}') - \frac{ng_{s+1}(\bar{R}', \bar{R}_1, \dots, \bar{R}_s)}{g_s(\bar{R}_1, \dots, \bar{R}_s)} \right] \rho_{i_1}(\bar{R}_1) \dots \rho_{i_s}(\bar{R}_s) \right\rangle_c \end{aligned} \quad (3.19)$$

Then it is easy to show that for any function $f(\bar{R})$,

$$\int P_s(\bar{R}, \bar{R}') f^*(\bar{R}) f(\bar{R}') dR dR' > 0,$$

which proves the theorem. For $n=0$, $g_n = g_{n+1} = 1$, and $P_0(\bar{R}, \bar{R}')$ is just $S(\bar{R}, \bar{R}')/n$.

Now if a Kirkwood decomposition is valid, then

$$g_s(\bar{R}_1, \dots, \bar{R}_s) = \prod_{i>j=1}^s g(\bar{R}_i - \bar{R}_j) \quad (3.20)$$

in which case we have

$$P_s(\bar{R}, \bar{R}') \cong n^{-1} \delta(\bar{R} - \bar{R}') \prod_{i=1}^s g(\bar{R} - \bar{R}_i) + h(\bar{R} - \bar{R}') \prod_{i,j=1}^s g(\bar{R} - \bar{R}_i) g(\bar{R}' - \bar{R}_j) \quad (3.21)$$

The Green's function can be written quite generally as

$$G = \sum_{s=0}^{\infty} n^s \int G^{(s)}(\bar{R}_1, \dots, \bar{R}_s) g_s(\bar{R}_1, \dots, \bar{R}_s) d\bar{R}_1, \dots, d\bar{R}_s \quad (3.22)$$

Where $G^{(0)} = G_0$ (with no integration). If we multiply each g_s by the corresponding positive quantity P_s the conjecture is that this leads to a Herglotz operator. Within the Kirkwood approximation, the PDF's in Eq. (3.22)

are just right to exclude ions at \bar{R} and \bar{R}' , so that the result is

$$K_{\sigma} = n^{-1} \delta(\bar{R} - \bar{R}') G_K^{\bar{R}} + h(\bar{R} - \bar{R}') G_K^{\bar{R}\bar{R}'} \quad (3.23)$$

where K is for Kirkwood. Thus to the extent that the modified Kirkwood approximation approaches the Kirkwood [Eq. (3.20)] and to the extent that the Kirkwood [Eq. (3.20)] is valid, our conjecture leads to analyticity for the EMA.

One case for which the Kirkwood approximation is exact is that of impurities distributed randomly on a crystalline lattice. For this case the EMA and SE theories both reduce to the alloy CPA.^{6,8,18} We must replace the continuous distributions by discrete distributions on the lattice, and replace n by x , the impurity concentration. For the lattice $g_{\bar{R}\bar{R}'} = 1 - \delta_{\bar{R}\bar{R}'}$ and $h_{\bar{R}\bar{R}'} = -\delta_{\bar{R}\bar{R}'}$, so that for EMA

$$K_{\sigma} = \delta_{\bar{R}\bar{R}'} (x^{-1} G^{\bar{R}} - G^{\bar{R}\bar{R}'}). \quad (3.24)$$

From the first line of Eqs. (3.16) and (2.12),

$$G^{\bar{R}\bar{R}'} = G_0 + G_0 \sum_{\bar{R}''\bar{R}'''} Q^{\bar{R}}(\bar{R}'', \bar{R}''') (G_0 - \delta_{\bar{R}''\bar{R}'''} G^{\bar{R}\bar{R}''}), \quad (3.25)$$

but $Q^{\bar{R}}(\bar{R}'', \bar{R}) = 0$, so that $G^{\bar{R}\bar{R}'}$ is simply $G^{\bar{R}}$ and thus

$$K_{\sigma} = \delta_{\bar{R}\bar{R}'} G^{\bar{R}} (1 - x)/x. \quad (3.26)$$

This holds also for the SE result. We expect $G^{\bar{R}}$ to be Herglotz, and this supports previous proofs of analyticity for the alloy CPA.

