Inelastic neutron scattering from amorphous solids. II. Interpretation of measurements*

J. M. Carpenter
Solid State Science Division, Argonne National Laboratory, Argonne, Illinois 60439
and Department of Nuclear Engineering, University of Michigan, Ann Arbor, Michigan 48105

C. A. Pelizzari
Solid State Science Division, Argonne National Laboratory, Argonne, Illinois 60439
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The one-phonon scattering law for a disordered harmonic system is related to a frequency-dependent displacement-displacement correlation function. We suggest a means of investigating this correlation function by means of a suitable transformation of inelastic neutron scattering data for such systems.

I. INTRODUCTION

In our first paper[1] (referred to below as I), we developed expressions for the one- and two-phonon terms in the scattering law for glassy solids, considering them to be isotropic, harmonically oscillating systems. The results provide practical means for calculating the inelastic neutron scattering from models of glassy solids, given atomic coordinates and normal mode frequencies and eigenvectors. Here, we investigate the use of those results in the interpretation of measurements. Notation in the present paper is the same as I.

II. FUNDAMENTALS

Frequently measurements of the inelastic neutron scattering are interpreted in the one-phonon incoherent approximation, to extract the density of lattice vibrational states, which is defined

$$g(\omega)\equiv\frac{1}{3N}\sum_{\lambda}\delta(\omega-\omega^{\lambda})\,, \tag{1}$$

where N is the number of scattering units, and which is normalized

$$\int_0^{\omega_{\max}} d\omega\, g(\omega)=n\,, \tag{2}$$

where n is the number of atoms in the scattering unit. The function thus extracted from measurements, when two-phonon contributions are ignored, is actually a generalized frequency distribution

$$G(Q,\omega)=\left(\frac{\hbar^2Q^2}{2\overline{m}}\,\mathrm{csch}(\hbar\omega/2k_BT)/2\hbar\omega\right)^{-1}S^{(1)}(Q,\omega)\,, \tag{3}$$

which is a function of Q as well as ω. Using Eq. (21) of I for the one-phonon scattering law $S^{(1)}(Q,\omega)$, we have

$$G(Q,\omega)=\frac{1}{N\overline{\sigma}}\sum_{\lambda}\delta(\omega-\omega^{\lambda})\sum_{\nu,\nu'}\sigma_{\nu\nu'}\frac{F_{\nu\nu'}(Q)}{Q^2}\,.$$

In the following, it will be useful to introduce the notion of the frequency average of any function f^{λ} of normal mode index λ: Let

$$\langle f\rangle_{\omega}\equiv\sum_{\lambda}\delta(\omega-\omega^{\lambda})f^{\lambda}/3Ng(\omega)\,. \tag{4}$$

Then $\langle f\rangle_{\omega}$ is just the average value of f^{λ} for all normal modes of frequency $\omega^{\lambda}=\omega$. $\langle f\rangle_{\omega}$ is not defined (and needs not be) when $g(\omega)=0$.

With this notation,

$$G(Q,\omega)=\sum_{\nu\nu'}\frac{\sigma_{\nu\nu'}}{\overline{\sigma}}\,3\overline{m}\left\langle\frac{F_{\nu\nu'}(Q)}{Q^2}\right\rangle_{\omega}g(\omega)\,. \tag{5}$$

III. INCOHERENT SCATTERING

In the case of purely incoherent scattering,

$$\begin{aligned}\sigma_{\nu\nu'}&=\sigma_{\nu}^{\mathrm{incoh}}\delta_{\nu\nu'}\\&=4\pi\langle a_{\nu}^2\rangle\delta_{\nu\nu'}\,,\end{aligned} \tag{6}$$

the double sum on atoms in Eq. (5) collapses to a single sum which represents the independent-atom scattering, so that

$$G(Q,\omega)=G^{\mathrm{incoh}}(\omega)=\sum_{\nu}\frac{\sigma_{\nu}^{\mathrm{incoh}}}{\overline{\sigma}}\,3\overline{m}\left\langle\frac{F_{\nu\nu}(Q)}{Q^2}\right\rangle_{\omega}g(\omega)\,. \tag{7}$$

