Influence of Ergodic Behavior on the Scattering of Slow Neutrons by a Harmonic Oscillator*

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Random quantum jumps of a harmonic oscillator in contact with a temperature bath are shown to give rise to a general broadening of the slow neutron scattering peaks. An exception occurs in the case of the elastic scattering peak, a major component of which remains unbroadened. In general, the broadening increases with the number of quanta transferred. The analysis is based on the "damped" oscillator model of Senitzky.

I. INTRODUCTION

THE effects of random movements of scatterers on the incoherent scattering of slow neutrons by disordered systems have recently been discussed by Vineyard[1] and by Singwi and Sjölander.[2] Both these investigators deduce a broadening of the slow-neutron elastic scattering peak as a consequence of the random motion. In the present work, the influence of another type of stochastic process on the scattering of slow neutrons is considered, namely, the ergodic behavior of a spatially localized scattering system in thermal equilibrium with a surrounding temperature bath. In this case, the random processes are jumps of the system from one quantum state to another owing to the coupling with the temperature bath. In order to gain insight into the influence of such random quantum jumps on slow neutron scattering, a relatively simple scattering system, the harmonic oscillator, is investigated. The analysis is facilitated by the appearance of the recent work of Senitzky[3] on the quantum-mechanical behavior of a harmonic oscillator with dissipation. Senitzky, in contrast to several previous investigators, has viewed the oscillator and the loss mechanism to which it is coupled as a single quantum system. The coupling is assumed linear, and the effect of the oscillator on the loss mechanism is treated as a perturbation, though not vice versa. Third- and higher-order quantum effects in the loss mechanism are neglected. The formalism then yields the quantum analog of the damped oscillator differential equation of classical mechanics but with an inhomogeneous forcing term which arises from statistical fluctuations in the loss mechanism. The solution of the differential equation appears as the sum of a term referring to the uncoupled oscillator which is exponentially damped in time, and another which builds up asymptotically to a value corresponding to a thermal distribution of states. A characteristic of Senitzky's model is that the oscillator retains its quantum character throughout the coupling process, as is manifested in the validity, at all times, of the usual commutation relation between oscillator coordinate and momentum. This result helps justify the application of techniques in scattering theory which were originally intended for uncoupled systems. From the point of view of the development presented here, the analogy with a classically damped harmonic oscillator need not be emphasized. Instead, the Senitzky analysis will be regarded as a description of the transition of the oscillator from an initial stationary state to one corresponding to a thermal distribution over stationary states. The dissipation constant β is then interpreted as the reciprocal of the time constant τ associated with the thermalization process.

II. THE SCATTERING LAW

The pertinent results of Senitzky's analysis will be summarized first. The oscillator coordinate q is given by

$$q=e^{-\beta t/2}q^{(0)}+R(t), \quad (t\geqslant 0), \tag{1}$$

where β is the dissipation constant, $q^{(0)}$ is the uncoupled harmonic oscillator coordinate, and

$$R(t)\equiv\alpha\int_0^t \Gamma^{(0)}(t_1)e^{-\beta(t-t_1)/2}\cos\omega(t-t_1)dt_1, \tag{2}$$

in which α is the coupling constant, ω is the angular frequency of the oscillator, and $\Gamma^{(0)}$ is the coordinate of the uncoupled loss mechanism. It is assumed that $\beta/\omega\ll 1$, i.e., that the coupling is "weak." Expressions analogous to (1) and (2) also apply to the oscillator momentum p. The usual commutation relation[4]

$$[q(t),p(t)]=i$$

is then obeyed, which is not the case in earlier models of the dissipative harmonic oscillator in quantum mechanics. For the expectation value of q^2, one finds

$$\langle q^2\rangle=\langle q^{(0)2}\rangle e^{-\beta t}+\frac{z+1}{2M\omega(z-1)}(1-e^{-\beta t}), \tag{3}$$

where M is the oscillator mass and $z\equiv e^{\omega/kT}$. From (1)

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[1] G. H. Vineyard, Phys. Rev. **110**, 999 (1958).
[2] K. S. Singwi and A. Sjölander, Phys. Rev. **119**, 863 (1960).
[3] I. R. Senitzky, Phys. Rev. **119**, 670 (1960).
[4] Units in which $\hbar=1$ are used throughout.

