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Quantum Corrections to the Neutron Transport Equation

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The singular behaviour of the neutron transport equation, in the limit of zero neutron velocity, comes into play in an essential manner when one wants to study the nature of its asymptotic solutions. From the physical point of view, the consistency of such a study can be checked only if one knows explicitly the behaviour of the quantum correction terms which are usually neglected. These terms are derived and explicitly exhibited using techniques of the statistical mechanics of irreversible processes. Neglecting terms of order greater than the second in the interaction potential between neutron and scattering centers and in the "short memory" approximation it is shown that the quantum correction terms can be expressed by means of Van Hove's scattering function $S(\vec{\kappa}, \omega)$. Some models for the dynamics of the scattering centers (moderators) are discussed, and it is found that the correction terms are critically dependent on the detailed balance condition being satisfied.

I. INTRODUCTION

The mathematical study of the neutron transport equation, developed particularly in connection with problems relevant to reactor theory and, more recently, to pulsed neutron experiments, has brought out a peculiar difficulty. Namely, to quote Nelkin,[1] "the singular behaviour of the transport equation, in a limit where the transport equation does not describe the physical situation, has been used to infer the nature of its asymptotic solutions".

Precisely the spectrum of the neutron transport operator[2–4] is in general constituted by a discrete part and by a continuous part. The whole spectrum becomes purely discrete if one assumes that the neutron-energy distribution is bounded from below.

Clearly in the very low-energy limit, one expects quantum corrections to be important. In this paper, we derive these corrections explicitly and begin the study of their importance in some physical situations. To this end, we develop a general formalism along the lines of Zwanzig's projection technique[5] which we present in Sec. II. In Sec. III, we introduce our basic approximations which are the following:

(i) "Born approximation": we neglect the terms of order greater than the second in the interaction potential between neutron and scattering centers;

(ii) "Short memory": we assume that the time during which the motion of the scattering centers is correlated and the time during which the neutron distribution varies appreciably, are well separated;

(iii) translational invariance of the Hamiltonian describing the scattering centers.

Within the limits of these approximations we derive, by means of the Wigner transformation, a kinetic equation for the neutron distribution, which turns out to be nonlocal. These nonlocal effects extend over a distance of the order of that traveled by a neutron having a momentum roughly equal to the inverse of the correlation distance of the scattering centers during a correlation time. Expansion of the neutron distribution in terms of this nonlocality parameter gives at the order zero the usual phenomenological neutron transport equation and, at the higher orders, the quantum corrections we are looking for. A study of these in some models for the dynamics of the scattering centers is given in Sec. IV. The difficulties encountered in finding a suitable model and the aspects of the problem still to be investigated are discussed in the last section.

II. GENERAL FORMALISM

Since the neutron density is always much smaller than that of the scattering centers, we may neglect neutron-neutron interactions. Therefore we can limit ourselves to the consideration of only one neutron interacting with N scattering centers via an interaction potential of the following type

$$V=\sum_{i=1}^{N} v(|\vec{R}-\vec{r}_i|), \tag{II.1}$$

where $\vec{R}$ is the position vector of the neutron and $\vec{r}_i$ is the position vector of the ith scattering center.

The time evolution of the density matrix $\rho(t)$ of the system (neutron plus scattering centers) is given by the quantum-mechanical Liouville equation

$$i\hbar\frac{\partial\rho(t)}{\partial t}=[H,\rho(t)]\equiv\mathcal{H}\rho(t) \tag{II.2}$$

with $$H=H_n+H_S+V, \tag{II.3}$$

where H_n and H_S are the Hamiltonians of the neutron and of the scattering centers, respectively.

