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Slow Neutron Scattering, the "Scattering Law," and $G(\mathbf{r},t)$*

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The general relationships between the energy moments of the inelastic cross section for slow-neutron scattering, and the so-called "Placzek moments," and the coefficients of the time expansion of the "pair-correlation function" $G(\mathbf{r},t)$ are derived. Also, a new method of determining $G(\mathbf{r},t)$ from slow-neutron scattering experiments is suggested.

I. INTRODUCTION

THE description of thermal neutron scattering is frequently given in terms of a function $S(\boldsymbol{\kappa},\omega)$ called the "scattering law."[1,2] Here $\hbar\boldsymbol{\kappa}$ and $\hbar\omega$ are, respectively, the neutron momentum and energy losses. The differential cross section is written in the form

$$\frac{\partial^2\sigma}{\partial\Omega\partial\epsilon}=a^2\frac{k}{\hbar k_0}S(\boldsymbol{\kappa},\omega)\,, \tag{1}$$

where $\mathbf{k}$ and $\mathbf{k}_0$ are, respectively, the outgoing and incoming wave vectors of the neutron; $\boldsymbol{\kappa}=\mathbf{k}_0-\mathbf{k}$; $\boldsymbol{\Omega}=\mathbf{k}/k$; $\hbar\omega=\epsilon=\hbar^2(k_0^2-k^2)/2m$; and a is the bound-atom scattering length.

Van Hove[1] introduced the function $G(\mathbf{r},t)$, which is the Fourier transform of $S(\boldsymbol{\kappa},\omega)$.

$$\begin{aligned} G(\mathbf{r},t)&=\frac{1}{(2\pi)^3N}\int \exp(-i\boldsymbol{\kappa}\cdot\mathbf{r}+i\omega t)S(\boldsymbol{\kappa},\omega)d^3\kappa d\omega \\ S(\boldsymbol{\kappa},\omega)&=\frac{N}{2\pi}\int \exp(i\boldsymbol{\kappa}\cdot\mathbf{r}-i\omega t)G(\mathbf{r},t)d^3r dt. \end{aligned} \tag{2}$$

N is the number of nuclei in the scattering system. Van Hove was then able to show that

$$G(\mathbf{r},t)=\frac{1}{N}\sum_i\frac{\exp(-E_i/\theta)}{z}\times\left\langle i\left|\sum_{j,l=1}^{N}\int d^3r\delta(\mathbf{r}+\mathbf{r}_l-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}_j(t))\right|i\right\rangle, \tag{3}$$

where θ is the absolute temperature in units of energy and $\mathbf{r}_j(t)$ is the usual Heisenberg operator.

In a scattering event, $\boldsymbol{\kappa}$, ω and the scattering angle, $\mathbf{k}_0\cdot\mathbf{k}/k_0k$, are related by energy and momentum conservation. This restricts the possible values of $\boldsymbol{\kappa}$ and ω in a scattering event to the following region.

$$-\infty<\omega\leq\frac{\hbar k_0^2}{2m}$$

$$\left\{2k_0^2-\frac{2m\omega}{\hbar}-2k_0\left(k_0^2-\frac{2m\omega}{\hbar}\right)^{1/2}\right\}^{1/2} \leq|\boldsymbol{\kappa}|\leq\left\{2k_0^2-\frac{2m\omega}{\hbar}+2k_0\left(k_0^2-\frac{2m\omega}{\hbar}\right)^{1/2}\right\}^{1/2}. \tag{4}$$

To write Eq. (2), we must define $S(\boldsymbol{\kappa},\omega)$ for all values of $\boldsymbol{\kappa}$ and ω. We can do this, in principle, by allowing $k_0\to\infty$. However, in practice, experiments are performed at a single incident energy and $\boldsymbol{\kappa}$ and ω are restricted by Eq. (4). For this reason, the determination of $G(\mathbf{r},t)$ from experiment is not particularly straightforward.

