PHYSICAL REVIEW B VOLUME 8, NUMBER 8 15 OCTOBER 1973

Comment on the Theory of Extended X-Ray-Absorption Fine Structure*

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(Received 20 April 1973)

The two theoretical approaches to extended x-ray-absorption fine structure, based on either "long-range order" or "short-range order" are critically examined within a muffin-tin-scatterer model. It is argued that the two apparently dissimilar theories will in practice yield essentially the same results. The argument is based on the implications of recent multiple scattering calculations on clusters of atoms.

INTRODUCTION

The theory of extended x-ray-absorption fine structure (EXAFS) has had a long and varied history.[1,2] However, this development has not led to a unified theoretical approach. Specifically, as applied to periodic materials, one supposedly has to decide between a "long-range order" theory or a "short-range order" theory. In both theories the extended structure in the x-ray absorption coefficient above a core-level threshold is considered to be a consequence of structure in the single-particle final states. In the "long-range order" approach one argues that this structure is a band-structure effect, due to the diffraction of the final-state electrons off the various periodic planes of atoms; while in the "short-range order" approach one again invokes scattering of the final-state electrons, but in this case scattering only from the near neighbors of the absorbing atom. Both theories predict extended oscillatory structure in the absorption coefficient, which roughly correlates with experimental data. Several experimental tests have been proposed to discriminate between the two theoretical approaches, but the sum of these tests have not allowed a definite conclusion to be drawn.[2]

We propose here to show that, within the limitations of a simplified single-particle model, the two theoretical approaches outlined above should yield essentially the same predictions. More precisely, we shall derive an expression for the absorption coefficient which can be evaluated in either a long-range order or short-range order limit and we shall show the close relation between these two limits.[3]

DERIVATION

Let us begin with a brief description of the simplified single-particle model we use. The essence of this model is to describe the potential seen by the final-state electrons as a nonoverlapping array of spherically symmetric spin-independent potentials, each centered about an atom. The potential between these muffin-tin scatterers is assumed constant and this level determines our zero of energy. We calculate the x-ray-absorption cross section from a deep core level of an atom, at which we place our coordinate origin, to final states above the Fermi level. Although the expression we derive could be evaluated for any energy above threshold, many-body effects are probably dominant close to threshold. Since these effects, such as singular behavior at threshold,[4] multiplet structure,[5] or plasma resonances,[6] are clearly beyond the scope of our model, we should expect our expressions not to become valid until somewhat beyond the threshold x-ray energy. Just how far beyond threshold is not clear, but a rough estimate would be a few times the plasma frequency. This limitation is inherent in any approach that is essentially a single-particle theory. The further approximation of a muffin-tin model is made to facilitate our analysis. In fact, the determination of the effective single-particle potential seen by the final-state electron is a very difficult problem involving the screening reaction of the electrons to the developing presence of a core hole. Though the relevant time scales for these relaxation processes are not precisely defined, it seems to us reasonable to assume in metals that the effective single-particle potential is that of a screened core hole, at least in the sense of presenting a localized potential. If this assumption is accepted then the further approximation of muffin-tin potentials is not an extreme step. We shall assume that only the muffin-tin potential at the origin is modified, though further modifications could be incorporated. Finally, we summarize our model description with the double comment that, first, a muffin-tin model should not be an unreasonable representation of the effective potential and second, that the use of a muffin-tin model greatly facilitates the analysis of the multiple scattering effects.

The quantity we wish to calculate is the contribution to the x-ray-absorption coefficient due to the excitation of a deep core level, μ_c. This may be expressed as

$$\mu_c = n_c \sigma_c , \qquad (1)$$

where n_c is the density of atoms with the core level of concern and σ_c is the relevant contribution to the absorption cross section of a single atom. We find σ_c from the golden rule transition rate per unit photon flux. The electronic perturbation is $-e\vec{\mathcal{E}}\cdot\vec{\mathrm{r}}\cos\omega t$, where $\vec{\mathcal{E}}\cos\omega t$ is the electric field of the monochromatic x-ray with angular frequency ω.[7] Hence the single-particle transition rate for absorption is

$$\tau^{-1}=(2\pi/\hbar)\sum_F\langle I\,|\,-(\tfrac{1}{2}e)\vec{\mathcal{E}}\cdot\vec{\mathrm{r}}\,|\,F\rangle \times\delta(E_I+\hbar\omega-E_F)\langle F\,|\,-\tfrac{1}{2}e\vec{\mathcal{E}}\cdot\vec{\mathrm{r}}\,|\,I\rangle\ , \tag{2}$$

