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Analytic approximation for random muffin-tin alloys

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The methods introduced in a previous paper under the name of "traveling-cluster approximation" (TCA) are applied, in a multiple-scattering approach, to the case of a random muffin-tin substitutional alloy. This permits the iterative part of a self-consistent calculation to be carried out entirely in terms of on-the-energy-shell scattering amplitudes. Off-shell components of the mean resolvent, needed for the calculation of spectral functions, are obtained by standard methods involving single-site scattering wave functions. The single-site TCA is just the usual coherent-potential approximation, expressed in a form particularly suited for iteration. A fixed-point theorem is proved for the general t-matrix TCA, ensuring convergence upon iteration to a unique self-consistent solution with the physically essential Herglotz properties.

I. INTRODUCTION

The development of efforts to apply and extend the coherent-potential approximation (CPA) for random substitutional alloys has followed two somewhat independent lines since the idea was first put forward in 1967, in different but logically equivalent forms, by Soven[1] and Taylor.[2] On the one hand there have been the more formal efforts, concentrating often on methods of graphical analysis,[3–5] looking for effective cluster-type approximations,[6] and finding a testing ground in simple models such as single-band systems. On the other hand there have been many efforts to work with realistic models, starting with Soven's use[7] of a CPA-type approximation for muffin-tin potentials (i.e., potential wells confined to a spherical region inside each unit cell of the lattice), and leading to various ways[8] of calculating physical properties of real systems using an on-the-energy-shell multiple-scattering approach, but not going beyond single-site approximations for the most part. We shall refer to this approach as the "t-matrix CPA".

The purpose of this paper is to present a systematic multiple-scattering version of the "traveling-cluster approximation" (TCA). The TCA is a formal extension of the CPA developed by Mills and Ratanavararaksa[5] (hereafter referred to as MR) which incorporates cluster effects in a way that preserves the necessary analyticity properties referred to collectively as the "Herglotz property" (see Sec. V). Such a multiple-scattering version of the TCA, in the case of a muffin-tin potential, would permit practical calculations using on-the-energy-shell t matrices, in the spirit of the t-matrix CPA. In the case of the CPA, the t-matrix approach proves to be exactly equivalent to the formal approach, as is implicit in the work of Bansil *et al.*[9] In the general TCA, in contrast, the two approaches are not equivalent, and we find that the t-matrix version is preferable on several grounds. In the first place, the formal approach, when reexpressed in terms of scattering operators, cannot be satisfactorily projected onto the energy shell, so that it is not suitable for practical calculations, and in the second place, when the t-matrix TCA is broken down into modified-cumulant-average (MCA) graphs in the manner of MR, it is found to include a few more graphs than the corresponding formal TCA using potential operators (see Sec. V). Off-shell components are needed for the t-matrix TCA as well, in order to calculate the mean resolvent and the spectral density function, but these can be handled much as in Faulkner and Stocks[10] by the use of single-scatterer wave functions as shown in Sec. II. Practical calculational procedures are described in Sec. III,

along with the results of a simple single-band calculation, which show only slight differences in the density of states between the formal TCA and the t-matrix TCA.

The t-matrix CPA can be seen as the single-site version of the TCA, giving rise to forms that seem to have some practical advantages over the standard procedures, and that allow one to see that the Faulkner and Stocks way of recovering the full mean resolvent agrees exactly with the formal CPA. This is discussed in Sec. IV.

The analysis of causality (related to the Herglotz property) in the t-matrix TCA is complicated by the following fact: The propagator in the multiple-scattering formulation consists of the off-diagonal parts of the electron Green's function, since the site-diagonal parts are absorbed in the single-site t matrix. Such a propagator lacks the Herglotz property, which is crucial to the analysis, so that in order to test this approximation for the causality condition, it is necessary to reduce it to an equivalent form involving potential operators and the full Green's function. This has been done, and the appropriate fixed-point theorem proved, showing that iteration of the equations for any complex energy converges to a unique, Herglotz solution of the self-consistent equations. This is described in Sec. V.

It is our intention that Secs. II and IV provide an outline of the structure of the theory including its implications in the single-site case. It is further our intention that the more mathematical and calculational details be contained in Secs. III and V, and the Appendices. For the sake of brevity the results of MR and Kaplan, Leath, Gray, and Diehl[5] (hereafter referred to as KLGD) are used extensively, often with little comment.

II. FORMALITIES

The Hamiltonian is

$$H=H^0+V\,, \tag{2.1}$$

where V is a sum of random single-site scattering potentials, centered at the sites R^i of a Bravais lattice,

$$V=\sum_i v^i\,, \tag{2.2}$$

and v^i is the random scattering potential, v^{iA} or v^{iB}, which occupies site i with probability c_A or c_B, respectively. Since we restrict ourselves to muffin-tin potentials, each localized within a single cell, the terms v^i are nonoverlapping, and it is often convenient to characterize a point r by its site index i and a local coordinate x to locate the point within the ith cell. Thus

$$r=R^i+x,\quad (r\in U^i,\ x\in U^0)\,, \tag{2.3}$$

where U^i is the unit cell centered at R^i. Note that R^0 is taken as zero.

The mean system scattering operator $\bar{\tau}$ is given by

$$\bar{\tau}=\overline{(V^{-1}-G^0)^{-1}}=[(V^c)^{-1}-G^0]^{-1}\,, \tag{2.4}$$

where the overbar indicates a configuration average, and V^c is an effective scattering potential for the system, defined by this equation. G^0 is the free-electron Green's function, given by

$$G^0=(E-H^0)^{-1}\,. \tag{2.5}$$

[In Eq. (2.4) and elsewhere, we use the compact expression $(a^{-1}-b)^{-1}$ to represent $a(1-ba)^{-1}$, even where a^{-1} may not be defined.]

In any given level of approximation in the TCA (see MR, Ref. 5, pp. 5296f) the effective potential V^c has the form [MR, Ref. 5, Eq. (4.5)]:

$$V^c=\bar{V}+V'MV'\,, \tag{2.6}$$

where

$$\bar{V}=\sum_i \bar{v}^i=\sum_i (c_A v^{iA}+c_B v^{iB})\,, \tag{2.7}$$

$$V'=\sum_i v'^i=\sum_i \sqrt{c_A c_B}(v^{iA}-v^{iB})\,. \tag{2.8}$$

The operator M is given by rather complicated expressions involving an augmented-vector space, with basis vectors labeled by the different sets of sites on which MCA lines are allowed to overlap, as described in Sec. III, and in greater detail by MR.