IV. RELATIVE COORDINATE REPRESENTATION

Some of the above results take a rather tidier form if we introduce a new representation which makes use of translational symmetry. Operators like $T(\bar{\tau}, \bar{\tau}', \bar{R}, \bar{R}')$ depend only on relative electron and ion coordinates. We can therefore write

$$\begin{aligned} Q(\bar{\tau}, \bar{\tau}', \bar{R}, \bar{R}') &= \hat{Q}(\bar{\tau} - \bar{R}, \bar{\tau}' - \bar{R}', \bar{R} - \bar{R}'), \\ \tilde{G}(\bar{\tau}, \bar{\tau}', \bar{R}, \bar{R}') &= \hat{G}(\bar{\tau} - \bar{R}, \bar{\tau}' - \bar{R}', \bar{R} - \bar{R}'), \text{ etc.}, \\ t_c(\bar{\tau}, \bar{\tau}', \bar{R}) \delta(\bar{R} - \bar{R}') &= \hat{t}_c(\bar{\tau} - \bar{R}, \bar{\tau}' - \bar{R}', \bar{R} - \bar{R}') \\ &= t_c(\bar{\tau} - \bar{R}, \bar{\tau}' - \bar{R}') \delta(\bar{R} - \bar{R}'). \end{aligned} \quad (4.1)$$

Note that t_c differs from $t_c(R)$ of Eq. (2.9) in that the origin is at 0. Equation (2.9) for the scattering path

operator becomes

$$\begin{aligned} \hat{Q}(\bar{\rho}, \bar{\rho}', \bar{R} - \bar{R}') &= nt_c(\bar{\rho}, \bar{\rho}') \delta(\bar{R} - \bar{R}') \\ &+ n \int t_c(\bar{\rho}, \bar{\rho}'') \hat{G}(\bar{\rho}'', \bar{\rho}''', \bar{R} - \bar{R}''') \\ &\times \hat{Q}(\bar{\rho}''', \bar{\rho}', \bar{R}'' - \bar{R}') d\bar{\rho}'' d\bar{\rho}''' d\bar{R}'' \quad (4.2) \end{aligned}$$

or, if we suppress the relative electron coordinates $\bar{\rho}$ and $\bar{\rho}'$

$$\begin{aligned} \hat{Q}(\bar{R} - \bar{R}') &= nt_c \left[\delta(\bar{R} - \bar{R}') \right. \\ &\left. + \int \hat{G}(\bar{R} - \bar{R}'') \hat{Q}(\bar{R}'' - \bar{R}') d\bar{R}'' \right]. \end{aligned} \quad (4.3)$$

This is a convolution product in the ion coordinates, so a Fourier transform yields a simple product. Thus if

$$\begin{aligned} \hat{Q}_{\bar{k}} &= \int e^{-i\bar{k} \cdot \bar{R}} \hat{Q}(\bar{R}) d\bar{R}, \\ \hat{Q}(\bar{R}) &= \int e^{i\bar{k} \cdot \bar{R}} \hat{Q}_{\bar{k}} \frac{d\bar{k}}{8\pi^3}, \end{aligned} \quad (4.4)$$

then we have

$$\hat{Q}_{\bar{k}} = nt_c (1 + \hat{G}_{\bar{k}} Q_{\bar{k}}). \quad (4.5)$$

In a similar way we have for the self-energy path operator

$$\hat{Q}_{\bar{k}} = nt_c [1 + (\hat{G}_{\bar{k}} - \hat{G}_{0\bar{k}}) \sigma_{\bar{k}}]. \quad (4.6)$$

