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LETTER TO THE EDITOR

The EMA for a two-band spatially disordered system: comparison of simulation with theory

Ian J Bush, David E Logan, Paul A Madden and Martyn D Winn
University of Oxford, Physical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, UK

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Abstract. An approximate but soluble single-site theory for the density of states of a two-band spatially disordered system, the single super-chain approximation/effective-medium approximation (SSCA/EMA), is compared with direct simulations on an off-diagonally disordered, two-level tight-binding model. The theory reproduces the simulations remarkably well.

There has recently been renewed interest in exploiting parallels with conventional liquid state theory to develop accurate but analytically tractable theories for the density of states (DOS) of a system characterised by quenched liquid-like disorder, at the level of a one-band, tight-binding model (TBM) (Winn and Logan 1988, 1989a, Stratt and Xu 1989a, b, Bush *et al* 1989). For many non-simple systems, however, several different bands may be important in determining electrical characteristics. It is thus desirable to extend previous theoretical work beyond the one-level TBM; and to compare the resultant predictions with 'exact' numerical simulations, which is the aim of this work.

Using the methods of liquid-state graph theory, a formally exact analysis of the ensemble averaged Green functions for a topologically disordered n-level per site TBM has recently been given (Winn and Logan 1989b). In particular a knowledge of the average diagonal (site and level) Green functions, $\bar{G}^{\alpha\alpha}(z)$, give the partial DOS $D_\alpha(E) = -\pi^{-1}\,\mathrm{Im}\,\bar{G}^{\alpha\alpha}(z)$ associated with level α, where $z = E + is\,(s \to 0+)$ is the energy. From this an approximate single-site theory for the averaged Green functions, the single super-chain approximation (SSCA), was systematically developed. The SSCA was shown to be mathematically equivalent to the effective medium approximation (EMA) of Roth (1974, 1976), but the simpler manner in which the SSCA is formulated enables further exploitation of parallels with conventional liquid-state problems: the exact equations governing the averaged off-diagonal Green functions (which enter a determination of $\bar{G}^{\alpha\alpha}(z)$ via an exact self-consistency equation) are closely related to the Ornstein–Zernike equations for a classical n-component liquid mixture; and the SSCA/EMA in essence provides an approximate closure condition to these equations, enabling solutions to be obtained. In particular, if the structural pair distribution function (PDF) $g(R)$, which enters the closure relation, is approximated as a step function $\theta(R - \sigma)$, corresponding to the low density limit for hard spheres of diameter σ, then the SSCA/EMA is formally related to the mean spherical approximation of liquid-state theory for the PDF of a classical n-component liquid mixture, for which analytical solutions are

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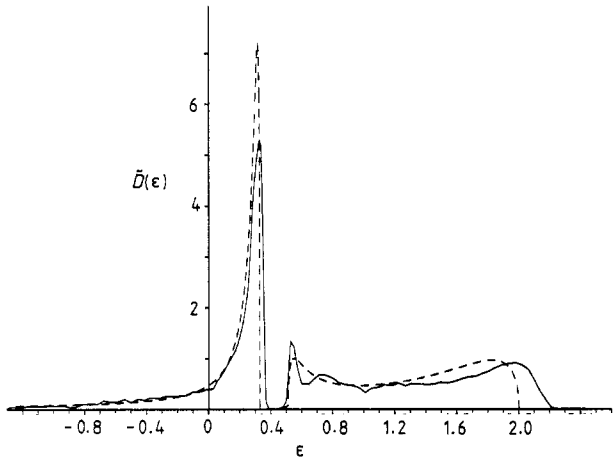

Figure 1. Total DOS, $\tilde{D}(\varepsilon)$ (reduced energy $\varepsilon = E/V_0^*$) for $\rho^* = 0.5$, $\sigma/a_H = 0.8$, $\Delta\varepsilon = 1 = a$. Broken curves, theoretical results; full curves, simulation.

known. From this, Winn and Logan (1989b) obtained solutions for the DOS in the case of a 2-level TBM with modified exponential (Yukawa) transfer matrix elements $V^{\alpha\beta}(R) = -(a^{\alpha\beta}V_0/R)\exp(-R/a_H)$, where $\alpha(=0, 1)$ and β denote the levels. Details for the reduced partial DOS, $\tilde{D}_\alpha(\varepsilon) = V_0^* D_\alpha(E)$, where $V_0^* = V_0/\sigma$, as a function of reduced energy $\varepsilon = E/V_0^*$, are given in Winn and Logan (1989b). The theory is characterised parametrically by: a reduced density $\rho^* = \rho\sigma^3$ (where ρ is the number density of particles); the ratio of length scales σ/a_H; $\Delta\varepsilon = [\varepsilon_1 - \varepsilon_0]/V_0^*$ where $\varepsilon_0(\varepsilon_1)$ denotes the unperturbed site energy of level 0(1); and the strength parameters a^{00}, $a^{01} = a^{10}$, a^{11}.