Note that the ω integration in Eq. (2) is defined along a line of constant $\boldsymbol{\kappa}$. This point leads to some difficulty in the comparison of the energy moments of the cross section with the energy moments of $S(\boldsymbol{\kappa},\omega)$. We attempt to clarify the comparison of these quantities in the next section.

The function $G(\mathbf{r},t)$ is of considerable importance in understanding the structure of scattering systems, since it is related to the time dependent-pair correlation function.[3] In fact, $G(\mathbf{r},0)$ is the familiar radial-distribution function, $\delta(\mathbf{r})+g(\mathbf{r})$. Thus, one would like to obtain $G(\mathbf{r},t)$ from neutron-scattering data.

An attempt has been made to circumvent the difficulty encountered in determining $G(\mathbf{r},t)$ from an experiment done at one incident neutron energy. Brockhouse[4] has introduced the procedure of measuring $S(\boldsymbol{\kappa},\omega)$ for constant values of $\boldsymbol{\kappa}$. By extending $S(\boldsymbol{\kappa},\omega)$ beyond the limits of Eq. (4) by some guess, the transformation in Eq. (2) can be made. Of course, the accuracy of $G(\mathbf{r},t)$ depends on the accuracy of the guess.

Pope[5] has determined $G(\mathbf{r},0)$ from measurements of $\partial\sigma/\partial\Omega$. His procedure can be understood by expanding $G(\mathbf{r},t)$ in a power series in t. This expresses $\partial^2\sigma/\partial\Omega\partial\epsilon$ in a series of derivatives of delta functions of the energy transfer. By integrating this expression over ϵ, a series expansion for $\partial\sigma/\partial\Omega$ is obtained. The first term of this series is proportional to the three-dimensional Fourier

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[1] L. Van Hove, Phys. Rev. 95, 249 (1954).
[2] G. Placzek, Phys. Rev. 86, 377 (1952).
[3] R. Aamodt, K. M. Case, M. Rosenbaum, and P. F. Zweifel, Phys. Rev. 126, 1165 (1962).
[4] B. N. Brockhouse, in Proceedings of the International Atomic Energy Agency Symposium on Inelastic Scattering of Neutrons in Solids and Liquids, Vienna, 1961 [International Atomic Energy Agency (to be published)].
[5] N. K. Pope, in Second Symposium on Melting, Diffusion, and Related Topics, Ottawa, 1957.

transform of $G(\mathbf{r},0)$; and the second term is proportional to $[\kappa^2 m/\kappa_0^2 M]$. If the higher terms can be estimated, $G(\mathbf{r},0)$ can be found. Pope assumes that all terms beyond the second vanish.

We suggest a method for obtaining $G(\mathbf{r},t)$ which is an extension of this procedure. The series expansion for $\partial^2\sigma/\partial\Omega\partial\epsilon$ is obtained.

$$\frac{\partial^2\sigma}{\partial\Omega\partial\epsilon}=a^2\frac{k}{\hbar k_0}\sum_{n=0}(-1)^n\bar{\omega}^n(\mathbf{k}_0-\mathbf{k})\delta^n(\omega). \tag{5}$$

The $\bar{\omega}^n$ are the moments of $S(\kappa\omega)$, "Placzek moments."[2] Using Eq. (5), the energy moments of the cross section, $\bar{\epsilon}^n$, can be expressed in an infinite series in the $\bar{\omega}^n$. The $\bar{\epsilon}^n$ can be determined from the scattering data, if the data are sufficiently accurate. By terminating the series expansion for the $\bar{\epsilon}^n$, it is possible to solve for the $\bar{\omega}^n$ in terms of the $\bar{\epsilon}^n$. Then the coefficients in the series expansion of $G(\mathbf{r},t)$,

$$\left\{\frac{\partial^n G(\mathbf{r},t)}{\partial t^n}\right\}_{t=0},$$

are proportional to the three-dimensional Fourier transforms of the $\bar{\omega}^n(\boldsymbol{\kappa})$.