To obtain the multiple-scattering form, we separate G^0_{ij} into site-diagonal and nonsite-diagonal parts:

$$G^0=G^{0D}+g^0\,, \tag{2.9}$$

where G^{0D} has matrix elements only between an r and r' in the same cell,

$$(R^i+x\,|\,G^{0D}\,|\,R^j+x')=\delta_{ij}(R^i+x\,|\,G^0\,|\,R^i+x')\,, \tag{2.10}$$

and g^0, only between an r and r' in different cells,

$$(R^i+x\,|\,g^0\,|\,R^j+x')=(1-\delta_{ij})(R^i+x\,|\,G^0\,|\,R^j+x')\,. \tag{2.11}$$

This immediately lets us recast the mean system scattering operator [Eq. (2.4)] in the multiple-scattering form:

$$\bar{\tau}=\overline{(V^{-1}-G^{0D}-g^0)^{-1}} \tag{2.12}$$

$$=\overline{(T^{-1}-g^0)^{-1}}=[(T^c)^{-1}-g^0]^{-1}\,, \tag{2.13}$$

where T is the sum of random single-site scattering operators,

$$T=(V^{-1}-G^{0D})^{-1}=\sum_i t^i , \tag{2.14}$$

and T^c is an effective local scattering operator analogous to V^c and related to it by

$$T^c=[(V^c)^{-1}-G^{0D}]^{-1} . \tag{2.15}$$

Note the role of G^{0D} in (2.15), in that while V^c_{ij} is not site diagonal, the propagation between one V^c and the next is localized within a single cell.

Since the potentials v^i are assumed to be muffin tins of radius c, and since g^0 is nonsite-diagonal, the latter can be expressed exactly in terms of on-energy-shell wave functions in x and x', so that the heart of the calculation takes place on-shell and involves only the on-shell matrix elements of t^i. It is not necessary, however, to project τ onto the energy shell, and indeed this would lose some of the information needed to construct the mean resolvent $\bar{G}$ [defined below in Eq. (2.23)].

The structure of (2.13) is identical to that of (2.4), with T and g^0 replacing, respectively, V and G^0. It follows that the analysis of MR (apart from the proof of uniqueness, convergence, and the Herglotz properties) can be carried through directly, yielding a form structurally the same as (2.6):

$$T^c=\bar{T}+T'MT' , \tag{2.16}$$

where

$$\bar{T}=\sum_i \bar{t}^i=\sum_i (c_A t^{iA}+c_B t^{iB}) , \tag{2.17}$$

$$T'=\sum_i t'^i=\sum_i \sqrt{c_A c_B}(t^{iA}-t^{iB}) , \tag{2.18}$$

and where M is constructed in the same way as before, but out of t^i and g^0 instead of v^i and G^0. In Sec. III we shall exhibit the appropriate equations in a form suitable for calculation.

At this point we expand g^0 in on-shell free-particle wave functions, in the usual fashion [see, e.g., Ref. 10, Eqs. (2), (7), and (16)]:

$$\begin{aligned}(R^i+x\,|\,g^0\,|\,R^j+x') &= \sum_{L,L'} j^L(x)g^0_{LL'}(R^i-R^j)j^{L'}(x') \\ &= \underline{j}(x)\underline{g}^0_{ij}\underline{j}(x') ,\end{aligned} \tag{2.19}$$

with

$$j^L(x)\equiv j^{l,m}(x)=j_l(\sqrt{E}\,|x|)Y_{l,m}(x) . \tag{2.20}$$

The substitution of (2.19) into M has the effect of replacing $t^{i\alpha}$, wherever it appears, by an on-shell t matrix $\underline{t}^\alpha$:

$$\int \underline{j}(x)(R^i+x\,|\,t^{i\alpha}\,|\,R^i+x')\underline{j}(x')dx\,dx' = \underline{t}^\alpha,\ \alpha=A,B \text{ (any } i) , \tag{2.21}$$

so that we can write

$$(R^i+x\,|\,M\,|\,R^j+x')=\underline{j}(x)\underline{M}_{ij}\underline{j}(x') , \tag{2.22}$$

where $\underline{M}_{ij}$ has the same structure as M but is made out of $\underline{t}^\alpha$ and $\underline{g}^0_{ij}$. At this point the only things in T^c (2.16) that are not on-shell are the single-site operators $\bar{t}^i$ and t'^i that appear explicitly, and are easy to deal with.

Our aim in this is to set up expressions for the mean resolvent $\bar{G}$, so that we can calculate physically meaningful quantities like the mean spectral-density function. The general expression,

$$\bar{G}=G^0+G^0\bar{\tau}G^0 , \tag{2.23}$$

must be broken down into terms in which the initial and final propagations G^0 are within a single cell ($i=j$) or between different cells ($i\neq j$). In the latter case Eq. (2.19) can be used, while in the former case we identify the initial or final scattering as being from an A or a B site, and describe it by means of a corresponding Schrödinger wave function. After inserting (2.9) into (2.23), and performing some manipulations, we end up with

$$\begin{aligned}\bar{G}=&G^{0D}+G^{0D}T^cG^{0D} \\ &+(1+G^{0D}T^c)\bar{g}(1+T^cG^{0D}) .\end{aligned} \tag{2.24}$$

Here $\bar{g}$ is the multiple-scattering analog of $\bar{G}$:

$$\bar{g}=[(g^0)^{-1}-T^c]^{-1} , \tag{2.25}$$

which can be expressed in terms of on-shell wave functions by the use of Eq. (2.19):

$$(R^i+x\,|\,\bar{g}\,|\,R^j+x')=\underline{j}(x)\underline{\bar{g}}_{ij}\underline{j}(x') , \tag{2.26}$$

with

$$\underline{\bar{g}}=[(\underline{g}^0)^{-1}-\underline{T}^c]^{-1} , \tag{2.27}$$

$$\underline{T}^c_{ij}=\int \underline{j}(x)(R^i+x\,|\,T^c\,|\,R^j+x')\,\underline{j}(x')dx\,dx' \tag{2.28}$$

$$=\bar{t}\delta_{ij}+\underline{t}'\underline{M}_{ij}\underline{t}' . \tag{2.29}$$

The definitions of $\underline{\bar{t}}$ and $\underline{t}'$ are implicit in Eqs. (2.17), (2.18), and (2.21).

Substituting (2.26) and (2.24) and taking everything on-shell that we can, we get the relation

$$\bar{G}=\bar{G}^D+\sum_{ij}\underline{\psi}^c_i\underline{M}_{ij}\underline{\psi}'_j+\sum_{ij}\underline{\psi}^c_i\underline{\bar{g}}_{ij}(\underline{\psi}^c_j)^\dagger \tag{2.30}$$

with the following definitions:

$$\bar{G}^D = G^{0D} + G^{0D}\bar{T}G^{0D} , \tag{2.31}$$

$$(R^i+x \mid \bar{G}^D \mid R^j+x') = \delta_{ij}\sum_a c_a (x \mid G^0 + G^0 t^{0\alpha} G^0 \mid x') \tag{2.32}$$

$$= \delta_{ij}\sum_\alpha c_\alpha \underline{\psi}^\alpha(x_<)\underline{\xi}^\alpha(x_>) , \tag{2.33}$$

$$(R^i+x \mid \underline{\psi}'_j) = \delta_{ij}\underline{\psi}'(x) = \delta_{ij}\sqrt{c_A c_B}[\underline{\psi}^A(x) - \underline{\psi}^B(x)] , \tag{2.34}$$

$$(R^i+x \mid \underline{\psi}^c_j) = \int (R^i+x \mid (1+G^{0D}T^c) \mid R^j+x')\underline{j}(x')dx' \tag{2.35}$$

$$= \delta_{ij}\bar{\underline{\psi}}(x) + \underline{\psi}'(x)\underline{M}_{ij}\underline{t}' , \tag{2.36}$$

$$((\underline{\psi}^c_i)^\dagger \mid R^j+x) = \delta_{ij}\bar{\underline{\psi}}(x) + \underline{t}'\underline{M}_{ij}\underline{\psi}'(x) , \tag{2.37}$$

$$\bar{\underline{\psi}}(x) = \sum_\alpha c_\alpha \underline{\psi}^\alpha(x) . \tag{2.38}$$