In Eq. (II.2) the script symbol $\mathcal{H}$ denotes as usual[6] an operator in the operator space of the system. To obtain a kinetic equation for the neutron one has, so to speak, to eliminate the degrees of freedom of the scattering centers. The situation, which one usually considers, is that of a sample in thermodynamical equilibrium at a given temperature T. Obviously the density matrix of the whole system cannot be described during the time evolution by the simple product of the canonical density matrix for the scattering centers and the density matrix of the neutron (because in this case no interaction could take place), but it is indeed possible to consider the "projection" of the complete time-dependent density matrix onto the "subspace" of the density matrices having such a factorized form. This can be achieved by means of Zwanzig's technique[5] if one uses the following explicit form for the "projection" operator

$$\mathcal{P}=\rho_{eq}(S)\mathrm{Tr}_S, \tag{II.4}$$

where $\rho_{eq}(S)$ denotes the canonical density matrix of the system (S) of the scattering centers, and Tr_S the trace over the degrees of freedom of S. If we now put

$$\rho(t)=\mathcal{P}\rho(t)+(1-\mathcal{P})\rho(t) \tag{II.5}$$

and assume[7]

$$(1-\mathcal{P})\rho(0)=0, \tag{II.6}$$

we obtain the following equation for $\rho_n(t)=\mathrm{Tr}_S\rho(t)$

$$\begin{aligned}\frac{\partial\rho_n(t)}{\partial t}=&-\frac{i}{\hbar}[\mathcal{H}_n+\mathrm{Tr}_S\mathcal{V}\rho_{eq}(S)]\rho_n(t)\\&-\frac{1}{\hbar^2}\int_0^t\mathrm{Tr}_S[\mathcal{V}\mathcal{U}(\tau)\mathcal{V}\rho_{eq}(S)]\rho_n(t-\tau)d\tau\\&+\frac{1}{\hbar^2}\int_0^t\mathrm{Tr}_S[\mathcal{V}\mathcal{U}(\tau)\rho_{eq}(S)\\&\times\mathrm{Tr}_S\mathcal{V}\rho_{eq}(S)]\rho_n(t-\tau)d\tau,\end{aligned} \tag{II.7}$$

where

$$\mathcal{U}(\tau)=\exp\{-(i/\hbar)[\mathcal{H}_n+\mathcal{H}_S+(1-\mathcal{P})\mathcal{V}]\tau\}, \tag{II.8}$$

and $\mathcal{H}_n$, $\mathcal{H}_S$, $\mathcal{V}$ are defined in analogy with $\mathcal{H}$. Use has been made also of the relations $\mathcal{P}\mathcal{H}_S=0$ and $\mathcal{P}\mathcal{H}_n=\mathcal{H}_n\mathcal{P}$. The second and fourth term in the right-hand side of Eq. (II.7) vanish as a consequence of the translational invariance of the system of scattering centers.

III. BASIC APPROXIMATIONS AND DERIVATION OF THE KINETIC EQUATION

To derive a kinetic equation for the neutron, we have to go over from a purely quantum-mechanical description to one which allows the introduction, at least in some approximate sense, of a distribution function in phase space. A method to perform such a transition is afforded by the Wigner[8] transformation. In spite of its shortcomings,[9] we have found this to be the most suitable way to obtain results in a reasonably straightforward and formally simple manner.[10] We apply this transformation in the following form:

$$F(\vec{R},\vec{P};t)=(1/\hbar\pi)^3\int d^3r\langle\vec{R}-\vec{r}|\rho_n(t)|\vec{R}+\vec{r}\rangle e^{(2i/\hbar)\vec{P}\cdot\vec{r}}, \tag{III.1}$$

and from Eq. (II. 7) we obtain

$$(\partial/\partial t)F(\vec{R},\vec{P};t)+(\vec{P}/m)\cdot \mathrm{grad}_{\vec{R}}F(\vec{R},\vec{P};t)$$
$$=-(1/\hbar^2)(1/\hbar\pi)^3\int_0^t d\tau\int d^3r\langle\vec{R}-\vec{r}|\mathrm{Tr}_S[\mathcal{V}\mathfrak{U}(\tau)\mathcal{V}\rho_{eq}(S)]\rho_n(t-\tau)|\vec{R}+\vec{r}\rangle e^{(2i/\hbar)\vec{P}\cdot\vec{r}}, \quad \text{(III. 2)}$$

where $\vec{R}$, $\vec{P}$, and m are the position, the momentum, and the mass of the neutron, respectively.