We can also use a momentum representation for the relative electron coordinates ρ and ρ' :

$$\begin{aligned} \hat{Q}_{\bar{k}}^{\bar{\rho}\bar{\rho}'} &= \int \exp(-i\bar{p} \cdot \bar{\rho} + i\bar{p}' \cdot \bar{\rho}' - i\bar{k} \cdot \bar{R}) \\ &\times \hat{Q}(\bar{\rho}, \bar{\rho}', \bar{R}) d\bar{\rho} d\bar{\rho}' d\bar{R} \quad (4.7) \end{aligned}$$

$$\begin{aligned} \hat{Q}(\bar{\rho}, \bar{\rho}', \bar{R}) &= \int \exp(i\bar{p} \cdot \bar{\rho} - i\bar{p}' \cdot \bar{\rho}' + i\bar{k} \cdot \bar{R}) \\ &\times Q_{\bar{R}}^{\bar{\rho}\bar{\rho}'} \frac{d\bar{k} d\bar{p} d\bar{p}'}{(2\pi)^9} \quad (4.8) \end{aligned}$$

In particular, since the unperturbed Green's function depends only on $\bar{\tau} - \bar{\tau}'$ we have

$$\begin{aligned} \hat{G}_0(\bar{\rho}, \bar{\rho}', \bar{R}) &= G_0(\bar{\rho} - \bar{\rho}' + \bar{R}) \\ &= \int \exp[i\bar{k} \cdot (\bar{\rho} - \bar{\rho}' + \bar{R})] G_{0\bar{k}} \frac{d\bar{k}}{8\pi^3} \quad (4.9) \end{aligned}$$

It follows that

$$\hat{G}_{0\bar{k}}^{\bar{\rho}\bar{\rho}'} = (2\pi)^6 \delta(\bar{\rho} - \bar{k}) \delta(\bar{\rho}' - \bar{k}) G_{0\bar{k}} \quad (4.10)$$

The same applies to the exact Green's function G .

Another quantity of interest is $T = \int Q(\bar{R}, \bar{R}') d\bar{R} d\bar{R}'$

$$T_{\bar{k}} = \int \left[\int \hat{Q}(\bar{r} - \bar{R}, \bar{r}' - \bar{R}', \bar{R} - \bar{R}') d\bar{R} d\bar{R}' \right] \times e^{i\bar{k} \cdot (\bar{r} - \bar{r}')} d\bar{r} = \hat{Q}_{\bar{k}}^{\bar{k}} \quad (4.11)$$

That is, to obtain the configuration-averaged total-scattering matrix we set the electron wave vectors \bar{p} and \bar{p}' in $Q_{\bar{k}}^{\bar{p}\bar{p}'}$ both equal to the ion wave vector \bar{k} . Also, we have for the self-energy and the medium Green's function.

$$G_{\bar{k}}^{-1} = \omega - \epsilon_{\bar{k}}^0 - \Sigma_{\bar{k}}, \quad \Sigma_{\bar{k}} = \sigma_{\bar{k}}^{\bar{k}} \quad (4.12)$$

The various results for Q and σ can be written in the new representation

$$\hat{Q}_{\bar{k}} = n\nu(1 + \hat{K}_{Q_{\bar{k}}} \hat{Q}_{\bar{k}}), \quad \sigma_{\bar{k}} = n\nu(1 + \hat{K}_{\sigma_{\bar{k}}} \sigma_{\bar{k}}) \quad (4.13)$$

Let us examine the GKM. We find that the σ kernel is given by

$$\hat{K}_{\sigma_{\bar{k}}}^{\text{GKM}} = \int \left[\frac{1}{n} + h(\bar{k} - \bar{k}') \right] \hat{G}_{\bar{k}} \frac{d\bar{k}'}{8\pi^3}, \quad (4.14)$$

or

$$(\hat{K}_{\sigma_{\bar{k}}}^{\text{GKM}})^{pp'} = 8\pi^3 \delta(\bar{p} - \bar{p}') \left[\frac{1}{n} + h(\bar{k} - \bar{p}) \right] G_{\bar{p}} \quad (4.15)$$

