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One-dimensional model for transition metals and their alloys*

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We develop the one-dimensional analogs of multiple-scattering theory and Korringa-Kohn-Rostoker band theory. The muffin-tin coherent-potential approximation turns out to be quite simple in one dimension when written in terms of the logarithmic derivatives of the radial Schrödinger equation. We develop a one-dimensional model for transition metals which includes the effects of hybridization and resonant scattering. Using this model we calculate the change in the density of states owing to the addition of a single impurity. A number of surprising effects which are outside the realm of tight-binding models and which seem to have three-dimensional analogs are observed.

I. INTRODUCTION

It is generally recognized that the coherent-potential approximation[1,2] (CPA) is an excellent single-site approximation for treating alloys. Unfortunately the CPA equations are only easy to solve for model Hamiltonians such as the tight-binding model which have severe limitations when applied to the alloy problem.

Probably the best model alloy Hamiltonian for which the CPA is tractable is the muffin-tin model discussed by Soven,[3] Shiba,[4] and Gyorffy.[5] No three-dimensional CPA calculations using this model have been achieved to date. Indeed, the computational difficulties are sufficiently great that some authors have suggested using less sophisticated non-self-consistent theories such as the average-t-matrix approximation as an alternative to the CPA.[6]

In this paper we present a formalism which is the one-dimensional analog of the muffin-tin CPA. We believe that one can understand a great deal about the three-dimensional muffin-tin CPA from the study of this model. Much of the calculation can be carried through by hand in closed form and the numerical parts of the calculation are not time consuming. From these calculations one can draw a number of qualitative conclusions which should apply in three dimensions as well as in one. One can also investigate other alloy theories such as the ATA and define the limits of their applicability. Finally one can obtain an exact density of states for this one-dimensional problem which one can use for comparison with the CPA and other approximate theories.

In this paper we set up the one-dimensional muffin-tin formalism and show that the CPA can be reduced to a single quartic equation. This simplicity is achieved because of the simple form of the Green's function in one dimension when expressed in terms of the logarithmic derivatives of the radial wave functions. We also show how one can mimic many of the characteristics of transition-metal energy bands with a simple one-dimensional model. We investigate the one impurity problem for this model in some detail. Several somewhat surprising effects which may have three-dimensional analogs are observed. A detailed numerical investigation of the CPA and comparison with the ATA is deferred to a later paper.

In Sec. II we develop the one-dimensional analog of KKR band theory. In Sec. III we derive a simple closed form expression for the Green's function for a periodic system in one dimension. In Sec. IV we derive the CPA equations. In Sec. V we present our model of a one-dimensional transition-metal alloy and show the results of calculations of the change in the density of states caused by a single impurity.

II. KKR THEORY IN ONE DIMENSION

We consider a one-dimensional system with Hamiltonian

$$H = -\frac{d^2}{dx^2} + \sum_n v(x - na) \ . \qquad (2.1)$$

We assume $v(x)$ to be symmetric and to vanish for $|x|$ greater than some radius (r_{mt}). We also assume that the distance between the centers of the potentials is great enough that they do not overlap:

$$v(x) = 0, \quad r \equiv |x| > r_{mt} \ , \qquad (2.2)$$

$$r_{mt} < \tfrac{1}{2} a \ . \qquad (2.3)$$

These assumptions are analogous to the use of nonoverlapping muffin-tin potentials in Korringa-Kohn-Rostoker (KKR) theory.

We shall expand the wave functions about the center of each potential in terms of symmetric and antisymmetric functions analogous to the spherical harmonics used in KKR theory. Thus we define the functions

$$Y_0(\hat{x}) = 1/\sqrt{2}\ ,$$
$$Y_1(\hat{x}) = 1/\sqrt{2}\ \operatorname{sgn}(x)\ . \tag{2.4}$$

We shall also need the one-dimensional analogs of the spherical Bessel functions. We define these as follows:

$$j_l(z) = \cos(z - \tfrac{1}{2}l\pi),\quad l = 0, 1\ ,$$
$$n_l(z) = \sin(z - \tfrac{1}{2}l\pi),\quad l = 0, 1\ , \tag{2.5}$$
$$h_l^+(z) = j_l(z) + in_l(z) = e^{i(z - l\pi/2)}\ .$$

Almost all of the familiar identities involving spherical harmonics and spherical Bessel functions have one-dimensional analogs. Some of these are listed in Appendix A for future reference.

One can use (2.4) and (2.5) to solve the single scatterer problem. If we have a single symmetric potential satisfying (2.2) centered at the origin, then

$$\left(-\frac{d^2}{dx^2} + v(x) - E\right)\psi(x) = 0\ . \tag{2.6}$$

We may let

$$\psi(x) = 2\sum_l a_l R_l(\sqrt{E}\,r) Y_l(\hat{x})\ , \tag{2.7}$$

where R_l may be expressed in terms of phase shifts for $r > r_{mt}$:

$$R_l(\sqrt{E}\,r) = j_l(\sqrt{E}\,r)\cos\delta_l - n_l(\sqrt{E}\,r)\sin\delta_l\ . \tag{2.8}$$

We may also write

$$\psi(x) = e^{ikx} + 2\sum_l f_l e^{i\sqrt{E}r} Y_l(\hat{x}) \tag{2.9}$$

for $r > r_{mt}$ and with $|k| = \sqrt{E}$. We then have [using (A5)]

$$a_l = i^l e^{i\delta_l}\ , \tag{2.10}$$
$$f_l = ie^{i\delta_l}\sin\delta_l\ . \tag{2.11}$$

Thus the partial wave analysis for the single scatter is almost identical in one and three dimensions.

Furthermore, one can easily show that, just as in three dimensions, the scattering amplitude f_l is simply related to the on-energy shell t matrix. Thus if $t(x, y)$ is the t matrix defined by

$$t(x, y) = v(x)\delta(x - y) + \int dz\, v(x) G_0(x - z) t(z, y)\ , \tag{2.12}$$

where G_0 is the free-space Green's function (A6) then

$$t_{ll'}(E) = \int_{-r_{mt}}^{+r_{mt}} dy \int_{-r_{mt}}^{r_{mt}} dz\, j_l(\sqrt{E}\,r_y)$$
$$\times Y_l(\hat{y}) t(y, z) j_{l'}(\sqrt{E}\,r_z) Y_{l'}(\hat{z})$$
$$= -\sqrt{E}\,e^{i\delta_l}\sin\delta_l\delta_{ll'} = t_l\delta_{ll'}\ . \tag{2.13}$$

Thus

$$f_l = -it_l/\sqrt{E}\ . \tag{2.14}$$

The theory for an assembly of scatterers is also very similar to that in three dimensions.[7] The Green's function for (2.1) satisfying

$$(E - H)G(x, x') = \delta(x - x') \tag{2.15}$$

can be developed in the familiar multiple-scattering expansion

$$G = G_0 + G_0 T G_0\ , \tag{2.16}$$

with

$$T = \sum_m t^m + \sum_m \sum_{n \neq m} t^m G_0 t^n$$
$$+ \sum_m \sum_{n \neq m} \sum_{p \neq n} t^m G_0 t^n G_0 t^p + \cdots\ , \tag{2.17}$$

where t^m is the t matrix for scattering off the mth potential.