Making the approximation of neglecting in the right-hand side of this equation terms of order greater than the second in the interaction potential, that is, putting

$$\mathfrak{U}(\tau)=\exp[-(i/\hbar)(\mathcal{H}_n+\mathcal{H}_S)\tau], \quad \text{(III. 3)}$$

and recalling the explicit expression of the operators $\mathcal{V}$ and $\mathfrak{U}$, we obtain

$$\mathrm{Tr}_S[\mathcal{V}\mathfrak{U}(\tau)\mathcal{V}\rho_{eq}(S)]\rho_n(t-\tau)$$
$$=\mathrm{Tr}_S[Ve^{-(i/\hbar)(H_n+H_S)\tau}V\rho_{eq}(S)\rho_n(t-\tau)e^{(i/\hbar)(H_n+H_S)\tau}-Ve^{-(i/\hbar)(H_n+H_S)\tau}\rho_{eq}(S)\rho_n(t-\tau)V$$
$$\times e^{(i/\hbar)(H_n+H_S)\tau}-e^{-(i/\hbar)(H_n+H_S)\tau}V\rho_{eq}(S)\rho_n(t-\tau)e^{(i/\hbar)(H_n+H_S)\tau}V+e^{-(i/\hbar)(H_n+H_S)\tau}$$
$$\times\rho_{eq}(S)\rho_n(t-\tau)Ve^{(i/\hbar)(H_n+H_S)\tau}V]. \quad \text{(III. 4)}$$

It is now a matter of simple algebra to work out the explicit expressions of the matrix elements of the four similar operators in (III. 4). Let us consider for example in some detail the first one

$$-\frac{1}{\hbar^2}\left(\frac{1}{\hbar\pi}\right)^3\sum_{i,j=1}^{N}\int_0^t d\tau\int d^3r\,d^3r'\,d^3r''\,d^3k\,d^3k'\langle v(|\vec{R}-\vec{r}-\vec{x}_i|)v[|\vec{R}-\vec{r}'-\vec{x}_j(-\tau)|]\rangle_T$$
$$\times\langle\vec{R}-\vec{r}'|\rho_n(t-\tau)|\vec{R}+\vec{r}''\rangle\exp[i\vec{k}\cdot(\vec{r}'-\vec{r})+i\vec{k}'\cdot(\vec{r}''-\vec{r})+(2i/\hbar)\vec{P}\cdot\vec{r}+(i/\hbar)(E_{k'}-E_k)\tau], \quad \text{(III. 5)}$$

where $\vec{x}_j(-\tau)=e^{-(i/\hbar)H_S\tau}\vec{x}_j e^{(i/\hbar)H_S\tau}$ and $\langle\circ\cdots\rangle_T=\mathrm{Tr}_S[\circ\cdots\rho_{eq}(S)]$.

Introducing the Fourier transform of the interaction potential, defined thus

$$v(\vec{r})=(2\pi)^{-3}\int d^3k v(\vec{k})e^{-i\vec{k}\cdot\vec{r}},$$

and making use once more of the translational invariance of the system of scattering centers (which gives

$$\langle e^{i\vec{k}\cdot\vec{x}_i}e^{i\vec{k}'\cdot\vec{x}_j(-\tau)}\rangle_T=\langle e^{-i\vec{k}'\cdot\vec{x}_i}e^{i\vec{k}'\cdot\vec{x}_j(-\tau)}\rangle_T\,\delta(\vec{k}+\vec{k}')(2\pi)^3/\Omega, \quad \text{(III. 6)}$$

where Ω is the normalization volume), expression (III. 5) becomes

$$-\frac{1}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^t d\tau\int d^3k\rho v^2\left(\left|\frac{\vec{P}}{\hbar}-\vec{k}\right|\right)\chi\left(\frac{P}{\hbar}-\vec{k},-\tau\right)e^{(i/\hbar)(E_P-E_k)\tau}F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\vec{k}+\frac{\vec{P}}{\hbar}\right),\vec{P};t-\tau\right]. \quad \text{(III. 7)}$$