where in the sum over final states $|\,F\rangle$ we must stay above the Fermi level. For the initial state $|\,I\rangle$ we use an atomic orbital; for simplicity we assume it to be an S state (K level):

$$\langle\vec{\mathrm{r}}\,|\,I\rangle=R_0(r)(4\pi)^{-1/2}\ . \tag{3}$$

Since the core level is deep, we assume $|\,I\rangle$ is finite only within the muffin-tin sphere, of radius R_{MT}, of the absorbing atom and we normalize it within this volume:

$$R_0(r)=0\ \text{ for }\ r>R_{\mathrm{MT}},\ \int_0^{R_{\mathrm{MT}}}r^2dr\,R_0^2(r)=1\ . \tag{4}$$

Also for simplicity, we apply the dipole approximation to $\vec{\mathcal{E}}$, neglecting its spatial dependence. These approximations are not essential, but do allow us to write our final result in a fairly simple form.[8] The only unknown now in Eq. (2) is a certain matrix element of the operator

$$\hat{\rho}=\sum_F|\,F\rangle\,\delta(E_I+\hbar\omega-E_F)\langle F\,|$$

$$=-(\mathrm{Im}/\pi)(E_I+\hbar\omega-H+i0^+)^{-1}\ , \tag{5}$$

where H is the effective single-particle muffin-tin Hamiltonian. An expression for $\hat{\rho}$ may in this model be derived as a straightforward application of multiple scattering theory.[9–11] Substituting the general expression for $\hat{\rho}$ into our special case of (2), we find

$$\mu_c=\frac{4\pi^2}{3}\,n_c\,\frac{e^2}{\hbar c}\,\hbar\omega\left[\frac{-1}{2\pi^2}\,\frac{E}{\sin^2\delta_1'}\left(\frac{2m}{\hbar^2}\right)^3\mathrm{Im}(\rho)\right] \times\left|\int_0^{R_{\mathrm{MT}}}r^3dr\,R_0(r)R_1(r)\right|^2\ ; \tag{6}$$

$$\rho=\langle R=0,\ l=1,\ m=0\,|\,(\underline{\mathrm{t}}^{-1}-\underline{\mathrm{G}})^{-1}\,|\,R=0,\ l=1,\ m=0\rangle\ . \tag{7}$$

Here $R_1(r)$ is a radial solution of the p-wave Schrödinger equation at energy E for the muffin-tin potential of the absorbing atom in the absence of all other muffin-tin potentials. It is regular at the origin and outside the muffin tin varies as

$$|\,R_1(r)\,|=4\pi\{j_1[(2mE/\hbar^2)^{1/2}r]\cos\delta_1' -n_1[(2mE/\hbar^2)^{1/2}r]\sin\delta_1'\}\ , \tag{8}$$

where j_l and n_l are spherical Bessel functions[12] and δ_1' is the $l=1$ phase shift of the absorbing atom's muffin-tin potential. As noted above, we assume the phase shifts for this potential δ_l' are distinct from those of the surrounding potentials δ_l. The matrices in Eq. (7) are defined in a space determined by the positions of all the scatterers $\{\vec{\mathrm{R}}\}$ and by the angular momentum $L=(l,m)$[11,13]:

$$\begin{aligned}\langle\vec{\mathrm{R}}L\,|\,\underline{\mathrm{t}}\,|\,\vec{\mathrm{R}}'L'\rangle&=\delta_{\vec{\mathrm{R}},\vec{\mathrm{R}}'}\delta_{L,L'}(-)(\hbar^2/2m)^{3/2}E^{-1/2}e^{i\delta_l}\sin\delta_l(1-\delta_{\vec{\mathrm{R}},0})\\&=\delta_{\vec{\mathrm{R}},\vec{\mathrm{R}}'}\delta_{L,L'}(-)(\hbar^2/2m)^{3/2}E^{-1/2}e^{i\delta_l'}\sin\delta_l'(\delta_{\vec{\mathrm{R}},0})\ ,\end{aligned} \tag{9}$$