Consider the case where both arguments of G, x, and x' are outside all muffin tins. The single scattering term in (2.16) may be written

$$\langle x | G_0 t^n G_0 | x' \rangle = \int dy \int dz\, G_0(x - y) t^n(y - R_n, z - R_n) G_0(z - x')$$
$$= \int dy' \int dz'\, G_0(x - y' - R_n) t^n(y', z') G_0(z' + R_n - x')\ . \tag{2.18}$$

Using (A6) and (2.13) we have

$$\langle x | G_0 t^n G_0 | x' \rangle = \sum_l (i\sqrt{E})^{-1} h_l(\sqrt{E}\,|x - R_n|) Y_l(x - R_n) t_l^n (i\sqrt{E})^{-1} h_l(\sqrt{E}\,|x' - R_n|) Y_l(x' - R_n)\ . \tag{2.19}$$

Similarly using (A6), (2.13), and (A11) one can write the third term in the expansion for G as

$$\langle x|G_0 t^m G_0 t^n G_0|x'\rangle = \sum_{l_1 l_2} (i\sqrt{E}\,)^{-1} h_{l_1}(\sqrt{E}\,|x-R_m|) Y_{l_1}(x-R_m) t^m_{l_1} G'_{l_1 l_2}(R_m - R_n)$$
$$\times t^n_{l_2}(i\sqrt{E}\,)^{-1} h_{l_2}(\sqrt{E}\,|x'-R_n|) Y_{l_2}(\hat{x}' - \hat{R}_n)\,, \tag{2.20}$$

and so on for the higher-order terms. Thus for x and x' outside all muffin tins we obtain

$$G(x,x') = G_0(x,x') + \sum_{\substack{mn\\ l_1 l_2}} (i\sqrt{E}\,)^{-1} h_{l_1}(\sqrt{E}\,|x-R_m|)\, Y_{l_1}(\hat{x}-\hat{R}_m) \tau^{mn}_{l_1 l_2}\, (i\sqrt{E}\,)^{-1} h_{l_2}(\sqrt{E}\,|x'-R_n|)\, Y_{l_2}(x'-R_n)\,, \tag{2.21}$$

where

$$\tau^{mn}_{l_1 l_2} = t^m_{l_1} \delta_{l_1 l_2} \delta_{mn} + \sum_{l_3} \sum_{p\neq m} t^m_{l_1} G'_{l_1 l_3}(R_m - R_p) \tau^{pn}_{l_3 l_2} \tag{2.22}$$

is the scattering-path operator introduced by Gyorffy and Stott.[8]

Equation (2.22) applies for any arrangement of nonoverlapping muffin-tin potentials. It is also valid in three dimensions with obvious redefinitions. Let us now restrict our consideration to identical scatterers on a lattice. Equation (2.22) may be solved in this case by means of a lattice Fourier transform.

$$\tau_{l_1 l_2}(k) = \frac{1}{N} \sum_m \sum_n e^{-ik(m-n)a} \tau^{mn}_{l_1 l_2}$$
$$= t_{l_1} \delta_{l_1 l_2} + \sum_{l_3} t_{l_1} G'_{l_1 l_3}(k) \tau_{l_3 l_2}(k)\,, \tag{2.23}$$

where

$$G'_{l_1 l_3}(k) = \sum_{p\neq 0} e^{-ikpa} G'_{l_1 l_3}(pa)\,. \tag{2.24}$$

Equation (2.23) is a two-by-two matrix equation for τ which has solution

$$(\tau^{-1})_{l_1 l_2} = t_{l_1} \delta_{l_1 l_2} - G'_{l_1 l_2}(k)\,. \tag{2.25}$$

Now the poles of τ are determined by $\det(\tau^{-1}) = 0$ and are also the poles of the Green's function (2.14) and are thus the eigenvalues of the Hamiltonian (2.1). Then

$$\det[t_l^{-1} \delta_{ll'} - G'_{ll'}(k)] = 0 \tag{2.26}$$

is the one-dimensional analog of the KKR equation.

In one dimension a closed-form solution to (2.26) may be obtained. Substituting from (2.13) and (A13) into (2.26) we have

$$\det(t_l^{-1}\delta_{ll'} - G'_{ll'}) = \frac{[\cot\delta_0(\cos\theta - \cos\phi) - \sin\phi][\cot\delta_1(\cos\theta - \cos\phi) - \sin\phi] - \sin^2\theta}{[E(\cos\theta - \cos\phi)^2]}\,. \tag{2.27}$$

There would appear to be two zeros and a second-order pole in det when considered as a function of $\theta(=ka)$ for fixed $\phi(=\sqrt{E}\,a)$. Such is not the case, however, since one of the roots (zeros of the numerator) is $\cos\theta = \cos\phi$. Thus (2.26) has one zero and one pole.

$$\det(t_l^{-1} - G'_{ll'}) = \frac{\cos\theta(1 + \cot\delta_0 \cot\delta_1) + \cos\phi(1 - \cot\delta_0\cot\delta_1) - \sin\phi(\cot\delta_0 + \cot\delta_1)}{E(\cos\theta - \cos\phi)}\,. \tag{2.28}$$

Thus the KKR determinant in one dimension has one root for a given E and a single simple free-electron pole. The root is given by

$$\theta = ka = \cos^{-1}[\cos(\sqrt{E}\,a + \delta_0 + \delta_1)/\cos(\delta_0 - \delta_1)]\,. \tag{2.29}$$

In three dimensions one will in general have several allowed k's (for a given direction) for fixed E. However, one can show that there is usually a single simple free-electron pole.

The Kronig-Penny formula for δ-function potentials can be obtained from (2.29) by setting $\delta_1 = 0$ and $\tan\delta_0 = -\lambda/2\sqrt{E}$, where λ is the strength of the δ function. It is also instructive to write (2.29) in terms of the logarithmic derivatives of the radial wave functions at the "Wigner-Seitz" radius, $r = \frac{1}{2}a$. We have

$$\gamma_0 = R_0'/R_0\,|_{r=a/2} = -\sqrt{E}\,\tan(\tfrac{1}{2}\phi + \delta_0)$$

and (2.30)

$$\gamma_1 = R_1'/R_1\,|_{r=a/2} = \sqrt{E}\,\cot(\tfrac{1}{2}\phi + \delta_1)\,.$$

It is easy to verify that

$$\cos\theta = -(\gamma_0 + \gamma_1)/(\gamma_0 - \gamma_1)\,. \tag{2.31}$$

Thus many of the approximate rules of thumb which are used in three dimensions are exact in one dimension, e.g., "$k=0$ when $\gamma_0=0$," or "at least one of the logarithmic derivatives must be negative for the density of states to be nonzero."

