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The influence of many-body properties on the excitation spectra of alloys: a model calculation within CPA

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Abstract. The influence of many-body effects on the excitation spectrum of a binary alloy is investigated at the hand of a simple model within CPA. It is found that the detail of the spectrum can be significantly altered by many-body self-energy although the average behaviour does not differ drastically from the single-particle approximation.

1. Introduction

The most reliable theoretical formalism for the description of the electronic properties of random alloys is the coherent potential approximation (CPA) [1]. In its current implementation CPA is based on density functional theory (DFT) [2] and is therefore not expected to yield accurate information on excitation spectra. Although it is well known that DFT applies in principle only to the calculation of ground-state properties [2] such as ground-state energy and electron density, DFT in its local density version has become a matter of routine for calculating the band structures of metals. Encouraging qualitative results have been obtained for metals, but for semiconductors and insulators appreciable departures from experiment are well known for DFT consistently underestimating the band gap in these materials [3]. Recently it has been demonstrated that it is possible to calculate band gaps accurately from first principles by going beyond DFT and including many-body effects [3]. In the case of metals it is also becoming clear that DFT electronic spectra generally deviate from experiment. Even for 'simple' metals DFT fails. The band widths of the alkali metals Na and K, for example, are overestimated by DFT [4] whereas the quasi-particle band widths give very good agreement with experiment [4]. For the simple metals Mg, Al and Be, Plummer [5] enumerated a number of discrepancies such as the underestimation of band gaps and poor correspondence for unoccupied states when experiment and single-particle approximations are compared. Horsch and co-workers have shown in a recent paper that a many-body analysis is crucial to achieve agreement between theory and experiment for the unoccupied states of Ag [6]. Schönhammer and Gunnarson in a recent publication [7] have shown that the DFT Fermi surface does not always correspond to the quasi-particle Fermi surface by constructing a counter-example. This suggests that an improvement of the local-density theory must still fail in the detailed description of excitation spectra. Godby and co-workers [3] have shown that the full DFT still underestimates the bandgap in semiconductors and that this is not a failure of the local-density approximation.

These examples show that although DFT can yield good qualitative results, it fails in

the quantitative description of electronic properties. This is not really surprising since there is no obvious relationship between the DFT eigenvalues and the true excitation energies of a system. It follows that a many-body analysis is necessary to describe the detail of electronic spectra.

The electronic spectra for binary alloys obtained from CPA calculations qualitatively compare quite well with experiment, but as in all other single-particle theories, quantitative discrepancies exist [1, 8]. Some of the questions that are still to be answered include the band width and the distribution of the projected densities of states [1, 8]. It may be that these questions cannot be answered with any accuracy within CPA which is really a mean-field approximation and strictly only applies to completely random systems, taking no account of possible local order. In the present work we explore at the hand of a simple model some of the consequences of the inclusion of many-body effects on the electronic spectra of random binary alloys within CPA.

In § 2 brief overview is given of the lowest-order approximation to the true many-body Green function and a system for including many-body effects in a simple CPA model is developed. In § 3 illustrative results of calculations are presented and in § 4 we summarise and discuss the model and calculations.

2. Background and model

The Green function method is ideal for describing the electronic excitation spectrum of an interacting system of electrons and nuclei [9]. Unfortunately this involves solving a complicated integro-differential equation,

$$[\omega - h(\mathbf{r})]G(\mathbf{r}, \mathbf{r}', \omega) - \int d\mathbf{r}_1 \Sigma(\mathbf{r}, \mathbf{r}_1, \omega)G(\mathbf{r}_1, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.1)$$

where (for a non-relativistic spin-independent Hamiltonian with the nuclei frozen at the equilibrium positions \mathbf{R}_n)

$$h(\mathbf{r}) = -\nabla^2 - \sum_n Z_n v(\mathbf{r} - \mathbf{R}_n) + \int d\mathbf{r}' v(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}') \quad (2.2)$$

with $v(\mathbf{r})$ the Coulomb interactions and $\rho(\mathbf{r})$ the ground-state charge density. The excitation energies are given by the poles of G , but the solution of equation (2.1) for realistic systems is not yet within reach. The 'best' alternative to data is the calculation of quasi-particle energies as discussed in [9]. This involves solving an expression of the form

$$h(\mathbf{r})\psi(\mathbf{r}) + \int d\mathbf{r}' \Sigma(\mathbf{r}, \mathbf{r}', \varepsilon)\psi(\mathbf{r}') = \varepsilon\psi(\mathbf{r}). \quad (2.3)$$

