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One-dimensional model of a liquid metal in the effective-medium approximation in the random limit

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In this paper it is shown that the effective-medium approximation (EMA) of Roth [Phys. Rev. B **9**, 2476 (1974)] corresponds to the approximation No. 5 of Klauder [Ann. Phys. **14**, 43 (1961)] in the random limit for the one-dimensional delta-function model of a liquid metal. The random EMA results are compared with the exact results obtained by Frisch and Lloyd [Phys. Rev. **120**, 1175 (1960)] for this model.

I. INTRODUCTION

Theoretical studies of one-dimensional models are useful because they provide a critical means to test a given approximation. If an approximation agrees well with exact available numerical studies of one-dimensional systems, it is a natural step to extend a certain theory to three-dimensional models of materials. Thus, the most successful random-alloy theory, the coherent-potential approximation (CPA) of Soven[1] and of Velický, Kirkpatrick, and Ehrenreich[2] has already been tested for one-dimensional models.[1,3]

Klauder[4] conducted a study on a system composed of randomly distributed impurities using diagrammatic perturbation methods from field theory. Klauder[4] arrived at a series of approximations to the average Green's function for the system of random impurities, the highest level of approximation he analyzed was similar to the Brueckner approximation of many-body theory. This approximation he called approximation No. 5. Klauder[4] compared the results of his approximations for the one-dimensional delta-function model of a liquid metal with the exact results of Frisch and Lloyd.[5]

Faulkner[6] investigated the case of a random liquid metal based on the coherent-potential approximation (CPA) of Soven[1] and of Velický *et al.*[2] and showed that the CPA in general corresponds to Klauder's approximation No. 5. This is an important result because it provides a connection between two different calculational schemes. It is also reassuring when an extension of the CPA reduces to Klauder's results in the random limit.

Roth[7] developed an effective-medium approximation (EMA) for liquid metals based on the CPA but designed to include short-range order. Roth[7,8] showed in her works that the EMA when applied to the alloy problem reduces to the CPA. Yonezawa, Roth, and Watabe[9] have shown that the EMA is the proper extension of the CPA to include short-range order such as found in liquid metals. The EMA has a tight-binding version due to Roth[10] and the interested reader is referred to the work of Hasbun and Roth[11] for a recent study of local effects in alloys using the EMA and further extensions to semiconductors.[12]

Singh and Roth[13] derived the full effective-medium approximation (EMA) equations for the correlated case of the one-dimensional delta-function model of a liquid metal. The authors compared their results with the exact Monte Carlo calculation of Peterson, Schwartz, and Butler.[14]

While the work of Singh and Roth[13] deals with the correlated case of a one-dimensional model, to date it has not been shown clearly that the EMA gives Klauder's results,[4] i.e., approximation No. 5, for the random limit case of the one-dimensional delta-function model of a liquid metal. The purpose of this paper is to show that indeed such correspondence exists. Below, in Sec. II the model is discussed; in Sec. III we present the full EMA, and its random limit case, followed by the results in Sec. IV, and the conclusion in Sec. V.

II. THE MODEL

The model consists of hard rods of length distributed randomly in one dimension.[13] A negative δ function is at the center of each rod. The one-electron Hamiltonian is given by

$$H=\frac{p^2}{2m_e}-\sum_{n=1}^{N}V_0\delta(x-X_n) \tag{2.1}$$

with $V_0>0$. From the work of Singh and Roth,[13] the pair distribution function of a correlated one-dimensional delta-function model[15] has an order parameter $\alpha=a/l$, where $l=L/N$ the average length per atom. For the case of complete randomness $\alpha\rightarrow 0$ and the pair distribution function becomes

$$g(X)=1\ . \tag{2.2}$$

This gives the probability of finding an ion at X given one at $X=0$. It has the value of unity since there is no minimum separation of sites required.[14]

