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Observability of stochastic resonance in neutron scattering

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The observability of the stochastic resonance phenomenon in a neutron scattering experiment is investigated, considering that the scatterer can hop between two sites. Under stochastic resonance conditions scattered intensity is transferred from the quasielastic region to two inelastic peaks. The magnitude of the signal-to-noise ratio is shown to be similar to that arising in the corresponding power spectrum. Effects of potential asymmetry are discussed in detail. Asymmetry leads to a reduction of the signal-to-noise ratio by a factor of $1-\xi^2$, where ξ is an asymmetry parameter which is zero for symmetric problems and equal to unity in a completely asymmetric case. [S1063-651X(99)50710-1]

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The last few years have seen the publication of a large body of work dealing with the phenomenon of stochastic resonance (SR) [1–3]. In this phenomenon the presence of noise amplifies the response of a nonlinear dynamical system to an input signal. Theoretical studies have usually concentrated on the analysis of the power spectrum, i.e., the time Fourier transform of the position-position correlation function. The power spectrum is the natural function to analyze due to its direct relation to the dynamical susceptibility. Although stochastic resonance has been predicted to occur in a manifold of dynamical systems, the paradigmatic example is that of a periodic signal acting on a particle moving in a two-well potential and under the influence of noise. A simplified version, the *two-state* system, has been shown to contain the main ingredients necessary for the discussion of SR [4].

For some systems, however, other experimental tools may be profitably used. Such is the case with glasses and proteins, whose dynamic properties can be advantageously investigated using neutron scattering techniques [5]. The purpose of this work is to investigate the signature of the SR phenomenon in a measurement of the incoherent neutron scattering cross section. Since this cross section is proportional to the dynamic structure factor (DSF), we will investigate the properties of the DSF for a two-state dynamical system subject to periodic forcing and noise. Because two-well potentials in glasses and proteins are often asymmetric [6], we will also analyze how asymmetry modifies the SR effect. In this connection, we remark that the influence of asymmetries on SR phenomena is a topic of current interest. For instance, Marchesoni, Apostolico, and Santucci have recently characterized the effects of asymetry in a low-noise Schmitt trigger [7].

In the absence of external forcing, stochasticity causes the transfer of part of the elastic intensity to a quasielastic (QE) line. The main results of this paper can be summarized as follows: Due to the external forcing, part of the QE intensity is transferred to inelastic, resonant lines, yielding a large signal-to-noise ratio. Asymmetry strongly reduces both the transfer to the QE region and the fractional transfer to the resonant lines.

To describe the dynamics of the scatterer center we consider a two-state model whose states x_+ and $-x_-(x_+,x_->0)$ are occupied with probabilities n_+ and n_- respectively [2,4]. The master equation for $n_\pm$ reads

$$\dot{n}_\pm(t)=-W_\mp(t)n_\pm(t)+W_\pm(t)n_\mp(t), \tag{1}$$

where $W_\pm(t)$ is the transition rate out of the $\pm$ state. Following McNamara and Wiesenfeld [4], we choose periodically modulated, Arrhenius-type transition rates,

$$W_\pm(t)=r_\pm \exp\left(\pm\frac{A_0 x_\pm \cos(\Omega t)}{D}\right), \tag{2}$$

where $r_\pm$ is the Kramers' rate and D is the noise strength.

Equations (1) can be solved by assuming that the modulation amplitude is small [2,4], $(x_\pm A_0/D)\ll 1$. We obtain,

$$\begin{aligned} n_+(t|x_0,t_0)=&e^{-\alpha(t-t_0)}\left[1-\frac{A_0\beta}{D\Omega}[\sin(\Omega t)-\sin(\Omega t_0)]\right]\\ &\times\delta_{n_+n_0}+\frac{r_+}{\alpha}(1-e^{-\alpha(t-t_0)})\\ &\times\left(1-\frac{A_0\beta}{D\Omega}\sin(\Omega t)\right)-\frac{\beta}{2\Omega^2 x_+}\\ &\times[\dot{K}(t)-e^{-\alpha(t-t_0)}\dot{K}(t_0)]\\ &+\frac{1}{2}[K(t)-e^{-\alpha(t-t_0)}K(t_0)], \end{aligned} \tag{3}$$

where $\alpha=r_++r_-$, $\beta=r_+x_+-r_-x_-$, and

$$K(t)=\frac{2r_+\alpha}{\alpha^2+\Omega^2}\left(\frac{A_0x_+}{D}\right)\left[\cos(\Omega t)-\frac{\Omega}{\alpha}\sin(\Omega t)\right]. \tag{4}$$