The eigenvalues of this expression approximate the poles of G . In (2.3) the self-energy operator $\Sigma(\mathbf{r}, \mathbf{r}', \omega)$ plays a central role in determining the quasi-particle energies. Equation (2.3) is formally equivalent to the DFT expression but with Σ energy independent and in the local-density version of density functional theory $\Sigma(\mathbf{r}, \mathbf{r}', \omega)$ is replaced by a local function $\delta(\mathbf{r} - \mathbf{r}')V_{XC}(\mathbf{r})$. The eigenvalues of (2.3) can be complex and the eigenfunctions are in general not orthogonal, which reflects the quasi-particle nature of the states described by the wavefunctions. A further simplification that is commonly made is to retain only the real part of the self-energy in (2.3). Excitation spectra which compare well to experiment have been calculated using equation (2.3) [3, 6].

As for the Green function the exact form of the self-energy operator Σ is not known.

A popular choice for Σ is the so-called GW approximation first introduced by Hedin [9, 10] where one sets

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega) = \frac{i}{2\pi} \int G(\mathbf{r}, \mathbf{r}', \omega - \omega') W(\mathbf{r}, \mathbf{r}', \omega') \exp(-i\delta\omega') d\omega' \quad (2.4)$$

where δ is an infinitesimal positive number. In this expression W represents the dynamically screened interaction given by

$$W(\mathbf{r}, \mathbf{r}', \omega) = \int d\mathbf{r}'' \varepsilon^{-1}(\mathbf{r}, \mathbf{r}'', \omega) v(\mathbf{r}'' - \mathbf{r}) \quad (2.5)$$

where $\varepsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$ is the inverse of the longitudinal dielectric response function and $v(\mathbf{r})$ the bare electron–electron interaction. The exact form for ε^{-1} is also not known, but a number of models exist in the literature [9–10]; see also [11]. The simplest is the so-called plasmon pole approximation [9, 10]

$$\varepsilon^{-1}(\mathbf{q}, \omega) = 1 + \omega_p^2 / (\omega^2 - \omega_1^2(\mathbf{q})). \quad (2.6)$$

This expression was successfully used in [9, 10] to calculate quasi-particle energies for a homogeneous electron gas, and it is quite adequate for the illustrative purposes that we have in mind in this work. If we now let

$$\omega_1^2(\mathbf{q}) = \omega_p^2(1 + q^2/\lambda^2) \quad (2.7)$$

it is a simple matter to determine the expression for the screened interaction in real space;

$$W(\mathbf{r}, \mathbf{r}', \omega) = v(\mathbf{r} - \mathbf{r}') \llbracket 1 + \omega_p^2 \{1 - \exp[i|\mathbf{r} - \mathbf{r}'|(\lambda/\omega_p)\sqrt{\omega^2 - \omega_p^2}] / (\omega^2 - \omega_p^2) \} \rrbracket \quad (2.8)$$

where λ is the screening length and the analytic nature of W requires that in the integral of (2.4) the branch cut is taken along $[-\infty, \omega_p]$ and $[\omega_p, \infty]$. The dispersion relation (2.7) for the plasmon pole is correct in the limit $q \rightarrow 0$, but not in the asymptotic limit where it would be more correct to have ω_1 proportional to q^2 . Within the plasmon pole approximation we only include the effects of plasmons on the self-energy and neglect the contribution from electron–hole excitations. These approximations may not always be satisfactory, but for the model calculations considered in this paper the simple expression (2.8) is deemed adequate.

