On a rotational-invariant dynamic susceptibility for dilute alloys

ON A ROTATIONAL-INVARIANT DYNAMIC SUSCEPTIBILITY FOR DILUTE ALLOYS

BY

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ABSTRACT

General conditions for a rotational invariant susceptibility are derived. The particular case of a single impurity is investigated and a phenomenological susceptibility is observed which is similar but not identical, to that used in localised spin fluctuation theories.

1. Several metallic systems containing spins (isolated impurity, spin glass) have full local rotational (or cubic) invariance at all temperatures. In other words, they never undergo a phase transition to some state of long range magnetic order. A field theoretical treatment of these systems presents important difficulties: One may write an expression in terms of Feynman diagrams, keeping rotational—or crossing—invariance at each order. Such diagrams are complicated to keep track of and no obvious way of isolating and summing a series of dominant diagrams has yet been found. Or one can attempt to find a summable series of diagrams dominating the scattering, but those diagrams are usually not rotationally invariant. An alternative approach, taken in the present paper, consists in looking for a phenomenological expression, which is manifestly rotational invariant but includes the physically dominant process.

This note has two purposes: First to derive generally the necessary and sufficient conditions for the dynamic susceptibility (or precisely the fluctuation or noise spectrum $K^{+-}(\omega)$ mentioned also by Dr. Götze in this conference) to be rotational invariant. Second to obtain this noise spectrum in a particular case, that of a damped spin $\frac{1}{2}$ impurity in a metal which corresponds to the single pole dominance or localized spin fluctuation (*LSF*) treatment of the Anderson model [1].

2. Consider first an impurity S, described by the fluctuation or noise correlation function

$$K^{+-}(t) = \tfrac{1}{2}\langle S^{+}(t)\, S^{-}(0) + S^{-}(0)\, S^{+}(t)\rangle \tag{1}$$

The fluctuation-dissipation theorem relates the Fourier transform of the noise spectrum $K^{+-}(\omega)$ to the imaginary part of the transverse susceptibility ($\hbar = 1$, $\beta = 1/kT$)

$$Im\,\chi^{+-}(\omega) = \tanh \tfrac{1}{2}(\beta\omega)\, K^{+-}(\omega) \tag{2}$$

where $\chi^{+-}(t) = i\,\theta(t)\langle [S^+(t), S^-(0)]_- \rangle$. $K^{+-}(\omega)$ satisfies the hermicity relations

$$K^{+-}(\omega) = K^{+-}(\omega)^* = K^{-+}(-\omega) \geqslant 0 \tag{3}$$

and must be non-negative at all frequencies to insure dissipation of energy. From eq. (2) and the Kramers-Kronig relations, one obtains the static transverse susceptibility

$$\chi^{+-}(0) = \int \frac{d\omega}{\pi} \tanh \frac{\beta\omega}{2} \frac{K^{+-}(\omega)}{\omega} \tag{4}$$

with $\mathrm{Im}\,\chi^{+-}(0) = 0$.

The longitudinal susceptibility is defined as the zero field derivitive of the magnetization $g\,\mu_B \langle S^z \rangle$

$$\chi^z(0) = g\,\mu_B \frac{\partial \langle S^z \rangle}{\partial H_e}\bigg|_{H_e=0} = \frac{\partial \langle S^z \rangle}{\partial \omega_e}\bigg|_{\omega_e=0} \tag{5}$$

where $\omega_e = g\mu_B H_e$. From the identities $-S^z = S^{x2} + S^{y2} - S^+ S^-$, $\langle (S^{x2} + S^{y2}) \rangle = = \int \frac{d\omega}{2\pi} K^{+-}(\omega)$, and a relation between $\langle S^+ S^- \rangle$ and the noise spectrum which can be obtained by a similar spectral decomposition as that used to prove the fluctuation-dissipation theorem (2),

$$\langle S^+ S^- \rangle = \int \frac{d\omega}{2\pi}\left(1 + \tanh \frac{\beta\omega}{2}\right) K^{+-}(\omega) \tag{6}$$

one obtains

$$\langle S^z \rangle = \int \frac{d\omega}{2\pi} \tanh \frac{\beta\omega}{2} K^{+-}(\omega) \tag{7}$$