Here, since $b_{\nu\nu}=0$, while $j_0(0)=1$ and $j_2(0)=0$,

$$\frac{F_{\nu\nu}^{\lambda}(Q)}{Q^2}=\frac{1}{3m_{\nu}N}\,|\gamma_{\nu}^{\lambda}|^2 \tag{8}$$

then

$$G_{(\omega)}^{\mathrm{incoh}}=\Gamma^2(\omega)g(\omega)\,, \tag{9}$$

where

$$\Gamma^2(\omega)\equiv\frac{1}{N}\sum_{\nu}\frac{\sigma_{\nu}^{\mathrm{incoh}}}{\overline{\sigma}}\frac{\overline{m}}{m_{\nu}}\langle|\gamma_{\nu}|^2\rangle_{\omega}\,. \tag{10}$$

$(\hbar/m_{\nu}\omega)\langle|\gamma_{\nu}^2|\rangle_{\omega}$ is the mean-squared vibrational amplitude of atom ν, averaged for all modes of frequency ω; therefore $(\hbar/\overline{m}\omega)\,\Gamma^2(\omega)$ is the scattering cross section weighted average of the mean-squared vibrational amplitudes of all atoms in the system, for modes of frequency ω.

$G^{\text{incoh}}(\omega)$ has the general features of $g(\omega)$; singularities, band gaps, etc., and where $\Gamma^2(\omega)$ is constant (as for frequencies corresponding to long-wavelength acoustic-wave modes) $G^{\text{incoh}}(\omega)$ has the same shape as $g(\omega)$. Equation (9) is similar in form and content to that describing superconducting tunneling measurements. Of course, $G^{\text{incoh}}(\omega)$ is independent of Q (except for variation of the Debye-Waller factor, which is ignored here), but is equal to $g(\omega)$ only under special circumstances.

In any crystalline system having one atom per primitive unit cell (all atoms the same and equivalent) it is easily shown, since $\sum_\nu |\gamma_\nu^\lambda|^2 = 1$, so that $\Gamma^2(\omega) = 1$, that therefore

$$G^{\text{incoh}}(\omega) = g(\omega) . \tag{11}$$

Under the less restrictive condition, for any system, that

$$M \sum_\nu \frac{\sigma_\nu}{m_\nu} |\gamma_\nu^\lambda|^2 = C , \tag{12}$$

where C is a constant independent of λ, it is also true that $\Gamma^2(\omega) = C$ and $G^{\text{incoh}}(\omega) = Cg(\omega)$.

In crystals with more than one atom per unit cell, equivalent atoms may be classed together. In glassy solids, all atoms are in principle in different environments, thus inequivalent; nevertheless, all atoms of the same chemical species may be classed together. Then, perhaps with some advantage, the general result for incoherent scattering can be cast in terms of the mean-squared displacements for each type. Let

$$\begin{aligned} &\sigma_\nu^{\text{incoh}} = \sigma_t^{\text{incoh}} \text{ if atom } \nu \text{ is of type } t , \\ &m_\nu = m_t \text{ if atom } \nu \text{ is of type } t , \\ &n_t \text{ is the number of atoms of type } t \text{ in the scattering unit} , \end{aligned} \tag{13}$$

so that $N_t = n_t N$ is equal to number of atoms of type t in the system.

Then decomposing the atom sum into a sum on species, and a sum on atoms within each species, one easily obtains

$$\Gamma^2(\omega) = \sum_t n_t \frac{\sigma_t^{\text{incoh}}}{\bar{\sigma}} \frac{\bar{m}}{m_t} \langle \gamma_t^2 \rangle_\omega , \tag{14}$$

where

$$\langle \gamma_t^2 \rangle_\omega \equiv \frac{1}{N_t} \sum_{\nu \in t} \langle \gamma_\nu^2 \rangle_\omega \tag{15}$$

is the mean-squared displacement for atoms of type t.