and (3), we find

$$\langle R^2(t)\rangle = \frac{z+1}{2M\omega(z-1)}(1-e^{-\beta t}). \quad (4)$$

Since $[q^{(0)}(t),\Gamma^{(0)}(t')]=0$, it follows that

$$[q^{(0)}(t),R(t')]=0. \quad (5)$$

The scattering is treated by the method of Zemach and Glauber,[5] which is based on the use of the Fermi pseudopotential approximation and the introduction of Heisenberg time-dependent operators in lieu of an explicit summation over final scatterer states. The differential cross section $\sigma(\theta,\epsilon)$ for scattering by a single spinless scatterer through an angle θ with energy gain ϵ is given by Z.G. as

$$\sigma(\theta,\epsilon)=a^2\frac{k}{2\pi k_0}\int_{-\infty}^{+\infty} e^{-i\epsilon t}\chi(\boldsymbol{\kappa},t)dt, \quad (6)$$

where a is the bound scattering length, k_0 and k are initial and final neutron momenta, and $\boldsymbol{\kappa}$ is the momentum gain of the neutron. The dynamics of the scatterer are contained in the function χ, which satisfies the basic relation

$$\chi^*(\boldsymbol{\kappa},t)=\chi(\boldsymbol{\kappa},-t), \quad (7)$$

thereby ensuring the reality of $\sigma(\theta,\epsilon)$.

When the scatterer is bound to a fixed center by a harmonic oscillator potential, χ assumes the form[5]

$$\chi=\prod_\lambda\langle\exp\{i[\kappa_\lambda(q_\lambda(t)-q_\lambda(0))]\}\times\exp\{\tfrac{1}{2}\kappa_\lambda^2[q_\lambda(t),q_\lambda(0)]\}\rangle, \quad (8)$$

where the κ_λ ($\lambda=1, 2, 3$) are the Cartesian components of the momentum gain of the neutron, $q_\lambda(t)$ is the component of the Heisenberg coordinate operator of the scatterer, and $\langle\cdots\rangle$ indicates expectation value in the initial scatterer state. For the problem at hand, (8) still holds and becomes, by (1) and (5),

$$\chi=\prod_\lambda\langle\exp\{i[\kappa_\lambda(e^{-\beta t/2}q_\lambda^{(0)}(t)-q^{(0)}(0)+R(t))]\}\times\exp\{\tfrac{1}{2}\kappa_\lambda^2e^{-\beta t/2}[q_\lambda^{(0)}(t),q_\lambda^{(0)}(0)]\}\rangle. \quad (9)$$

Taking thermal averages in (9), we find

$$\langle\chi\rangle_T=\prod_\lambda\langle\exp[i\kappa_\lambda R(t)]\rangle_T\exp\left\{\frac{\kappa_\lambda^2}{4M\omega}e^{-\beta t/2}[e^{-i\omega t}-e^{i\omega t}]\right\}\times\langle\exp\{i\kappa_\lambda[e^{-\beta t/2}q_\lambda^{(0)}(t)-q_\lambda^{(0)}(0)]\}\rangle_T \quad (10)$$

since

$$[q_\lambda^{(0)}(t),q_\lambda^{(0)}(0)]=(e^{-i\omega t}-e^{i\omega t})/2M\omega.$$

In (10), $\langle\cdots\rangle_T$ indicates an average over a thermal distribution of initial states of the complete system of scatterer plus loss mechanism (or temperature bath).

Now, by a theorem of Bloch,[6]

$$\begin{aligned}\langle\exp\{i\kappa[e^{-\beta t/2}q^{(0)}(t)-q^{(0)}(0)]\}\rangle_T &=\exp[-\tfrac{1}{2}\kappa^2\langle e^{-\beta t}q^{(0)2}(t)+q^{(0)2}(0)\\ &\quad -e^{-\beta t/2}\{2q^{(0)}(t)q^{(0)}(0)+[q^{(0)}(0),q^{(0)}(t)]\}\rangle_T],\end{aligned} \quad (11)$$

where the subscript λ is omitted for the sake of brevity. Now

$$\langle q^{(0)}(t)q^{(0)}(0)\rangle_T=\frac{ze^{-i\omega t}+e^{i\omega t}}{2M\omega(z-1)}, \quad (12)$$

where

$$z=e^{\omega/kT}, \quad (13)$$

and

$$\langle q^{(0)2}(t)\rangle_T=\langle q^{(0)2}(0)\rangle_T=\frac{z+1}{2M\omega(z-1)}. \quad (14)$$

Also, since third- and higher-order quantum effects in the loss mechanism are neglected, we have,[7] by (4),

$$\langle\exp[i\kappa R(t)]\rangle_T=\exp[-\tfrac{1}{2}\kappa^2\langle R^2(t)\rangle_T]=\exp\left[-\frac{\kappa^2}{4M\omega}\frac{z+1}{z-1}(1-e^{-\beta t})\right]. \quad (15)$$

Combining (10), (11), (12), (14), and (15) yields finally

$$\langle\chi\rangle_T=\exp\left\{-\frac{\kappa^2}{2M\omega}\left[\frac{z+1}{z-1}-\frac{ze^{-i\omega t}+e^{i\omega t}}{z-1}e^{-\beta t/2}\right]\right\},\quad (t\geqslant 0), \quad (16)$$

where $\kappa^2=\sum_\lambda\kappa_\lambda^2$.