Since the $\bar{\omega}^n(\boldsymbol{\kappa})$ can be obtained from experiment only for κ in the range $0\leq\kappa\leq 2k_0$, we must extend $\bar{\omega}^n(\boldsymbol{\kappa})$ to $\kappa>2k_0$. The effects of different extensions of $\bar{\omega}^n(\boldsymbol{\kappa})$ can be more readily determined, than can the effects of different extensions of $S(\boldsymbol{\kappa},\omega)$. Pope's results indicate that the Fourier transforms of $\bar{\omega}^n$ are not too sensitive to the extension used, at least for $\bar{\omega}^0$.

Our method clearly will have greatest practical application for small t. However, for liquids, this is the most interesting time range. It is reasonably well established that the motions of liquids over long time intervals is diffusive, and the structure should be largely determined by the short and intermediate time behavior.

In Sec. II, we discuss the moments, $\bar{\omega}^n$ and $\bar{\epsilon}^n$, in some detail. In Sec. III, we discuss the analysis of experimental data.

II. THE CROSS SECTION AND THE "SCATTERING LAW"

In the Fermi approximation,[6] the cross section is given by Eqs. (1), (2), and (3). Following Wick,[7] we expand $G(\mathbf{r},t)$ in a Maclaurin's series in t.

$$G(\mathbf{r},t)=\sum_n\frac{t^n}{n!}\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}. \tag{6}$$

For a scattering system with spherical symmetry the first three terms in this series are

$$G(\mathbf{r},0)=\delta(\mathbf{r})+g(\mathbf{r}) \tag{7}$$

$$\left\{\frac{\partial G(\mathbf{r},t)}{\partial t}\right\}_{t=0}=-\frac{i\hbar}{2M}\nabla^2\delta(\mathbf{r}) \tag{8}$$

$$\begin{aligned}\left\{\frac{\partial^2 G(\mathbf{r},t)}{\partial t^2}\right\}_{t=0}=&-\frac{\hbar^2}{4M^2}\nabla^2\nabla^2[\delta(\mathbf{r})+g(\mathbf{r})]\\&+\frac{\hbar^2}{3M^2}\nabla^2\delta(\mathbf{r})\sum_m\langle m|\sum_l\nabla_l^2|m\rangle\frac{e^{-E_m/\theta}}{z}\\&+\frac{\hbar^2}{3M^2}\nabla^2\sum_m\langle m|\sum_{l\neq n}\delta(\mathbf{r}+\mathbf{r}_l-\mathbf{r}_n)\nabla_l^2|m\rangle\\&\times\frac{e^{-E_n/\theta}}{z}\end{aligned} \tag{9}$$

$g(\mathbf{r})$ is the usual time-independent pair correlation function. Applying this expansion in Eq. (2), we obtain

$$S(\boldsymbol{\kappa},\omega)=N\sum_{n=0}^{\infty}\frac{(-i)^n\delta^n(\omega)}{n!}\times\int\exp(i\boldsymbol{\kappa}\cdot\mathbf{r})\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}d^3r. \tag{10}$$

Using Eq. (10), we can show that the "Placzek moments,"

$$\bar{\omega}^n(\boldsymbol{\kappa})=\int_{-\infty}^{\infty}\omega^n S(\boldsymbol{\kappa},\omega)d\omega \tag{11}$$

are proportional to the Fourier transforms of the

$$\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}.$$

Notice that the integration in Eq. (11) is carried out for constant $\boldsymbol{\kappa}$.

$$\bar{\omega}^n(\boldsymbol{\kappa})=N(-i)^n\int\exp(i\boldsymbol{\kappa}\cdot\mathbf{r})\times\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}d^3r \tag{12a}$$

$$\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}=\frac{(i)^n}{(2\pi)^3N}\int\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})\bar{\omega}^n(\boldsymbol{\kappa})d^3\kappa. \tag{12b}$$

Using Eqs. (10) and (12) in Eq. (1), we obtain a series expansion for the cross section,

$$\frac{\partial^2\sigma}{\partial\Omega\partial\epsilon}=a^2\frac{k}{\hbar k_0}\sum_{n=0}^{\infty}(-1)^n\bar{\omega}^n(\mathbf{k}_0-\mathbf{k})\delta^n(\omega). \tag{13}$$

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[6] E. Fermi, Ric. Sci. **7**, 13 (1936).