The function $\chi(\vec{k},\tau)$ is defined as follows

$$\chi(\vec{k},\tau)=\frac{1}{N}\sum_{i,j=1}^{N}\langle e^{-i\vec{k}\circ\vec{x}_i}e^{i\vec{k}\cdot\vec{x}_j(\tau)}\rangle_T \quad \text{(III. 8)}$$

and $\rho=N/\Omega$. This definition makes, as usual,[11] $\chi(\vec{k},\tau)$ independent of N and is therefore suitable for the passage to the limit $N\to\infty$, $\Omega\to\infty$, and $N/\Omega=\mathrm{const}$, which will be understood in the following. The expression analogous to (III. 7) for the remaining three terms in (II. 4) is as follows

$$\frac{1}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^t d\tau\int\frac{d^3P'}{\hbar^3}\rho v^2\left(\left|\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar}\right|\right)\chi\left(\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar},\tau\right)e^{(i/\hbar)(E_P-E_{P'})\tau}F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\frac{\vec{P}}{\hbar}+\frac{\vec{P}'}{\hbar}\right),P';t-\tau\right], \quad \text{(III. 9)}$$

$$\frac{1}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^t d\tau\int\frac{d^3P'}{\hbar^3}\rho v^2\left(\left|\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar}\right|\right)\chi\left(\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar},-\tau\right)e^{-(i/\hbar)(E_P-E_{P'})\tau}F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\frac{\vec{P}}{\hbar}+\frac{\vec{P}'}{\hbar}\right),\vec{P}';t-\tau\right], \quad \text{(III. 10)}$$

$$-\frac{1}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^t d\tau\int d^3k\rho v^2\left(\left|\frac{\vec{P}}{\hbar}-\vec{k}\right|\right)\chi\left(\frac{\vec{P}}{\hbar}-\vec{k},\tau\right)e^{(i/\hbar)(E_k-E_P)\tau}F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\vec{k}+\frac{\vec{P}}{\hbar}\right),\vec{P};t-\tau\right]. \quad \text{(III.11)}$$

Collecting the terms in (II. 7, III. 9, III. 10, III. 11) and making use of the property[12]

$$\chi(\vec{k},-\tau)=\chi^*(\vec{k},\tau), \quad \text{(III.12)}$$

where the star denotes the complex conjugate, we arrive at the following equation for the neutron distribution function

$$\frac{\partial}{\partial t}F(\vec{R},\vec{P};t)+\frac{\vec{P}}{m}\cdot\operatorname{grad}_{\vec{R}}F(\vec{R},\vec{P};t)+\frac{1}{\hbar^2(2\pi)^3}\int d^3k\int_0^t d\tau\rho v^2\left(\left|\frac{\vec{P}}{\hbar}-\vec{k}\right|\right)$$
$$\times\left[\chi\left(\frac{\vec{P}}{\hbar}-\vec{k},\tau\right)e^{-(i/\hbar)(E_P-E_k)\tau}+\text{c.c.}\right]F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\vec{k}+\frac{\vec{P}}{\hbar}\right),\vec{P};t-\tau\right]=\frac{1}{\hbar^2(2\pi)^3}\int\frac{d^3P'}{\hbar^3}\int_0^t d\tau\rho v^2\left(\left|\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar}\right|\right)$$
$$\times\left[\chi\left(\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar},\tau\right)e^{-(i/\hbar)(E_{P'}-E_P)\tau}+\text{c.c.}\right]F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\frac{\vec{P}}{\hbar}+\frac{\vec{P}'}{\hbar}\right),\vec{P}';t-\tau\right]. \quad \text{(III.13)}$$

From this equation, one can see explicitly the role played by the assumption mentioned in the introduction on the separation of the two times: the time during which the motion of the scattering centers is correlated, which is the relaxation time of the intermediate scattering function $\chi(\vec{k},t)$, and the time during which the neutron distribution function $F(\vec{R},\vec{P},t)$ varies appreciably. The general problem of justifying and, possibly, taking into systematic account the successive approximations to equation (III. 13) in an approximation scheme, the zeroth order of which is a Markoffian equation, has received much attention in the literature (Lanz *et al.*,[13] Résibois,[14] Prigogine[15]). It is generally believed that non-Markoffian corrections are not very significant because either there is a clear-cut separation between the two characteristic times entering the problem, in which case the Markoffian approximation is sufficient, or there are other parameters in the problem, like external fields and then the non-Markoffian corrections are irrelevant. We believe that in our case such non-Markoffian corrections could become important, at least for some scattering systems. In this paper we are interested in presenting and examining the quantum corrections, therefore we do not attempt a detailed analysis of this point; but limit ourselves to the Markoffian approximation, that is to say, to the consideration of scattering systems for which one is allowed to extend the time integrations appearing in Eq. (III. 13) to infinity, and to approximate the time evolution of the neutron distribution during the time interval $t-\tau$ to t by the free evolution. Equation (III. 13) becomes then