We work with a dimensionless density parameter[4] ε given by

$$\varepsilon\equiv n/\kappa_0,\quad \kappa_0\equiv\frac{m_eV_0}{h^2}\ , \tag{2.3}$$

where n is the number of ions per length. The energy is in units of binding energy[4] ε_b given by

$$\varepsilon_b = \frac{h^2\kappa_0^2}{2m_e} . \tag{2.4}$$

III. THE EMA

We begin with the full self-consistent equations for the one-dimensional delta-function model from the work of Singh and Roth,[13] which we restate for clarity. The total Green's function for the system is given in $\mathbf{k}$ space by

$$G_k = G_{0k} + G_{0k} T_k G_{0k} , \tag{3.1}$$

where

$$G_{0k} = \left[\bar{w} - \frac{h^2 k^2}{2m_e} + i\delta \right]^{-1} \tag{3.2}$$

is the free-electron Green's function. The T matrix is given by

$$T_k = nt_c/(1 - nt_c \tilde{G}_k) , \tag{3.3}$$

where

$$\tilde{G}_k = \tilde{G}_{0k} + \int_{-\infty}^{\infty} \hbar(k-k')\tilde{G}\,{}_{k'}^{2} T_{k'}\, dk'/2\pi \tag{3.4}$$

and

$$\tilde{G}_{0k} \equiv \int_{-\infty}^{\infty} G_0(x) g(x) e^{ikx}\, dx , \tag{3.5a}$$

$$G_0(x) = \left[\frac{m_e}{ih^2 k_0} \right] e^{-ik_0|x|} , \quad k_0 \equiv \left[\frac{2m_e \bar{w}}{h^2} \right]^{1/2} . \tag{3.5b}$$

The single-site scattering matrix is given by

$$t_c^{-1} = t_0^{-1} - nt_c \int_{-\infty}^{\infty} \tilde{G}_{0k}(G_{0k} + \tilde{G}\,{}_k^2 T_k)\, dk/2\pi , \tag{3.6}$$

where

$$t_0 = -V_0/(1 + m_e V_0/ih^2 k_0) . \tag{3.7}$$

The quantity $\hbar(k-k')$ in Eq. (3.4) is defined by

$$\hbar(k-k') \equiv \int_{-\infty}^{\infty} [g(x) - 1] e^{i(k-k')x} dx , \tag{3.8}$$

and carries information on the site exclusion property of the EMA.[9]

The differential density of states is obtained from the imaginary part of the energy $\bar{w}$-dependent Green's function of Eq. (3.1) by

$$\bar{n}(\bar{w}) = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} G_k\, dk/2\pi , \tag{3.9}$$

and the integrated density of states per atom is given by

$$N(\bar{w}) = \frac{1}{n} \int_{-\infty}^{\bar{w}} \bar{n}(\bar{w}')\, d\bar{w}' \tag{3.10}$$

We note that, in general, the most difficult part of the EMA is the coupled iterative nature of Eqs. (3.4) and (3.6), which need to be iterated self-consistently in order to determine the Green's function Eq. (3.1) completely in the full EMA.

A. The random EMA

In this limit, we recall Eq. (2.2) which when substituted into Eq. (3.8) gives

$$\hbar(k-k') \rightarrow 0 . \tag{3.11}$$

We also have from the above section, using Eqs. (2.2) and (3.11), that

$$\tilde{G}_k \rightarrow \tilde{G}_{0k} \rightarrow G_{0k} , \tag{3.12}$$

$$T_k \rightarrow nt_c/(1 - nt_c G_{0k}) , \tag{3.13}$$

and

$$t_c^{-1} \rightarrow t_0^{-1} - nt_c \int_{-\infty}^{\infty} \frac{G_{0k}^2}{(1 - nt_c G_{0k})} \frac{dk}{2\pi} , \tag{3.14}$$

reducing the EMA equations to one self-consistent energy-dependent quantity t_c of Eq. (3.14).