[7] G. C. Wick, Phys. Rev. **94**, 1228 (1954). Wick does not expand $G(\mathbf{r},t)$, but rather $\chi(\boldsymbol{\kappa},t)=\int\exp(i\boldsymbol{\kappa}\cdot\mathbf{r})G(\mathbf{r},t)d^3r$.

We can now compare the "Placzek moments" and the energy moments of the cross section, $\bar{\epsilon}^n$.

$$\bar{\epsilon}^n=\frac{1}{a^2}\int_{-\infty}^{\hbar^2k_0^2/2m}\epsilon^n\frac{\partial^2\sigma}{\partial\Omega\partial\epsilon}d\epsilon \quad (14a)$$

$$\bar{\epsilon}^n=\sum_{l=n}^{\infty}\frac{\hbar^l}{k_0}\left\{\frac{\partial^{(l-n)}}{\partial\epsilon^{(l-n)}}k\bar{\omega}^l(\mathbf{k}_0-\mathbf{k})\right\}_{\omega=0}. \quad (14b)$$

Notice that the integration in Eq. (14a) is carried out for constant scattering angle. This is a different path of integration from that in Eq. (11). If the cross section is strongly peaked about zero energy transfer, this time expansion procedure should be applicable.

The first "Placzek moment" is particularly simple,

$$\hbar\bar{\omega}^1(\boldsymbol{\kappa})=\hbar^2N\kappa^2/2M. \quad (15)$$

This result has been interpreted as the average neutron energy loss in the approximation that[8] $k\sim k_0$ and for scatterers with a mass number much greater than unity.[9] Actually Eq. (15) represents the average energy loss only when $\bar{\omega}^n$ and $\bar{\epsilon}^n$ vanish for $n>1$. It is difficult to interpret this condition in terms of the physical details of the scattering system. Simple conditions such as those mentioned above do not appear to be precisely correct. We can understand this point more fully by examining the average energy loss for a heavy gas.[10]

$$\bar{\epsilon}_{\text{hg}}=N\left\{\frac{\hbar^2(\mathbf{k}_0-\mathbf{k})^2}{2M}-\theta\frac{m(\mathbf{k}_0-\mathbf{k})^2}{Mk_0^2}\right\}_{\omega=0}. \quad (16)$$

The second term in Eq. (16) may give the dominant contribution to $\bar{\epsilon}_{\text{hg}}$ although a heavy gas seems to fit both of the conditions given for the interpretation of the first term of Eq. (16) above as the average energy loss.

III. INTERPRETATION OF EXPERIMENTS

As was discussed in the Introduction, one subject of the analysis of neutron scattering data is the determination of $G(\mathbf{r},t)$. It would seem that the easiest way to do this would be to Fourier transform $S(\boldsymbol{\kappa},\omega)$. This certainly would be the case if $S(\boldsymbol{\kappa},\omega)$ would be determined for all values of $\boldsymbol{\kappa}$ and ω.