$$\langle\vec{\mathrm{R}}L\,|\,\underline{\mathrm{G}}\,|\,\vec{\mathrm{R}}'L'\rangle=-4\pi i(2m/\hbar^2)^{3/2}E^{1/2}\sum_{L_1}(i)^{l_1}C_{L,L'}^{L_1}h_{l_1}^{+}[(2mE/\hbar^2)^{1/2}\,|\,\vec{\mathrm{R}}-\vec{\mathrm{R}}'\,|\,] \times Y_{L_1}[(\vec{\mathrm{R}}-\vec{\mathrm{R}}')/\,|\,\vec{\mathrm{R}}-\vec{\mathrm{R}}'\,|\,](1-\delta_{\vec{\mathrm{R}},\vec{\mathrm{R}}'})\ , \tag{10}$$

$$C_{LL'}^{L_1}=\int d\hat{k}\,Y_{L_1}^{*}(\hat{k})Y_L^{*}(\hat{k})\,Y_{L'}(\hat{k})\ , \tag{11}$$

where $h_l^{+}=j_l+in_l$ and Y_L is a spherical harmonic function.[14] Note that the m in (6), (9), and (10) is the electron mass, not the magnetic quantum number, and that $\delta_{\vec{\mathrm{R}},\vec{\mathrm{R}}'}$ is a Kronecker δ, not a phase shift. The energy E that appears explicitly in the above equations [and implicitly in the phase shifts and $R_1(r)$] equals $E_I+\hbar\omega$; we have assumed it to be positive. Equation (6) is our most general expression for μ_c. We now concentrate on ρ to derive alternative expressions in various limits.

First we consider a long-range order limit. For this case we formally include all the scattering centers in the evaluation of ρ. Such formulas for ρ were first derived by Beeby[9]; we quote two cases. First in the special case $\delta_l'=\delta_l$, and with the assumption of one atom per unit cell,

$$\rho=\tau^{-1}\int_{\mathrm{BZ}}d\vec{\mathrm{k}}\,\langle l=1,\ m=0\,|$$

$$\times[\underline{t}^{-1}-\underline{G}(\vec{k},E)]^{-1}\,|\,l=1,\ m=0\rangle$$

$$=\langle l=1,\ m=0\,|\,\underline{S}\,|\,l=1,\ m=0\rangle\ , \quad (12)$$

where

$$\langle L\,|\,\underline{G}(\vec{k},E)\,|\,L'\rangle=N^{-1}\sum_{\alpha,\beta}e^{i\vec{k}\cdot(\vec{R}_\alpha-\vec{R}_\beta)}\langle\vec{R}_\alpha L\,|\,\underline{G}\,|\vec{R}_\beta L'\rangle. \quad (13)$$

Here the matrices $\underline{G}(\vec{k},E)$, $\underline{t}$, and $\underline{S}$ are in angular-momentum space only. The integration in (12) is over the Brillouin zone, whose volume is τ; the sums in (13) are over the N atomic sites in the material. Since $(\underline{t}^{-1}-\underline{G})$ is the real Korringa-Kohn-Rostoker (KKR) matrix,[15] the contribution to Imρ comes from the solutions of

$$\det[\underline{t}^{-1}-\underline{G}(\vec{k},E)]=0 \quad (14)$$

and hence are determined by the band structure. The second case for which a simple answer is possible is when $\delta_l'\neq\delta_l$:

$$\rho=\langle l=1,\ m=0\,|\,(\underline{t}'^{-1}-\underline{t}^{-1}+\underline{S}^{-1})^{-1}\,|\,l=1,\ m=0\rangle\ , \quad (15)$$

where t and $\underline{t}'$ are the angular-momentum matrices corresponding to the first and second line of Eq. (9), respectively. Harris[16] has shown how such formulas as (12) and (14) may be numerically evaluated, given the muffin-tin potentials. We only wish to emphasize that definite long-range order expressions for ρ do exist.