which has a particularly simple structure. Considering the self-energy relationship, from Eqs. (2.13) and (3.7) we have

$$\Sigma_{\bar{k}} - \Sigma_{\bar{k}}^* = \int \sigma_{\bar{k}}^{\bar{p}\bar{k}'} \left(K_{\sigma_{\bar{k}}}^{\bar{p}\bar{p}'} - K_{\sigma_{\bar{k}}}^{\bar{p}'\bar{p}^*} \right) \sigma_{\bar{k}}^{\bar{p}'\bar{k}} \frac{d\bar{p} d\bar{p}'}{(2\pi)^6} \quad (4.16)$$

For the GKM this gives

$$\Sigma_{\bar{k}} - \Sigma_{\bar{k}}^* = \int |\sigma_{\bar{k}}^{\bar{k}\bar{k}'}|^2 \left[\frac{1}{n} + h(\bar{k} - \bar{k}') \right] \times (G_{\bar{k}'} - G_{\bar{k}'}^*) \frac{d\bar{k}'}{8\pi^3} \quad (4.17)$$

The quantity

$$|\sigma_{\bar{k}}^{\bar{k}\bar{k}'}|^2 [1/n + h(\bar{k} - \bar{k}')] = W(\omega + i\epsilon, \omega - i\epsilon, \bar{k}, \bar{k}')$$

is the GKM result for the vertex function which appears in the conductivity problem. Specifically Rubio²⁹ postulated a Bethe-Salpeter type equation for the quantity

$$\pi^{\mu}(z, z') = \langle \mathcal{G}(z) j^{\mu} \mathcal{G}(z') \rangle,$$

where j_{μ} is a component of the current operator. The integral equation for π is

$$\pi_{\bar{k}}^{\mu}(z, z') = G_{\bar{k}}(z) \times \left[j_{\bar{k}}^{\mu} + \int W(z, z', \bar{k}, \bar{k}') \pi_{\bar{k}}^{\mu}(z, z') \right] G_{\bar{k}}(z') \quad (4.18)$$

Equation (4.17) corresponds to a Ward identity discussed by Popielawski³⁰ and Velicky.³¹ Popielawski derived Eq. (4.18) and showed that the GKM theory is the basis for the work of Ashcraft and Schaich³² on an extension of the Ziman formula for the conductivity.

For the EMA we can write

$$K_{\sigma_{\bar{k}}} = \int \left[\frac{1}{n} \hat{G}_{1\bar{k}'} + h(\bar{k} - \bar{k}') \hat{G}_{2\bar{k}'} \right] \frac{d\bar{k}'}{8\pi^3}, \quad (4.19)$$

where

$$\hat{G}_{1\bar{k}} = (1 + \hat{G}_{\bar{k}} \hat{Q}_{\bar{k}}) \hat{G}_{0\bar{k}}, \quad \hat{G}_{2\bar{k}} = \hat{G}_{0\bar{k}} + \hat{G}_{\bar{k}} \hat{Q}_{\bar{k}} \hat{G}_{\bar{k}} \quad (4.20)$$

It is possible to write G_{1k} and G_{2k} entirely in terms of medium quantities as follows

$$\hat{G}_{1\bar{k}} = (1 + \hat{W}_{\bar{k}} \sigma_{\bar{k}}) \hat{G}_{\bar{k}}, \quad \hat{G}_{2\bar{k}} = (1 + \hat{W}_{\bar{k}} \sigma_{\bar{k}}) \hat{G}_{\bar{k}} (1 + \hat{\sigma}_{\bar{k}} \hat{W}_{\bar{k}}) + \hat{W}_{\bar{k}} \hat{\sigma}_{\bar{k}} \hat{W}_{\bar{k}}, \quad (4.21)$$

where

$$\hat{W}_{\bar{k}} = \hat{G}_{\bar{k}} - \hat{G}_{0\bar{k}} = \int h(\bar{k} - \bar{k}') \hat{G}_{2\bar{k}'} \quad (4.22)$$