IV. COHERENT SCATTERING

In the general case including coherent scattering,

$$\sigma_{\nu\nu'} = \sigma_{\nu\nu'}^{\text{coh}} = 4\pi \langle a_\nu \rangle \langle a_{\nu'} \rangle , \qquad \nu \neq \nu'$$

$$= (\sigma_{\nu\nu}^{\text{coh}} + \sigma_{\nu\nu}^{\text{incoh}}) = 4\pi \langle a_\nu^2 \rangle \qquad \nu = \nu' \tag{16}$$

and the generalized frequency distribution is a function of Q as well as ω:

$$G(Q, \omega) = \frac{1}{N\bar{\sigma}} \sum_\lambda \delta(\omega - \omega^\lambda) \sum_{\nu,\nu'} \sigma_{\nu\nu'} \frac{F_{\nu\nu'}^\lambda(Q)}{Q^2} , \tag{17}$$

where the one-phonon structure factor $F_{\nu\nu'}(Q)$ was expressed in Eqs. (22) and (23) of I. It is useful to cast this in the form of a structure factor averaged over all modes of frequency ω which we define

$$\Gamma^2(Q, \omega) = \sum_{\nu,\nu'} \frac{\sigma_{\nu\nu'}}{\bar{\sigma}} 3\bar{m} \left\langle \frac{F_{\nu\nu'}(Q)}{Q^2} \right\rangle_\omega , \tag{18}$$

so that

$$G(Q, \omega) = \Gamma^2(Q, \omega) g(\omega) . \tag{19}$$

Recalling Eqs. (22) and (23) of I, it is clear that $\Gamma^2(Q, \omega)$ is sensitive to the structure in a way similar to that in which the static and elastic structure factors are. In the one-phonon structure factor, however, the contributions from different pairs ν, ν' are weighted by vibrational displacements γ_ν^λ as well as by scattering lengths. Thus $\Gamma^2(Q, \omega)$ contains information about the pair density of the product of vibrational displacements and scattering lengths, just as the static structure factor provides the pair density of scattering lengths through the Zernike-Prins relation. $\Gamma^2(Q, \omega)$ is in fact the displacement-displacement correlation function for modes of frequency ω.

The function $G(Q, \omega)$ has been examined by De Wette and Rahman[2] for polycrystals. $G(Q, \omega)$ varies significantly with both Q and ω, and changes dramatically at ω's which correspond to singularities in $g(\omega)$.

It remains a significant question at which values of Q, $\Gamma^2(Q, \omega)$ becomes nearly enough constant with Q and ω, to allow interpretation of measurements in the incoherent approximation, $G(Q, \omega) \propto g(\omega)$. The answer depends entirely on the details of the structure, and the nature of the motions at each frequency. Since for some materials, the diffraction pattern varies significantly with Q as large as 20 Å^{-1} and more, it is expected that for some ω's, $\Gamma^2(Q, \omega)$ is not constant with Q even for such large Q's.

For local modes involving only one atom (say the λ_ith mode), $\vec{\gamma}_\nu^\lambda = 0$ for all except one atom (say the ν_ith). Then

$$F_{\nu\nu'}^{\lambda_i}(Q) \propto \delta_{\nu\nu'} \delta_{\nu\nu_i} , \tag{20}$$

that is, $F_{\nu\nu'}^{\lambda_i}(Q)$ is diagonal and zero for all except the ν_ith atom. If there is a band of frequencies which contains nothing but such local modes, the incoherent approximation applies in that band, i.e.,

$\Gamma^2(Q, \omega) = \text{const}$ for all Q.