We write the self-energy as

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega) = \Sigma_{\text{se}}(\mathbf{r}, \mathbf{r}', \omega) + \Sigma_{\text{coh}}(\mathbf{r}, \mathbf{r}', \omega) \quad (2.9a)$$

where the screened exchanged term is given by

$$\Sigma_{\text{se}}(\mathbf{r}, \mathbf{r}', \omega) = - \sum_s^{\text{occ}} \varphi_s(\mathbf{r}) \varphi_s(\mathbf{r}') W(\mathbf{r}, \mathbf{r}', \omega - \varepsilon_s) \quad (2.9b)$$

and the Coulomb hole term by

$$\begin{aligned} \Sigma_{\text{coh}}(\mathbf{r}, \mathbf{r}', \omega) &= \frac{\omega_p}{2\pi} v(\mathbf{r} - \mathbf{r}') \int_{\omega_p}^{\infty} G(\mathbf{r}, \mathbf{r}', \omega - \omega') \\ &\times \frac{\sin(|\mathbf{r} - \mathbf{r}'|(\lambda/\omega_p)\sqrt{\omega'^2 - \omega_p^2})}{\omega'^2 - \omega_p^2} d\omega'. \end{aligned} \quad (2.9c)$$

As a first approximation in an iteration loop we may choose the Green function as

$$G(\mathbf{r}, \mathbf{r}', \omega) = \sum_s \frac{\psi_s(\mathbf{r}) \psi_s(\mathbf{r}')}{\omega - \varepsilon_s - i\delta_s} \quad (2.10)$$

where $\delta_s = 0^+$ for $\varepsilon_s < \mu$ and $\delta_s = 0^-$ for $\varepsilon_s > \mu$, with μ being the chemical potential. The initial values for the eigenenergies ε_s and eigenfunctions $\psi_s(\mathbf{r})$ can be generated by the DFT Hamiltonian. The self-energy is then evaluated and equation (2.3) is solved. In the next iteration ψ_s and ε_s in (2.10) are replaced by the solutions of (2.3) and the cycle is repeated until consistency is achieved.

For a regular lattice it is always possible to find a complete set of functions $\{\varphi_\alpha(\mathbf{r})\}$, Wannier functions for example, that are localised at the lattice sites (the suffix α is a compound symbol that includes the orbital type as well as position). Equation (2.1) can then be expressed in matrix notation as:

$$[\omega \mathbf{I} - \mathbf{h} - \Sigma(\omega)]\mathbf{G}(\omega) = \mathbf{I} \quad (2.11)$$

where

$$h_{\alpha\beta} = \int d\mathbf{r} \varphi_\alpha^*(\mathbf{r}) h(\mathbf{r}) \varphi_\beta(\mathbf{r})$$

$$\Sigma_{\alpha\beta}(\omega) = \int d\mathbf{r} d\mathbf{r}' \varphi_\alpha^*(\mathbf{r}) \Sigma(\mathbf{r}, \mathbf{r}', \omega) \varphi_\beta(\mathbf{r}')$$

and similarly for $G_{\alpha\beta}(\omega)$.

Within CPA the Green function $\mathbf{G}(\omega)$ for a random binary alloy with atom types A and B, is approximated by imposing the CPA condition

$$c_A \mathbf{G}_A(\omega) + c_B \mathbf{G}_B(\omega) = \mathbf{G}(\omega) \quad (2.12)$$

where c_A (c_B) is the concentration of atom A (B). The Green functions $\mathbf{G}_{A(B)}$ are obtained by solving equation (2.1) with an effective potential, the so-called coherent potential, extending throughout the system except in the vicinity of the central cell where the correct potential for atom A (B) is retained. This procedure effectively determines the coherent potential through the implied consistency requirement (2.12) and \mathbf{G} is the solution where the coherent potential extends throughout the system.