Here $\underline{\psi}^\alpha$ and $\underline{\xi}^\alpha$ are regular and irregular solutions, respectively, of the single-scatterer Schrödinger equation, defined by

$$\underline{\psi}^\alpha = \underline{j} + G^0 v^{0\alpha}\underline{\psi}^\alpha = \underline{j} + G^0 t^{0\alpha}\underline{j} , \tag{2.39}$$

with asymptotic behavior:

$$(x \mid \underline{\psi}^\alpha) = \underline{j}(x) - i\sqrt{E}\,\underline{h}(x)\underline{t}^\alpha \quad (\mid x \mid > c) , \tag{2.40}$$

$$(x \mid \underline{\xi}^\alpha) = -i\sqrt{E}\,\underline{h}(x) \quad (\mid x \mid > c) , \tag{2.41}$$

$$h^L(x) = h_l^{(1)}(\sqrt{E}\mid x \mid)Y_{l,m}(x) . \tag{2.42}$$

In practice we work with the Bloch-Fourier transforms $\bar{G}(k)$, etc., the lattice transforms appropriate to the crystal symmetry of configuration-averaged quantities:

$$(x \mid \bar{G}(k) \mid x') = \sum_i e^{-ik\cdot R^i}(R^i+x \mid \bar{G} \mid x') \tag{2.43}$$

$$= (x \mid \bar{G}^D \mid x') + \underline{\psi}'(x)\underline{M}(k)\underline{\psi}'(x') + \underline{\psi}^c(x,k)\underline{\bar{g}}(k)\underline{\psi}^{c+}(x',k) , \tag{2.44}$$

$$\underline{\bar{g}}(k) = \sum_i e^{-ik\cdot R^i}\underline{\bar{g}}_{i0} = [\underline{g}^0(k)^{-1} - \underline{T}^c(k)]^{-1} , \tag{2.45}$$

$$\underline{T}^c(k) = \underline{\bar{t}} + \underline{t}'\underline{M}(k)\underline{t}' . \tag{2.46}$$

Here

$$\underline{\psi}^c(x,k) = \sum_i e^{-ik\cdot R^i}(R^i+x \mid \underline{\psi}^c_0) = \bar{\underline{\psi}}(x) + \underline{\psi}'(x)\underline{M}(k)\underline{t}' , \tag{2.47}$$

$$[\underline{\psi}^c(x,k)]^\dagger = \sum_i e^{-ik\cdot R^i}(\underline{\psi}^c_i \mid x) = \bar{\underline{\psi}}(x) + \underline{t}'\underline{M}(k)\underline{\psi}'(x) . \tag{2.48}$$

The mean Bloch spectral-density function or "reduced spectral density function," introduced by Soven,[10,11] and the mean density of states per site are obtained from $\bar{G}(k)$:

$$\tilde{\rho}(k,E) = -\frac{1}{\pi\Omega}\mathrm{Im}\int_{U^0} dx (x \mid \bar{G}(k) \mid x) , \tag{2.49}$$

$$n(E) = \int_{\mathrm{BZ}} \tilde{\rho}(k,E)dk , \tag{2.50}$$

where the integration is made over the first Brillouin zone (BZ), with volume Ω. The regular mean spectral-density function, for unrestricted momentum p, is given by

$$\rho(p,E) = -\frac{1}{8\pi^4}\mathrm{Im}\int_{U^0} dx\,dx' e^{-ip\cdot(x-x')} \times (x \mid \bar{G}(k) \mid x') , \tag{2.51}$$

where k is the reduced-wave vector that relates p to a reciprocal-lattice vector P_n:

$$p = P_n + k . \tag{2.52}$$

III. PRACTICALITIES

The central part of the calculation is the kernal $\underline{M}(k)$ which is found self-consistently via $\underline{t}^c(k)$ and $\underline{\bar{g}}(k)$, the latter [Eq. (2.45)] being the effective propagator that appears self-consistently in the intermediate "states" in $\underline{M}(k)$. The calculation, following closely the patterns of MR, gives $\underline{M}(k)$ as one central submatrix of a matrix $\underline{F}_{\mu\nu}^{\sigma\sigma'}$ whose rows and columns are labeled by three indices, L, μ, and σ. L is the familiar partial-wave index, μ is a local, or relative, site index, confined to a neighborhood of a local origin at $\mu=0$, and σ labels the different inequivalent (not translation-equivalent) MCA overlap sets included in the family T defining the approximation. To see what this means, look at the inverse Bloch transform $\underline{F}_{\mu\nu}^{\sigma\sigma'}(R^i,R^j)$: i is a reference site anywhere in the sample, $i+\sigma$ (i.e., the set σ displaced by R^i) is the actual overlap set, and $i+\mu$ (i.e., the site at R^i+R_μ) is the actual scattering site.

The equations determining $\underline{M}(k)$ are as follows:

$$\underline{M}(k)=\underline{F}_{00}^{00}(k) \tag{3.1}$$

(a superscript 0 indicates the single-site set located at $i=0$), where $F_{\mu\nu}^{\sigma\sigma'}(k)$ is a matrix of finite dimension, determined by

$$[\underline{F}^{-1}(k)]_{\mu\nu}^{\sigma\sigma'}=\underline{\Delta}_{\mu\nu}^{\sigma}\delta_{\sigma\sigma'}-\underline{\tilde{T}}_{\mu\nu}^{\sigma\sigma'}(k)\ , \tag{3.2}$$

$$\underline{\tilde{T}}_{\mu\nu}^{\sigma\sigma'}=\delta_{\sigma\sigma'}\delta_{\mu\nu}[\underline{\tilde{t}}\theta(\mu\in\sigma)+\underline{\bar{t}}\theta(\mu\in\tilde{\sigma})]+e^{ik\cdot(R^\mu-R^\nu)}\underline{t}'\delta(0;\sigma-\mu,\sigma'-\nu)\ , \tag{3.3}$$

$$\underline{\Delta}^{\sigma}=[\underline{I}+\underline{T}^c\underline{\bar{g}}]_+[\underline{\bar{g}}^{-1}]_+[\underline{I}+\underline{\bar{g}}\,\underline{T}^c]_+-[\underline{T}^c+\underline{T}^c\underline{\bar{g}}\,\underline{T}^c]_+\ . \tag{3.4}$$

[cf. MR, Ref. 5 Eqs. (7.32), (7.31), and (7.7)]. Here $\theta(S)$ is a truth function for the statement S, equal to 1 if S is true and to 0 if not:

$$\delta(\mu;\sigma,\sigma')=\theta(\sigma\neq\sigma')[\theta((\mu\cup\sigma)=\sigma')+\theta((\mu\cup\sigma')=\sigma)]\ , \tag{3.5}$$