Equations (2.29) or (2.31) determine the dispersion relation for a periodic system in one dimension. In Sec. III we will show that $\tau^{mn}_{l_1 l_2}$ may also be obtained in closed form so that the Green's function is in principle determined by (2.21). In practice however a multicenter expansion of this type is not very useful. We are mainly interested in the Green's function $G(x, x')$ when x and x' are both within the same Wigner-Seitz cell. Let us suppose that x and x' are both within the Wigner-Seitz cell at the origin (but for the time being still in the zero potential muffin-tin plateau region). One can now use (A9) to express all terms in (2.21) as spherical harmonic expansions about the origin[9]

$$\begin{aligned}G(x,x') = G_0(x,x') &+ \sum_{l_1 l_2} (i\sqrt{E})^{-1} h_{l_1}(\sqrt{E}\,|x|) Y_{l_1}(\hat{x}) \tau^{00}_{l_1 l_2} (i\sqrt{E})^{-1} h_{l_2}(\sqrt{E}\,|x|) Y_{l_2}(\hat{x}') \\ &+ \sum_{l_1 l_2 l_3} \sum_{n\neq 0} (i\sqrt{E})^{-1} h_{l_1}(\sqrt{E}\,|x|) Y_{l_1}(\hat{x}) \tau^{0n}_{l_1 l_2} G'_{l_2 l_3}(R_n) j_{l_3}(\sqrt{E}\,|x'|) Y_{l_3}(\hat{x}') \\ &+ \sum_{l_1 l_2 l_3} \sum_{m\neq 0} j_{l_1}(\sqrt{E}\,|x|) Y_{l_1}(\hat{x}) G'_{l_1 l_2}(R_m) \tau^{m0}_{l_2 l_3} (i\sqrt{E})^{-1} h_{l_3}(\sqrt{E}\,|x'|) Y_{l_3}(\hat{x}') \\ &+ \sum_{\substack{l_1 l_2 \\ l_3 l_4}} \sum_{\substack{m\neq 0 \\ n\neq 0}} j_{l_1}(\sqrt{E}\,|x|) Y_{l_1}(\hat{x}) G'_{l_1 l_2}(R_m) \tau^{mn}_{l_2 l_3} G'_{l_3 l_4}(R_n) j_{l_4}(\sqrt{E}\,|x'|) Y_{l_4}(\hat{x}') \,. \end{aligned} \tag{2.32}$$

Using the facts that

$$\tau^{00}_{l_1 l_2} = t^0_{l_1} \delta_{l_1 l_2} + t^0_{l_1} G^{00}_{l_1 l_2} t^0_{l_2} \,, \tag{2.33a}$$

$$\sum_{l_2} G'_{l_1 l_2}(R_m) \tau^{m0}_{l_2 l_3} = G^{00}_{l_1 l_2} t^0_{l_2} , \tag{2.33b}$$

and

$$\sum_{l_2} \tau^{0n}_{l_1 l_2} G'_{l_2 l_3}(R_n) = t^0_{l_1} G^{00}_{l_1 l_3} \,, \tag{2.33c}$$

where

$$G^{00}_{l_1 l_2} = t^{-1}_{l_1} (\tau^{00}_{l_1 l_2} - t_{l_1} \delta_{l_1 l_2}) t^{-1}_{l_2} \,, \tag{2.34}$$

we have

$$\begin{aligned}G(x,x') = G_0(x,x') &+ \sum_{l} (i\sqrt{E})^{-2} h_l(\sqrt{E}\,|x|) h_l(\sqrt{E}\,|x'|) t^0_l Y_l(\hat{x}) Y_l(\hat{x}') + \sum_{l_1 l_2} [j_{l_1}(\sqrt{E}\,|x|) \\ &+ (i\sqrt{E})^{-1} t_{l_1} h_{l_1}(\sqrt{E}\,|x|)] Y_{l_1}(\hat{x}) G^{00}_{l_1 l_2} [j_{l_2}(\sqrt{E}\,|x'|) + (i\sqrt{E})^{-1} t_{l_2} h_{l_2}(\sqrt{E}\,|x'|) Y_{l_2}(x')] \,. \end{aligned} \tag{2.35}$$

Equation (2.35) can also be written

$$G(x,x') = G^{(1)}(x,x') + \sum_{l_1 l_2} R_{l_1}(\sqrt{E}\,|x|)(\exp i\delta_{l_1}) Y_{l_1}(\hat{x}) G^{00}_{l_1 l_2} R_{l_2}(\sqrt{E}\,|x'|)(\exp i\delta_{l_2}) Y_{l_2}(\hat{x}') \,, \tag{2.36}$$

where $R_l(\sqrt{E}\,|x|)$ is given by (2.8), and $G^{(1)}$ is the Green's function for one potential at the origin. Our derivation of (2.36) applies only in the region of the cell at the origin where $v=0$. However, (2.36) satisfies (2.15) everywhere inside the cell and has the correct boundary conditions so that it is in fact valid at all points within the cell at the origin. Equation (2.35) is also valid in three dimensions with appropriate redefinitions.

It is also useful to note that

$$\operatorname{Im} G(x,x') = \sum_{l_1 l_2} [R_{l_1}(\sqrt{E}\,r) R_{l_2}(\sqrt{E}\,r') / \sin\delta_{l_1} \sin\delta_{l_2}] \times \operatorname{Im} \tau^{00}_{l_1 l_2} Y_{l_1}(\hat{x}) Y_{l_2}(x') \,. \tag{2.37}$$

Thus the density of states is determined directly by τ^{00}.

III. EVALUATION OF THE GREEN'S FUNCTION

Soven,[3] Shiha,[4] and Gyorffy[5] have shown that in order to treat the single impurity problem in a partial wave representation (and thus also to perform a muffin-tin CPA calculation) one needs $\tau^{00}_{l_1 l_2}$, i.e., the scattering path operator for a path which leaves from and returns to the origin. From (2.23) and (2.25) this is

$$\tau^{00}_{l_1 l_2}=\frac{a}{2\pi}\int dk\,\tau_{l_1 l_2}(k)$$

$$=\frac{a}{2\pi}\int dk\,(t^{-1}-G'(k))^{-1}_{l_1 l_2}\ . \tag{3.1}$$

In one dimension, (3.1) can be evaluated exactly by means of a contour integral. Substituting from (2.13) and (A17) we have

$$\tau^{00}=\frac{-1}{2\pi}\int_{-\pi}^{\pi} d\theta \begin{pmatrix} \cot\delta_0(\cos\theta-\cos\phi)+\sin\phi & -i\sin\theta \\ i\sin\theta & \cot\delta_1(\cos\theta-\cos\phi)+\sin\phi \end{pmatrix}^{-1} \sqrt{E}\,(\cos\theta-\cos\phi)\ , \tag{3.2}$$