To determine $G(\mathbf{r},t)$ in this way, one must assume some behavior for $S(\boldsymbol{\kappa},\omega)$ outside the region defined by Eq. (4), since it cannot be measured outside of this region. The assumption must be made such that $S(\boldsymbol{\kappa},\omega)$ satisfies Eq. (15), but this still does not determine $S(\boldsymbol{\kappa},\omega)$ uniquely. Using the data and satisfying Eq. (15), it may be possible to construct two functions, $G_1(\mathbf{r},t)$ and $G_2(\mathbf{r},t)$, that are quite different. Certainly this possibility should be considered. Even when $S(\boldsymbol{\kappa},\omega)$ is spherically symmetric, checking the uniqueness of $G(\mathbf{r},t)$ entails considering the possible extensions of $S(\boldsymbol{\kappa},\omega)$ into an infinite region of the (κ,ω)-plane.

Brockhouse[4] describes a method for extending the data, in which $S(\boldsymbol{\kappa},\omega)$ is chosen to be the ideal gas result or the result obtained by inserting the $G(\mathbf{r},t)$ for a classical liquid into Eq. (2). As shown by Schofield,[11] the cross section obtained by using a classical $G(\mathbf{r},t)$ in Eq. (2) does not satisfy detailed balance. An $S(\boldsymbol{\kappa},\omega)$ that is more realistic than the classical liquid result used by Brockhouse is the quasiclassical result of Aamodt *et al.*[3]

We now present an alternative method of determining $G(\mathbf{r},t)$. From the measured values of the cross section, we can determine, in principle, the first $R+1$ energy moments, $\bar{\epsilon}^n$, at particular values of the scattering angle. Truncating Eq. (14b) at $l=R$, we have a set of $R+1$ equations.[12]

$$\begin{aligned}
\bar{\epsilon}^R&=\hbar^R\bar{\omega}^R(k_0(2-2\mu)^{1/2}),\\
\bar{\epsilon}^1&=\sum_{l=1}^{R}\frac{\hbar^l}{k_0}\left\{\frac{\partial^{l-1}}{\partial\epsilon^{l-1}}k\bar{\omega}^l(|\mathbf{k}_0-\mathbf{k}|)\right\}_{\epsilon=0}\\
&\vdots\\
\bar{\epsilon}^0&=\sum_{l=0}^{R}\frac{\hbar^l}{k_0}\left\{\frac{\partial^{l}}{\partial\epsilon^{l}}k\bar{\omega}^l(|\mathbf{k}_0-\mathbf{k}|)\right\}_{\epsilon=0},
\end{aligned} \quad (17)$$

where $\mu=\mathbf{k}_0\cdot\mathbf{k}/k_0k$. The following equation is an identity, which can be used to relate the derivatives with respect to ϵ of the $\bar{\omega}^l(\kappa)$ to the derivatives with respect to κ.

$$\frac{\partial}{\partial\epsilon}\omega(|\mathbf{k}_0-\mathbf{k}|)=\frac{k_0\mu-k}{k|\mathbf{k}_0-\mathbf{k}|}\frac{m}{\hbar^2}\omega'(|\mathbf{k}_0-\mathbf{k}|). \quad (18)$$

The first of Eqs. (17) determines $\bar{\omega}^R(\kappa)$ for $0\leq\kappa\leq 2k_0$. Using Eq. (18) and $\bar{\omega}^R(\kappa)$, we can determine $\bar{\omega}^{R-1}(\kappa)$ for $0\leq\kappa\leq 2k_0$ from the second of Eqs. (17). We can proceed in the same way to determine all $R+1$ of the "Placzek moments."[13] The first "Placzek moment" is $\hbar\kappa^2/2M$. We can use this fact to check the accuracy of our results and to insure that R is sufficiently large.

The coefficients of the time expansion in Eq. (6) are proportional to the Fourier transforms of the "Placzek moments."

$$\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}=\frac{i^n}{2\pi^2Nr}\int_0^\infty\kappa\sin\kappa r\bar{\omega}^n(\kappa)d\kappa. \quad (19)$$

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[8] M. Nelkin, in Proceedings of the International Atomic Energy Agency Symposium on Inelastic Scattering of Neutrons in Solids and Liquids, Vienna, 1961 [International Atomic Energy Agency (to be published)].