$\underline{\bar{t}}$ and $\underline{t}'$ are defined in Sec. II, and

$$\underline{\tilde{t}}=c_B\underline{t}^A+c_A\underline{t}^B\ . \tag{3.6}$$

In Eq. (3.4), the quantities are all matrices in i,j; the square brackets with subscript "+" denote a projection onto the subspace σ^+, i.e., a restriction to $i=\mu\in\sigma^+$, $j=\nu\in\sigma^+$, and $\tilde{\sigma}$ and σ^+ are sets related to σ and defined by

$$\sigma^+=\{\mu\mid(\mu\cup\sigma)\in T\}\ , \tag{3.7}$$

$$\tilde{\sigma}=\sigma^+\cap\bar{\sigma}\ . \tag{3.8}$$

In the expression $\mu\cup\sigma$, μ represents the single-site set $\{\mu\}$; $\bar{\sigma}$ is the complement of σ. One could think of σ^+ as a "neighborhood" of σ, and extension of σ to include the sites one might add to σ without going outside the family of sets T that defines the approximation (MR, Ref. 5, p. 5297). For the nearest-neighborhood pair approximation on a two-dimensional square lattice, the different sets σ, $\tilde{\sigma}$, and σ^+ are illustrated in Fig. 1. The bracketed expressions in (3.4) can be evaluated by means of Bloch transforms. The choice of an initial form for $\underline{T}^c$ to start the iteration procedure is discussed at the end of Sec. V.

The t-matrix TCA can be applied readily to the single-band tight-binding model, where the calculation closely resembles the TCA using potential strengths worked out by MR. Results for the t matrix and potential form of the TCA for a linear chain with nearest-neighbor hopping are shown in Fig. 2. It is evident that the differences in the two approaches are indeed slight. A comparison of the potential TCA calculation given in Fig. 2 with exact results can be found in Fig. 5 of Kaplan *et al.*[5]

IV. THE SINGLE-SITE APPROXIMATION

It is shown by MR (Ref. 5) that the single-site TCA, in the formal version using potentials, is exactly equivalent to the formal CPA. It also turns out that the t matrix and formal versions of the TCA are equivalent in the single-site approximation, since the extra terms in the t matrix TCA (discussed in Sec. V) do not occur in that case. So the single-site t matrix TCA provides an alternative formula-

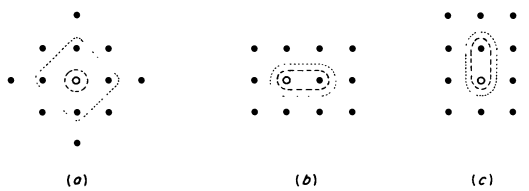

FIG. 1. The inequivalent overlap sets σ for the nearest-neighbor two-site TCA in two dimensions, with the associated sets $\tilde{\sigma}$ and σ^+. The site at the origin is indicated by an open circle. The dashed line encloses σ, the dotted line encloses σ^+, and the sites between the dashed and dotted lines comprise $\tilde{\sigma}$. In cases (b) and (c), where σ is a two-site set, $\tilde{\sigma}=\emptyset$, the null set.

tion of the CPA, which has some advantages over some conventional procedures. In the first place, the fixed-point theorem discussed below guarantees convergence on iteration, for any complex value of the energy, to the self-consistent Herglotz solution. In the second place, the TCA provides an explicit expression for $\underline{t}^c$ at each iteration, as contrasted with the implicit expressions that arise from the standard CPA approach.

Specifically, $\underline{T}^c_{ij}$ [Eq. (2.28)] is site-local in the single-site approximation, so that $\underline{T}^c(k)=\underline{t}^c$ is independent of k, and is given at each iteration, by Eq. (2.46):

$$\underline{t}^c=\underline{\bar{t}}+\underline{t}'\underline{M}\underline{t}' , \tag{4.1}$$

where $\underline{M}$, by the procedures of Sec. III, turns out to be

$$\underline{M}=(\underline{\bar{g}}_{00}^{-1}+\underline{t}^c-\underline{\tilde{t}})^{-1} . \tag{4.2}$$

To see this, note that the $\underline{\bar{t}}$ and $\underline{t}'$ terms in (3.3) vanish in this case, while from (3.7), σ^+ is just σ, a single-site set, and all four matrices in (3.4) projected onto σ^+ are 1×1. So $\underline{\Delta}^{\sigma}_{\mu\nu}$ and $\underline{\tilde{T}}^{\sigma\sigma'}_{\mu\nu}$ reduce to

$$\underline{\Delta}^0_{00}=\underline{\bar{g}}_{00}^{-1}\,\underline{t}^c , \tag{4.3}$$

$$\underline{\tilde{T}}^{00}_{00}=\underline{\tilde{t}} . \tag{4.4}$$

This statement of the t-matrix CPA is completed by the equation for $\underline{\bar{g}}_{00}$:

$$\underline{\bar{g}}_{00}=\frac{1}{\Omega}\int_{\mathrm{BZ}} dk\,\underline{\bar{g}}(k) , \tag{4.5}$$

$$\underline{\bar{g}}(k)=[\underline{g}^0(k)^{-1}-\underline{t}^c]^{-1} . \tag{4.6}$$

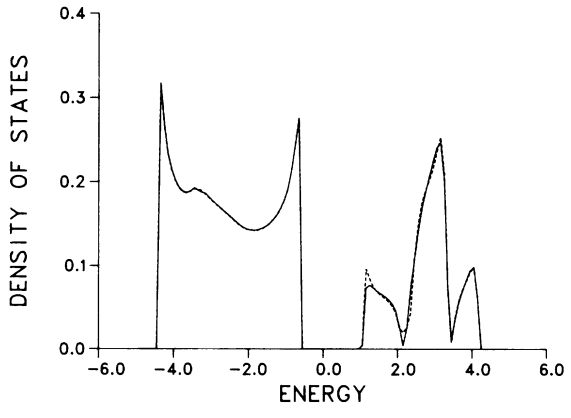

FIG. 2. The electronic density of states for a single-band tight-binding one-dimensional A-B alloy with nearest-neighbor hopping; site-diagonal energies, $v^A=-2.5$, $v^B=2.5$, hopping integral equal to 1.0, and $c_B=0.3$. Comparison of the t-matrix (solid line) and potential (dashed line) forms of the TCA in the pair approximation. For a comparison of this calculation with exact results see Fig. 5 of KLGD (Ref. 5).

The Bloch-transformed mean resolvent $\bar{G}(k)$ is given directly by Eq. (2.44).

The forms (4.1) and (4.2) are quite similar to those used by Bansil *et al.*, as is the procedure for obtaining the full mean resolvent. The two methods have the same self-consistent solution, but do not correspond to the same iteration procedure, since the $\underline{M}$ of Eq. (4.2) differs from their expression [Ref. 9, Eq. (2.33)] by terms that vanish only when $\underline{t}^c$ (in our notation) has its correct value.

It is also possible (but not very illuminating) to show that the t-matrix CPA derived here is equivalent to the version of Faulkner and Stocks, which requires an additional ansatz [their Eq. (2.41)] in order to obtain the nonsite-diagonal components of the mean resolvent. Again, while their equations and the single-site TCA have the same self-consistent solution, the iteration procedures are not equivalent.