V. RELATIONSHIP OF THE ONE-PHONON STRUCTURE FACTOR TO THE STRUCTURE

In the following, we consider the Q variation of the inelastic structure factor at constant ω. Therefore we may deal with $\Gamma^2(Q, \omega)$ (which is not accessible from measurements) rather than $G(Q, \omega)$ (which is, if multiphonon effects are accounted for). Recalling Eq. (23) of I,

$$F^{\lambda}_{\nu\nu'}(Q) = \frac{Q^2}{N\sqrt{m_\nu m_{\nu'}}} \{\tfrac{1}{3}(\vec{\gamma}^{\lambda}_{\nu} \cdot \vec{\gamma}^{\lambda *}_{\nu'}) j_0(Qb_{\nu\nu'}) + [\tfrac{1}{3}(\vec{\gamma}^{\lambda}_{\nu} \cdot \vec{\gamma}^{\lambda *}_{\nu'}) - (\hat{b}_{\nu\nu'} \cdot \vec{\gamma}^{\lambda}_{\nu})(\hat{b}_{\nu\nu'} \cdot \vec{\gamma}^{\lambda *}_{\nu'})] j_2(Qb_{\nu\nu'})\},$$

we now explore the relationship between the one-phonon structure factor and the structure of the system. We may express, as in Eq. (18) above

$$\Gamma^2(Q, \omega) = \sum_{\nu\nu'} \frac{\sigma_{\nu\nu'}}{\bar{\sigma}} 3\bar{m} \left\langle \frac{F_{\nu\nu'}(Q)}{Q^2} \right\rangle_\omega = \frac{1}{N} \sum_{\nu\nu'} \frac{\sigma_{\nu\nu'}}{\bar{\sigma}} \frac{\bar{m}}{\sqrt{m_\nu m_{\nu'}}} \{\langle \vec{\gamma}_\nu \cdot \vec{\gamma}^{*}_{\nu'} \rangle_\omega j_0(Qb_{\nu\nu'}) + [\langle \vec{\gamma}_\nu \cdot \vec{\gamma}^{*}_{\nu'} \rangle_\omega - 3\langle (\hat{b}_{\nu\nu'} \cdot \vec{\gamma}_\nu)(\hat{b}_{\nu\nu} \cdot \vec{\gamma}_{\nu'}) \rangle_\omega] j_2(Qb_{\nu\nu'})\} . \tag{21}$$

Proceeding in a fashion similar to that followed in relating the static structure factor to the structure through the radial density function, we now introduce two new functions related to the radial density function:

$$4\pi r^2 A(r, \omega) \equiv \frac{1}{N} \sum_{\nu,\nu';\nu\neq\nu'} \frac{\sigma_{\nu\nu'}}{\bar{\sigma}} \frac{\bar{m}}{\sqrt{m_\nu m_{\nu'}}} A_{\nu\nu'}(\omega)\, \delta(r - b_{\nu\nu'}), \tag{22}$$

$$4\pi r^2 B(r, \omega) \equiv \frac{1}{N} \sum_{\nu,\nu';\nu\neq\nu'} \frac{\sigma_{\nu\nu'}}{\bar{\sigma}} \frac{\bar{m}}{\sqrt{m_\nu m_{\nu'}}} B_{\nu\nu'}(\omega)\, \delta(r - b_{\nu\nu'}), \tag{23}$$

where

$$A_{\nu\nu'}(\omega) = \langle \vec{\gamma}_\nu \cdot \vec{\gamma}^{*}_{\nu'} \rangle_\omega \tag{24}$$

and

$$B_{\nu\nu'}(\omega) = 3\langle (\hat{b}_{\nu\nu'} \cdot \vec{\gamma}_\nu)(\hat{b}_{\nu\nu'} \cdot \vec{\gamma}^{*}_{\nu'}) \rangle_\omega . \tag{25}$$