Inverting the matrix and canceling one of the roots of the determinant against the factor $\cos\theta-\cos\phi$, we obtain

$$\tau^{00}_{00}=\frac{-\sqrt{E}}{2\pi}\,\frac{\tan\delta_0}{1+\tan\delta_0\tan\delta_1}\int_{-\pi}^{\pi}\frac{\cos\theta-f_1}{\cos\theta-x}\,d\theta\ , \tag{3.3a}$$

$$\tau^{00}_{11}=\frac{-\sqrt{E}}{2\pi}\,\frac{\tan\delta_1}{1+\tan\delta_0\tan\delta_1}\int_{-\pi}^{\pi}\frac{\cos\theta-f_0}{\cos\theta-x}\,d\theta\ , \tag{3.3b}$$

$$\tau^{00}_{01}=-\tau^{00}_{10}=\frac{-\sqrt{E}}{2\pi}\,\frac{\tan\delta_0\tan\delta_1}{1+\tan\delta_0\tan\delta_1}\int_{-\pi}^{\pi}\frac{i\sin\theta}{\cos\theta-x}\,d\theta\ , \tag{3.3c}$$

where

$$x=\cos(\phi+\delta_0+\delta_1)/\cos(\delta_0-\delta_1)\ , \tag{3.3d}$$

$$f_0=\cos\phi-\tan\delta_0\sin\phi\ , \tag{3.3e}$$

$$f_1=\cos\phi-\tan\delta_1\sin\phi\ . \tag{3.3f}$$

Note first that $\tau^{00}_{10}=-\tau^{00}_{10}=0$ due to the odd parity of the integrand. This means that the matrix τ^{00} is diagonal in one dimension. A similar thing occurs in three dimensions as well, for cubic systems; there the point symmetry is such that, through $l_{\max}=2$, cubic harmonics are equivalent to spherical harmonics so that the matrix τ^{00} is diagonal.

Integrals (3.3a) and (3.3b) may be performed by making a change of variables, $z=\exp(i\theta)$, and integrating around the unit circle:

$$I=\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{\cos\theta-f}{\cos\theta-x}\,dx=\frac{1}{2\pi i}\int\frac{dz}{z}\,\frac{z^2-2fz+1}{z^2-2xz+1}\ . \tag{3.4}$$

The integrand of (3.4) has three simple poles, $z=0$, $z=z_<$, and $z=z_>$, where

$$z_< z_>=1\ . \tag{3.5}$$

For x real and less than 1 both $z_<$ and $z_>$ will lie on the unit circle. However if we let E have a small positive imaginary part one of the pair $z_<$ and $z_>$ will move outside and the other inside the unit circle since (3.5) must be satisfied. Thus

$$I=1+(x-f)/(x^2-1)^{1/2} \tag{3.6}$$

and

$$\tau^{00}_{00}=-\sqrt{E}\,\frac{\tan\delta_0}{1+\tan\delta_0\tan\delta_1}\,I(x,f_1)\ , \tag{3.7a}$$

$$\tau^{00}_{11}=-\sqrt{E}\,\frac{\tan\delta_1}{1+\tan\delta_0\tan\delta_1}\,I(x,f_0)\ . \tag{3.7b}$$

Equations (3.7a) and (3.7b), although simple, are not easy to interpret physically. An extremely simple and physically interesting expression can be derived for the partial wave decomposition of the Green's function, (2.35), for the case where x and x' are both at one of the boundaries of the cell at the origin. If

$$G(x,x')=\sum_l G_l(r,r')Y_l(\hat{x})Y_l(\hat{x}')\ , \tag{3.8}$$

then a little algebra yields

$$G_l(r,r')=\frac{R_l(\sqrt{E}r_<)}{\sqrt{E}\sin\delta_l}\left(j_l(\sqrt{E}r_>)+\frac{R_l(\sqrt{E}r_>)}{\sqrt{E}\sin\delta_l}\,\tau^{00}_{ll}\right), \tag{3.9}$$

setting $r=r'=r_s=\frac{1}{2}a$ and using some results peculiar to one dimension, (2.29), (2.30), (3.6), and (3.7) we have

$$G_0(r_s,r_s)=-\frac{1+(\gamma_1/\gamma_0)^{1/2}}{\gamma_0-\gamma_1}=\frac{-1}{\gamma_0-(\gamma_0\gamma_1)^{1/2}} \tag{3.10a}$$

$$G_1(r_s,r_s)=+\frac{1+(\gamma_0/\gamma_1)^{1/2}}{\gamma_0-\gamma_1}=\frac{-1}{\gamma_1-(\gamma_0\gamma_1)^{1/2}}\ . \tag{3.10b}$$

If we substitute (3.10a) and (3.10b) into (3.8) we see that

$$G(\tfrac{1}{2}a,\tfrac{1}{2}a)=1/[2(\gamma_0\gamma_1)^{1/2}] \tag{3.11a}$$

and

$$G(\tfrac{1}{2}a,\,-\tfrac{1}{2}a)=G(\tfrac{1}{2}a,\tfrac{1}{2}a)e^{ik(E)a}\ . \tag{3.11b}$$

The density of states at the cell boundary is proportional to the imaginary part of (3.11a) and is seen to be nonzero for a periodic system of real potentials if and only if one and only one of the logarithmic derivatives is negative.

Equations (3.10) can also be used to show that within the cell at the origin, the Green's function for the periodic system is identical to the Green's function for a single cell surrounded by a uniform medium, $\Sigma = E + \gamma_0\gamma_1$. From (A14) we see that the one potential Green's function is

$$G_l^{(1)}(r, r') = (1/i\sqrt{E})R_l(r_<)F_l(r_>) \ . \tag{3.12}$$

Applying the Wronskian condition, $(R_l' F_l - F_l' R_l) = -i\sqrt{E}$, we have

$$G_l(r, r) = -(R_l'/R_l - F_l'/F_l)^{-1}, \quad r \le r_s \tag{3.13}$$

and

$$G_l(r_s, r_s) = -(\gamma_l - F_l'/F_l \,|_{r_s})^{-1} \ . \tag{3.14}$$

Now F_l must match onto outgoing waves in the medium Σ outside the cell. Hence

$$F_l'/F_l \,|_{r_s} = (d/dr)h_l(\kappa r)/h_l(\kappa r)_{r=r_s} \,| = i\kappa \ , \tag{3.15}$$

where

$$\kappa = (E - \Sigma)^{1/2} \ . \tag{3.16}$$

Comparison of (3.14) with (3.10) gives the desired result

$$i\kappa = (\gamma_0\gamma_1)^{1/2} \quad \text{or} \quad \Sigma = E + \gamma_0\gamma_1 \ . \tag{3.17}$$

We will use this result to derive a very simple form of the muffin-tin CPA in Sec. IV.

The result that the Green's function within the Wigner-Seitz cell at the origin for a periodic system is equal to that for a single scatterer in a uniform medium is reminiscent of a suggestion due to Anderson and McMillan[10] for treating liquid metals. Anderson and McMillan chose their uniform exterior medium by requiring that the *forward* scattering off the cell in the medium vanish. (3.17) on the other hand can be obtained by requiring that the *backward* scattering vanish.