V. FIXED-POINT THEOREM

We now wish to show that the t-matrix TCA equations have a unique analytic solution. As mentioned in the Introduction, a straightforward analysis is hindered by the propagator g^0, which fails to satisfy $\mathrm{Im}g^0\leq 0$; as g^0 is not Herglotz, the proofs[5] used for the potential equations are not directly applicable. In order to circumvent this difficulty, it is shown in this section that the multiple-scattering equations have an equivalent expression in terms of potential operators (Eq. 5.10) in which the full Herglotz[12] Green's function appears. Some algebraic manipulation of this equation yields a form (Eq. 5.30) for which the analyticity proof in Kaplan *et al.*[5] can be repeated almost verbatim. This latter part of the argument is relegated to Appendix B.

For the discussion in this section, it is convenient to be able to express the Hilbert space, Ψ, of the single-electron system as a product space, based upon the separation of Eq. (2.3):

$$\Psi=\Phi\otimes\Psi_0 , \tag{5.1}$$

with the natural bases $\{|i)\}$ and $\{|x)\}$:

$$|R_i+x)=|i)|x) . \tag{5.2}$$

We deal explicitly with the site-index space, Φ, which is all that is relevant here, so that we can write, for example,

$$(i\,|\,V^c\,|\,j)=V^c_{ij} , \tag{5.3}$$

where V^c_{ij}, for given i and j, is an operator on Ψ_0, the space of functions over U^0.

In the formal TCA, self-consistent propagators

are defined which are specified by conditional self-energy operators W^σ [see MR, Ref. 5, Eqs. (5.1) and (7.3)] given (in current notation) by

$$W^\sigma = P^{\hat{\sigma}} V^c P^{\hat{\sigma}} , \tag{5.4}$$

where $P_{ij}^{\hat{\sigma}} = \delta_{ij}\theta(i \in \hat{\sigma})$ and $\hat{\sigma} = \overline{\sigma^+}$ [see Eq. (3.7)]. Now the t-matrix TCA can be recast in terms of potentials by the use of Eq. (2.14), in which case it takes exactly the same form as the formal TCA, except that W^σ takes on a different value, which we now determine.

Since the formal TCA and the t-matrix TCA are identical in structure [Eq. (2.4) vs Eq. (2.13)], it follows that self-consistent propagators of the same type as $\bar{g}$ [Eq. (2.25)] for the t-matrix TCA are determined by analogous self-energy operators Z^σ given by

$$Z^\sigma \equiv P^{\hat{\sigma}} T^c P^{\hat{\sigma}} . \tag{5.5}$$

From Eq. (2.15) we have

$$\begin{aligned} Z^\sigma &= P^{\hat{\sigma}}(V^{c\,-1} - G^{0D})^{-1} P^{\hat{\sigma}} \\ &= P^{\hat{\sigma}}(V^{c\,-1} - G^{0D}P^{\sigma^+} - G^{0D}P^{\hat{\sigma}})^{-1} P^{\hat{\sigma}} , \end{aligned} \tag{5.6}$$

where $P_{ij}^{\sigma^+} = \delta_{ij}\theta(i \in \sigma^+)$ and obviously, $P^{\sigma^+} + P^{\hat{\sigma}} = I$. Now, by the properties of P^σ as a projection, one finds that

$$\begin{aligned} &P^{\hat{\sigma}}(A - G^{0D}P^{\hat{\sigma}})^{-1} P^{\hat{\sigma}} \\ &\quad = [(P^{\hat{\sigma}} A^{-1} P^{\hat{\sigma}})^{-1} - G^{0D} I]^{-1} , \end{aligned} \tag{5.7}$$

and thus, from (5.6) we see that

$$Z^\sigma = \{[P^{\hat{\sigma}}(V^{c\,-1} - G^{0D}P^{\sigma^+})^{-1} P^{\hat{\sigma}}]^{-1} - G^{0D} I\}^{-1} . \tag{5.8}$$

Now it turns out (see Appendix A) that Z^σ and W^σ obey the same form of scattering equation as T^c and V^c [Eq. (2.15)], namely

$$Z^\sigma = (W^{\sigma\,-1} - G^{0D} I)^{-1} , \tag{5.9}$$

and therefore Eq. (5.8) implies that

$$W^\sigma = P^{\hat{\sigma}}(V^{c\,-1} - G^{0D}P^{\sigma^+})^{-1} P^{\hat{\sigma}} . \tag{5.10}$$

This is the desired result, in that it expressed the t-matrix TCA in terms of a new definition of the conditional self-energies W^σ.

The additional terms that are included in the t-matrix TCA and not in the formal TCA are a consequence of the extra term $G^{0D}P^{\sigma^+}$ in Eq. (5.10), as compared with Eq. (5.4). The difference between the t-matrix TCA and the formal TCA thus lies in the details of the conditional self-energy operators W^σ used in the calculation of $\underline{M}(k)$ to describe the effective environment. However, for the single-site approximation, V^c is diagonal, and thus Eq. (5.10) reduces to Eq. (5.4), showing that the formal and t-matrix CPA calculations are the same. In the development of the TCA by MR, self-consistency did not arise in a natural way, as it does in the n-site CPA,[4] where the logical structure is just like that of quantum-field theory and one replaces G^0 by $\bar{G}$ in the process of summing only over "irreducible self-energy graphs." In the TCA, as explained by MR, Ref. 5, Sec. V, as many graphs were included in a conditional effective potential as could be managed without overcounting or violation of the Herglotz property. The analysis of the t-matrix TCA shows that in the formal approach, a few graphs that might have been included were missed, and that these are in fact included naturally in the multiple-scattering version. An example of such a graph is shown in Fig. 3, in the graphical notation introduced by MR, with the dots representing potential operators v. The bracketed subgraph is an improper subgraph in terms of potentials, but arises as a proper subgraph involving operators t (the two successive scatterings from v^j in this case) within the t-matrix formulation. The return to the site j in the intermediate state of the self-energy subgraph does not in fact cause overcounting, as explained by MR, in connection with Fig. 8.

Since the form of Eq. (5.10) is rather different from that of Eq. (5.4), we must now cast it into a form more amenable to analysis. To do so, we require the augmented-space notation (with minor changes) found in KLGD. Our discussion here will be as brief as possible; we ask the reader to see the above-mentioned paper for a more complete presentation. Note that the main change from KLGD is that now the self-energy (here called V^c) is defined relative to the free-particle Green's function, and not the virtual crystal.