[9] P. De Gennes, Physica 25, 825 (1959).

[10] H. Hurwitz, Jr., M. S. Nelkin, and G. J. Habetler, Nucl. Sci. Eng. 1, 280 (1956).

[11] P. Schofield, Phys. Rev. Letters 4, 239 (1960).

[12] We assume spherical symmetry.

[13] It appears that to solve Eqs. (17) we must solve a set of differential equations. However, the equation for $\bar{\epsilon}^R$ involves no derivatives, and in succeeding equations the only derivatives are of moments that have been previously determined.

The general form of $\bar{\omega}^n(\boldsymbol{\kappa})$ will be

$$\bar{\omega}^n(\boldsymbol{\kappa})=f(\boldsymbol{\kappa})+\sum_{l=0} a_l(\boldsymbol{\kappa}^2)^l,$$

where the Fourier transform of $f(\boldsymbol{\kappa})$ is well defined. The terms in $\bar{\omega}^n(\boldsymbol{\kappa})$ that are proportional to $(\boldsymbol{\kappa}^2)^l$ will produce terms in the expression for $\{(\partial^n/\partial t^n)G(\mathbf{r},t)\}_{t=0}$ that are proportional to $(\nabla^2)^l\delta(\mathbf{r})$, cf. Eqs. (7)–(9). Since this analysis requires numerical integration, one should subtract that part of $\bar{\omega}^n(\boldsymbol{\kappa})$ that goes as $(\boldsymbol{\kappa}^2)^l$ before applying Eq. (19).

Since $\bar{\omega}^n(\kappa)$ can only be determined for $0\leq\kappa\leq 2k_0$, we must still extend the $\bar{\omega}^n(\kappa)$ to values of κ greater than $2k_0$. However, it is easier to determine the uniqueness of

$$\left\{\frac{\partial^n}{\partial t^n}G(\mathbf{r},t)\right\}_{t=0}$$

considering different extensions of $\omega^n(\kappa)$ than it is to examine the possible extensions of $S(\boldsymbol{\kappa},\omega)$.

The validity of Eq. (17) is based on the assumption that the higher moments, $\bar{\epsilon}^n$, do not contribute significantly to $G(\mathbf{r},t)$. This assumption can be tested directly by an analysis of the data. Pope[5] has analyzed neutron diffraction data from liquid argon using this method for $R=1$. Pope used a measurement of $\bar{\epsilon}^0$, and

$$\bar{\omega}^1(\boldsymbol{\kappa})=\hbar\boldsymbol{\kappa}^2/2M$$

and Eqs. (17) for $R=1$ to write

$$\bar{\epsilon}^0=\{\bar{\omega}^0(|\mathbf{k}_0-\mathbf{k}|)\}_{\epsilon=0}+\frac{\hbar^2}{k_0}\left\{\frac{\partial}{\partial\epsilon}k\frac{|\mathbf{k}_0-\mathbf{k}|^2}{2M}\right\}_{\epsilon=0}.$$

Using Eq. (7) and performing the subtraction of the constant term as discussed above, we have

$$g(\mathbf{r})=\frac{1}{2\pi^2Nr}\int_0^\infty dKK\sin Kr \times\left[\bar{\epsilon}^0-N-\frac{\hbar^2}{k_0}\left\{\frac{\partial}{\partial\epsilon}k\frac{|\mathbf{k}_0-\mathbf{k}|^2}{2M}\right\}_{\epsilon=0}\right],$$

where

$$K=\{|\mathbf{k}_0-\mathbf{k}|\}_{\epsilon=0}.$$

The results of this calculation showed that the main features of $g(\mathbf{r})$ were not very sensitive to the way in which $\bar{\omega}^0(K)$ was extended.