To examine the validity of the above SSCA/EMA, numerical simulations were performed on an off-diagonally disordered TBM, with quenched disorder characteristic of a hard-sphere fluid. For a given configuration, direct diagonalisation of the two-level, tight-binding Hamiltonian yields the eigenvalues of the system. The resultant configurationally averaged DOS is smoothed by averaging over an energy interval large enough to give adequate statistics and small enough to preserve detail. Results reported here refer to 12 configurations of a 250-particle system; computational details are given in Gibbons *et al* (1988) and Bush *et al* (1989).

One theoretical prediction is that for the case of identical transfer matrix elements ($a^{\alpha\beta} = a$, $\forall_{\alpha,\beta}$), and regardless of the remaining physical parameters, there is always a band gap in the total DOS, $\tilde{D} = \tilde{D}_0 + \tilde{D}_1$, lying between the zero-order site energies ε_0 and $\varepsilon_1 > \varepsilon_0$. An explanation for this, in terms of a repulsion between the sub-bands arising from the inter-level couplings, $V^{01}(R)$, has been given (Winn and Logan 1989b), and for $a^{01} \geqslant a^{00}$, a^{11}, band crossing does not occur. This is confirmed from simulation over a wide range of parameters; an example is given in figure 1 for $\rho^* = 0.5$, $\sigma/a_H = 0.8$, $\Delta\varepsilon = 1$ and $a = 1$. The separate sub-bands are each normalised to unity in both theory and simulation, all features of the lower (upper) sub-bands are reproduced excellently (well) by the SSCA/EMA, and for an $m = 2$ electron-per-site system the Fermi energy, ε_F, lies in the band gap and the system is an insulator.

To investigate band overlap, figure 2 shows the case $\rho^* = 0.3$, $\sigma/a_H = 0.8$, $\Delta\varepsilon = 1$, $a^{00} = 0.7 = a^{01}$ and $a^{11} = 1$. Simulation and theory again agree quite well, but in this case the sub-bands overlap. For $m = 2$ the SSCA Fermi energy, $\varepsilon_F \simeq 0.26$, agrees well with simulation, $\varepsilon_F \simeq 0.29$, and it is noteworthy that in each case ε_F lies in a high DOS region close to the peak in the lower band: states at ε_F are thus likely to be extended,

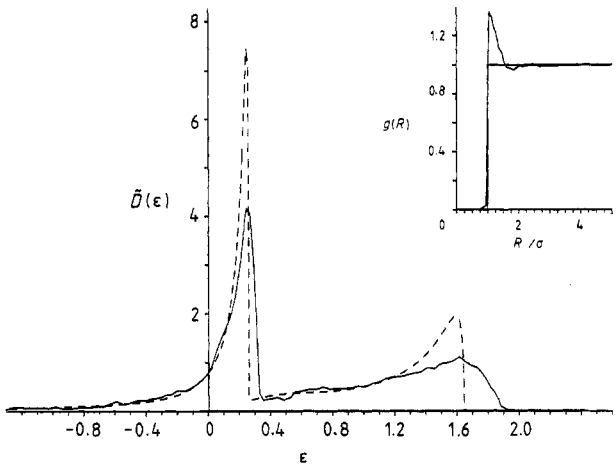

Figure 2. As figure 1 but with $\rho^* = 0.3$, $a^{00} = 0.7 = a^{01}$ and $a^{11} = 1$. Inset: the PDF from simulation compared to a step function.

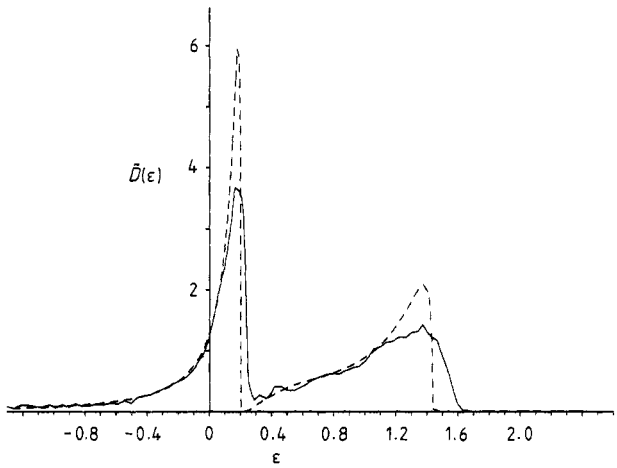

Figure 3. As figure 2 but with $\sigma/a_H = 1.2$.