The Hamiltonian for the problem is an operator, given by Eq. (2.1), on the Hilbert space Ψ. The con-

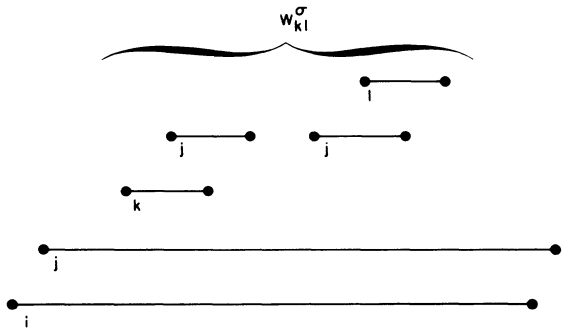

FIG. 3. A typical self-consistent self-energy subgraph W^σ_{kl} included in the t-matrix TCA but not in the formal TCA. The overlap set σ is $\{i,j\}$.

figurationally averaged Green's function is given by

$$\bar{G}=[(G^0)^{-1}-V^c]^{-1} . \tag{5.11}$$

The augmented space is $\Omega=\Psi\otimes\Theta$, with an orthonormal basis in $\Phi\otimes\Theta$, the part we deal with explicitly, being denoted by $|if_\sigma\rangle$, where i is a site label and σ is any finite collection of sites; if $\sigma=\emptyset$, the null set, we write $|if\rangle$, and we normally use σ to represent sets other than $\emptyset$. On Ω, there is a "Hamiltonian" $\hat{H}=\hat{H}^0+\hat{V}$ such that

$$\bar{G}_{ij}=\langle if|(E\hat{I}-\hat{H})^{-1}|jf\rangle , \tag{5.12}$$

where $\hat{I}$ is the identity on Ω. We now write our augmented-space operators as operator-valued matrices, with rows and columns labeled by f and f_σ, and components which are operators on Ψ. In block form,

$$\hat{K}=(E-H^0)\hat{I}-\hat{V}=\begin{bmatrix}\bar{K} & K^L\\ K^R & \tilde{K}\end{bmatrix},\quad \hat{V}=\begin{bmatrix}\bar{V} & V^L\\ V^R & \tilde{V}\end{bmatrix} , \tag{5.13}$$

where [cf. Eq. (3.3)]

$$\bar{V}_{ij}=\langle if|\hat{V}|jf\rangle=\bar{v}\delta_{ij} , \tag{5.14}$$

$$V^{L\sigma}_{ij}=\langle if|\hat{V}|jf_\sigma\rangle=v'\delta_{ij}\delta_{i\sigma}=V^{R\sigma}_{ij} , \tag{5.15}$$

$$\tilde{V}^{\sigma\sigma'}_{ij}=\langle if_\sigma|\hat{V}|jf_{\sigma'}\rangle =\delta_{\sigma\sigma'}(\bar{v}P^\sigma_{ij}+\bar{v}P^{\bar{\sigma}}_{ij})+\delta_{ij}v'\delta(i;\sigma,\sigma') . \tag{5.16}$$

Here $\bar{v}$, v', and $\tilde{v}$ represent operators on Ψ_0, with the obvious definitions [see Eqs. (2.7), (2.8), and (3.6)]:

$$\bar{v}=\sum_\alpha c_\alpha v^\alpha , \tag{5.17}$$

$$v'=\sqrt{c_Ac_B}(v^A-v^B) , \tag{5.18}$$

$$\tilde{v}=c_Bv^A+c_Av^B , \tag{5.19}$$

$$v^\alpha=(i|v^{i\alpha}|i),\quad \alpha=A,B\ (\text{any } i) . \tag{5.20}$$

In any given approximation, $\tilde{K}$ is renormalized to include self-consistency, as discussed below. Using Eqs. (5.11) and (5.12), we find

$$V^c=\bar{V}+K^LFK^R , \tag{5.21}$$

$$F=\tilde{K}^{-1} . \tag{5.22}$$

[Note that $\tilde{V}$ as defined by Eq. (5.13) and (5.16) is different from the $\tilde{V}$ in KLGD.] In both the formal TCA and the t-matrix TCA, self-consistency can be expressed by the use in Eq. (5.21) of a renormalized F:

$$F=[\{(G^\sigma)^{-1}\}_T-P_T\tilde{V}P_T]^{-1} . \tag{5.23}$$

Here the subscript T denotes the subsets of sites which define the approximation; P_T is the projection onto all vectors of the form $|if_\sigma\rangle$ such that $i\in\sigma^+$ and $\sigma\in T$, i.e.,

$$(P_T)^{\sigma\sigma'}_{ij}=\delta_{\sigma\sigma'}P^{\sigma^+}_{ij}\theta(\sigma\in T) . \tag{5.24}$$

The expression $\{X^\sigma\}_T$, where X^σ is an operator on Ψ for each σ, represents the operator $\sum_{\sigma\in T}X^\sigma P_\sigma$, where P_σ is the projection onto all vectors of the form $|if_\sigma\rangle$, and finally, the conditional propagator is defined as

$$G^\sigma=[(G^0)^{-1}-W^\sigma]^{-1} . \tag{5.25}$$

For the t-matrix TCA, W^σ is given by Eq. (5.10), and combining this with Eq. (5.21) we have

$$W^\sigma=P^{\hat{\sigma}}[(\bar{V}+K^LFK^R)^{-1}-G^{0D}P^{\sigma^+}]^{-1}P^{\hat{\sigma}} . \tag{5.26}$$

For diagonal disorder, which is the case we are considering, K^R is an operator which maps $|if\rangle$ onto $|if_i\rangle$ (with a matrix element v'), and K^L maps $|if_i\rangle$ onto $|if\rangle$. Denote by J^R the operator which maps $|if\rangle$ onto $|if_i\rangle$ for all i, with matrix element 1, and let J^L be its transpose. We can write

$$K^L=v'J^L , \tag{5.27}$$

and

$$J^LJ^R=I , \tag{5.28}$$

where I is the identity operator on Φ. Thus,

$$\bar{V}+K^LFK^R=J^L(\bar{v}I+v'Fv')J^R , \tag{5.29}$$

where I is here the identity on Θ. From Eqs. (5.26)–(5.29) we see that

$$W^{\hat{\sigma}}=P^\sigma\{[J^L(\bar{v}I+v'Fv')J^R]^{-1}-G^{0D}P^{\sigma^+}\}^{-1}P^{\hat{\sigma}} =P^{\hat{\sigma}}J^L[(\bar{v}I+v'Fv')^{-1}-G^{0D}\tilde{P}^{\sigma^+}]^{-1}J^RP^{\hat{\sigma}} , \tag{5.30}$$

where $\tilde{P}^{\sigma^+}=J^RP^{\sigma^+}J^L$. This equation is close enough in form to Eq. (A7) of KLGD so that the proof of analyticity, with appropriate modification, does work. The details can be found in Appendix B.

The theorem assures that, for any choice of the family T that defines the approximation, the self-consistent equations have a unique Herglotz solution for V^c to which the iterated solution converges regardless of the initial choice of V^c, provided only that it is Herglotz. How to choose initial forms of T^c (Sec. III) that are consistent with a Herglotz V^c [Eqs. (2.15) and (2.28)] is not quite obvious, but the choice $\underline{T}^c=0$ is certainly all right.

VI. DISCUSSION

The t-matrix traveling-cluster approximation provides a form of the approximation developed by MR which is appropriate for muffin-tin random alloys. The fixed-point theorem guarantees physically reasonable solutions and good behavior on iteration. In addition the single-site TCA gives a convenient form to the coherent-potential approximation, and ties together some of the different approaches to the CPA that have been presented previously.

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APPENDIX A: JUSTIFICATION OF EQUATION (5.9)

Equation (5.9) gives the relationship between the conditional operators W^σ of the formal TCA and the conditional operators Z^σ of the t-matrix TCA, in the case that the formal TCA has been modified to give the same answer as the t-matrix TCA. In order to establish this result, we employ the augmented-space notation briefly introduced in Sec. V, and more fully explained in KLGD. As in Sec. V it is implicit that all matrix elements are operators on the Hilbert space of electronic states.