$$\frac{\partial}{\partial t}F(\vec{R},\vec{P};t)+\frac{\vec{P}}{m}\cdot\operatorname{grad}_{\vec{R}}F(\vec{R},\vec{P};t)+\frac{1}{\hbar^2(2\pi)^3}\int d^3k\int_0^\infty d\tau\rho v^2\left(\left|\frac{\vec{P}}{\hbar}-\vec{k}\right|\right)$$
$$\times\left[\chi\left(\frac{\vec{P}}{\hbar}-\vec{k},\tau\right)e^{-(i/\hbar)(E_P-E_k)\tau}+\text{c.c.}\right]F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\vec{k}-\frac{\vec{P}}{\hbar}\right),\vec{P};t\right]=\frac{1}{\hbar^2(2\pi)^3}\int\frac{d^3P'}{\hbar^3}\int_0^\infty d\tau\rho v^2\left(\left|\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar}\right|\right)$$
$$\times\left[\chi\left(\frac{\vec{P}'}{\hbar}-\frac{\vec{P}}{\hbar},\tau\right)e^{-(i/\hbar)(E_{P'}-E_P)\tau}+\text{c.c.}\right]F\left[\vec{R}-\frac{\hbar\tau}{2m}\left(\frac{\vec{P}}{\hbar}-\frac{\vec{P}'}{\hbar}\right),\vec{P}';t\right]. \quad \text{(III.14)}$$

This is the kinetic equation for the neutron distribution we were looking for.

IV. DISCUSSION OF QUANTUM CORRECTIONS

If we now expand the distribution function F around the local value $\vec{R}$,

$$F(\vec{R}+\hbar\tau\vec{\kappa}/2m,\vec{P};t)=\sum_{n=0}^{\infty}\left(\frac{\hbar\tau}{2m}\right)^n\frac{1}{n!}(\vec{\kappa}\cdot\operatorname{grad}_{\vec{R}})^nF(\vec{R},\vec{P};t), \quad \text{(IV.1)}$$

and insert this expansion in Eq. (III. 14) we obtain

$$\frac{\partial}{\partial t}F(\vec{R},\vec{P};t)+\frac{\vec{P}}{m}\cdot\operatorname{grad}_{\vec{R}}F(\vec{R},\vec{P};t)+\sum_{n=0}^{\infty}A_n[F]=\sum_{n=0}^{\infty}B_n[F],$$

where

$$A_n[F]=\frac{1}{\hbar^2(2\pi)^3}\int d^3\kappa\int_0^\infty d\tau\left(\frac{\hbar\tau}{2m}\right)^n\frac{1}{n!}\rho v^2(|\vec{\kappa}|)[\chi(\vec{\kappa},\tau)e^{-i\omega\tau}+\text{c.c.}](\vec{\kappa}\cdot\operatorname{grad}_{\vec{R}})^nF(\vec{R},\vec{P};t), \quad \text{(IV.2)}$$

$$\hbar\vec{\kappa} = \vec{P} - \hbar\vec{\kappa}, \quad \hbar\omega = E_P - E_k;$$

$$B_n[F] = \frac{1}{\hbar^2(2\pi)^3}\int d^3\kappa' \int_0^\infty d\tau \left(\frac{\hbar\tau}{2m}\right)^n \frac{1}{n!}\rho v^2(|\vec{\kappa}'|)[\chi(\vec{\kappa}', \tau)\, e^{-i\omega'\tau} + \text{c. c.}]\,(\vec{\kappa}' \circ \operatorname{grad}_{\vec{R}})^n F(\vec{R}, \vec{P} + \hbar\vec{\kappa}'; t), \tag{IV.3}$$

