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QUANTUM PROTECTORATE AND MICROSCOPIC MODELS OF MAGNETISM

A. L. KUZEMSKY

Bogoliubov Laboratory of Theoretical Physics,
Joint Institute for Nuclear Research,
141980 Dubna, Moscow Region, Russia
kuzemsky@thsun1.jinr.ru
http://thsun1.jinr.ru/∼kuzemsky

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Some physical implications involved in a new concept, termed the "quantum protectorate" (QP), are developed and discussed. This is done by considering the idea of quantum protectorate in the context of quantum theory of magnetism. It is suggested that the difficulties in the formulation of quantum theory of magnetism at the microscopic level, that are related to the choice of relevant models, can be understood better in the light of the QP concept. We argue that the difficulties in the formulation of adequate microscopic models of electron and magnetic properties of materials are intimately related to dual, itinerant and localized behaviour of electrons. We formulate a criterion of what basic picture describes best this dual behaviour. The main suggestion is that quasi-particle excitation spectra might provide distinctive signatures and good criteria for the appropriate choice of the relevant model.

Keywords: Quantum theory of magnetism; conservation laws; neutron scattering.

1. Introduction

It is well known that there are many branches of physics and chemistry where phenomena occur which cannot be described in the framework of interactions amongst a few particles.[1] As a rule, these phenomena arise essentially from the cooperative behavior of a large number of particles. Such many-body problems are of great interest not only because of the nature of phenomena themselves, but also because of the intrinsic difficulty in solving problems which involve interactions of many particles in terms of known Anderson statement that "more is different".[2] It is often difficult to formulate a fully consistent and adequate microscopic theory of complex cooperative phenomena. In Ref. 3, the authors invented an idea of a quantum protectorate, "a stable state of matter, whose generic low-energy properties are determined by a higher-organizing principle and nothing else".[3] This idea brings into physics the concept that reminds the uncertainty relations of quantum mechanics. The notion of QP was introduced to unify some generic features of complex physical systems on different energy scales, and is a certain reformulation of the conservation laws and

symmetry breaking concepts.[4] As typical examples of QP, the crystalline state, the Landau-Fermi liquid, the state of matter represented by conventional metals and normal ^{3}He (cf. Refs. 6 and 7), and the quantum Hall effect were considered. The sources of quantum protection in high-T_c superconductivity and low-dimensional systems were discussed in Refs. 8–10. According to Anderson,[8] "the source of quantum protection is likely to be a collective state of the quantum field, in which the individual particles are sufficiently tightly coupled that elementary excitations no longer involve just a few particles, but are collective excitations of the whole system. As a result, macroscopic behavior is mostly determined by overall conservation laws". In the same manner the concept of a spontaneous breakdown of symmetry enters through the observation that the symmetry of a physical system could be lower than the symmetry of the basic equations describing the system.[4,5] This situation is encountered in non-relativistic statistical mechanics. A typical example is provided by the formation of a crystal which is not invariant under all space translations, although the basic equations of equilibrium mechanics are. In this article, I will attempt to relate the term of a quantum protectorate and the foundations of quantum theory of magnetism. I will not touch the low-dimensional systems that were discussed already comprehensively in Refs. 8–10. I concentrate on the problem of choosing the most adequate microscopic model of magnetism of materials and, in particular, related to the duality of localized and itinerant behavior of electrons where the microscopic theory meets the most serious difficulties. To justify this statement and to introduce all necessary notions that are relevant for the present discussion, we very briefly recall the basic facts of the microscopic approach to magnetism.