Let us consider the simplest possible model for a binary alloy, the so called single-band tight-binding model with diagonal randomness [12, 13]. In this model it is assumed that only the one basis function is of interest for each atom type A and B. The wavefunctions and eigenvalues for each atom are

$$(-\nabla^2 + v_A(r))\varphi_A(r) = \varepsilon_A \varphi(r)$$

$$(-\nabla^2 + v_B(r))\varphi_B(r) = \varepsilon_B \varphi(r). \quad (2.13)$$

It is further assumed that the wavefunctions on different sites are orthogonal. The diagonal matrix elements $h_{\alpha\alpha}$, $\alpha = A(B)$, in principle depends on the distribution of atoms in its neighbourhood, but in this model this effect is ignored;

$$h_{\alpha\alpha} = \begin{cases} \varepsilon_A & \text{A atom on site } \alpha \\ \varepsilon_B & \text{B atom on site } \alpha \end{cases} \quad (2.14)$$

If we further ignore randomness in the off-diagonal matrix elements $h_{\alpha\beta}$ we have a particularly simple model which is easy to use but still substantial enough to give physical insight for a number of systems [13].

Henceforth all matrix elements given are diagonal ones. If $\mathbf{G}_0(\varepsilon)$ is the Green function for an ordered system, that is for $\varepsilon_A = \varepsilon_B = 0$, the Green function for an ordered system with diagonal matrix elements $h_{\alpha\alpha} = w$ at each site is [13] $\mathbf{G}_w(\varepsilon) = \mathbf{G}_0(\varepsilon - w)$. Invoking

the CPA condition equation (2.12) and ignoring for the moment the many-body self-energy, we have

$$w = c_A \varepsilon_A + c_B \varepsilon_B - (\varepsilon_A - w)G_w(\varepsilon_B - w) \tag{2.15}$$

where $G_w(\varepsilon)$ is the diagonal matrix element of \mathbf{G}_w . The average density of states per atom for the alloy is given by

$$\rho_w(\varepsilon) = (1/\pi) \text{Im } G_w(\varepsilon). \tag{2.16}$$

From equation (2.12) it follows that

$$c_A \rho_A(\varepsilon) + c_B \rho_B(\varepsilon) = \rho_w(\varepsilon). \tag{2.17}$$

This indicates that we may think of $\rho_{A(B)}(\varepsilon)$ as the average density of states in the vicinity of atom type A(B).

The self-energy is short ranged in $|\mathbf{r} - \mathbf{r}'|$ [10, 11] consequently it should be a reasonable approximation to retain only the diagonal matrix elements in Σ . Hybertsen and Louie [3] found that retaining only the diagonal terms of the self-energy did not change the quasi-particle energies significantly in their calculations for semiconductors. The short-range nature of Σ leads one to expect that the self-energy depends mainly on the local electronic structure, and we take

$$\Sigma_{A(B)}(\omega) = \frac{i}{2\pi} \int G_{A(B)}(\omega - \omega')W(\omega') d\omega' \tag{2.18}$$

where Σ and G are diagonal matrix elements. In order to have an expression for $\Sigma_{A(B)}(\omega)$ we choose a normalised Gaussian basis,

$$\varphi(\mathbf{r}) = (\alpha/\pi)^{3/4} \exp(-\alpha r^2).$$

If we replace the complete set of states in (2.10) by a sum over the Gaussian basis, we obtain the diagonal matrix elements

$$\begin{aligned} \Sigma_{\text{se}A(B)}(\omega) = & - \int_{-\infty}^{\mu} \rho_{A(B)}(\omega') \left\{ \frac{1}{4} \sqrt{\frac{\alpha}{\pi}} - \frac{1}{8} \frac{\lambda}{\sqrt{\gamma(\omega - \omega')}} \right. \\ & \left. \times \exp\left(-\frac{\lambda^2 \gamma(\omega - \omega')}{4\alpha}\right) \left[1 - \text{erf}\left(\sqrt{\frac{\gamma(\omega - \omega')}{4\alpha}}\right) \right] \right\} d\omega' \end{aligned}$$