$$\hbar\vec{\kappa}' = \vec{P}' - \vec{P}, \quad \hbar\omega' = E_{P'} - E_P .$$

At this point, recalling the relation

$$\int_{-\infty}^{+\infty} d\tau\, v^2(|\vec{k}' - \vec{k}|)\chi(\vec{k}' - \vec{k}, \tau)\, e^{-(i/\hbar)(E_{k'} - E_k)\tau} = \frac{8\pi^3\hbar^3 k'}{m}\,\sigma(\vec{k}' \to \vec{k}) \tag{IV.4}$$

we see that, to the zeroth order, Eq. (III. 14) reduces to the usual neutron transport equation.

For the evaluation of the correction terms, we have to compute the following quantities:

$$\int_0^\infty d\tau\, \tau^n [\chi(\vec{\kappa}, \tau)\, e^{-i\omega\tau} + \text{c. c.}] . \tag{IV.5}$$

All these quantities can be obtained, at least in principle, from the knowledge of the scattering function

$$S(\vec{\kappa}, \omega) = (2\pi)^{-1}\int_0^\infty d\tau\, [\chi(\vec{\kappa}, \tau)\, e^{-i\omega\tau} + \text{c. c.}] . \tag{IV.6}$$

In fact we have

$$(i) \quad \frac{1}{2\pi}\int_0^\infty d\tau\, \tau^n [\chi(\vec{\kappa}, \tau)\, e^{-i\omega\tau} + \text{c. c.}] = \frac{\partial^n}{\partial\omega^n} S(\vec{\kappa}, \omega), \quad n \text{ even}, \tag{IV.7}$$

$$(ii) \quad \frac{1}{2\pi}\int_0^\infty d\tau\, \tau^n [\chi(\vec{\kappa}, \tau)\, e^{-i\omega\tau} + \text{c. c.}] = (-1)^{\frac{1}{2}(n+1)} \frac{\partial^n}{\partial\omega^n} I(\vec{\kappa}, \omega), \quad n \text{ odd}, \tag{IV.8}$$

where $$S(\vec{\kappa}, \omega) + iI(\vec{\kappa}, \omega) = \pi^{-1}\int_0^\infty d\tau\, \chi(\vec{\kappa}, \tau)\, e^{-i\omega\tau} , \tag{IV.9}$$

and $I(\vec{\kappa}, \omega)$ is in turn related to $S(\vec{\kappa}, \omega)$ by the following dispersion relation

$$I(\vec{\kappa}, \omega) = (1/\pi)\int_{-\infty}^{+\infty} [S(\vec{\kappa}, \omega')/(\omega' - \omega)]\, d\omega' . \tag{IV.10}$$

Let us now discuss specific physical models by considering explicit expressions for the intermediate scattering function $\chi(\vec{\kappa}, \tau)$. As for the interaction potential $v(\vec{R} - \vec{r}_i)$, we use the Fermi pseudopotential[16] which gives

$$v^2(|\vec{\kappa}|) = 4\pi^2 a^2\hbar^4/m^2 , \tag{IV.11}$$

where a is the scattering length.

1. Free Gas

This is the only case in which a tractable exact expression for $\chi(\vec{\kappa}, \tau)$ is available, namely,

$$\chi(\vec{\kappa}, \tau) = \exp[-(\kappa^2/2M)(\tau^2 T - i\hbar\tau)] , \tag{IV.12}$$

where T is the absolute temperature in energy units and M is the mass of the particles of the gas. The resulting expressions for $S(\vec{\kappa}, \omega)$ and $I(\vec{\kappa}, \omega)$ are[17]

$$S(\vec{\kappa}, \omega) = (M/2\pi T\kappa^2)^{1/2} \exp[-M(\omega - \hbar\kappa^2/2M)^2/2T\kappa^2] , \tag{IV.13}$$

$$I(\vec{\kappa}, \omega) = -i\,(M/2\pi T\kappa^2)^{1/2} \exp[-M(\omega - \hbar\kappa^2/2M)^2/2T\kappa^2]\, \operatorname{erf}[\tfrac{1}{2}i\,(2M/T\kappa^2)^{1/2}(\hbar\kappa^2/2M - \omega)] . \tag{IV.14}$$