The result of Eq. (4.21) is obtained by using Eqs. (2.14) and (2.15) which become simply $\hat{Q}_{\bar{k}} = \hat{\sigma}_{\bar{k}} (1 + \hat{G}_{\bar{k}} \hat{\sigma}_{\bar{k}})$ and $\hat{Q}_{\bar{k}} \hat{G}_{0\bar{k}} = \hat{\sigma}_{\bar{k}} \hat{G}_{\bar{k}}$. This is the same result for σ as was obtained by Watabe and Yonezawa.¹⁸

The conductivity problem is more difficult in the EMA and Eq. (4.18) becomes a set of coupled integral equations. We are investigating these equations and expect to report our findings in a future publication.

Another interesting use for relative coordinates is the angular momentum representation for the muffin-tin model. In fact the work of Lloyd,⁴ Schwartz *et al.*¹⁰ and subsequent authors²⁰⁻²² is all based on a relative coordinate approach.

V. SOME RESULTS FOR THE TIGHT-BINDING MODEL

We recall here some results for the one-orbital tight-binding model, for which the T matrix is replaced by a medium Green's function

$$G_{\bar{k}} = \frac{n}{\omega - n\hat{H}_{\bar{k}} - \Sigma_{\bar{k}}}, \quad (5.1)$$

where $n\tilde{H}_{\bar{k}}$ is given by

$$n\tilde{H}_{\bar{k}} = \int nH(\bar{R})g(\bar{R})e^{i\bar{k}\cdot\bar{R}}d\bar{R}, \quad (5.2)$$

with $H(\bar{R})$ a transfer energy, and $\Sigma_{\bar{k}}$ is a self-energy which has different forms for the various theories.

The results for $\Sigma_{\bar{k}}$ can be put in the form

$$\Sigma_{\bar{k}} = \int [F_{1\bar{k}'} + nh(\bar{k} - \bar{k}')F_{2\bar{k}'}] \frac{d\bar{k}'}{8\pi^3} = \Sigma_d + \Sigma_{1\bar{k}}, \quad (5.3)$$

with $F_{1\bar{k}}$ and $F_{2\bar{k}}$ given for several theories in Table II. To ensure the analyticity of G , $\Sigma_{\bar{k}}$ must be analytic and have a negative imaginary part in the upper half ω plane.

For QCA, the Green's function is obviously analytic. For the GKM theory the positive definite character of the structure factor ensures that $\text{Im} \Sigma_{\bar{k}}$ has the same sign as $\text{Im} G_{\bar{k}}$, and this implies analyticity. We have in fact proved analyticity²⁵ for the random case ($h=0$). In this case all the self-consistent theories are equivalent to the GKM. The proof also holds for the IY theory in the case of a square PDF for which $g^2=g$.

We have also discussed a necessary condition for analyticity. If the spectral weight function is positive, then the mean-squared frequency deviation or width function

$$\gamma_{\bar{k}}^2 = \int (\omega - \bar{\omega})^2 \left[-\frac{1}{\pi} \text{Im} G_{\bar{k}} \right] d\omega \quad (5.4)$$

must be positive. In terms of distribution functions

the exact result for $\gamma_{\bar{k}}^2$ is given by

$$\gamma_{\bar{k}}^2 = \int \left(\int P_2(\bar{R}, \bar{R}', \bar{R}_1) H(\bar{R} - \bar{R}_1) \times H(\bar{R}' - \bar{R}_1) d\bar{R}_1 \right) e^{i\bar{k}\cdot(\bar{R} - \bar{R}')} d\bar{k}, \quad (5.5)$$

where P_2 is defined in Eq. (3.17), and has been shown to be a positive semidefinite operator in R and R' . The operator in square brackets is also positive semidefinite, and $\gamma_{\bar{k}}^2$ is an eigenvalue of it and is, therefore, non-negative.

