Comment on "Absence of Impurity Bands in Conjugated Polymers"

In a recent Letter,[1] Harigaya, Wada, and Fesser used the coherent-potential approximation (CPA) to study the effect of impurities on the density of electronic states in conducting polymers. They reached the conclusion that the qualitative nature of the density of states is determined by the quantity $J-I$, with J the site impurity strength and I the bond impurity strength.

It is the purpose of this Comment to note that the model studied in Ref. 1 can, in fact, be solved exactly by using the supersymmetric techniques of Xu and Trullinger.[2] The exact calculation shows the density of states to be governed by the quantity $v=2\Delta I+I^2-2EJ$, with E the energy and 2Δ the unperturbed band gap, rather than by $J-I$, and to lack the singularities predicted by use of the CPA.

The treatment of a Gaussian distribution of disorder given in Refs. 2 and 3 is simply adapted to handle without any approximation the Poisson distribution of the model used in Ref. 1. The resulting exact density of states for the model of Harigaya, Wada, and Fesser,[1] i.e., Poisson distributed disorder, is related to the solution of equation

$$\phi''(r)-\left(E^2-\Delta^2+\frac{c(1-e^{ivr})}{ir}\right)\phi(r)=0\,, \qquad (1)$$

with boundary conditions

$$\phi(0)=1,\quad \phi(\pm\infty)=0\,, \qquad (2)$$

and with c the concentration. Explicitly, the density of states is

$$\rho(E)=-\frac{\partial}{\pi\partial E}\left[\mathrm{Re}\left(\frac{\partial\phi(r)}{\partial r}\bigg|_{r=0}\right)\right], \qquad (3)$$

the functional form of which can be expressed as

$$\rho(E)=\rho_1(E,\Delta,c,v)+J\rho_2(E,\Delta,c,v)\,. \qquad (4)$$

The qualitative nature of the density of states at given E, Δ, and c is thus seen to be dependent only on v, which may be restated as a dependence on $J-I(2\Delta+I)/2E$. The conclusion of Ref. 1 that $\rho(E)$ depends on $J-I$ is thus an approximation valid only for certain ranges of I, Δ, and E.

The differential equation (2) was studied some years ago by Frisch and Lloyd.[4] The resulting density of states is analytic. The inverse-square-root singularities are smoothed out and instead one finds exponential band tails within the original gap region in accord with the more general conclusions of Wegner.[5] The semicircular band shape, algebraic band tails, exact zeros, and singularities found in Ref. 1 are thus most likely an artifact of the CPA which is known to be less accurate when applied to low-dimensional systems than to higher-dimensional systems.[6]

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[1]K. Harigaya, Y. Wada, and K. Fesser, Phys. Rev. Lett. **63**, 2401 (1989).
[2]B. C. Xu and S. E. Trullinger, Phys. Rev. Lett. **57**, 3113 (1986).
[3]B. C. Xu, Ph.D. thesis, University of Southern California, 1987 (unpublished).
[4]H. L. Frisch and S. P. Lloyd, Phys. Rev. **120**, 1175 (1960).
[5]F. Wegner, Z. Phys. B **44**, 9 (1981).
[6]E. N. Economou, *Green's Functions in Quantum Physics* (Springer-Verlag, Berlin, 1983).