Corresponding to the scattering operator τ, there is an augmented-space operator $\hat{\tau}$ such that [see Eq. (2.4)] the mean scattering operator $\bar{\tau}$ is given by

$$\bar{\tau}=[(V^c)^{-1}-G^0]^{-1}=\langle f\,|\,\hat{\tau}\,|\,f\rangle\ , \tag{A1}$$

$$\hat{\tau}=(\hat{V}^{-1}-G^0)^{-1}\ , \tag{A2}$$

where $\hat{V}$ is the augmented-space potential operator. In both the formal TCA and the potential formulation of the t-matrix TCA, the renormalization expressed in Eq. (5.23) is equivalent to replacing $\hat{V}$ [using the notation of Eq. (5.23)] by

$$\hat{V}+\hat{W}=\begin{bmatrix}\bar{V} & V^L\\ V^R & \tilde{V}\end{bmatrix}+\begin{bmatrix}0 & 0\\ 0 & W\end{bmatrix}\ , \tag{A3}$$

where $\bar{V}$ is given by Eq. (5.14) and

$$W=\{W^\sigma\}_T=\sum_{\sigma\in T}W^\sigma P_\sigma\ , \tag{A4}$$

with an appropriate choice for W^σ. Substituting into Eq. (A2) gives

$$\begin{aligned}\hat{\tau}&=[(\hat{V}+\hat{W})^{-1}-G^0]^{-1}\\ &=[(\hat{V}+\hat{W})^{-1}-G^{0D}-g^0]^{-1}\ .\end{aligned} \tag{A5}$$

We now wish to determine $\hat{W}$ by comparison with the t-matrix equations. In the manner of Eqs. (A1) and (A2), we recast Eq. (2.13) into the form

$$\bar{\tau}=\langle f\,|\,\hat{\tau}\,|\,f\rangle=\langle f\,|\,(\hat{T}^{-1}-g^0)^{-1}\,|\,f\rangle\ , \tag{A6}$$

where $\hat{T}$ is the augmented-space operator corresponding to the random operator T of Eq. (2.14). Analogously to Eqs. (A3) and (A4), $\hat{T}$ is renormalized to the form

$$\hat{T}+\hat{Z}=\begin{bmatrix}\bar{T} & T^L\\ T^R & \tilde{T}\end{bmatrix}+\begin{bmatrix}0 & 0\\ 0 & Z\end{bmatrix}\ , \tag{A7}$$

$$Z=\sum_{\sigma\in T}Z^\sigma P_\sigma\ , \tag{A8}$$

so that

$$\hat{\tau}=[(\hat{T}+\hat{Z})^{-1}-g^0]^{-1}\ . \tag{A9}$$

Comparing this with Eq. (A5), we see that

$$(\hat{T}+\hat{Z})^{-1}=(\hat{V}+\hat{W})^{-1}-G^{0D}\ , \tag{A10}$$

or

$$\hat{V}+\hat{W}=[(\hat{T}+\hat{Z})^{-1}+G^{0D}]^{-1}\ . \tag{A11}$$

Now it follows from the definitions of $\hat{T}$ and $\hat{Z}$ that $\hat{T}\,|\,if_\sigma\rangle$ is zero unless $i\in\sigma^+$, while $\hat{Z}\,|\,if_\sigma\rangle$ is zero unless $i\in\hat{\sigma}$ $(=\overline{\sigma^+})$. Thus $\hat{T}$ and $\hat{Z}$ act on orthogonal spaces, and the right side of Eq. (A11) can be separated out to give

$$\hat{V}+\hat{W}=(\hat{T}+G^{0D})^{-1}+(\hat{Z}^{-1}+G^{0D})^{-1}\ . \tag{A12}$$

But the relation (2.14) between T and V implies the same relation between $\hat{T}$ and $\hat{V}$,

$$\hat{T}=(\hat{V}^{-1}-G^{0D})^{-1}\ , \tag{A13}$$

so that

$$\hat{W}=(\hat{Z}^{-1}+G^{0D})^{-1}\ , \tag{A14}$$

or

$$\hat{Z}=(\hat{W}^{-1}-G^{0D})^{-1}\,, \tag{A15}$$

the promised result [Eq. (5.9)].

APPENDIX B: PROOF OF CONVERGENCE

The additional terms (as compared with the formal TCA) in Eq. (5.30) do not alter the basic structure of the analyticity proof in KLGD. Substituting the expression (5.30) for W^{σ} into Eq. (A4), we have

$$\begin{aligned} W=\{W^{\sigma}\}_T&=\{P^{\hat{\sigma}}J^L[(\bar{v}I+v'Fv')^{-1}\\ &\quad -G^{0D}\tilde{P}^{\sigma^+}]^{-1}J^RP^{\hat{\sigma}}\}_T\\ &\equiv\mathcal{F}(W)\,. \end{aligned} \tag{B1}$$

For a suitable starting guess W^0, iterating Eq. (B1) produces a sequence which converges to the required fixed point. To prove this, the following assumptions are required. The variable E is restricted to a compact subset D of the upper half-plane, and $G^0(E)$ is a Herglotz function on D. Furthermore, for any $E\in D$, $\mathrm{Im}[(G^0)^{-1}]$ is uniformly bounded away from 0, (i.e., $\mathrm{Im}([G^0(E)]^{-1})\geq y>0$, while $\mathrm{Im}G^{0D}<0$. By the compactness of D it then follows that $\mathrm{Im}G^{0D}\leq-\eta$, with $\eta>0$ a constant. We also assume that $\hat{V}$ is a bounded, Hermitian operator, independent of E; thus $\bar{V}$ and v' are Hermitian.

We first show that $\mathrm{Im}\mathcal{F}(W)\leq 0$ if $\mathrm{Im}W\leq 0$. Letting

$$\Gamma=[(\bar{v}I+v'Fv')^{-1}-G^{0D}\tilde{P}^{\sigma^+}]^{-1}$$

and $\Delta=(\bar{v}I+v'Fv')^{-1}$ we have (using the dagger to denote the Hermitian conjugate)

$$\begin{aligned} \mathrm{Im}\mathcal{F}(W)&=\frac{1}{2i}\{P^{\hat{\sigma}}J^L(\Gamma-\Gamma^{\dagger})J^RP^{\hat{\sigma}}\}_T\\ &=\frac{1}{2i}\{P^{\hat{\sigma}}J^L\Gamma[(\Delta-G^{0D}\tilde{P}^{\sigma^+})^{\dagger}-(\Delta-G^{0D}\tilde{P}^{\sigma^+})]\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T\\ &=\frac{1}{2i}\{P^{\hat{\sigma}}J^L\Gamma(\Delta^{\dagger}-\Delta)\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T+\{P^{\hat{\sigma}}J^L\Gamma\mathrm{Im}(G^{0D})\tilde{P}^{\sigma^+}\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T\,. \end{aligned} \tag{B2}$$

The second term is negative definite because $\mathrm{Im}G^{0D}\leq 0$, so we now look only at the first term:

$$\begin{aligned} \frac{1}{2i}\{P^{\hat{\sigma}}J^L\Gamma(\Delta^{\dagger}-\Delta)\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T&=\frac{1}{2i}\{P^{\hat{\sigma}}J^L\Gamma\Delta[(\bar{v}I+v'Fv')-(\bar{v}I+v'Fv')^{\dagger}]\Delta^{\dagger}\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T\\ &=\frac{1}{2i}\{P^{\hat{\sigma}}J^L\Gamma\Delta v'(F-F^{\dagger})v'\Delta^{\dagger}\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T\\ &=\{P^{\hat{\sigma}}J^L\Gamma\Delta v'F\{-\mathrm{Im}[(G^{\sigma})^{-1}]\}_TF^{\dagger}v'\Delta^{\dagger}\Gamma^{\dagger}J^RP^{\hat{\sigma}}\}_T\,, \end{aligned} \tag{B3}$$

and this term is also negative definite.