for $(\omega - \omega')^2 < \omega_p^2$ and

$$\begin{aligned} \Sigma_{\text{se}A(B)}(\omega) = & - \int_{-\infty}^{\mu} \rho_{A(B)}(\omega') \left\{ \frac{1}{4} \sqrt{\frac{\alpha}{\pi}} - \frac{1}{2} \sqrt{\frac{\alpha}{\pi}} \frac{1}{\gamma(\omega - \omega')} \left[\exp\left(-\frac{\lambda^2 \gamma(\omega - \omega')}{4\alpha}\right) - 1 \right] \right. \\ & \left. - \frac{i}{8} \frac{1}{\sqrt{\gamma(\omega - \omega')}} \exp\left(-\frac{\lambda^2 \gamma(\omega - \omega')}{4\alpha}\right) \right\} d\omega' \end{aligned}$$

for $(\omega - \omega')^2 > \omega_p^2$.

$$\Sigma_{\text{coh}A(B)}(\omega) = \frac{1}{8\pi} \int_{\omega_p}^{\infty} \frac{\exp(-\lambda^2 \sqrt{\gamma(\omega')}/4\alpha)}{\sqrt{\gamma(\omega')}} G_{A(B)}(\omega - \omega') d\omega' \tag{2.19}$$

where

$$\gamma(\omega) = (\omega^2 - \omega_p^2)/\omega_p^2.$$

The results presented in the next section do not depend qualitatively on the screening length λ and the orbital extent α . In all the calculations $\lambda = 1.8 \text{ \AA}^{-1}$, an average for metallic densities, and $\alpha = 1.0 \text{ \AA}^{-2}$ were used.

As we are interested in the quasi-particle spectrum, we retain the only real part of the shelf-energy in the calculations. Retaining only the diagonal self-energy matrix elements, the Green function for our model of a random alloy system can be determined from equation (2.15) by replacing $\varepsilon_{A(B)}$ by $\eta_{A(B)} = \varepsilon_{A(B)} + \Sigma_{A(B)}$. We use an elliptical density of states as is normal in model calculations [12]. If the band width is $2b$, the Green function corresponding to an elliptical density of states is given by

$$G_0(\omega) = (2/b^2)(\omega - \sqrt{\omega^2 - b^2}).$$

We take the band as filled, that is the Fermi level is at $\omega = b$. Substituting G_0 and $\eta_{A(B)}$ into (2.15) yields a cubic polynomial in G_w ;

$$G_w^3 + (4/b^2)(\eta_A + \eta_B - 8\omega)G_w^2 + (16/b^4)[(\omega - \eta_A)(\omega - \eta_B) + b^2/4]G_w + (16/b^2)[(1 - c_A)\eta_A + (1 - c_B)\eta_B - \omega] = 0 \quad (2.20)$$

where we have suppressed the energy dependence of G and η . The appropriate root of G_w can be selected by inspection. The quasi-particle energies are associated with the solution of a Dyson equation $\omega - \varepsilon_s - \text{Re } \Sigma_s(\omega) = 0$. In addition to the quasi-particle energies, other solutions to the Dyson equation, such as the so-called plasmarons [9], are possible and care must be taken to exclude these in each iteration. The quasi-particle density of states is normalised to the number of electrons per atom (two electrons per atom) in each cycle. Convergence was usually achieved after four or five iterations.

3. Results

As there are effectively two units of energy involved in the model, the band width and the plasmon energy, it is necessary to assign a numerical value to at least one of these. In the calculations presented in this section the plasmon energy was set to 8 eV and ω_p was used as the unit of energy. The atomic energy levels were set to $\varepsilon_B = -\varepsilon_A$ and we use the dimensionless parameter

$$\delta = (\varepsilon_A - \varepsilon_B)/b$$

consistent with the notation of [12].