Now we consider the opposite short-range order limit. This we treat by expanding ρ in a power series in $\underline{t}$:

$$\rho=\langle\vec{R}=0,\ l=1,\ m=0\,|\,(\underline{t}+\underline{t}\underline{G}\underline{t}+\underline{t}\underline{G}\underline{t}\underline{G}\underline{t}+\cdots)$$

$$\times\,|\,\vec{R}=0,\ l=1,\ m=0\rangle\ . \quad (16)$$

Most short-range order theories to date effectively terminate this series at the third-order term and with some further approximations deduce a simple expression for ρ. To illustrate this approach, we assume that only δ_0 is significant for the surrounding atoms and evaluate the first three terms in (16). We need

$$\langle\vec{R}=0,\ l=1,\ m=0\,|\,\underline{G}\,|\,\vec{R}_\alpha,\ l=0,\ m=0\rangle=(2m/\hbar^2)(2mE/\hbar^2)^{1/2}\,Y_{10}(-\hat{R}_\alpha)(4\pi)^{1/2}h_1^+[R_\alpha(2mE/\hbar^2)^{1/2}]$$

$$=-\langle\vec{R}_\alpha,\ l=0,\ m=0\,|\,\underline{G}\,|\,\vec{R}=0,\ l=1,\ m=0\rangle\ . \quad (17)$$

Using the asymptotic form of h_1^+ plus an *ad hoc* damping factor[17]

$$h_1^+[R(2mE/\hbar^2)^{1/2}]\rightarrow R^{-1}(2mE/\hbar^2)^{-1/2}e^{iR(2mE/\hbar^2)^{1/2}}e^{-\lambda R},\quad R(2mE/\hbar^2)^{1/2}\gg 1\ , \quad (18)$$

we find for the expression in square brackets in Eq. (6),

$$-\frac{1}{2\pi^2}\,\frac{E}{\sin^2\delta_1'}\left(\frac{2m}{\hbar^2}\right)^3\mathrm{Im}\rho=\frac{m}{\pi^2\hbar^2}\left(\frac{2mE}{\hbar^2}\right)^{1/2}\left(1-\sum_{\vec{R}_\alpha}3(\hat{R}_\alpha\cdot\hat{z})^2\,\frac{\sin[2R_\alpha(2mE/\hbar^2)^{1/2}+2\delta_1'+\delta_0]}{R_\alpha^2(2mE/\hbar^2)}\,\sin\delta_0\,e^{-2\lambda R_\alpha}\right)\ , \quad (19)$$

where $\hat{z}$ is a unit vector in the polar direction. The damping factor roughly accounts for the inelastic scattering that occurs between elastic scatterings from the muffin-tin potentials. As long as the inelastic scattering only leads to a mild blurring of the energy (as appears to be the case, aside from discrete plasmon loss effects[18]), its inclusion solely as a damping factor is reasonable.[19] The result (19) is the typical form of short-range order theories,[2,20] aside from the lack of a Debye-Waller factor in the sum over $\vec{R}_\alpha$, which one would obtain from a thermal average of (19).[21] Most of these theories make the further approximation of assuming that the scattering represented by δ_0 is weak so that δ_0 may be obtained in Born approximation. We consider this is a dubious approximation, even for energies several hundred volts above threshold. Our reasoning is based on Levinson's theorem, which states that δ_l must decrease by n_l multiples of π as E increases from zero to infinity. Here n_l is the number of bound states of l symmetry in a single muffin tin, and is roughly the number of core levels of l symmetry. Thus, the necessary occurrence of antiresonances, as δ_l passes through an odd multiple of $\frac{1}{2}\pi$, is inconsistent with weak scattering. Furthermore, Pendry has shown that these antiresonances occur at surprisingly high energy.[22] Finally, we note that except for the light elements, our argument implies that the truncation of the expansion (16) at only third order and the neglect of δ_l for $l\geq 1$ in the subsequent reduction, are generally incorrect approximations. We do not, however, wish to imply that the short-range order approach is invalid. The essence of this approach lies in the introduction of the damping factor and the physical justification of this term (that the final-state electron can only propagate a limited distance before inelastic effects destroy its single-particle character) is very reasonable. Our point is merely that the elastic scattering is generally strong.

DISCUSSION

Let us now examine the relation between a long-range order and a short-range order evaluation of EXAFS. As argued above, the only difference between these two approaches is whether the damping coefficient λ is zero or finite. In a short-range order approach as $\lambda \to 0$, one must end up with the long-range order result, essentially by definition. The interesting question is how small must λ become before the results are essentially independent of λ; or, in other words, how large a cluster of atoms is necessary to essentially reproduce a bulk density of states. The answer to this question may be inferred from the results of recent calculations at Bristol of the multiple scattering properties of clusters of atoms.[23] The implication of this work is that the essential structure of the density of states is obtainable in small clusters of atoms (less than thirty) and, more tentatively, that the configuration and scattering properties of the nearest neighbors may be sufficient information. One way to understand these results is to note that the introduction of λ in the calculation of the density of states, which is essentially the quantity on the left-hand side of Eq. (19), is roughly equivalent[24] to the calculation of a Lorentzian averaged density of states where the half-width of the Lorentzian Γ centered at energy E is