IV. THE CPA

The CPA can be derived by requiring that the Green's function for a system having scattering amplitude t_A or t_B at the origin and the coherent scattering amplitude t_C at all other sites be equal on the average to the Green's function for a system having t_C on all sites. This is equivalent to

$$c_A\tau_{C,A}^{00} + c_B\tau_{C,B}^{00} = \tau_C^{00} \ , \tag{4.1}$$

where τ_C^{00} is given by (3.7) with $\tan\delta_l = \tan\delta_l^C$ and $\tau_{C,A}^{00}$ is given by

$$\tau_{C,A,ll}^{00} = (\tau_{C,ll}^{00-1} + t_{A,l}^{-1} - t_{C,l}^{-1})^{-1} \ . \tag{4.2}$$

In the following we shall drop the superscripts on τ and the angular-momentum subscripts on τ and t.

Substitution of (4.2) into (4.1) yields an equation for t_C:

$$t_C^{-1} = c_At_A^{-1} + c_Bt_B^{-1} + (t_C^{-1} - t_A^{-1})\tau_C(t_C^{-1} - t_B^{-1}) \ . \tag{4.3}$$

It should be remembered that (4.3) represents two equations in two unknowns $t_{C,0}$ and $t_{C,1}$. These equations are coupled since $\tau_{C,ll}$ depends on both $t_{C,0}$ and $t_{C,1}$. Equation (4.3) can be manipulated to yield several equivalent forms which may be useful in certain cases:

$$t_C = c_At_A + c_Bt_B + (t_C - t_A)G_C(t_C - t_B) \ , \tag{4.4a}$$

$$G_C = t_C^{-1}(\tau_C - t_C)t_C^{-1} \ , \tag{4.4b}$$

$$\cot\delta_C = c_A\cot\delta_A + c_B\cot\delta_B + (\cot\delta_C - \cot\delta_A)\tau_C'(\cot\delta_C - \cot\delta_B) \ , \tag{4.5a}$$

$$\tau_C' = -(1/\sqrt{E})\tau_C \ , \tag{4.5b}$$

$$\tan\delta_C = c_A\tan\delta_A + c_B\tan\delta_B + (\tan\delta_C - \tan\delta_A)G_C'(\tan\delta_C - \tan\delta_B) \ , \tag{4.6a}$$

$$G_C' = \cot\delta_C(\tau_C' - \tan\delta_C)\cot\delta_C \ , \tag{4.6b}$$

$$\gamma_C = c_A\gamma_A + c_B\gamma_B + (\gamma_C - \gamma_A)G_C^\gamma(\gamma_C - \gamma_B) \ , \tag{4.7a}$$

$$G_{C,l}^\gamma = -\frac{R_l^C(r_s)}{\sqrt{E}\,\sin\delta_l^C}\left(j_l(r_s) + \frac{R_l^C(r_s)\tau_{C,ll}^{00}}{\sqrt{E}\,\sin\delta_l^C}\right). \tag{4.7b}$$

Now according to (3.9),

$$G_{C,l}^\gamma = -G_{C,l}(r_s, r_s) \ , \tag{4.8}$$

so that using (3.10) we have

$$G_{C,l}^\gamma = +1/[\gamma_l^C - (\gamma_0^C\gamma_1^C)^{1/2}] \ . \tag{4.9}$$

Equations (4.1) through (4.7) have three-dimensional analogs, however (4.9), because of the use of (3.10), is peculiar to one dimension.

Equation (4.7) stands for the set of equations

$$\gamma_0^C = c_A\gamma_0^A + c_B\gamma_0^B + (\gamma_0^C - \gamma_0^A)(\gamma_0^C - \gamma_0^B)/[\gamma_0^C - (\gamma_0^C\gamma_1^C)^{1/2}] \tag{4.10a}$$

and

$$\gamma_1^C = c_A\gamma_1^A + c_B\gamma_1^B + (\gamma_1^C - \gamma_1^A)(\gamma_1^C - \gamma_1^B)/[\gamma_1^C - (\gamma_0^C\gamma_1^C)^{1/2}]. \tag{4.10b}$$

Equations (4.10) can be converted into a single equation in one unknown $Z = (\gamma_0^C\gamma_1^C).^{1/2}$

A substantial amount of algebraic manipulation applied to (4.10a) and (4.10b) yields

$$\frac{-1}{Z} = \frac{c_A}{\gamma_0^A - Z} + \frac{c_A}{\gamma_1^A - Z} + \frac{c_B}{\gamma_0^B - Z} + \frac{c_B}{\gamma_1^B - Z} \ , \tag{4.11a}$$

where

$$Z=(\gamma_0^C\gamma_1^C)^{1/2} . \qquad (4.11b)$$

Equations (4.11) are equivalent to the equation

$$c_A\overline{G}_A^{(1)}(\tfrac{1}{2}a, \tfrac{1}{2}a, -iZ)+c_B G_B^{(1)}(\tfrac{1}{2}a, \tfrac{1}{2}a, -iZ) = \overline{G}(x, x, -iZ) , \qquad (4.12)$$

where $\overline{G}_A^{(1)}(\frac{1}{2}a, \frac{1}{2}a, -iZ)$ is the Green's function for a system consisting of a single scatterer surrounded by a medium $\Sigma = E+Z^2$ evaluated at the cell boundary and $\overline{G}$ is the Green's function for the medium only. Thus we see that the muffin-tin CPA in one dimension is equivalent to the SCBS criterion[11] in which one determines a uniform self-consistent medium by setting the average Green's function at the boundary of a cell equal to the Green's function for a uniform medium.

The CPA is not complete until one specifies how the density of states is to be obtained. Since the quantity Z (4.11b) acts as a uniform, self-consistent, medium replacing all scatterers outside the central cell, the partial Green's functions, $G_l^{i,C}(i=A$ or $B)$, for a system with an A or B atom on the central site and self-consistent scatterers outside can be obtained from (3.12) and (3.14):

$$G_l^{i,C}(r, r)=(1/i\sqrt{E})R_l^i(r_<)F_l^i(r_>) , \qquad (4.13)$$

where

$$F_l^i(r)=N_l^i+a_l R_l^i . \qquad (4.14)$$

Here N_l is the real "other" solution to the Schrödinger equation for an A or B potential. N_l satisfies the same Wronskian condition with R_l as F_l. a_l is determined by the boundary condition on F_l. Thus the density of states of angular momentum l at r is

$$\rho_l^{i,C}(r)=(1/\pi)\,\mathrm{Im}(a_l/i\sqrt{E})R_l^{i2}(r) , \qquad (4.15)$$

but from (3.14) we have

$$\rho_l^{i,C}(r_s)=(1/\pi)\,\mathrm{Im}[1/(\gamma_l^i-Z)] . \qquad (4.16)$$

Hence

$$\rho_l^{i,C}(r)=(1/\pi)\,\mathrm{Im}[1/(\gamma_l^i-Z)]R_l^{i2}(r)/R_l^{i2}(r_s) . \qquad (4.17)$$

In addition we can use the relation between the integral of the square of the radial wave function and the energy derivative of its logarithmic derivative,

$$\int_0^{r_s} R_l^2(r)\,dr=-R_l^2(r_s)\,\frac{d\gamma_l^i}{dE} \qquad (4.18)$$

to obtain an equation for the partial density of states

$$n_l^{i,C}=\int_0^{r_s}\rho_l^{i,C}(r)dr = (1/\pi)\,\mathrm{Im}[1/(\gamma_l-Z)](-d\gamma_l^i/dE) . \qquad (4.19)$$

V. ONE-DIMENSIONAL MODEL FOR A TRANSITION METAL

Although the formulas of Sec. I–IV are applicable to any set of nonoverlapping, symmetric potentials, we would especially like to mimic in one dimension the resonant scattering behavior typical of three-dimensional transition-metal potentials. Rather than concoct a one-dimensional potential which exhibits resonant scattering we find it more convenient to introduce phase shifts with the desired energy dependence directly.

