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Excitations in Modulated (Quasi-Periodic) Systems: Collision Induced Effects

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EXCITATIONS IN MODULATED (QUASI-PERIODIC) SYSTEMS: COLLISION INDUCED EFFECTS

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Abstract

It is argued that collision damping of excitations in a modulated (quasi-periodic) system has a pronounced effect on results for the frequency and wave vector dependent response function observed in scattering experiments. Even a relatively small damping can remove all vestige of some of the striking features predicted for the undamped model. Results are obtained for a model that can be solved without approximation in the absence of damping. The latter is introduced by extending the frequency to complex values, and the magnitude of the imaginary component is viewed as the damping control parameter.

1. INTRODUCTION

Systems that essentially depend on two or more length scales display various intriguing properties. In condensed matter and materials research, the best known examples of modulated (quasi-periodic) systems are electrons in a crystal subject to an applied magnetic field, incommensurate crystal phases, and magnets with a longitudinally modulated configuration of the moments. Intriguing properties include an energy spectrum that as a function of the ratio of length scales forms a fractal diagram (Hofstadter butterfly). The fragmentation of the energy spectrum is a key element in the integer Quantum Hall Effect; wave functions of states in a gap are localized while those for a band are extended, the localized states being characterized by a Lyapunov exponent. In view of this, the density of states is highly structured. Similar structure appears in response functions which describe scattering experiments and depend on frequency and wave vector transfers.

In confronting predictions for standard models of modulated systems with experimental data there naturally arises a question as to what extent predicted structure might be degraded by collisions, both between excitations and of excitations with impurities and defects. In an incommensurate crystal the latter can be viewed as generating a finite distribution of length scales, and an energy spectrum which is a union of many similar spectra. Hence, singular features in response functions for simple systems might be blurred by collisions, together with some filling of the band gaps. Since all materials contain impurities and defects to some greater or lesser extent, and thermally activated collisions between excitations are usually present, there is interest in gauging the influence of collisions on response functions for modulated (quasi-periodic) systems.

The existence of closed analytic expressions for response functions of some models of modulated systems affords a route to a first step toward appreciating the nature of collision induced effects. The proposed modification of the theory is accomplished by adding to the excitation energy an imaginary part. The form for including collision damping satisfies causality, and therefore ensures that the poles of the propagator (Green function) occur only in the lower half-plane of the complex frequency. It is found that a modest value for the collision damping parameter (γ) leads to significant changes in the shape and structure of response functions.

An alternative calculation to the proposed use of a phenomenological damping parameter is to solve a specific model of a mixed system, with an underlying modulated structure. For example, a realistic model for lattice vibrations in a mixed mass incommensurate crystal can be constructed from the solution of a model with a single mass defect (Lovesey and Westhead 1990) combined with the average T-matrix approximation. However, findings from studies of mixed commensurate systems lead us to expect the phenomenological approach to produce the salient features induced by collisions.

One motivation for the present study is the marked discrepancy between predictions for a standard model of a modulated magnet and available experimental data; erbium metal possibly supports a longitudinally modulated phase when the temperature is fractionally less than the critical temperature. Experimental data for this phase, obtained by inelastic neutron scattering (Nicklow and Wakabayashi 1982), bears little resemblance to results for a standard model (Lantwin 1990). The predicted dynamic structure is remarkably robust with respect to reasonable variations in the parameters (exchange and anistropy energies) and Lantwin (1990) was unable to find satisfactory agreement between theoretical and experimental findings. While the quality of the experimental data can be much improved, using state of the art instrumentation and data analysis methods (R.M. Nicklow and J.A. Fernandez-Baca, private communication), nonetheless it is likely that in erbium at an elevated temperature there is some effect on the neutron scattering response from thermally activated collisions between spin excitations. Collision damping is predicted to modify the dynamic structure such that it is more like the experimental data than without damping, but reservations about the quality of the data and precise magnetic structure of erbium metal (R.A. Cowley, private communication) mean that, at this moment, a confrontation of theory and experimental results has minimal value. Rather, the present work will be useful in analysing future data on well characterized modulated magnets. In this context, the compound $Pr\ Ni_2\ Si_2$ orders at 20K in a modulated structure which remains stable to extremely low temperatures owing to the existence of a non-magnetic singlet as the crystal-field ground state (Blanco et al. 1991).