$$\Gamma = \lambda(\hbar^2/m)(2mE/\hbar^2)^{1/2} . \qquad (20)$$

The Bristol calculations actually imply a stronger result—that the effective blurring of the density of states in their range of E due to the finite size of the cluster is less than that suggested by (20). However, the point we wish to extract is that the evaluation of ρ, though done with a short-range order technique (i.e., using only several layers of atoms), should reproduce the basic structure of the long-range order evaluation. It is in this sense that short-range order and long-range order theories are essentially equivalent.

Finally, we conclude with some brief remarks on the extension of our discussion to nonperiodic materials. We consider two classes of disordered materials: microscopic disordered systems, such as isolated molecules, and macroscopic disordered systems, such as amorphous materials. In the first class the only order is short range, since there is only a small total number of neighbors. The muffin-tin model might be less believable here (though it is used for such systems[25]), but at least there is no dichotomy between long-range and short-range approaches. For the second class, bulk amorphous materials, the two approaches are possible and distinct in detailed method, though in both it is necessary to average the absorption coefficient over the environment of the absorbing atom. The long-range approach would concentrate on the conditional average density of states of the bulk, as for instance, in the work by Gyorffy and Stott on disordered alloys.[10] The average is conditional on the absorbing atom retaining its position and identity. On the other hand, in the short-range method one would essentially replace, say, the sum in Eq. (19) by an integral

$$\sum_{R_\alpha} \to n_s \int d\vec{R}\, g(R) , \qquad (21)$$

where n_s is the density of surrounding atoms (here assumed identical) and $g(R)$ is the pair correlation function of atomic positions.[26] The implications of the Bristol calculations should still apply, however, and we would expect the long-range and short-range methods to yield essentially the same predictions on the same model. This may not be evident in practice, though, due to the considerably greater difficulty of finding the bulk density of states in disordered systems. In fact, one aim of the Bristol calculations was to determine long-range bulk density of states by doing only a short-range calculation.

ACKNOWLEDGMENT

I wish to thank Professor E. A. Stern for several interesting discussions.

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[*] Research supported by the Air Force Office of Scientific Research (AFSC) under Grant No. AFOSR-72-2156 Mod. 1.

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[1] R. A. Van Nordstrand, in *Handbook of X-Rays*, edited by E. F. Kaelble, (McGraw-Hill, San Francisco, 1967), Chap. 43.

[2] L. V. Azaroff, Rev. Mod. Phys. **35**, 1012 (1963).

[3] There is a certain analogy between the dichotomy discussed here and that between "dynamical" and "kinematical" theories of electron diffraction. In LEED for instance, the resolution lies in the strong inelastic scattering, which effectively limits the extent of multiple elastic scattering. One finds that the inclusion of strong inelastic scattering in the "dynamical" theories is necessary for agreement with the "kinematical" theories and experiments. See for discussion R. O. Jones and J. A. Strozier, Jr. [Phys. Rev. B **3**, 3228 (1971); Phys. Rev. Lett. **22**, 1186 (1969)] and C. B. Duke and C. W. Tucker, Jr. [Surf. Sci. **15**, 231 (1969)]. We note, however, that since in EXAFS the final-state electron is not collected, the magnitude of EXAFS should not show such a strong dependence on the inelastic mean free path as in LEED.

[4] B. Roulet, J. Gavoret, and P. Nozieres, Phys. Rev. **178**, 1072 (1969); P. Nozieres, J. Gavoret, and B. Roulet, Phys. Rev. **178**, 1084 (1969); P. Nozieres and C. T. De Dominicis, Phys. Rev. **178**, 1097 (1969).

[5] See Ref. 1 and L. G. Parrett, Rev. Mod. Phys. **31**, 616 (1959).

[6] L. Hedin and S. Lundqvist, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol. 23, p. 1.

[7] We note that since in the single-particle model used here the

states $|I\rangle$ and $|F\rangle$ are eigenstates of different Hamiltonians, the choice of the electronic perturbation is not obvious. To illustrate, coupling the vector potential to the electronic current would yield a somewhat different result in (6). This ambiguity is another limitation of the use of an effective single-particle model.