For the various theories we find

$$\gamma_{\bar{k}}^2 = \int [f_{1\bar{k}'} + nh(\bar{k} - \bar{k}')f_{2\bar{k}'}] \frac{d\bar{k}'}{8\pi^3}, \quad (5.6)$$

where $f_{1\bar{k}}$ and $f_{2\bar{k}}$ are given in Table II, and correspond essentially to different approximations for P_2 . For the EMA P_2 is evaluated in the Kirkwood approximation. It is clear that IY and GKM give positive width functions. For other cases one can test theories by calculating $\gamma_{\bar{k}}^2$. We have plotted the width function for several theories for an exponential overlap and a hard-sphere Percus-Yevich PDF³³ in Fig. 1(a), using a packing fraction of $\eta=0.45$ appropriate for liquid metals. We see that the EMA gives a positive width function while the SE result goes negative. This has been discussed previously.³³ While the IY and GKM width functions are positive, they are not very realistic and in particular the GKM width function is quite large. This is because no correlations are included in $H(R)$ in Eq. (5.5) as we can see in Table II. We can modify the GKM in several ways to improve the situation. We can multi-

TABLE II. Functions for Eqs. (5.3) and (5.6) for various theories.

	F_1	F_2	f_1	f_2
QCA	0	0		
GKM	$H^2 G_{\bar{k}}$	$= F_1$	$H_{\bar{k}}^2$	$= f_1$
SCA	$H_{\bar{k}} M_{\bar{k}} G_{\bar{k}}$	$= F_1$	$H_{\bar{k}} \tilde{H}_{\bar{k}}$	$= f_1$
IY	$\tilde{H}_{\bar{k}}^2 G_{\bar{k}} + n\tilde{H}_{\bar{k}} \frac{(H_{\bar{k}} - \tilde{H}_{\bar{k}})}{\omega - \Sigma_d}$	0	$H_{\bar{k}} \tilde{H}_{\bar{k}}$	0
EMA	$H_{\bar{k}} M_{\bar{k}} G_{\bar{k}}$ $M_{\bar{k}} = \tilde{H}_{\bar{k}} + \Sigma_{1\bar{k}}/n$	$M_{\bar{k}}^2 G_{\bar{k}}$	$H_{\bar{k}} \tilde{H}_{\bar{k}}$	$\tilde{H}_{\bar{k}}^2$

ply $H(R)$ in Table II by $g(R)$ or $[g(R)]^{1/2}$. The first choice gives the EMA result for f_2 but overmultiplies f_1 , by $g(R)$. The second choice is correct for f_1 but not f_2 . We can also cut $H(R)$ off at the hard-sphere diameter. These three possibilities are included in Fig. 1(b).

The EMA result is given for larger packing fractions in Fig. 2. We see that there is a tendency for the width function to go negative for larger packing fractions. There is some dependence on the Bohr radius relative to the hard-sphere diameter. Introducing a large R cutoff tends to reduce the tendency to go negative as is shown in the dashed curve in Fig. 2. We have earlier defined²⁵ an effective coordination number

$$z = \left(\int n\bar{H}(\bar{R}) d\bar{R} \right)^2 / \int n\bar{H}(\bar{R})H(\bar{R}) d\bar{R}$$

and we see that negativity of γ_k^2 is connected somewhat with too many neighbors. Of course if the width function in the EMA is negative for any form of $H(R)$ for a given packing fraction, this implies that P_2 is not a positive definite operator in the Kirkwood approximation for that packing fraction. This suggests that there may be problems with the Percus-Yevick hard-sphere model for larger packing fractions simulating amorphous metals.