For computational convenience we rewrite the above equations in terms of dimensionless units.[4] The energy parameter becomes in terms of Eqs. (2.3) and (2.4)

$$\bar{w} = w\varepsilon_b, \quad w = y_0^2, \quad y_0 \equiv k_0/\kappa_0 . \tag{3.15}$$

With the above definitions we obtain the random EMA Green's function in terms of dimensionless quantities

$$G_y = G_{0y}/(1 + bG_{0y}) , \tag{3.16a}$$

$$G_{0y} = (y_0^2 - y^2 + i\delta)^{-1} , \tag{3.16b}$$

where the single-site scattering matrix b is given by

$$b^{-1} = b_0^{-1} - \frac{b}{\varepsilon} \int G_{0y} G_y\, dy/2\pi , \tag{3.17a}$$

with

$$b_0 \equiv -nt_0/\varepsilon_b = 2\varepsilon \Big/ \left[1 + \frac{1}{iy_0} \right] , \tag{3.17b}$$

and where we have made use of

$$b \equiv -nt_c/\varepsilon_b, \quad y \equiv k/\kappa_0 , \tag{3.18a}$$

and

$$G_{0y} \equiv \varepsilon_b G_{0k}, \quad G_y \equiv \varepsilon_b G_k . \tag{3.18b}$$

The differential density of states is now given by

$$\bar{n}(\bar{w}) = \frac{\kappa_0}{\varepsilon_b} n(w), \quad n(w) = -\frac{1}{\pi} \mathrm{Im} \int G_y\, dy/2\pi , \tag{3.19}$$

and the integrated density of states per site becomes

$$N(w) = \frac{1}{\varepsilon} \int_{-\infty}^{w} n(w')\, dw' . \tag{3.20}$$

Equations (3.16)–(3.20) are the EMA equations for the one-dimensional delta-function model in the random limit.

We note that while it is not so obvious, this result for the random EMA is the CPA of Soven[1] and Velický *et al.*[2] In fact, the purpose of this paper is to show this by demonstrating, in the next section, that the above equations give Klauder's approximation No. 5.[4] The connection with the CPA follows from the work of Faulkner.[6]

IV. RESULTS

We first discuss briefly, and for completeness, the simple quasicrystalline approximation (QCA) of Lax.[16] For this case Eq. (3.17a) becomes

$$b \rightarrow b_0 \ , \tag{4.1}$$

where b_0 is given by Eq. (3.17b). By substituting Eq. (4.1) into Eq. (3.16a) and performing the integral in Eq. (3.19) we obtain

$$n(w)=\frac{1}{\pi}\mathrm{Im}\left[\frac{i}{(q^2+i\Delta)^{1/2}}\right] , \tag{4.2}$$

where

$$q^2 \equiv w+\frac{2\varepsilon w}{1+w}, \quad \Delta \equiv \delta+\frac{2\varepsilon y_0}{1+w} . \tag{4.3}$$

This is as far as we discuss the QCA since it has been well documented in the literature.[17] Furthermore, it corresponds to Klauder's[4] approximation No. 4 in that work.

The result for the random EMA is obtained by substituting in the Green's functions of Eqs. (3.16) into Eq. (3.17a) and performing the integration. We find that the single-site scattering matrix obeys the equation

$$(w+b)^{3/2}-i(w+b)-(2\varepsilon+w)(w+b)^{1/2}+iw=0 , \tag{4.4}$$

which is a cubic.

If we make the substitution

$$b=-w-\frac{1}{\Sigma_K^2} , \tag{4.5}$$

where Σ_K is Klauder's self-energy Σ_5 in that work,[4] into Eq. (4.4) we obtain

$$w\Sigma_K^3-(2\varepsilon+w)\Sigma_K^2+\Sigma_K=1 . \tag{4.6}$$

Equation (4.6) is Klauder's self-consistent expression for his approximation No. 5 if we note that Klauder's energy variable ε is related to our energy variable by

$$w=2\varepsilon . \tag{4.7}$$

Finally, we make complete correspondence between the random EMA and Klauder's approximation No. 5 by noting that

$$n(w)=2\rho_K(\varepsilon) , \tag{4.8}$$

where ρ_K is Klauder's differential density of states.

Finally, for completeness, we compare our random EMA results with the exact results for the one-dimensional delta-function potential model of Frisch and Lloyd.[5] We note that the density of states variable in Ref. 5 is y_0 of Eq. (3.15) and we can easily compare our density of states Eq. (3.20) with Ref. 5.