[8] Our aim here is merely to circumvent a discussion of the effects due to the polarization of the x-ray or the possible off-diagonal (in L space) character of $\hat{\rho}$.

[9] J. L. Beeby, Proc. R. Soc. A **302**, 113 (1967).

[10] B. L. Gyorffy and M. J. Stott, Solid State Commun. **9**, 613 (1971).

[11] P. Lloyd and P. V. Smith, Adv. Phys. **21**, 69 (1972).

[12] M. Abramawitz and I. A. Stegun, *Handbook of Mathematical Functions*, Applied Mathematics Series No. 55, Natl. Bur. Std. (U.S. GPO, Washington, D.C., 1965), p. 437. Their y_n is our n_l.

[13] We assume (in order to write t^{-1}) that $l \leq l_{\max}$ and that $\sin\delta_l \neq 0$ for $l \leq l_{\max}$. As the expansion (16) shows, this is only a formal limitation.

[14] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1966), p. 494.

[15] J. L. Beeby, Proc. R. Soc. A **279**, 82 (1964).

[16] R. Harris, J. Phys. C **3**, 172 (1970).

[17] This could perhaps be chosen by the same procedure used in LEED calculations, where $\lambda(E)$ is related to the imaginary part of the self-energy $\Sigma(k, E)$, of the homogeneous electron gas evaluated at $k=(2mE/\hbar^2)^{1/2}$. See the references in footnote 3.

[19] There are two basic approximations here. First, we assume that the blurring of the energy due to electron-electron self-energy effects can be satisfactorily represented by a complex energy ($E \rightarrow E + i\Gamma$). Second, we retain the effects of Γ only in the exponential factors which involve spatial separations, $R \sim |\vec{\mathbf{R}}_\alpha - \vec{\mathbf{R}}_\beta|$. Hence the contribution of multiple scattering is significantly reduced since

$$\exp[iR(2m/\hbar)^{1/2}(E+i\Gamma)^{1/2}] \approx \exp[iR(2mE/\hbar^2)^{1/2}] \times \exp[-\Gamma R(m/2\hbar^2E)^{1/2}] \ll \exp[iR(2mE/\hbar^2)^{1/2}],$$

for large R; while the free-electron contribution (the factor outside the parenthesis on the right-hand side of Eq. (19) is not significantly modified: $(E+i\Gamma)^{(1/2)} \approx E^{(1/2)}$ since $\Gamma \ll E$ by assumption. Similarly, we use the phase shifts evaluated at energy E, not $E+i\Gamma$.

[20] D. E. Sayers, F. W. Lytle, and E. A. Stern, Adv. X-Ray Anal. **13**, 248 (1970).

[21] V. V. Schmidt, Akademia Nauk SSSR **25**, 988 (1961); Bull. Acad. Sci. USSR **27**, 392 (1963).

[22] J. B. Pendry, J. Phys. C **1**, 1065 (1968); J. Phys. C **2**, 1215 (1969).

[23] J. Klima and T. C. McGill, J. Phys. C **3**, 1163 (1970); J. Klima, T. C. McGill, and J. M. Ziman, Discuss. Faraday Soc. **50**, 20 (1970); T. C. McGill and J. Klima, Phys. Rev. B **5**, 1517 (1972); J. Keller, J. Phys. C **4**, 3143 (1971); J. Keller and R. Jones, J. Phys. F **1**, *L*33 (1971); D. House, P. V. Smith, and B. L. Gyorffy, J. Phys. F **3**, 745 (1973); D. House and P. V. Smith, J. Phys. F **3**, 753 (1973).

[24] Strictly speaking the Lorentzian average of $\hat{\rho}$ replaces the positive infinitesimal 0^+ in Eq. (5) with Γ. However, in the subsequent evaluation of $\hat{\rho}$, we only retain the significant effects of Γ [in the assumed limit $\Gamma \lessdot E$, $\delta_l(d\delta_l/dE)^{-1}$] as described in footnote 19.

[25] K. H. Johnson and F. C. Smith, Jr., Phys. Rev. Lett. **24**, 139 (1970), and references therein.

[26] D. E. Sayers, E. A. Stern, and F. W. Lytle, Phys. Rev. Lett. **27**, 1204 (1971); J. Non-Cryst. Solids **8–10**, 401 (1972).