The first-order correction to the total cross section turns out to be zero. The corresponding second-order correction $A_2[F]$, if we take the z axis along the direction of $\vec{P}$, has only three nonvanishing terms, those containing the second derivatives of $F(\vec{R}, \vec{P}, t)$ with respect to x, y, and z. For symmetry reasons, the coefficients of the x and y derivatives are equal, and their common value is given by

$$\sqrt{\pi}\,\rho(a^2\hbar^2/m^4\beta^2)\{(\sqrt{\alpha}/\mu^2)\, e^{-\mu^2/4\alpha} - (1/\mu)[(2\alpha/\mu^2 + 1)\operatorname{erf}(\mu/2\sqrt{\alpha})]\} , \tag{IV.15}$$

where $\alpha = T/2M$, $\beta = 1/M + 1/m$, $\mu = P/m$.

The corresponding expression for the z derivative is

$$\sqrt{\pi}\,\rho(a^2\hbar^2/m^4\beta^2)[(2\sqrt{\alpha}/\mu^2)e^{-\mu^2/4\alpha} - (4\alpha/\mu^3)\,\mathrm{erf}(\mu/2\sqrt{\alpha})]\,. \tag{IV.16}$$

The first-order correction to the energy-transfer cross section $B_1[F]$ is given by[17]

$$\rho(a^2\hbar^3/2\pi m^3)(M/T)\int d^3\kappa'/\kappa'^2\,\Phi(1;\tfrac{1}{2};-M(\hbar\kappa'^2/2M-\omega')^2/2T\kappa'^2)\,\vec{\kappa}'\cdot\mathrm{grad}_{\vec{R}}F(\vec{R},\vec{P}+\hbar\kappa';t) \tag{IV.17}$$

2. Diffusive Model

A model which is often considered to describe slow neutron scattering by liquids is the diffusive model. For definiteness let us consider the scattering function corresponding to this model as given in Ref. 18

$$S(\vec{\kappa},\omega) = e^{\hbar\omega/2T}(2\pi)^{-1}\int_{-\infty}^{+\infty}d\tau\,e^{-i\omega\tau}\chi_c(\vec{\kappa},\tau)\,, \tag{IV.18}$$

where $\chi_c(\vec{\kappa},\tau)$ is understood to be some sort of classical limit. Several expressions for this classical limit have been proposed; the simplest one is the following:

$$\chi_c(\vec{\kappa},\tau) = \exp(-D\kappa^2|\tau|)\,. \tag{IV.19}$$

For our purposes this is not satisfactory, since its Fourier transform, when multiplied by the factor $e^{\hbar\omega/2T}$ to obtain a scattering function $S(\vec{\kappa},\omega)$ which satisfies the detailed balance condition, leads to a divergent expression for $I(\vec{\kappa},\omega)$.

Other forms of $\chi_c(\vec{\kappa},\omega)$ which do not have this unpleasant feature can be devised,[19] such as for instance

$$\chi_c(\vec{\kappa},\omega) = \exp[-\kappa^2\gamma(\tau)],\quad \gamma(\tau) = D[(\tau^2+M^2D^2/T^2)^{1/2} - MD/T]\,. \tag{IV.20}$$

This reproduces the correct behavior for small τ, which should be like $\kappa^2\tau^2(T/2M)$, and for large $\tau(\sim D\tau)$. Unfortunately it leads to an expression for $I(\vec{\kappa},\omega)$ which is not possible to handle analytically if one wants to perform the $\vec{\kappa}$ integration and obtain the final expression for the correction term.

Instead, if one uses expression (IV.2) directly in Eq. (IV.6), one can perform analytically the desired integration, and one finds that the first- and second-order corrections have a dependence on the neutron velocity which is clearly unreasonable. Namely, the first-order correction turns out to be independent of μ and the second-order correction inversely proportional to μ.