Thus we shall study a model potential which has a smoothly varying $l=0$ phase shift and a resonant $l=1$ phase shift analogous to the d resonance typical of transition metals. The specific forms which we take are somewhat arbitrary:

$$\tan\delta_0(E)=\lambda/(2\sqrt{E}) , \qquad (5.1a)$$

$$\tan\delta_1(E)=\Gamma/(E_1-E)-\Gamma/E_1 . \qquad (5.1b)$$

The chosen forms are consistent with the requirement that $\delta_0(E=0)=\frac{1}{2}\pi$ and $\delta_1(E=0)=0$. In addition, $\delta_1(E)$ exhibits a resonance at $E=E_1$, rising rapidly over an energy range of 2Γ from approximately zero to approximately π. We shall say nothing more about the potential which yields (5.1) except to specify that if it is energy dependent this energy dependence must be such that

$$\int_0^{a/2}[\partial V(r, E)/\partial E]R_l^2(r)dr=0 . \qquad (5.2)$$

(5.2) is necessary if the density of states obtained from the Green's function is to agree with that obtained from the dispersion relation. Thus we assume that over a limited energy range there exists a potential such that (5.1) and (5.2) are approximately satisfied.

Figure 1(a) (solid line) shows the energy bands for $\lambda=2$, $E_1=2.05$, $\Gamma=0.5$ as the parameters in (5.1). In the following we shall take the lattice parameter a to be unity. There is a gap in the density of states extending from $E=1.74$ to $E=2.67$. This is the energy interval over which γ_0 and γ_1 are both negative. If γ_0 had been positive in this energy range, the resonant behavior of δ_1 would have induced an $l=1$ band over the region of the gap of Fig. 1(a). The dashed line in Fig. 1(a) shows the energy bands resulting from setting δ_1 equal to zero. One can see that the gap is due to $l=0$, $l=1$ hybridization.

Hybridization is a less dominant feature of the d bands of three-dimensional systems since there are five d bands and only one s band. The general

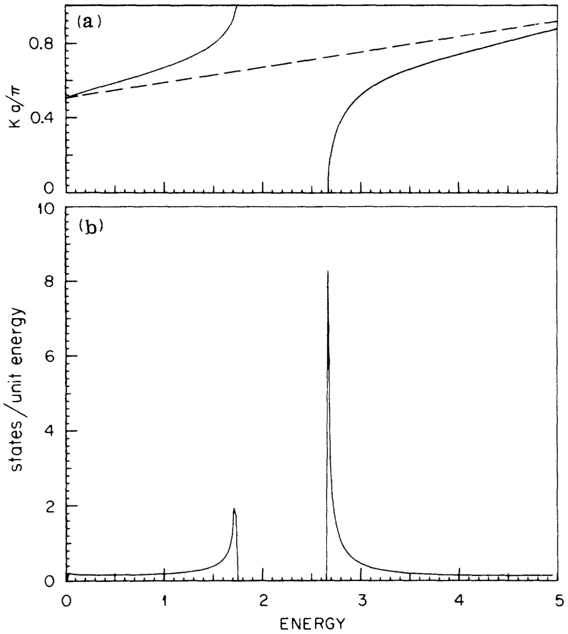

FIG. 1. (a) Energy bands for a one-dimensional model of a transition metal. Solid line is for $\lambda = 2.0$, $E_1 = 2.05$, $\Gamma = 0.5$ [see Eq. (5.1) of text]. Dashed line has $\lambda = 2$ but $\delta_1(E)$ identically zero. (b) Density of states [derivative of the solid curve of (a)] .

picture is that of a broad, parabolic $s-p$ band hybridizing with one of the narrow d bands in such a way as to create a gap over the approximate energy range of the original unhybridized d band. Superimposed on this hybridization structure are the unhybridized or weakly hybridized d bands. It is these unhybridized bands which are missing in our one-dimensional model. The hybridized bands of Fig. 1(a) are, in fact, quite similar to the Δ_1 bands of bcc transition metals. The density of states for our model transition metal is shown in Fig. 1(b).

A formula for the change in the integrated density of states induced by a substitutional impurity has been derived by Lasseter and Soven[12] and an equivalent formula has been obtained by Holzwarth.[13] The derivation is straightforward so we only quote the result, as adapted to one dimension.

$$\Delta N(E) = -\frac{1}{\pi}\ \mathrm{Im} \sum_{l} \ln[1 - G_l(\gamma_l^i - \gamma_l^h)]. \tag{5.3}$$

Here γ_l^i and γ_l^h are logarithmic derivatives of the impurity and host radial wave functions. Using (3.10) for G_l we have

$$\Delta N_l = -(1/\pi)\,\mathrm{Im}\ln\{[\gamma_l^i - (\gamma_0^h\gamma_1^h)^{1/2}]/[\gamma_l^h - (\gamma_0^h\gamma_1^h)^{1/2}]\} \tag{5.4}$$

or

$$\Delta N_l = (1/\pi)(\phi_l^i - \phi_l^h)\ , \tag{5.5}$$

with

$$\tan\phi_l^{i(h)} = (-\gamma_0^h\gamma_1^h)^{1/2}/\gamma_l^{i(h)}. \tag{5.6}$$

Figures 2(a) and 2(b) show the change in the $l = 1$ component of the integrated density of states and density of states, respectively, due to the replacement of one potential of the metal of Fig. 1 by a potential having parameters $\lambda = 1.0$, $E_1 = 4.05$, $\Gamma = 0.5$. Points worthy of note are the large subtraction of states at the Van Hove peaks of the host, the localized state in the gap, and the virtual bound state peak centered at $E = 4.38$.

The behavior of $\Delta N_1(E)$ at the host band edge is interesting. If the lower band edge is denoted by E_L and the upper band edge by E_U, then ΔN_1 tends to $-\frac{1}{2}$ as E approaches E_L from below or E_U from above. There is an additional, discontinuous, jump of $-\frac{1}{2}$ state per atom at $E = E_L$ and $E = E_U$. Also surprising is the state in the gap which increases $\Delta N_1(E)$ from -1 to 0.