The method outlined above is not applicable for large R since the higher energy moments cannot be measured accurately. However, it has been very successful in Pope's analysis of the measured values of $\bar{\epsilon}^0$, and we can extend it somewhat using currently available data. The first moment can be measured with some accuracy. In fact, Randolph[14] has determined such quantities. Knowing the first moment, $\bar{\epsilon}^1$, we can write

$$\bar{\epsilon}^1=\hbar^2\left\{\frac{|\mathbf{k}_0-\mathbf{k}|^2}{2M}\right\}_{\epsilon=0}+\frac{\hbar^2}{k_0}\left\{\frac{\partial}{\partial\epsilon}k\bar{\omega}^2(|\mathbf{k}_0-\mathbf{k}|)\right\}_{\epsilon=0} \quad (20a)$$

$$\bar{\epsilon}^0=\{\bar{\omega}^0(|\mathbf{k}_0-\mathbf{k}|)\}_{\epsilon=0}+\frac{\hbar^2}{k_0}\left\{\frac{\partial}{\partial\epsilon}k\frac{|\mathbf{k}_0-\mathbf{k}|^2}{2M}\right\}_{\epsilon=0} +\frac{\hbar^2}{k_0}\left\{\frac{\partial^2}{\partial\epsilon^2}k\bar{\omega}^2(|\mathbf{k}_0-\mathbf{k}|)\right\}_{\epsilon=0}. \quad (20b)$$

Using Eqs. (20a) and (18), we can determine the numerical values of $(\partial/\partial K)\bar{\omega}^2(K)$. Using these values of $(\partial/\partial K)\bar{\omega}^2(K)$ and Eq. (18), we can determine the numerical values of $\{(\partial^2/\partial\epsilon^2)k\bar{\omega}^2(|\mathbf{k}_0-\mathbf{k}|)\}_{\epsilon=0}$ and thus solve Eq. (20b) for $\bar{\omega}^0(K)$, $0\leq K\leq 2k_0$.

$$\{\bar{\omega}^0(|\mathbf{k}_0-\mathbf{k}|)\}_{\epsilon=0}=\bar{\epsilon}^0-\frac{\hbar^2}{k_0}\left\{\frac{\partial}{\partial\epsilon}k\frac{|\mathbf{k}_0-\mathbf{k}|^2}{2M}\right\}_{\epsilon=0} -\frac{\hbar^2}{k_0}\left\{\frac{\partial^2}{\partial\epsilon^2}k\bar{\omega}^2(|\mathbf{k}_0-\mathbf{k}|)\right\}_{\epsilon=0}. \quad (21)$$

Then $g(\mathbf{r})$ is given by

$$g(\mathbf{r})=\frac{1}{2\pi^2Nr}\int_0^\infty dKK\sin Kr\{\bar{\omega}^0(K)-N\}, \quad (22)$$

where $\bar{\omega}^0(K)$ is given by Eq. (21). Equation (21) should yield a more accurate $g(\mathbf{r})$ than Pope's calculation. The results of this calculation will be reported in a future work. Notice that this calculation of $g(\mathbf{r})$ involves a slight change in the general method we have previously described. The difference between the two methods is that, in the latter, we have explicitly used the known value of $\bar{\omega}^1(\mathbf{K})=\hbar\mathbf{K}^2/2M$.

IV. DISCUSSION

We have shown the relationship between time expansion of $G(\mathbf{r},t)$, and the moment expansion of the cross section, and the moment expansion of $S(\boldsymbol{\kappa},\omega)$. Our discussion should prove useful in clarifying the relationships between these quantities.

Also, we have described a method for determining $G(\mathbf{r},t)$ from slow neutron scattering data. This method should yield better results for small t than directly Fourier-transforming $S(\boldsymbol{\kappa},\omega)$ since $S(\boldsymbol{\kappa},\omega)$ is not completely determined in a scattering experiment. However, the method neglects the higher energy moments, and thus eliminates the possibility of determining the long-time behavior of $G(\mathbf{r},t)$.

[14] P. D. Randolph, Bull. Am. Phys. Soc. 8, 42 (1963).