Then the one-phonon structure factor may be written

$$\Gamma^2(Q, \omega) - \Gamma^2_\infty(\omega) = \int_0^\infty 4\pi r^2 A(r, \omega) j_0(Qr)\, dr + \int_0^\infty 4\pi r^2 [A(r, \omega) - B(r, \omega)]\, j_2(Qr)\, dr, \tag{26}$$

where $\Gamma^2_\infty(\omega) = \lim_{Q\to\infty} \Gamma^2(Q, \omega)$. Here, also,

$$\Gamma^2_\infty(\omega) = \frac{1}{N} \sum_{\nu} \frac{\sigma_{\nu\nu}}{\bar{\sigma}} \frac{\bar{m}}{m_\nu} A_{\nu\nu}(\omega)$$

since $\lim j_0(x)$ as $x \to \infty = \lim j_2(x)$ as $x \to \infty = 0$, and since $j_0(0) = 1$ and $j_2(0) = 0$, while there are no atom pairs at distances less than some $b_{\min} > 0$. $\Gamma^2_\infty(\omega)$ is just the independent-atom contribution and of course, $\sigma_{\nu\nu} = 4\pi \langle a^2_\nu \rangle$. The expression Eq. (26) is similar to the result of Zernike and Prins, [3] relating the static structure factor to the radial density function $\rho(r)$.

$A(r, \omega)$ is the function describing the density distribution of the quantity

$$\frac{\sigma_{\nu\nu'}}{\bar{\sigma}} \frac{\bar{m}}{\sqrt{m_\nu m_{\nu'}}} \langle \vec{\gamma}_\nu \cdot \vec{\gamma}_{\nu'} \rangle_\omega .$$

The information in $A(r, \omega)$ becomes more clear when one recalls that the radial density function $\rho(r)$ derived from diffraction, is the density distribution of the scattering power $\sigma_{\nu\nu'}/\bar{\sigma}$. Thus $A(r, \omega)$ describes the density distribution of the product of scattering power, and the (frequency average) scalar product of mass-weighted displacement vectors, $(\bar{m}/\sqrt{m_\nu m_{\nu'}}) \langle \vec{\gamma}_\nu \cdot \vec{\gamma}^{*}_{\nu'} \rangle_\omega$.

$B(r, \omega)$ is similarly the density distribution of the quantity

$$\frac{\sigma_{\nu\nu'}}{\bar{\sigma}} \frac{\bar{m}}{\sqrt{m_\nu m_{\nu'}}} \langle 3(\hat{b}_{\nu\nu'} \cdot \vec{\gamma}_\nu)(\hat{b}_{\nu\nu'} \cdot \vec{\gamma}^{*}_{\nu'}) \rangle_\omega ,$$

which is the product of scattering power and the projections of the normal mode displacements upon the unit interdistance vectors $(\hat{b}_{\nu\nu'} \cdot \vec{\gamma}_\nu)$. $A(r, \omega)$ and $B(r, \omega)$ are the real-space displacement-displacement correlation functions for modes of frequency ω. A and B depend parametrically upon the frequency ω; the r dependence is expected to differ for different frequencies.

Both $A(r, \omega)$ and $B(r, \omega)$ have similar behavior to $\rho(r)$, the radial density function; where $\rho(r)$ exhibits a peak, as due to a coordination shell, $A(r, \omega)$ and $B(r, \omega)$ also may exhibit peaks, either positive going or negative. Where $\rho(r) = 0$, $A(r, \omega)$ and $B(r, \omega)$ also vanish. The amplitudes and signs of peaks in A and B however are modified according

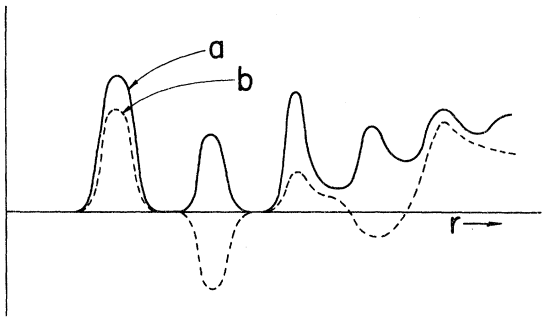

FIG. 1. Schematic representation of a, $\rho(r)$ and of b, either $A(r, \omega)$ or $B(r, \omega)$. Where $\rho(r) = 0$, $A = B = 0$. Even though $\rho(r)$ may be everywhere positive, A and B may be either positive or negative, depending on whether displacements of atoms at distance r have parallel or antiparallel components.

to the nature of the displacement vectors $\vec{\gamma}_{\nu}^{\lambda}$.