In figure 1(a) the conventional CPA density of states without the inclusion of the many-body self-energy is illustrated for a range of concentrations and for $\delta = 0.6$. In figure 1(b) the many-body self-energy is included and the half band width $b = 0.375\omega_p$. The results are typical for the situation where $b < \omega_p$. We note the following over the whole range of concentrations: (i) the overall band width decreases, (ii) the separation between the two bands associated with the two types of atom is enhanced. This separation is the consequence of the offset between the self-energies associated with the different component density of states, reminiscent of the opening of the band gap in semiconductors [3]. In the region of interest, Σ_A and Σ_B are almost parallel but separated by an interval that is related to the separation between the centre of mass of the component densities of states ρ_A and ρ_B . This is not an artefact of the model; the diagonal elements of the self-energy operator in the valence band, at least in the GW approximation, tend to scale as the eigenvalues of the states of h_0 with which they must be associated. This is illustrated in figure 8 of [3] for a number of semiconductors. One would therefore also expect to observe the enhancement of the separation between the component densities of states in more realistic calculations for split band systems.

The negative slope of the self-energy in the region of the quasi-particle band is similar to the jellium model [9] and is also consistent with the calculations of [3]. The overall

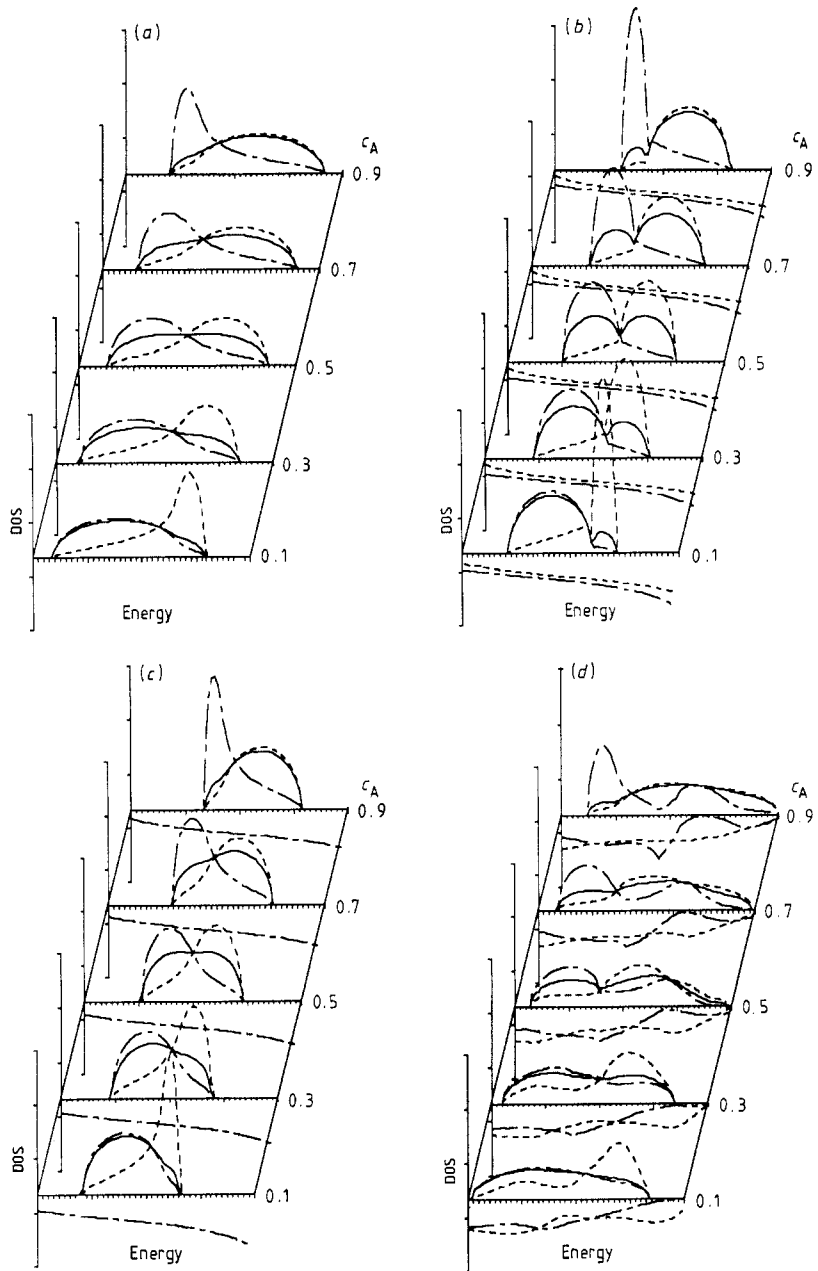


Figure 1. Densities of states and self-energies for a model binary alloy system within CPA. Graphs above the x axis refer to densities of states while the lines below the x axis refer to self-energies. Arbitrary units are used but they are scaled such that units correspond for each set of graphs. Full curves refer to average quantities while the broken curves correspond to atom type A and chain curves to atom type B. (a) No self-energy effects; $\delta = 0.6$. (b) As (a) but with self-energy included according to equation (2.18) and with $b = 0.375 \omega_p$. (c) As (b) but with an average self-energy for atom types A and B. (d) As (b) but with $b = 1.0 \omega_p$.

narrowing of the band is a consequence of the negative slope of the self-energy over the quasi-particle band.

In figure 1(c) the same situation as in (b) is portrayed, but in this case the same self-energy is used for both types of atom; $G_{A(B)}$ in (2.18) is replaced by G_w . In this instance the only effect the self-energy has is to scale the band. This illustrates that the enhanced split-band effect depends on the distinction between the two types of atom in calculating the self-energy. This distinction relies on the assumption that the self-energy is short ranged, and from (2.5) this appears to be reasonable for metallic systems with short-range screening [9]. In fact it turns out that even for semiconductors the self-energy is very localised as illustrated in [14].