The virtual bound state also has surprising fea-

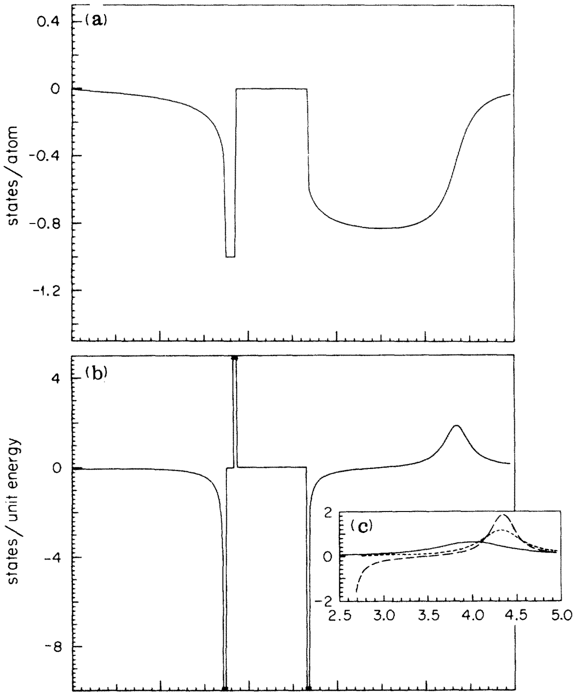

FIG. 2. (a) Change in the integrated density of states due to one substitutional impurity. The host atom is the same as in Fig. 1. The impurity atom parameters are $\lambda = 1.0$, $E_1 = 4.05$, $\Gamma = 0.5$. (b) Change in the density of states. (c) Solid line: impurity potential in free-electron matrix ($\delta_0^h = \delta_1^h = 0$). Dotted line: impurity potential in host matrix with δ_1^h set to zero. Dashed line: impurity potential in host matrix.

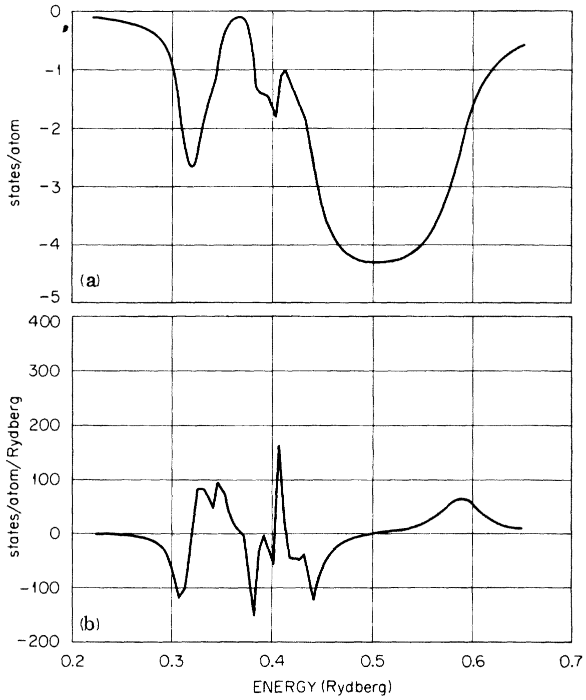

FIG. 3. Three-dimensional cluster calculations. (a) Change in the integrated density of states when Ni is substituted for Cu at the center of a 13-atom Cu cluster. (b) Change in density of states.

tures. There is a substantial shift in the position of the peak from $E = 4.05$ (for a free-electron host matrix) to $E = 4.38$ for the matrix of Fig. 1. In addition the total number of states under the virtual-bound-state peak is substantially less than one. It is difficult to find a simple formula for the position of the virtual-bound-state maximum. The shift does not seem to be a simple band repulsion effect, in fact, most of the shift in this case is due to the host $l = 0$ phase shift [Fig. 2(c)]. The host $l = 1$ phase shift has the effect of sharpening the virtual bound state.

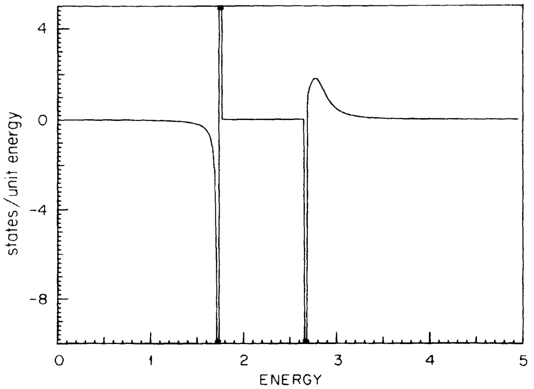

FIG. 4. Change in density of states. The host is that of Fig. 1. The impurity has parameters $\lambda = 1.0, E_1 = 2.30$, $\Gamma = 0.5$.

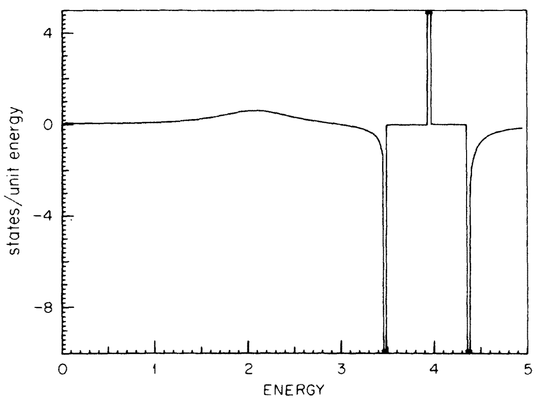

FIG. 5. Change in density of states. The host parameters are $\lambda = 1.0$, $E_1 = 4.05$, $\Gamma = 0.5$. The impurity parameters are $\lambda = 2.0, E_1 = 2.05$, $\Gamma = 0.5$.

Certain qualitative features of these one-dimensional model spectra seem to persist in three dimensions. Figures 3(a) and 3(b) show the changes in the integrated density of states and density of states, respectively, when an Ni atom is substituted for a Cu atom at the center of a 13-atom cluster of Cu atoms. The cluster is surrounded by a zero-potential background equal to the muffin-tin zero, and the geometry of the cluster is that of a Cu atom with its 12 nearest neighbors in metallic Cu. Figure 3 may be compared with Fig. 2 since in both cases the impurity resonance occurs at a somewhat higher energy than that of the host. In both cases there is a subtraction of states near the band edge, and ΔN_l goes to zero within the band. In both cases the virtual bound state is shifted to higher energy and reduced in width by the host.

Figures 4 and 5 show results analogous to those of Fig. 2 for two additional alloys. In Fig. 4, the host is the same as in Fig. 2 and the impurity parameters are $\lambda = 1.0$, $E_1 = 2.30$, and $\Gamma = 0.5$. For this alloy the host and impurity resonances are much closer together. The results are qualitatively similar, however. Note that there is still a virtual bound state maximum, even though E_1 is well within the host gap.