At large r, $A(r, \omega)$ and $B(r, \omega)$ approach zero if the modes of frequency ω have finite coherence length. For lowest frequencies, corresponding to those of infinitely propagating acoustic-wave modes, $A(r, \omega)$ and $B(r, \omega)$ oscillate at large r. Figure 1 shows $\rho(r)$, and $A(r, \omega)$ or $B(r, \omega)$ schematically.

VI. EXTRACTING $A(r,\omega)$ AND $B(r,\omega)$ FROM $\Gamma^2(Q,\omega)$

It is rewarding to explore what may be obtained from Fourier transforms of the one-phonon structure factor. By expressing[6]

$$j_n(x) = \frac{(-i)^n}{2}\int_{-1}^{1} e^{ix\mu} P_n(\mu)\, d\mu \ , \tag{27}$$

where $P_n(\mu)$ are the Legendre polynomials, the Fourier cosine transform of $\Gamma^2(Q, \omega) - \Gamma_\infty^2(\omega)$ can be shown to be

$$\frac{2}{\pi}\int_0^\infty \cos Qr'[\Gamma^2(Q, \omega) - \Gamma_\infty^2(\omega)]\, dQ$$

$$= \int_{r'}^\infty 4\pi r\left[A(r, \omega) P_0\left(\frac{r'}{r}\right) \right.$$

$$\left. - [A(r, \omega) - B(r, \omega)] P_2\left(\frac{r'}{r}\right) \right] dr \ . \tag{28}$$

By differentiating Eq. (28),

$$\frac{1}{r'}\frac{2}{\pi}\int_0^\infty Q \sin Qr'[\Gamma^2(Q, \omega) - \Gamma_\infty^2(\omega)]\, dQ$$

$$= \frac{2}{\pi}\int_0^\infty Q^2 j_0(Qr')[\Gamma^2(Q, \omega) - \Gamma_\infty^2(\omega)]\, dQ$$

$$= 4\pi B(r', \omega) + 3\int_{r'}^\infty 4\pi \frac{A(r, \omega) - B(r, \omega)}{r}\, dr \ . \tag{29}$$

Perhaps more readily interpretable, the result

$$4\pi P(r'; \omega) \equiv \frac{2}{\pi}\int_0^\infty Q^2 j_2(Qr')[\Gamma^2(Q, \omega) - \Gamma_\infty^2(\omega)]\, dQ$$

$$= -4\pi B(r', \omega) + \frac{3}{r'^3}\int_0^{r'} 4\pi r^2 A(r, \omega)\, dr \tag{30}$$

can be obtained using recurrence relations among the $j_n(x)$. Other transforms can also be generated which yield results of similar appearance. The transforms (28)–(30) may be calculated for many values of the frequency.

It is useful to note that Eq. (30) implies an integral-normalization condition on $\Gamma^2(Q, \omega)$ due to the fact that both $A(r, \omega)$ and $B(r, \omega)$ must vanish for r much smaller than the first-neighbor distance. Such integral normalizations are commonly applied to liquid and glass diffraction data, as discussed by Krogh-Moe,[8] Rahman,[9] and others. In the present case we have

$$P(r, \omega) = 0, \qquad r < b_{\min} \ , \tag{31}$$

which leads to the condition

$$\Gamma_\infty^2(\omega) = \lim_{Q\to\infty} \frac{5}{Q^5}\int_0^Q Q'^4 \Gamma^2(Q', \omega)\, dQ' \ . \tag{32}$$

Use of the value of $\Gamma_\infty^2(\omega)$ determined via Eq. (32) will ensure that the transform in Eq. (30) is well behaved near $r = 0$ [although spurious oscillations in $P(r, \omega)$ will in general be induced by inadequacies in the measured scattering law]. The function $\Gamma_\infty^2(\omega)$ contains only contributions from independent-atom scattering, as does the function derived from incoherent scattering.