The phenomenological treatment of collisions discussed here should be useful in the interpretation of response functions for any modulated system. In general, the damping parameter will depend on the system's characteristics and temperature, magnetic field etc. Before giving details of the calculation it is perhaps worth mentioning that the present treatment produces collision induced features which depend on both the frequency and wave vector, i.e. they have a non-trivial structure. Moreover, because of the singular nature of the spectrum of undamped fluctuations, it is not sufficient to calculate the collisional self-energy to leading-order in the damping parameter. Such a scheme, while adequate for most conventional systems, when applied to a modulated system produces spurious effects. Couched in a slightly different language, it is essential to preserve the full algebraic structure of the response function.

A theory for the response function of a standard model of a modulated system is briefly surveyed in the following section. A minimum of detail is given since the theory has recently been reviewed (Lovesey, Watson and Westhead 1991). The phenomenological treatment of collision damping is given in §3, and an example developed in §4. Results are discussed in §5.

2. RESPONSE FUNCTION

In order to minimize the textual material, it seems wise to focus on just one of the models mentioned in the introduction. We choose a standard model for transverse spin fluctuations in a modulated magnet, and follow the notation used by Lovesey (1988). In the absence of the longitudinal modulation of the configuration of magnetic moments, the transverse spin fluctuation spectrum is exhausted by spin wave excitations which are strongly dispersive. Even a very long range modulation of the magnetic moments removes the strong dispersion, and produces a finite intensity at zero frequency and a singular fragmented structure at finite frequencies.

When the external wave vector $\boldsymbol{q}$ is parallel to the modulation wave vector $\boldsymbol{Q}$, the equation of motion for spin-flip operators reduces to a second-order difference equation with coefficients (n an integer)

$$W_n = 1 + \alpha\, cos(q+nQ) + \beta\, cos2(q+nQ)\ , \tag{2.1}$$

in which the energy parameters α, β are related through

$$\alpha / \beta = -4\, cos\, Q\ . \tag{2.2}$$

The response function is obtained from a propagator, or Green function, expressed in terms of two infinite continued fractions in which the coefficients are,

$$t_n^2 = W_n W_{n+1}\ . \tag{2.3}$$

Manipulation of the continued fractions is made easier by expressing them in terms of two sets of polynomials (in the frequency of ω) derived from the common recursion relation,

$$R_n = \omega\, R_{n-1} - t_{n-1}^2\, R_{n-2}\ . \tag{2.4}$$

The two sets of polynomials $\{A_n\}$, $\{B_n\}$ are distinguished by their initial values, namely,

$$A_{-1} = B_o = 1 \quad and\; A_o = B_{-1} = O \;. \tag{2.5}$$

At this juncture it might be observed that the problem defined is very amenable to numerical methods. Efficient algorithms exist for the diagonalization of tri-diagonal matrices, or the straightforward calculation of $\{A_n\}$, $\{B_n\}$ from (2.4). Such a method inevitably means that results are for a rational value of Q, and presumably approximate closely to those for an irrational (incommensurate) value. This is confirmed in calculations made with numbers from a Fibonacci sequence which converge to an irrational. Use of successively higher order rational approximates generate increasingly fine structure in the response function. Hence, beyond a certain point the additional structure is possibly of only mathematical interest, since it is not likely to be resolved in an experiment. Hofstadter's viewpoint was that common sense tells that there can be no physical effect stemming from the irrationality of some parameter (Hofstadter 1976).

A numerical method is tantamount to using

$$Q = 2\pi M / N \tag{2.6}$$

where M and N are (coprime) integers. With this representation for the modulation wave vector t_n is N-fold periodic, i.e. $t_n = t_{n+N}$. In consequence, the continued fractions required for the propagator are fixed points of a fractional linear transformation, and the propagator can be expressed in closed analytic form. Note that the algebraic method referred to makes no use of translational invariance of the lattice on which the magnetic atoms are arranged, for this invariance is not present in the incommensurate magnet that is being modelled. Use of translational invariance and the representation (2.6) for Q leads to a response function which is zero everywhere except at the N normal mode frequencies.