The dot over the function $K(t)$ denotes its time derivative, and the factor $\delta_{n_+n_0}$ is equal to 1 if the scatterer is initially $(t=t_0)$ at site x_+. To obtain Eq. (3) we have made two approximations: (i) as mentioned above, the modulation amplitude must be small, $(x_\pm A_0/D)\ll 1$, and (ii), due to the time-integrated accumulation of asymmetry effects for very small values of Ω, we must also introduce an additional condition: $(\beta A_0/D\Omega)\ll 1$. Of course, this second condition does not apply for symmetric $(\beta=0)$ problems. We remark that if it were necessary to keep higher orders in the modulation amplitude, it may be useful to expand the transition rates in terms of modified Bessel functions [8].

The probability distribution at time t is given by

$$P(x,t|x_0,t_0)=n_+(t,t_0)\,\delta(x-x_+)+n_-(t,t_0)\,\delta(x-x_-). \tag{5}$$

In general the dynamic correlation function associated with the dynamic variable $f[x]$ is given by

$$\frac{1}{2\pi}\mathrm{Re}\int_{-\infty}^{+\infty}d\tau\, e^{-i\omega\tau}\overline{\langle f^*(t+\tau)f(t)\rangle}\ , \tag{6}$$

where $f(t)\equiv f[x(t)]$. The angular brackets represent a statistical average, while the overbar stands for an average over the initial conditions, that is, over the phase of the input signal,

$$\overline{\langle f^*(t+\tau)f(t)\rangle}=\frac{\Omega}{2\pi}\int_0^{2\pi/\Omega}dt\bigg[\int dx\int dy\, f^*(x)f(y)\times P(x,t+\tau|y,t)P(y,t|x_0,t_0\to-\infty)\bigg]. \tag{7}$$

It should be noted that we are considering the stationary limit, i.e., $t_0\to-\infty$. By choosing $f(t)=x(t)$ in expression (6) we obtain the power spectrum, while by taking $f(t)=e^{ikx(t)}$ we get the DSF, $S(k,\omega)$, where k is the momentum transferred to the scatterer.

A direct generalization of the McNamara-Wiesenfeld formula is

$$\begin{aligned}\langle f^*(t+\tau)f(t)\rangle=&[f(x_+)f^*(x_+)-f(-x_-)f^*(x_+)]n_+^+n_+\\&+[f(x_+)f^*(-x_-)-f(-x_-)f^*(-x_-)]\\&\times n_+^-+[f(-x_-)f^*(-x_-)-f(x_+)\\&\times f^*(-x_-)n_+^-n_++[f(-x_-)f^*(x_+)\\&-f(-x_-)f^*(-x_-)]n_+\\&+f(-x_-)f^*(-x_-).\end{aligned} \tag{8}$$

Here $n_+^+\equiv n_+(t+\tau|+,t)$ is the conditional probability that the particle is at x_+ at time $t+\tau$, given that it was at state $+$ at time t. Since the most complicated part of the calculation is the evaluation of the averages $\overline{n_+^+n_+}$, etc., Eq. (8) implies an important simplification: once these averages are calculated, we can evaluate an arbitrary autocorrelation function with minimum work.

The signal-to-noise ratio $\mathcal{R}$ is a suitable indicator of the intensity of the SR effect. [2] We generalize the definition in Ref. [2] and write

$$\mathcal{R}=2\left[\lim_{\epsilon\to0}\int_{\Omega-\epsilon}^{\Omega+\epsilon}S(\omega,\ldots)d\omega\right]\Big/\ S_B(\Omega,\ldots), \tag{9}$$

where $S(\omega,\ldots)$ is the Fourier transform of the correlation function under consideration and $S_B(\Omega,\ldots)$ is the value of the background component evaluated at the frequency Ω of the output signal.