It seems impossible to extract both $A(r, \omega)$ and $B(r, \omega)$ separately from $\Gamma^2(Q, \omega)$, at least without introducing further information. We make no attempt here to explore the difficulties of actually performing the Fourier integrals of Eqs. (28)–(30) which are subject to termination errors. Presumably the techniques of introducing modification functions and/or of peak function analysis[4,5] [which would have to be modified to fit the form of Eq. (30)] will be found useful. We note that Cochrane[7] has suggested an analysis similar to the present one, to obtain related information from the one-phonon scattering in single crystals.

By way of interpreting the function $P(r, \omega)$ of Eq. (30), and effecting something of a separation of the two terms, we note that the second term is just the average value of $A(r, \omega)$ in the sphere of radius r'. Thus if $A(r, \omega)$ contains a peak at $r = r_0$ [so also may $B(r, \omega)$], then the second term will rise up in a step at $r' = r_0$, then fall off as $(r')^{-3}$. The expected behaviors of $\rho(r')$, $A(r', \omega)$, $B(r', \omega)$, and $(3/r'^3)\int_0^{r'} 4\pi r^2 A(r, \omega) dr$ are shown schematically in Fig. 2.

For systems in which $\rho(r)$ has several isolated peaks (as at small r), the values of both A and B can apparently be obtained separately at each value of r where there is a peak. Thus for such systems, the nature of the displacements among near neighbors can be extracted from measured one-phonon

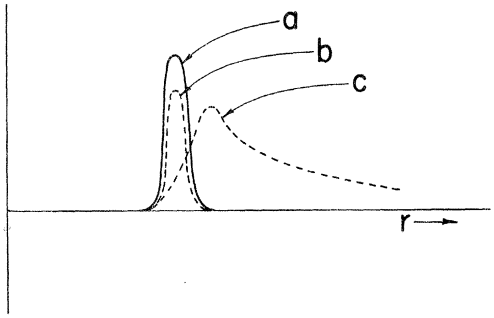

FIG. 2. Schematic representation of a, $\rho(r)$, b, $A(r, \omega)$, and c, $(1/r^3)\int_0^r 4\pi r'^2 A(r', \omega) dr'$ in the neighborhood of an isolated peak in $\rho(r)$.

scattering. It is not apparent to us how to do this where peaks in $\rho(r)$ overlap.

Now, $\Gamma^2(Q, \omega)$ is not accessible from measurement, while $G(Q, \omega)$ can be extracted from data according to Eq. (3). In terms of measurable quantities, Eq. (30) becomes

$$4\pi P(r', \omega)g(\omega) = \frac{2}{\pi}\int_0^\infty Q^2 j_2(Qr')[G(Q, \omega) - G_\infty(\omega)]\,dQ$$

$$= -4\pi B(r', \omega)g(\omega) + \frac{3}{r'^3}\int_0^{r'} 4\pi r^2 A(r, \omega)g(\omega)\,dr\ , \tag{33}$$

where

$$G_\infty(\omega) = \lim_{Q\to\infty} G(Q, \omega)\ . \tag{34}$$

The normalization condition (32) then reads

$$G_\infty(\omega) = \lim_{Q\to\infty} \frac{5}{Q^5}\int_0^Q Q'^4 G(Q', \omega)\,dQ'\ . \tag{35}$$

VII. CONCLUSIONS

The neutron scattering law can yield detailed information as to the nature and characteristic frequencies of atomic motions in amorphous solids. In the case of incoherent scattering, the generalized frequency distribution $G(Q, \omega)$ is independent of Q and is related to the density of lattice modes by a multiplicative factor which is the mean-squared displacement for modes of each frequency. For coherent scattering, $G(Q, \omega)$ depends on Q in a way related to the structure of the system and the nature of the atomic displacements. We have proposed a method by which, through a certain transformation of $G(Q, \omega)$, the real-space displacement-displacement correlations may be obtained for each frequency.

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