The alloy of Fig. 5 has host parameters $\lambda = 1$, $E_1 = 4.05$, $\Gamma = 0.5$ and the impurity potential has parameters $\lambda = 2$, $E_1 = 2.05$, $\Gamma = 0.5$. In this case the host seems to be acting very much like a free-electron matrix in the energy range of the virtual bound state since the virtual bound state is very broad and not perceptively shifted.

The results of these model calculations emphasize the importance of the proper treatment of resonant scattering and hybridization. Contrast the density of states shown in Fig. 2(a) with the predictions of the two level tight-binding model. In this model one takes a Hamiltonian of the form

$$H=\sum_i E_1^h |i\rangle\langle i| + \sum_{i,j=i} W |i\rangle\langle j| \tag{5.7}$$

for the host. E_1^h would generally be taken to be the host atom resonance energy (2.05 in this case) and W would be adjusted to give the correct band width, ($W=0.47$), in this case. The two level tight-binding model prediction for the change in the integrated density of states is

$$\Delta N(E)=-(1/\pi)\,\mathrm{Im}\ln\{1-(E_1^i-E_1^h)/[(E-E_1)^2 - W^2]^{1/2}\} . \tag{5.8}$$

The host band is centered at E_1 and extends from E_1-W to E_1+W in the two-level tight-binding model whereas the results of Fig. 2 yield a gap in this range. Furthermore, the two-level tight-binding model predicts an infinitely sharp localized state at approximately

$$E=E^i+W^2/2(E_1^i-E_1^h) . \tag{5.9}$$

The resonant scattering model however gives a virtual bound state whose width and position depend on the behavior of the $l=0$ and $l=1$ host logarithmic derivatives. The shift in peak position does not scale as W^2 as we verified by changing the width of the host bands in Fig. 2 by reducing Γ. When Γ and hence W was reduced by a factor of two, the shift was reduced by only 7%.

One must be careful in drawing conclusions about three-dimensional systems from one-dimensional models. It is clear that hybridization effects will not be quite so dominant in three dimensions as in one. However, these calculations do illustrate the need for three-dimensional muffin-tin CPA calculations, and the danger of naive acceptance of tight-binding CPA calculations which ignore hybridization.

ACKNOWLEDGMENTS

We thank J. S. Faulkner and B. L. Gyorffy for helpful discussions. We also thank J. S. Faulkner for permission to use his unpublished derivation of (2.36).

APPENDIX A

We collect here some useful relations involving the "one-dimensional spherical harmonics and spherical Bessel functions" defined in (2.4) and (2.5). Orthonormality of "spherical harmonics"

$$\sum_{\hat{x}=\pm} Y_l(\hat{x})Y_{l'}(\hat{x})=\delta_{ll'} . \tag{A1}$$

Closure:

$$\sum_{l=0,1} Y_l(\hat{x})Y_l(\hat{x}')=\delta(\hat{x},\hat{x}') . \tag{A2}$$

Wronskian relation for "spherical Bessel functions":

$$j_l(z)(dn_l/dz)-n_l(z)(dj_l/dz)=1 . \tag{A3}$$

Sum rule:

$$\sum_{l=0,1} j_l^2(z)=1 . \tag{A4}$$

Plane-wave expansion:

$$e^{ikx}=2\sum_{l=0,1} i^l j_l(kr)Y_l(\hat{x})Y_l(\hat{k}) . \tag{A5}$$

Free-particle propagator partial-wave expansion:

$$G^0(x,x')=(1/2i\sqrt{E})e^{i\sqrt{E}(|x-x'|)}$$

$$=(1/i\sqrt{E})\sum_l j_l(\sqrt{E}\,r_<)h_l(\sqrt{E}\,r_>)Y_l(\hat{x})Y_l(\hat{x}') . \tag{A6}$$

Two-center expansions:

$$j_l(k|x-y|)Y_l(x-y)$$

$$=2\sum_{l_1,l_2} i^{l_1-l_2-l} j_{l_1}(k|x|)j_{l_2}(k|y|) \times Y_{l_1}(\hat{x})Y_{l_2}(\hat{y})C(l,l_1,l_2) , \tag{A7}$$

where

$$C(l,l_1,l_2)=\sum_{\hat{k}=\pm} Y_{l_1}(\hat{k})Y_{l_2}(\hat{k})Y_l(\hat{k})$$

$$=(1/\sqrt{2})\,\delta_{l_1,l_2} \quad l=0 ,$$

$$=(1/\sqrt{2})(1-\delta_{l_1,l_2}), \quad l=1 , \tag{A8}$$

$$(1/i\sqrt{E})h_{l_1}(\sqrt{E}|x-y|)Y_{l_1}(x-y)$$

$$=\sum_{l_2} G'_{l_1 l_2}(y)j_{l_2}(\sqrt{E}|x|)Y_{l_2}(\hat{x}), \quad |y|>|x| \tag{A9}$$

where

$$G'_{l_1 l_2}(y)=(2/i\sqrt{E})\sum_{l_3} h_{l_3}(\sqrt{E}|y|) \times Y_{l_3}(\hat{y})i^{l_1-l_2+l_3}C(l_1,l_2,l_3) , \tag{A10}$$

$$G^0(x-x'+y)=\sum_{l_1l_2} G'_{l_1l_2}(y)j_{l_1}(\sqrt{E}\,|x|)\times Y_{l_1}(\hat{x})j_{l_2}(\sqrt{E}\,|x'|)Y_{l_2}(\hat{x}'),$$

$$\begin{array}{lcl} |x|<|x'-y|, & & |x'|<|x+y|, \\ |x'|<|y|, & \text{or} & |x|<|y|. \end{array} \tag{A11}$$

Explicit forms for $G'_{ll'}$:

$$G'(y)=\frac{e^{i\sqrt{E}|y|}}{i\sqrt{E}}\begin{pmatrix} 1 & i^{-1}\,\mathrm{sgn}(\hat{y}) \\ i\,\mathrm{sgn}(\hat{y}) & 1 \end{pmatrix}, \tag{A12}$$

$$G'(k)=\frac{1}{i\sqrt{E}}\begin{pmatrix} -1+\dfrac{i\sin\phi}{\cos\theta-\cos\phi} & \dfrac{\sin\theta}{\cos\theta-\cos\phi} \\ \dfrac{-\sin\theta}{\cos\theta-\cos\phi} & -1+\dfrac{i\sin\phi}{\cos\theta-\cos\phi} \end{pmatrix}.$$

$$\phi=\sqrt{E}\,a \qquad \theta=ka \tag{A13}$$

One-scatterer Green's function[10]:

$$G^{(1)}(x,x')=(1/i\sqrt{E})\sum_{l} R_l(r_<)F_l(r_>)Y_l(\hat{x})Y_l(x'), \tag{A14}$$

where R_l is the regular solution to the radial Schrödinger equation and F_l is a linear combination of regular and irregular solutions satisfying

$$R_lF_l'-R_l'F_l=i\sqrt{E}\,. \tag{A15}$$

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