The propagator which describes transverse spin fluctuations in a modulated magnet is conveniently expressed in terms of the function,

$$L_N(\omega) = (2\Omega_N)^2 - (A_{N-1}(\omega) + B_N(\omega))^2 \;, \tag{2.7}$$

where

$$\Omega_N = t_o t_1 \ldots t_{N-1} \;,\; N \geq 2 \;. \tag{2.8}$$

If we denote the propagator by $G(\omega)$ then the response function observed in an experiment is,

$$Im.\,G(\omega)=\begin{cases} O & ;\ L_N(\omega)\le O \\ (-\omega\chi/2)\left|B_{N-1}(\omega)\right|\left\{L_N(\omega)\right\}^{-\frac{1}{2}}; & L_N(\omega)>O\ . \end{cases} \tag{2.9}$$

In this expression, $\chi = 2S/W_o$ is the wave vector dependent susceptibility (S is the magnitude of the spin moment) and the imaginary part of G is calculated with the rule $\omega \to \omega + i\eta$ and $\eta \to O^+$.

$L_N(\omega)$ is a polynomial in ω of degree $2N$ and $L_N(\omega) = O$ has only real roots. A band (gap) is defined by $L_N(\omega) > O(\le O)$. For N even (odd) there are N-1(N) bands, and $B_{N-1}(\omega)$ is of one sign in a band. Additional properties of the spectrum together with several specific examples of $Im.G(\omega)$ can be found in papers by Lovesey (1988) and Lantwin (1990). It is usually the case that $Im.G(\omega)$ is singular at the band edges; such behaviour is difficult to extract from numerical work, and indeed the existence of the singularities makes the correct calculation of $Im.G(\omega)$ quite a subtle numerical problem. One example of the spectrum of spin fluctuations in an (undamped) modulated magnet is provided in Fig. (1).

3. COLLISION DAMPING

As mentioned in §1, it is entirely possible to convincingly analyse some specific models of collision damping, such as that generated by substitutional defects. Damping due to collisions between excitations is usually a more demanding theoretical task. An alternative viewpoint is to introduce into the theory a phenomenological damping parameter (γ) and model collisional effects by complexification $\omega \to \omega + i\gamma$ of the exact analytic expressions provided in §2. Such a scheme is justified when there is no experimental evidence to favour a specific mechanism. In the present case, of fluctuations in modulated (quasi-periodic) system, it is a sensible method by which to gauge effects of collision damping in models of observed response functions. It will be shown that our treatment of damping predicts non-trivial changes in the spectra.

The choice of sign for $\gamma \ge O$ in complexification of the theory ensures that the poles of the propagator (Green function) occur only in the lower half-plane of the complex frequency. Introduction of a damping parameter is, of course, very familiar in quantum mechanics in the form of pole-avoidance. In the present context, it is worth mentioning that, $\gamma > O$ ensures convergence of the temporal Fourier-Laplace transform of the causal Green function used in our formulation of the theory.

The appropriate prescription for the response function is relatively simple. Let us define

$$b(\omega) = b_1(\omega) + ib_2(\omega) = -L_N(\omega + i\gamma) \ , \tag{3.1}$$

and

$$a(\omega) = a_1(\omega) + ia_2(\omega) = B_{N-1}(\omega + i\gamma) \ . \tag{3.2}$$

Straightforward algebra then yields for the spectrum the following result,

$$Im.\left(a/\sqrt{b}\right) = (a_2 e_1 - a_1 e_2)\left\{b_1^2 + b_2^2\right\}^{-\frac{1}{2}} \ , \tag{3.3}$$

where

$$e_1 = (b_2 / 2e_2) \ , \tag{3.4}$$

and

$$e_2 = \left\{\tfrac{1}{2}\left[\sqrt{}\left(b_1^2 + b_2^2\right) - b_1\right]\right\}^{\frac{1}{2}} \ . \tag{3.5}$$

Note that a_2, b_2 and e_1 vanish in the limit $\gamma \to O$, in which case we recover the expression used in previous studies. For e_1 and e_2 there is a common phase factor (± 1) not displayed in (3.4) and (3.5) about which we have more to say later.

The functions b_1 (ω) = - L_N (ω) and a_1 (ω) = $B_{N\text{-}1}$ (ω) are derived by using the recursion relations provided in the previous section. It seems that the easiest way to find b_2 (ω) and a_2 (ω) is to expand L_N $(\omega + i\ \gamma)$ and $B_{N\text{-}1}$ $(\omega + i\ \gamma)$ in γ ; b_2 (ω) and a_2 (ω) are polynomials in γ of order ($2N$ - 1) and (N - 2), respectively. It is readily shown that approximating b_2 (ω) and a_2 (ω) by expressions correct to first-order in γ generates spurious effects in the response function. As a result of the dependence of b_2 and a_2 on γ and ω (and the external wave vector q) the contribution of the collision damping to the response function is non-trivial; an example is provided in the following section.