We have calculated the integrated density of states using Eq. (3.20) with the help of Eqs. (3.16) after solving for the single-site scattering matrix b of Eq. (4.4) by the standard method for cubics. Our results for $\varepsilon=0.1$ and $\varepsilon=1.0$ are shown in Figs. 1 and 2, respectively, and they are labeled random EMA. Frisch and Lloyd[5] results are labeled FL in the figures. The curves labeled FE correspond to the free-electron results which we provide for comparison.

We see in Fig. 2 that for the high-density $\varepsilon=1.0$ case the random EMA, which as shown above corresponds to the CPA, is in very good agreement with the exact results.[5] For the low density $\varepsilon=0.1$ case, Fig. 1, however, the agreement is not so good. These results appear in the work of Klauder[4] as well. The low-density problem has been discussed by Roth[8] and Singh and Roth.[13] In general, the CPA was shown by Schwartz and Siggia[18] to correspond in some sense to an expansion of $1/z$, where z is the number of neighbors in a nearest-neighbor tight-binding model. For certain energies terms in the self-energy of the order z^{-2} are omitted in the CPA.[8] For low concentration the impurity band is not well described by the CPA because z, which is the number of impurity neighbors, becomes small in this region. Similarly the EMA for liquid metals has been shown to be best for a large number of neighbors, i.e., at high density.[8]

V. CONCLUSION

In this work it has been shown that the effective medium approximation (EMA) of Roth[7] corresponds to the approximation No. 5 of Klauder[4] in the random limit for the one-dimensional delta-function model of a liquid metal. We have compared our EMA results with the exact results of Frisch and Lloyd[5] for this model. Our results for the high-density $\varepsilon=1.0$ case are in very good agreement with the exact results.[5] For the low-density case $\varepsilon=0.1$, the agreement is apparently not quite so good.[4,5]

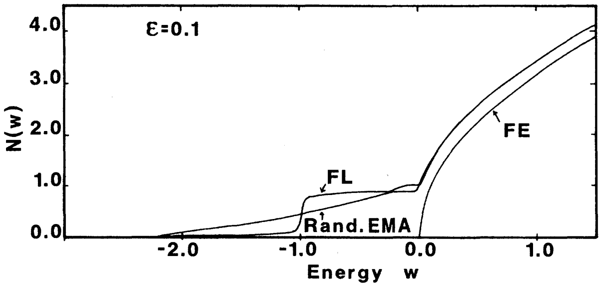

FIG. 1. The density of states $N(w)$ vs energy w, labeled Rand. EMA, from Eqs. (3.20), and the solution of Eq. (4.4) is compared with the exact results of Frisch and Lloyd, Ref. 5, labeled FL for the case of $\varepsilon=0.1$. The free-electron results FE are shown for comparison.

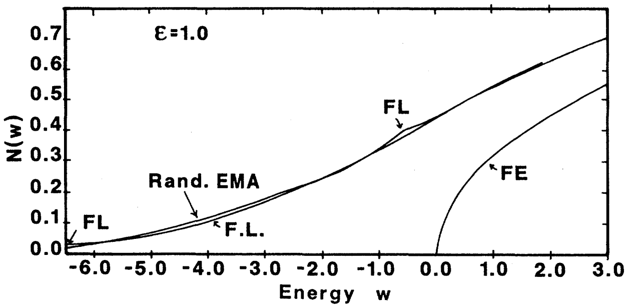

FIG. 2. The density of states $N(w)$ vs energy w, as in Fig. 1, for the case of $\varepsilon = 1.0$.

The self-consistent theories which are extensions of the CPA as is the EMA are not expected to be good in this region.[13]

While this work provides conclusive evidence that the EMA of Roth[7] for a random liquid is equivalent to Klauder's approximation No. 5, it also follows from the work of Faulkner[6] that the EMA for the random liquid case is equivalent to the coherent-potential approximation (CPA) of Soven[1] and Velický *et al.*[2]

Further investigation on the full EMA equations of Sec. III above for the correlated one-dimensional model of a liquid metal is needed. Suggestions have been proposed[13] to account for the fact that the EMA has too many pair-distribution functions in it in this one-dimensional case. We hope to continue work in this area where exact results are available.[14]

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