3. Critical Scattering

A physical situation in which quantum corrections might conceivably be relevant is neutron scattering in a gas at the critical point. The expression for $\chi(\vec{\kappa},\tau)$ that one can use in this case suffers from the same drawbacks as (IV.19). The calculation of the corresponding first-order correction $A_1[F]$ performed using Van Hove's model[11] leads to the following type of velocity dependence:

$$(1/\mu^2)\{\ln[(\alpha\beta+\mu)^2+\beta^2\lambda^2]/\beta^2(\alpha^2+\lambda^2) - (2\alpha/\lambda)\arctan\lambda\mu/[\alpha\mu+\beta(\alpha^2+\lambda^2)]\}\,, \tag{IV.21}$$

where $\mu = P/m$, $\lambda = \hbar/2m$, and α and β are constants related to Λ_0 and $\kappa_0\gamma_0$ of Ref. 11, respectively.

V. CONCLUDING REMARKS

As we have seen, the evaluations and the quantitative estimates of our correction terms are severely limited by the inadequacy of the available physical models for the dynamics of the scattering centers. In particular, as the example of the naive diffusive model has shown, our formulas are critically dependent on the fact that the detailed balance condition be satisfied. In fact, *a priori* one could have expected sensible results from a model in which the long-time behavior of the intermediate scattering function is represented fairly well, since we were interested in small neutron energy transfers.

The situation is even worse from the point of view of performing analytical evaluations in the case of solids. It would, of course, be possible to compute numerically the quantities of interest, but this, in our opinion, is justified only if one has already decided that in a specific problem quantum corrections are important. In conclusion, we believe that we have performed the first step towards an understanding of this particularly interesting problem, other aspects of which, such as the relevance of the initial condition and the role played by the non-Markoffian corrections, are worthwhile investigating.

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Spin Echoes in Terms of Spin Waves*

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A general theory of linearized spin echoes in an interacting Fermi liquid is developed by expressing the results of the usual type of echo experiment directly in terms of the spin-wave normal modes of the liquid as derived from the Landau theory. The possibility of obtaining further information by observing the echoes produced by a spatially nonuniform magnetization is briefly discussed.

I. DISCUSSION

A characteristic property of interactions between particles in a neutral Fermi liquid is that they lead to a whole spectrum of spin-wave–like excitations in the presence of a uniform magnetic field.[1] (In metals these also mix with cyclotron modes of the system.)

For some time spin echoes have been used as a tool to investigate spin excitations in liquid He^3 and dilute He^3-He^4 solutions.[2] Recently Leggett and Rice[3] have shown that a variation of the usual spin-echo experiment should yield further information about the Fermi liquid parameters.

The question therefore arises as to the explicit relationship between spin-echo experiments and the natural spin-wave–like modes of the Fermi liquid.

In this paper we give a general derivation of this relationship valid for long waves (low field gradient) under conditions where a linear approximation in the echo magnetization may be applied.

We also show how it can be further generalized to deal with a rather idealized echo experiment in which a nonuniform polarizing pulse ("90°" pulse) could be used to study diffusion of shorter wavelength modes of the system.

The gist of the derivation is as follows: The linearized Landau kinetic equation derived by Silin[1] for a Fermi liquid in a uniform magnetic field may be solved for long and medium long waves in terms of a set of eigenmodes with frequencies $\Omega_l(q)$ of different wave numbers q and different spherical harmonic character l measuring the phase relations between precessing spins on different parts of the Fermi surface. In the spin-echo experiment a magnetic field with a small gradient along the field direction (z axis) is applied to the liquid. The effect of this field, $H_z(z) = H_0 + Gz$, is to mix up modes of different wave number q, since the Gz term may be rewritten as $iG\,\partial/\partial q_z$. The effect of the mixing is to modify the time dependence of the mode q, l, from $\exp[i\Omega_l(q)t]$ to a more complicated time dependence containing a factor $\exp[\psi(q, l, t)]$. In the long-wave limit $\psi(q, l, t)$ is given directly in terms of $d^2\Omega_l(q)/dq^2$, and in fact only depends on the $l = 0$ mode in this limit. For an interacting system $d^2\Omega/dq^2$ is, in general, com-