Next we present the results for the symmetrical two-state problem and compare them with the well known predictions for the power spectrum, which was studied by McNamara and Wiesenfeld [4]. Under these conditions, $x_-=x_+=x_m$ and $r_-=r_+=r$, i.e., $\beta=0$. A straightforward evaluation of the averages in Eq. (6) leads to the following expression for the power spectrum:

$$S(\omega)=[1-M(\Omega)]\frac{2rx_m^2}{\pi(4r^2+\omega^2)}+\frac{M(\Omega)x_m^2}{2}[\delta(\omega-\Omega)+\delta(\omega+\Omega)], \tag{10}$$

where

$$M(\Omega)=\left(\frac{rA_0x_m}{D}\right)^2\frac{2}{4r^2+\Omega^2}.$$

If there is no forcing, $S(\omega)$ is simply a Lorentzian, due to the interstate jumps generated by the noise. Forcing transfers power from the noisy background to the spikes. The total output power, obtained by integrating over ω, equals x_m^2, while the signal-to-noise ratio (SNR) is

$$\mathcal{R}=\pi r\left(\frac{A_0x_m}{D}\right)^2+O\left(\frac{A_0x_m}{D}\right)^4. \tag{11}$$

Using the prescription (8) for $f(t)=e^{ikx(t)}$ the DSF is easily obtained,

$$\begin{aligned}S(k,\omega)=&\cos^2(kx_m)\,\delta(\omega)\\&+\frac{2r}{\pi(4r^2+\omega^2)}[1-M(\Omega)]\sin^2(kx_m)+\frac{M(\Omega)}{2}\\&\times[\delta(\omega-\Omega)+\delta(\omega+\Omega)]\sin^2(kx_m).\end{aligned} \tag{12}$$

The SNR obtained from the DSF is exactly the same as that corresponding to the power spectrum. Therefore, the DSF exhibits the SR effect as strongly as the power spectrum does. In both cases the inelastic intensity emerges directly from a decrease in the quasielastic component. The DSF contains, however, a purely elastic component which is not affected by the external forcing. This elastically scattered intensity is independent of noise strength, as long as there is some noise: if we take the $r\to0$ limit, the quasielastic component disappears and $S(k,\omega)\to\delta(\omega)$. This is in agreement with the older proof of the nonexistence of a quasielastic component for motion in nonstochastic potentials [9].

The wave-vector dependence of the DSF is obvious form expression (12). If $kx_m=n\pi$, for any integer n, an integer number of wavelengths fits exactly between the two states and there is only a strong elastic line. Therefore, the modulation cannot affect neutron scattering. If $kx_m=(n+\frac{1}{2})\pi$, the elastic line disappears, the whole intensity emerges as a quasielastic component and is available for transference to the inelastic lines, i.e., for the stochastic resonance phenomenon.

The asymmetric problem, for which $x_+\neq x_-$ and $r_+\neq r_-$, is much more involved. To properly understand the effects of asymmetry we first review the solution to the problem in the absence of the periodic excitation [5]. Since the stronger asymmetry effects are naturally those arising from having different jump rates, we introduce an asymmetry parameter,

$$\xi=\frac{r_+-r_-}{r_++r_-},\quad |\xi|\leqslant 1. \tag{13}$$

In terms of this asymmetry parameter, of the intersite distance $\Delta=x_++x_-$, and of the rate $\alpha=r_++r_-$, which is a measure of noise strength, the DSF is given by

$$S(k,\omega;A_0=0)=\left[1-(1-\xi^2)\sin^2\left(\frac{k\Delta}{2}\right)\right]\times\delta(\omega)+\frac{\alpha(1-\xi^2)}{\pi(\alpha^2+\omega^2)}\sin^2\left(\frac{k\Delta}{2}\right). \tag{14}$$

The main effect of the asymmetry is to reduce the total quasielastic intensity I_Q,

$$I_Q(A_0=0)=(1-\xi^2)\sin^2(k\Delta/2). \tag{15}$$

Since intensity can be transferred by the input signal to the inelastic peak solely out of the quasielastic (QE) region, the resonance effect will be correspondingly weakened. Note that in the completely asymmetric case, $|\xi|=1$, the particle is localized in one of the sites and there is only elastic scattering. The DSF for the $A_0\neq 0$ problem is,

$$S(k,\omega)=\left[1-(1-\xi^2)\sin^2\left(\frac{k\Delta}{2}\right)\right]\delta(\omega)+\sin^2\left(\frac{k\Delta}{2}\right)\times\left\{\left(\frac{A_0\Delta}{4D}\right)^2\frac{(1-\xi^2)^2}{1+(\Omega/\alpha)^2}[\delta(\omega-\Omega)+\delta(\omega+\Omega)]+\frac{1-\xi^2}{\pi\alpha[1+(\omega/\alpha)^2]}+\left(\frac{A_0\Delta}{D}\right)^2H(\omega)\right\}, \tag{16}$$

where H is a complicated function. Since the last term is only a small correction to the QE background, we omit its full expression. The integral of $S(k,\omega)$ over all frequencies satisfies the sum rule