corresponding to a metallic system. Figure 3 has the same parameters as figure 2 except that σ/a_H is increased to 1.2, so the transfer matrix elements are spatially shorter ranged. This has the expected effect of diminishing band overlap, with a consequent contraction of the constituent sub-bands. The SSCA/EMA predicts that a gap opens up (just), while simulation shows diminished overlap with ε_F lying in the low DOS 'pseudo-gap' region. As ρ^* is decreased one expects the sub-bands to separate further. This is seen in figure 4 which has the same parameters as figure 3 except that $\rho^* = 0.1$, and both theory and simulation predict a band gap in the DOS. Even at this low density, agreement between theory and simulation is adequate, particularly in the lower sub-band. As ρ^* is reduced below 0.1, however, agreement becomes progressively poorer: as discussed by Winn and Logan (1989b), the SSCA does not reproduce correctly the $\rho^* \to 0$ limit, a proper description of which requires a non-single-site theory. Finally, a representative example of the partial DOS, $\tilde{D}_0(\varepsilon)$ and $\tilde{D}_1(\varepsilon)$ is shown in figure 5 for the same parameters as figure 1; ($\tilde{D}_0$ and $\tilde{D}_1$ each contribute to both the upper and lower sub-bands). Agreement is again good: note in particular confirmation of the prediction that $\tilde{D}_0$ ($\tilde{D}_1$) should vanish for ε corresponding to the unperturbed site energy of level 1(0).

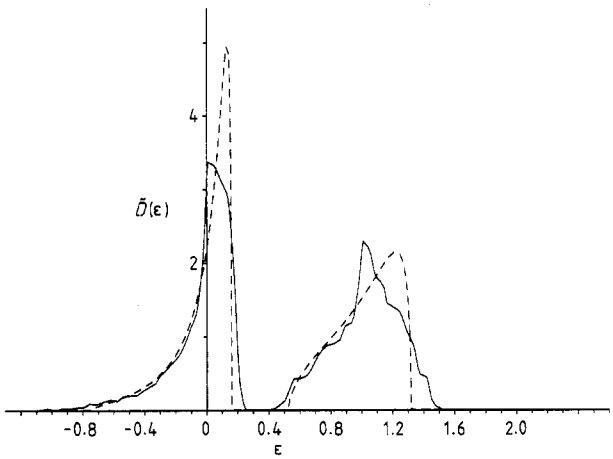

Figure 4. As figure 3 but with ρ^* reduced to 0.1.

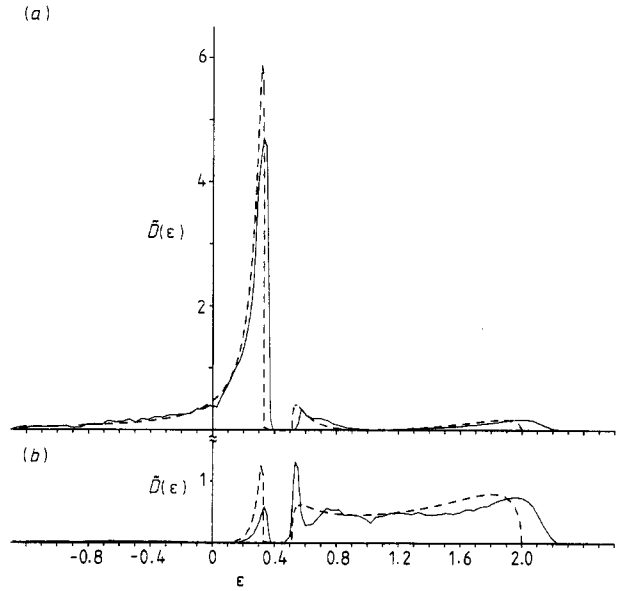

Figure 5. The partial DOS: (*a*) $\tilde{D}_0(\varepsilon)$ and (*b*) $\tilde{D}_1(\varepsilon)$, with parameters as in figure 1. Broken curves, theory; full curves, simulation.

The principal discrepancy between theory and simulation arises in the behaviour of $\tilde{D}(\varepsilon)$ near the upper edge of the upper sub-band: see figures 1–5. States near the upper edges of both sub-bands are in general strongly influenced by near-neighbour interactions, and the mean number of nearest neighbours is underestimated by the model PDF used in the SSCA/EMA, as illustrted in figure 2. Inter-band repulsions will, however, reduce this discrepancy for states near the upper edge of the lower sub-band, as such repulsions are stronger in simulation by virtue of the larger number of nearest neighbours. The main discrepancy thus occurs for states near the upper edge of the higher sub-band.

This study suggests that (for $\rho^* \geqslant 0.1$) a simple analytical theory, the SSCA/EMA, describes well the DOS of a two-band TBM characterised by quenched liquid-like disorder.

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