As the ratio between the band width and the plasmon pole increases, the affect the self-energy has on the density of states alters. In figure 1(d) we illustrate the situation where $b = \omega_p$ and $\delta = 0.6$. This situation may not arise in a realistic calculation; in the jellium model, for example, the magnitude of the plasmon pole is always larger than the band width for realistic charge densities. The example is included here for completeness. In figure 1(d) we notice that over the whole range of concentrations the band width is increased and the component densities of states are redistributed. This is in contrast with the previous examples where the component densities more or less scaled with the overall change in the band width. The redistribution of the component densities of states is especially pronounced for $c_A > 0.5$. The peak in ρ_B near the top of the band is a consequence of the peak in Σ_B in the same region. This peak comes from a combination of the square-root singularities in W at $\omega - \varepsilon_s = \omega_p$ in (2.9b) and in the integrand of equation (2.9c) at $\omega' = \omega_p$. The high density of states in ρ_B near the bottom of the band gives rise to the sharp peak in Σ_B towards the top of the band. As c_B increases ρ_B becomes smooth, the peak in Σ_B is pushed to higher energies and is smoothed at the same time. A similar feature can be noted in Σ_A where a peak appears above the band as c_A decreases and the density ρ_A becomes more peaked near the top of the band. There is no evidence of a band gap opening in the density of states as for the first example. The reason for this difference is the different behaviour of the self-energy. In this case Σ_A and Σ_B cross each other at least two points within the range of the band. In contrast to the first example where the self-energy effectively pushed the atomic levels apart over the whole range of interest, here the atomic levels are pushed apart over part of the range and pulled closer together over the rest of the interval.

4. Summary and conclusion

We have, for the first time, calculated the quasi-particle spectrum for a model of a binary alloy within CPA. The calculations show that the inclusion of the many-body self-energy can significantly influence the detail of the excitation spectrum. We illustrated that it is possible to stretch or contract the quasi-particle band width with respect to the single-particle band width depending on the ratio between the plasmon pole and the single-particle band width. For a band width less than twice the magnitude of the plasmon pole, a band gap opens up between the component densities of states. This is similar to what happens in semiconductors, but in this instance the gap opens in the valence band and not between the valence and conduction bands.

At this point it is not possible to state whether the quasi-particle spectrum, within CPA, will improve the correspondence between theory and experiment. A comparison of the self-consistent KKR CPA calculations of [15] and the XPS spectra measured in [16],

however, suggests that the enhanced split-band effect may improve the correspondence between the bare spectra, but in the final analysis only a detailed calculation for a realistic system can address these questions.

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