We now show that $\mathcal{F}(W)$ is bounded; that is, for all W for which $\mathrm{Im}W\leq 0$, there is a constant γ such that $||\mathcal{F}(W)||\leq\gamma$. Using $||J^2||=||J^R||=1$ and Eq. (5.7) we find

$$\begin{aligned} ||\mathcal{F}(W)||&=\sup_{\sigma}||P^{\hat{\sigma}}J^L\Gamma J^RP^{\hat{\sigma}}||=\sup_{\sigma}||J^L\tilde{P}^{\hat{\sigma}}\Gamma\tilde{P}^{\hat{\sigma}}J^R||=\sup_{\sigma}||\tilde{P}^{\hat{\sigma}}\Gamma\tilde{P}^{\hat{\sigma}}||\\ &=\sup_{\sigma}||\tilde{P}^{\hat{\sigma}}[(\bar{V}+v'Fv')^{-1}-G^{0D}I+G^{0D}\tilde{P}^{\hat{\sigma}}]^{-1}\tilde{P}^{\hat{\sigma}}||=\sup_{\sigma}||\{\tilde{P}^{\hat{\sigma}}[\bar{V}+v'Fv')^{-1}-G^{0D}I]^{-1}\tilde{P}^{\hat{\sigma}}\\ &\qquad +G^{0D}I\}^{-1}||\,, \end{aligned} \tag{B4}$$

where $\tilde{P}^{\hat{\sigma}}=J^RP^{\hat{\sigma}}J^L$. From $\mathrm{Im}W\leq 0$ and $\mathrm{Im}G^{0-1}\geq 0$, it follows that $\mathrm{Im}F^{-1}\geq 0$; applying Kato's theorem,[13] we obtain in succession $\mathrm{Im}F\leq 0$,

$$\mathrm{Im}(\bar{V}+v'Fv')^{-1}\geq 0\,,$$

and finally,

$$\mathrm{Im}\tilde{P}^{\hat{\sigma}}[(\bar{V}+v'Fv')^{-1}-G^{0D}I]^{-1}\tilde{P}\,\hat{\sigma}\leq 0\,.$$

Since $\mathrm{Im}G^{0D}\leq-\eta$, the operator in curly brackets in (B4) has a negative definite imaginary part, bounded above by $-\eta$. Hence,

$$||\mathcal{F}(W)||\leq\frac{1}{\eta}=\gamma\,,$$

as desired. If we defined the set $\hat{D}$ of augmented-space operators by

$$\hat{D}=\{X\,|\,X=\{X^{\sigma}\}_T,\ \mathrm{Im}X^{\sigma}\leq 0,\ ||X^{\sigma}||\leq\gamma\}\,, \tag{B5}$$

then we can summarize the above results as showing that $\mathcal{F}$: $\hat{D}\rightarrow\hat{D}$.

We next prove that the sequence $W^{n+1}=\mathcal{F}(W^n)$

is a Cauchy sequence. Let $\Delta W_n = W^{n+1} - W^n$; then using the same manipulations as above,

$$\Delta W_n = \mathcal{F}(W^n) - \mathcal{F}(W^{n-1})$$
$$= \{ P^{\hat{\sigma}} J^L \Gamma_n \Delta_n v' F_n (\Delta W_{n-1}) F_{n-1} \times v' \Delta_{n-1} \Gamma_{n-1} J^R P^{\hat{\sigma}} \}_T . \quad \text{(B6)}$$

Let

$$g_n = \mathrm{Im}[\{(G^\sigma)^{-1}\}_T^n - P_T \tilde{V} P_T]$$
$$= \mathrm{Im}(G^{0-1}) P_T - \mathrm{Im}\{W^\sigma\}_T^n \geq y .$$

Since g_n is positive definite, there is a positive-definite square root $\sqrt{g_n}$, and we have

$$\Delta W_n = \left\{ (Y_n'^\sigma)^\dagger \frac{1}{\sqrt{g_n}} \Delta W_{n-1} \frac{1}{\sqrt{g_{n-1}}} Y_{n-1}^\sigma \right\}_T , \quad \text{(B7)}$$

where

$$Y_n^\sigma = \sqrt{g_n} F_n v' \Delta_n \Gamma_n J^R P^{\hat{\sigma}} ,$$
$$Y_n'^\sigma = \sqrt{g_n} F_n^\dagger v' \Delta_n^\dagger \Gamma^\dagger J^R P^{\hat{\sigma}} . \quad \text{(B8)}$$

[In KLGD this part of the proof is not done correctly because the transpose (+) was interpreted as conjugate transpose. One must define separate operators for the left- and right-hand side of the expression in Eq. (B7), as is done here.] Let $Y_n^\sigma = S_n^\sigma L_n^\sigma$ be the polar decomposition of Y^σ; $L_n^\sigma = [(Y_n^\sigma)^\dagger Y_n^\sigma]^{1/2}$, and S_n^σ is a partial isometry from the range of L_n^σ [equal to the range of $Y_n^{\sigma\dagger} \subset P = P_\emptyset$; see just below Eq. (5.24)] to the range of Y_n^σ. In the same manner, $Y_n'^\sigma = S_n'^\sigma L_n'^\sigma$. Since L^σ maps P into P, Eq. (B7) becomes

$$\Delta W_n = \{ L_n'^\sigma \}_T \left\{ (S_n'^\sigma)^\dagger \frac{1}{\sqrt{g_n}} \Delta W_{n-1} \frac{1}{\sqrt{g_{n-1}}} S_{n-1}^\sigma \right\}_T \times \{ L_{n-1}^\sigma \}_T . \quad \text{(B9)}$$

By defining $X_n = \{ L_n^\sigma \}_T$, $X_n' = \{ L_n'^\sigma \}_T$ and

$$A_n = \left\{ (S_n'^\sigma)^\dagger \frac{1}{\sqrt{g_n}} \Delta W_{n-1} \frac{1}{\sqrt{g_{n-1}}} S_{n-1}^\sigma \right\}_T , \quad \text{(B10)}$$

we can write $\Delta W_n = X_n A_n X_{n-1}$, and substituting this back into (B10) we find

$$A_n = \left\{ (S_n'^\sigma)^\dagger \frac{1}{\sqrt{g_n}} X_{n-1}' A_{n-1} X_{n-2} \frac{1}{\sqrt{g_{n-1}}} S_{n-1}^\sigma \right\}_T . \quad \text{(B11)}$$

This equation is in exactly the same form as Eq. (A17) of KLGD. The remainder of the proof follows precisely as in that paper, and will not be repeated here.

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