Rotational invariance implies $\langle S^z \rangle = 0$ in the absence of an external field, at any temperature, hence our first condition,

$$K^{+-}(\omega;\, \omega_e = 0) = K^{+-}(-\omega;\, \omega_e = 0) \tag{I}$$

Moreover,

$$\chi^z = \int \frac{d\omega}{2\pi} \tanh \frac{\beta\omega}{2} \frac{\partial K^{+-}(\omega)}{\partial \omega_e}\bigg|_{\omega_e=0} \tag{9}$$

Rotational invariance requires that $\chi^z(0) = \frac{1}{2}\chi^{+-}(0)$ at all temperatures, thus,

$$K^{+-}(\omega)\Big|_{\omega_e=0} = \omega \frac{\partial K^{+-}(\omega)}{\partial \omega_e}\Bigg|_{\omega_e=0} \tag{II}$$

Equations I and II form the general conditions of rotational invariance on the noise spectrum.

3. Consider now the particular case of a spin $\frac{1}{2}$ impurity precessing in an external field and losing correlation at a rate Γ (which varies with the external field at most as $\Gamma = \Gamma_0 + 0(\omega_e^2)$). With the initial condition $K^{+-}(t{=}0) = \frac{1}{2}$ for spin $\frac{1}{2}$, the simplest noise correlation function can be written as

$$K^{+-}(t) = \tfrac{1}{2}\, e^{-i\omega_e t}\, e^{-\Gamma|t|} \tag{10}$$

and the spectrum is

$$K^{+-}(\omega) = \frac{\Gamma}{(\omega - \omega_e)^2 + \Gamma^2} \tag{11}$$

Clearly, this is *not* rotational invariant. Indeed, from (4) and (9), and after integrating term by term the expansion of the tanh around its poles, one obtains ($\Gamma = \Gamma_0$)

$$\chi^z = \frac{\beta}{2\pi^2}\psi'\left(\tfrac{1}{2} + \frac{\beta\Gamma}{2\pi}\right) \tag{12}$$

which remains finite at $T = 0$, whereas

$$\tfrac{1}{2}\chi^{+-} = \frac{1}{\pi\Gamma}\left[\psi\left(\tfrac{1}{2} + \frac{\beta\Gamma}{2\pi}\right) - \psi\left(\tfrac{1}{2}\right)\right] \tag{13}$$

diverges logarithmically at $T = 0$. ψ is the logarithmic derivative of Euler's gamma function. The two susceptibilities are similar only when $kT > \Gamma$ where they follow a Curie-Weiss law. There is however, a factor 2 discrepancy in their respective Curie temperatures which are $\theta^z = 2\theta^{+-} = -\Gamma\,|\,\psi''(\tfrac{1}{2})\,|\,/\,\pi^3 \simeq -\tfrac{1}{2}\Gamma$. When $kT < \Gamma$, χ^z falls below the Curie-Weiss curve whereas χ^{+-} rises above it.

4. The spectral density (11) is identical to that introduced in the localised spin fluctuation approximation of the Anderson model in an attempt to solve the Kondo problem [2, 3] [1]. A single pole dominating the scattering of a d electron and a d hole of opposite spin is equivalent to a unique lifetime for a transverse spin fluctuation described by (10). The relation between fluctuation spectrum and transverse susceptibility has been actually the original approach to *LSF* by Lederer and Mills [4].

[1] The *LSF* thermal propagator $(i\omega_n \pm i\Gamma)^{-1}$ is written in term of the spectral density $\rho(\omega)$ as $(i\omega_n \pm i\Gamma)^{-1} = \int d\omega \rho(\omega)/(i\omega_n - \omega)$ It then follows that $\pi\rho(\omega) = K^{+-}(\omega)$.