The observed response function is, of course, a quantity which is positive or possibly zero. In our notation, the observed response function is proportional to $\{-\,Im.\ G(\omega)\}$. Now it is easy to show that (3.3) as a function of $\omega \geq O$ is not of one sign. This feature is not a consequence of introducing collision damping, and it persists for $\gamma \to O$. A positive result for $\{-\,Im.\ G(\omega)\}$ is related to the phase factor (± 1) common to e_1 and e_2, which in turn is related to the convergence of the continued fractions in the formal solution for the propagator. This topic is thoroughly discussed by Lovesey and Westhead (1990) and Lovesey, Watson and Westhead (1991). For the present it suffices to say that the correct prescription for the phase of e_2 (and hence e_1) is that which renders $\{-\,Im.\ G(\omega)\}$ positive.

4. EXAMPLE

Consequences of collision damping introduced in §3 have been investigated for several systems. Our findings are illustrated by reporting results for one case, and some of these are displayed in Fig. (1).

We have chosen to report results for the modulated magnetic discussed in §2, taking the particular case $N = 5$. In the absence of damping ($\gamma = O$) the response function ($L_N > O$),

$$F(q,\omega) = -\,Im.G(\omega)/\omega = (\chi/2)\,|B_{N-1}(\omega)|\{L_N(\omega)\}^{-\frac{1}{2}} \tag{4.1}$$

considered as a function of frequency (ω) for a fixed wave vector (q) consists of five bands of intensity. The spectrum is symmetric about $\omega = O$. An example is shown in Fig. (1); additional examples can be found in papers by Lovesey (1988) and Lantwin (1990).

For the set of parameters chosen the undamped spectrum shows inverse square-root singularities at each band edge. It is possible with some special values of q to find the value zero at a band edge. This arises when as the band edge is approached B_{N-1} (ω) vanishes with a power law dependence strong enough to cancel the square-root behaviour of the denominator. The finite value of the spectrum at $\omega = O$ is a universal feature for modulated magnets.

Given that the maximum band edge frequency is 2.00 in our reduced units, a value of $\gamma = 0.10$ is viewed as a relatively small damping parameter. Even so we see in Fig. (1) that, such a damping has a pronounced effect on the spectrum. In particular, there is no vestige of the singular structure at the lowest two band edges (0.570 and 0.641), and the singular structure at 1.466 and 1.749 in the undamped spectrum are reduced to modest sized peaks.

Observe that there is next to no change in the magnitude of the spectrum at $\omega = O$. Turning to results for a larger damping $\gamma = 0.5$, results in Fig. (1) show that the spectrum is reduced to a featureless landscape. Results for other parameter sets, including different values of the periodicity number N, show that results given in Fig. (1) are quite typical, in as much that a small damping profoundly effects low frequency structure found in the undamped spectrum and a modest damping removes most of the structure at all frequencies.

5. DISCUSSION

Results for a model of a modulated (quasi-periodic) system including a collision damping show that damping has a pronounced effect on the frequency spectrum of excitations. While it is to be expected that singular structure in the undamped model is rendered smooth, it is perhaps a surprise that a small damping parameter has quite the dramatic influence demonstrated in Fig. (1). The damping mechanism is a strong function of frequency and the damping parameter. It is shown that a small damping influences low frequency structure more strongly than it does high frequency structure.

A specific (microscopic) model for collision damping is required to estimate the damping parameter γ. Such a model would most likely make γ a function of the external wave vector q. Certainly, it is expected that in representing behaviour in a real material γ must be allowed to depend on temperature, magnetic field, etc.

A recent analysis of the transverse spin fluctuation spectrum of thulium metal at a temperature, close to the ordering temperature, where the structure is thought to be modulated makes no mention of the fundamental signatures predicted for this phase (McEwen et al. 1991). Rather, an interpretation is offered in terms of an approximate analysis of a magnetic model to which phenomenological damping is added. Results from the model are then convoluted with a Gaussian whose width is varied so as to obtain agreement with the data sets, and the total width parameter is at least 20% of the width of the spectrum. In light of the findings based on the exact analysis of a quasi-periodic model provided here (damping) and by Lantwin (1990) (Gaussian resolution broadening) it is clear that a 20% degradation of spectra likely masks distinct signatures of the fundamental fragmented structure. In particular, it would not seem possible to have confidence in a weakly dispersive peak being labelled a crystal-field transition, for just such a feature has been shown to arise in the spectrum of a simple modulated (quasi-periodic) magnet.