To obtain $\langle\chi\rangle_T$ for $t<0$, we invoke (7), obtaining for all t

$$\langle\chi\rangle_T=\exp\left\{-\frac{\kappa^2}{2M\omega}\left[\frac{z+1}{z-1}-\frac{ze^{-i\omega t}+e^{i\omega t}}{z-1}e^{-\beta|t|/2}\right]\right\}. \quad (17)$$

To facilitate the calculation of the Fourier transform of (17), as required by (6), we expand the time-dependent factor in (17) in a series of modified Bessel functions I_n, following Z.G. The result is

$$\langle\chi\rangle_T=\exp\left[-\frac{\kappa^2}{2M\omega}\frac{z+1}{z-1}\right]\sum_{n=-\infty}^{\infty}e^{in\omega t}z^{-n/2}I_n(\gamma e^{-\beta|t|/2}), \quad (18)$$

where $\gamma\equiv\kappa^2/[2M\omega\sinh(\omega/2T)]$. For $\beta=0$, this yields the expected delta function contributions to the cross section; the nth term in (18), which corresponds to the transfer of n quanta ω, gives a term proportional to $\delta(\epsilon-n\omega)$. For $\beta>0$, a general broadening of the delta-

[5] A. C. Zemach and R. J. Glauber, Phys. Rev. **101**, 118 (1956). This paper will be referred to as Z.G.

[6] See, for example, reference 5.

[7] A discussion of the first equality in (15) will be published by I. R. Senitzky.

function peaks occurs, which can be seen in the following way. We consider first the case $\gamma \ll 1$, which holds in many cases of practical interest. If $I_n(\gamma e^{-\beta|t|/2})$ be expanded in a power series and only the leading term

$$I_n \approx \frac{(\gamma e^{-\beta|t|/2})^{|n|}}{2^{|n|}|n|!} \tag{19}$$

retained, we find from (6), (18), and (19)

$$\sigma(\theta,\epsilon)=\sum_{-\infty}^{+\infty}\sigma_n(\theta,\epsilon),$$

with

$$\sigma_n(\theta,\epsilon)\approx\frac{a^2k}{2\pi k_0}\frac{\exp\left[-\frac{\kappa^2}{2M\omega}\frac{z+1}{z-1}\right]\gamma^{|n|}}{2^{|n|}|n|!z^{n/2}} \times\frac{\beta|n|}{(\beta|n|/2)^2+(\epsilon-n\omega)^2}. \tag{20}$$

Thus, in the approximation represented by (19), the width of the line corresponding to the transfer of n quanta is $\beta|n|$; in particular, for elastic scattering, i.e., $n=0$, *there is no broadening at all*, $\sigma_0(\theta,\epsilon)$ remaining proportional to $\delta(\epsilon)$ and with an integrated value equal to that obtained with $\beta=0$.

For the case of arbitrary γ, the use of the complete expansion of I_n results in power series representation of $\sigma_n(\theta,\epsilon)$ whose leading term is proportional to $\gamma^{|n|}$, as shown in (20). Each term of the expansion contributes, in the case $\beta=0$, a delta function, which becomes broadened when $\beta>0$, except in the case $n=0$. For $n=0$, the leading term is unbroadened when $\beta>0$, but all higher order terms are broadened. The complete expression for the differential cross section is

$$\sigma(\theta,\epsilon)=\frac{a^2k}{2\pi k_0}\exp\left[-\frac{\kappa^2}{2M\omega}\frac{z+1}{z-1}\right]\sum_{n=-\infty}^{\infty}\sum_{p=0}^{\infty}\frac{\gamma^{|n|+2p}}{2^{|n|}|n|!z^{n/2}} \times\frac{\beta(|n|+2p)}{[\beta(|n|+2p)/2]^2+(\epsilon-n\omega)^2}. \tag{21}$$

III. DISCUSSION

Both Vineyard[1] and Singwi and Sjölander[2] have considered dynamical models in which the random forces result in the ever increasing separation of the scattering system from its initial position. As Vineyard has noted, by inference from a number of specific models, a nonlocalized scattering system will not possess infinitely sharp neutron elastic peaks, whereas a well-localized system will. The present work has been concerned with the effects of interactions of the scattering system with a surrounding temperature bath which cause fluctuations in its energy state but not in its spatial position. Thus, a broadening of the elastic neutron peak is not to be expected. The results of the present investigation with the Senitzky oscillator model bear out this prediction.

The formalism presented here may be applied to the scattering of slow neutrons by a crystal lattice. The mass-point harmonic oscillator is replaced by a lattice oscillator, while the coupling to a temperature bath corresponds to the coupling of a lattice oscillator to other lattice oscillators via anharmonic terms in the lattice potential energy.

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