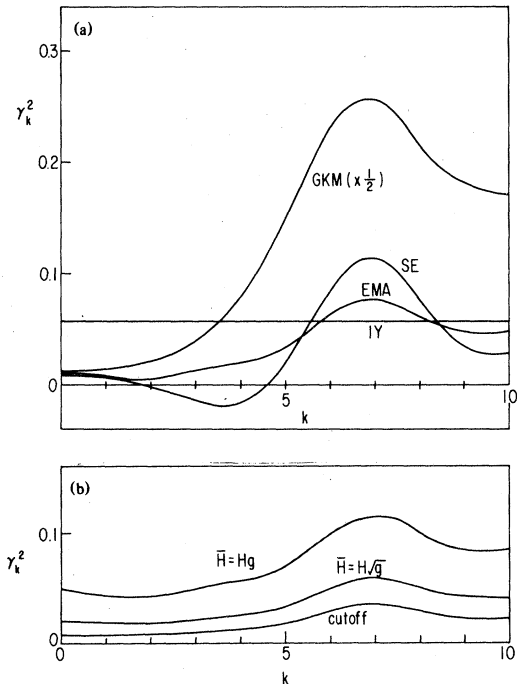


FIG. 1. Width function vs k for hard-sphere Percus-Yevick PDF, with Hopping integral $H(R) = H_1 e^{-\lambda R} [1 + \lambda R + \frac{1}{3}(\lambda R)^2]$ with $\lambda = 4.8$, and hard-sphere packing fraction $\eta = 0.45$, in units for which the hard-sphere diameter $\sigma = 1$. (a) Comparing several theories; (b) showing modifications of GKM in which $H(R) \rightarrow \bar{H}(R)$.

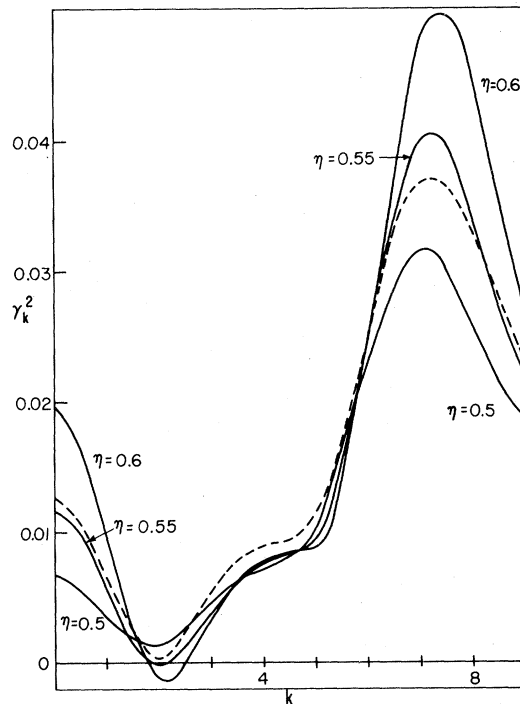


FIG. 2. Width function for the EMA for Percus-Yevick hard-sphere PDF for several packing fractions and $H(R)$ as in Fig. 1 with $\lambda = 4.8$. For dashed curve $H(R)$ has been cut off at $R = 1.6\sigma$.

VI. CONCLUSIONS

We have formulated a criterion for analyticity of the Green's function for liquid metals, in terms of the kernel of an integral equation obeyed by the self-energy path operator. It is shown that the GKM theory, which can be described as a renormalized QCA is analytic. For the random case ($g = 1$) all of the single-site self-consistent theories reduce to the GKM, so this implies analyticity for these theories in the random case. The inclusion of correlation makes it difficult to prove anything conclusive in regard to analyticity for the EMA, etc., but the tight-binding results suggest that the EMA is more accurate than the GKM while remaining analytic for not-too-large packing fractions. It would certainly be desirable to combine the analytic property of the GKM with the accuracy of the EMA, but so far we have not found a way to do this. Meanwhile, we must rely on experience in actual calculations.

ACKNOWLEDGMENTS

The author wishes to thank Dr. Vijay Singh for kindly providing Figs. 1 and 2. This research was supported by the NSF under Grant No. DRM75-18104.

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