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Figure Caption

The frequency spectrum $(-2Im.G(\omega)/\omega\chi)$ of a modulated (quasi-periodic) system is displayed as a function of ω for three values of the damping parameter, namely $\gamma = 0$, 0.1 and 0.5. Other quantities required to specify the model system are $N = 5$, $q = 0.25\pi$, and $\beta = 0.15$ with α determined by (2.2). The data in the figure are generated by (3.3) using the appropriate signs for e_1 and e_2 to yield positive values for the displayed quantity.

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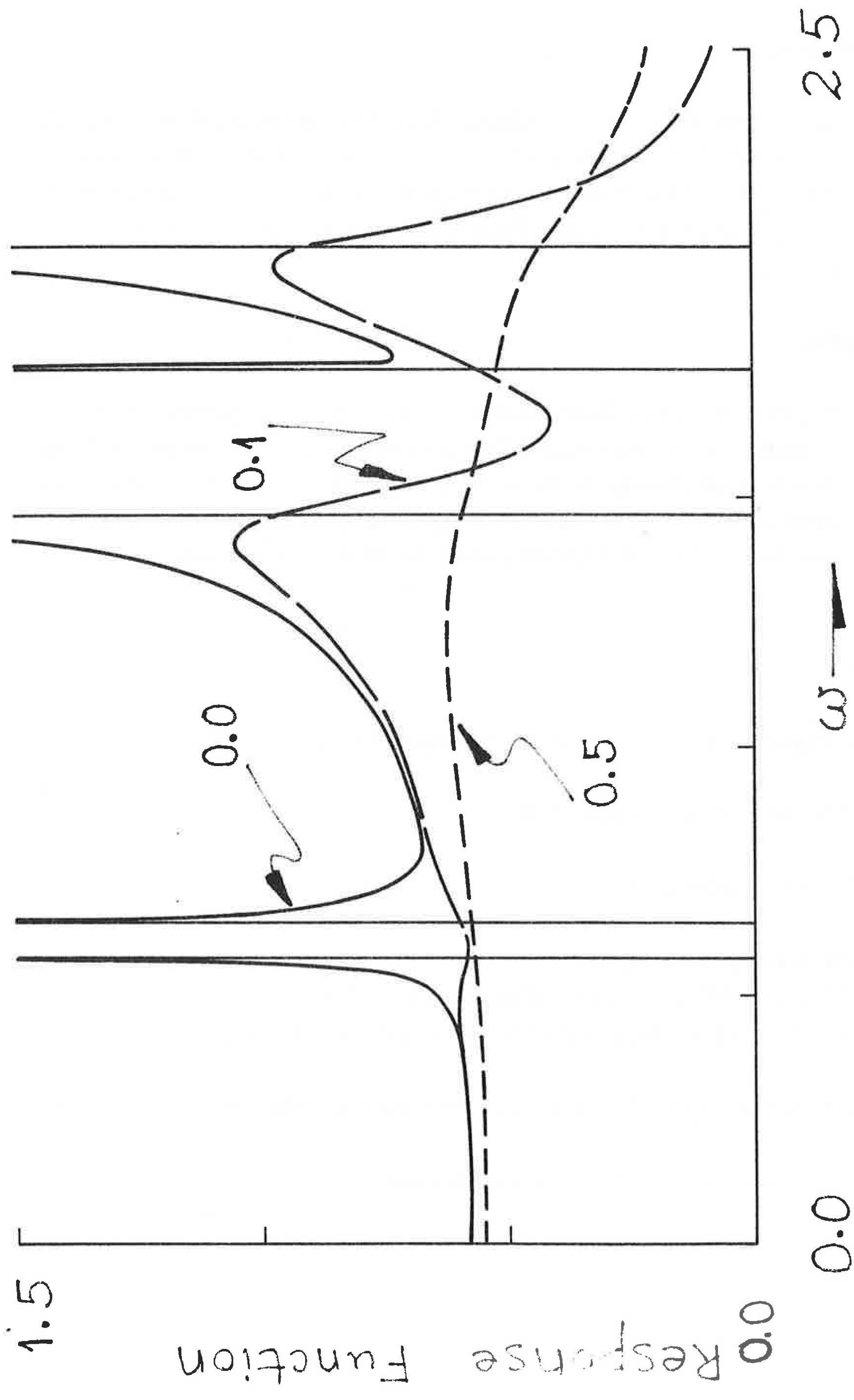

Fig. (1)