It can be shown [5] that the single pole dominance approximation describes satisfactorily the physics of the Kondo problem. Moreover, in the $U = 0$ limit of the Anderson model, the susceptibility is given *exactly* by eq. (12) ([3], p. 58; see also [6]). Indeed, the susceptibility for $U = 0$ can be written as

$$\chi^z = \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \mathcal{N}(\omega) \tag{14}$$

as in any non-interacting electron gas, where $\mathcal{N}(\omega) = \Delta / \pi (\omega^2 + \Delta^2)$ is the electronic density of states including a virtual bound state of width Δ and $f(\omega) = \frac{1}{2}\left(1 - \tanh \frac{\beta\omega}{2}\right)$ is the Fermi distribution function. Integrating by part, one obtains eq. (12) with the spin correlation time Γ^{-1} corresponding to the life time Δ^{-1} of an electron in the virtual bound state. These facts have enabled the author to write the same susceptibility for $U \neq 0$, i.e. when $\Gamma < \Delta$ [2, 3]. Subsequently, scaling from the Toulouse limit [7] of the $J\,S.\sigma$ model where, for some value of the coupling constant J this model is thermodynamically identical to the $U = 0$ Anderson model, *K D.* and *U.* Schotte [6] have reached the same conclusion.

We have therefore in the single pole dominance an approximation which

(i) includes most of the physics of the Kondo effect

(ii) yields an exact expression for χ^z in the $U = 0$ limit. But the simplest spectrum (11) is *not* rotational invariant and this precludes renormalizability of the theory [1]. We want therefore a spectrum which combines rotational invariance with simple scaling to the $U = 0$ limit and with the simple physical interpretation summarized by (10). Thus, writing, to preserve the form (12) of the susceptibility,

$$K^{+-}(\omega) = \frac{\Gamma}{(\omega - \omega_e)^2 + \Gamma^2} + \text{even function of } \omega_e \tag{15}$$

we obtain unambiguously, using condition II, the rotational invariant spectrum,

$$K^{+-}(\omega)\Big|_{\omega_e = 0} = \frac{2\,\Gamma\,\omega^2}{(\Gamma^2 + \omega^2)^2} \tag{16}$$

and the susceptibility

$$\chi^z = \tfrac{1}{2}\chi^{+-} = \frac{\beta}{2\pi^2}\,\psi'\left(\tfrac{1}{2} + \frac{\beta\Gamma}{2\pi}\right) \tag{17}$$

[1] Rotational invariance is associated to crossing invariance in the Anderson model since the longitudinal susceptibility belongs to the *t* channel when the transverse susceptibility dominates the *s* channel. The *u* channel describes then the scattering of two *d* electrons of opposite spins and is a self-regulating mechanism renormalizing *U*. A self-consistent theory must therefore be crossing invariant.

An identical expression is obtained for the susceptibility of some spin glasses [9], where Γ is the width of the distribution of local molecular fields $P(H)$.

By Fourier transform, one obtains the correlation function,

$$K^{+-}(t) = \tfrac{1}{2}(1 - \Gamma \mid t \mid) e^{-\Gamma |t|} \tag{18}$$

where the unique relaxation term is apparent. Eq. (18) is no longer a solution of the Bloch equation, but that of the second order differential equation representing a harmonic oscillator critically damped at a rate Γ, with initial condition and the requirement that the fluctuations average to zero, i.e. $\int dt\, K^{+-}(t) = K^{+-}(\omega=0) = 0$. Finally, for $\Gamma = 0$, one checks that (16) reduces to the well-known spectrum $K^{+-}(\omega) = -\omega \dfrac{d\,\delta(\omega)}{d\omega} = \delta(\omega)$.

5. We have obtained in (16) a simple phenomenological expression for the noise spectrum of a rotational invariant system. The importance of this result is that it enables us to construct a propagator for some collective excitation of the many-body system (the *LSF*) which has the required symmetry of the system. This symmetry requirement on the propagator is essential for the self-consitence or renormalizability of a field theory which includes this propagator. The spectrum (16) should yield a renormalizable theory of the Kondo effect, but this last step remains to be done.

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Note added in proof.

Recently, J. R. G. Armytage (Thesis, Cambridge 1974) has obtained by scaling the $J\, S.\sigma$ model an expression for χ^z at all temperatures. It differs from our eq. (12) at high temperatures where χ^z deviates first above the Curie-Weiss curve before falling below it, a deviation which could be obtained by perturbation theory. See also the Mössbauer measurements of P. Steiner (Proc. Disk. Kondo Effekt, F. U. Berlin, Dec. 73, fig. 6) on *Cu* Fe.

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