$$\int_{-\infty}^{\infty}S(k,\omega)d\omega=1. \tag{17}$$

The signal-to-noise ratio is decreased by the asymmetry,

$$\mathcal{R}=\pi\alpha\left(\frac{A_0\Delta}{4D}\right)^2(1-\xi^2). \tag{18}$$

The strong reduction $[\sim(1-\xi^2)^2]$ of the resonant intensity I_R due to the asymmetry (see Fig. 1) arises from two causes: the smaller QE intensity and the weaker transfer from the QE region to the resonant line. The relative transferred intensity is

$$\frac{I_R(\Omega)}{I_R(\Omega)+I_Q(\Omega)}=2\left(\frac{A_0\Delta}{4D}\right)^2(1-\xi^2)\frac{1}{1+(\Omega/\alpha)^2}. \tag{19}$$

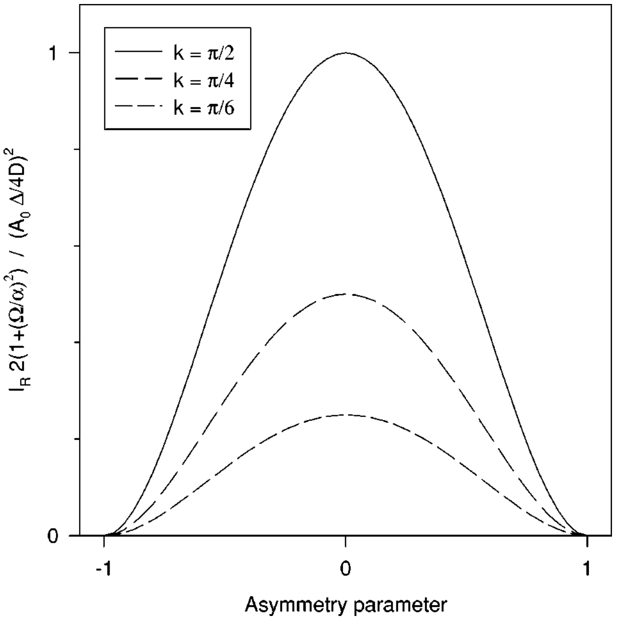

FIG. 1. Resonant intensity as a function of the asymmetry parameter $\xi=(r_+-r_-)/(r_++r_-)$ for the values of $(k\Delta/2)$ specified in the box.

The preceding results deserve a few remarks.

(i) The SR effect itself has no k dependence. The k dependence in the output signal is due exclusively to the varying size of the QE component when $A_0=0$.

(ii) The total intensity in the QE component when $A_0=0$ does not depend on the noise, but the amount transferred to the inelastic output signal grows with increasing α.

(iii) The magnitude of the SR effect increases with the square of the intensity of the output signal, and with the square of the intersite distance.

In the case of a glass, the periodic modulation can be introduced by using either an acoustic wave or a microwave field [6] (techniques for generating ultrasonic waves with Ω's of the order of the hundreds of GHz are currently standard [10]). A measurement of the intensity of the SR line would give us information about the strength of the coupling between the modulation and the scatterer. In a given sample we will usually have a distribution of parameters characterizing the potential where the scatterer oscillates, but all scattering centers will contribute constructively to the same SR line. In a future publication we will discuss how the detailed distribution of scatterer potential parameters influences the intensity of the SR effect.

The Kramers' rates are of the form $r_\pm=r_0\exp[(-V\pm\delta)/D]$, where $D=k_BT$, and V and δ are the barrier height and asymmetry, respectively. For vitreous silica, $r_0\approx 5\times 10^{13}$ Hz, $V=570$ K, and δ has been taken to be up to half the barrier height [11]. We can easily estimate the size of the asymmetry parameters: by assuming that $\delta\delta\approx D\approx 100$ K and that $x_+\approx x_-\approx 0.025$ nm, we obtain $\xi\approx 0.76$ and $\beta\approx 10$ m/s. Finally, let us remark that the range of frequencies and momentum transfers available for neutron scattering experiments is extensive: values of k up to several

$(\text{Å})^{-1}$ and values of ω ranging from the hundreds of MHz well into the THz range are usual. The effective ranges and accuracies of several instruments are described in detail in Ref. [5].

In summary, we have shown that the stochastic resonance phenomenon can be observed in neutron scattering, and that the corresponding signal-to-noise ratio is similar to the one predicted for the power spectrum. We have also determined how potential anisotropies reduce the SR effect.

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