2. Magnetic Degrees of Freedom

The discussion in this paper is concentrated on the right definition of the fundamental "magnetic" degrees of freedom and their correct model description for complex magnetic systems. We shall first describe the phenomenology of the magnetic materials to look at the physics involved. The problem of identification of the fundamental "magnetic" degrees of freedom in complex materials is rather nontrivial. Let us discuss briefly, to give a flavor only, the very intriguing problem of the electron dual behavior. The existence and properties of localized and itinerant magnetism in insulators, metals, oxides and alloys and their interplay in complex materials is an interesting and not yet fully understood problem of quantum theory of magnetism.[11,12] The central problem of recent efforts is to investigate the interplay and competition of the insulating, metallic, superconducting, and heavy fermion behavior versus the magnetic behavior, especially in the vicinity of a transition to a magnetically ordered state. The behavior and the true nature of the electronic and spin states and their quasi-particle dynamics are of central importance to the understanding of the physics of strongly correlated systems such as magnetism and metal–insulator transition in metals and oxides, heavy fermion

states, superconductivity and their competition with magnetism.[13] The strongly correlated electron systems are systems in which electron correlations dominate. An important problem in understanding the physical behavior of these systems was the connection between relevant underlying chemical, crystal and electronic structure, and the magnetic and transport properties which continue to be the subject of intensive debates.[14] Strongly correlated d and f electron systems are of special interest.[15] In these materials electron correlation effects are essential and, moreover, their spectra are complex, i.e. have many branches. Importance of the studies on strongly correlated electron systems are concerned with a fundamental problem of electronic solid state theory, namely, with a tendency of $3(4)d$ electrons in transition metals and compounds and $4(5)f$ electrons in rare-earth metals and compounds and alloys to exhibit both localized and delocalized behavior.[11,16] Many electronic and magnetic features of these substances relate intimately to this dual behavior of the relevant electronic states. For example, there are some alloy systems in which radical changes in physical properties occur with relatively modest changes in chemical composition or structural perfection of the crystal lattice.[15] Due to competing interactions of comparable strength, more complex ground states than usually supposed may be realized. The strong correlation effects among electrons, which lead to the formation of the heavy fermion state take part to some extent in formation of a magnetically ordered phase, and thus imply that the very delicate competition and interplay of interactions exist in these substances.[17] For most of the heavy fermion superconductors, cooperative magnetism, usually some kind of antiferromagnetic ordering was observed in the "vicinity" of superconductivity. In the case of U-based compounds, the two phenomena, antiferromagnetism and superconductivity coexist on a microscopic scale, while they seem to compete with each other in the Ce-based systems.[18] For a Kondo lattice system, the formation of a Néel state via the RKKY intersite interaction compete with the formation of a local Kondo singlet. Recent data for many heavy fermion Ce- or U-based compounds and alloys display a pronounced non-Fermi-liquid behavior. A number of theoretical scenarios have been proposed and they can be broadly classified into two categories which deal with the localized and extended states of f-electrons. Of special interest is the unsolved controversial problem of the reduced magnetic moment in Ce- and U-based alloys and the description of the heavy fermion state in the presence of the coexisting magnetic state. In other words, the main interest is in the understanding of the competition of intra-site (Kondo screening) and inter-site (RKKY exchange) interactions. Depending on the relative magnitudes of the Kondo and RKKY scales, materials with different characteristics are found which are classified as non-magnetic and magnetic concentrated Kondo systems. The latter, "Kondo magnets", are of main interest.[15] Furthermore, there are effects which have a very complicated and controversial origin. There are some experimental evidences that peculiar magnetism of some quasi-ternary heavy fermion alloys is not that of localized systems, but have some features of band magnetism. Thus, in

addition to the pronounced non-Fermi-liquid effects in thermodynamic and transport properties, the outstanding problems include small magnetic moments and possible transitions from a localized moment ordered phase to a kind of "heavy fermion band magnet".[19–21] These features reflect the very delicate interplay and competition of interactions and changes in a chemical composition. As a rule, very little intuitive insight could be gained from this very complicated behavior. The QP is an umbrella term for a theoretical approach which seems designed specifically to analyze such problems.

3. Microscopic Picture of Magnetism in Materials

In this section we recall the foundations of the quantum theory of magnetism in a sketchy form. Magnetism in materials such as iron and nickel results from the cooperative alignment of the microscopic magnetic moments of electrons in the material. The interactions between the microscopic magnets are described mathematically by the form of the Hamiltonian of the system. The Hamiltonian depends on some parameters, or coupling constants, which measure the strength of different kinds of interactions. The magnetization, which is measured experimentally, is related to the average or mean alignment of the microscopic magnets. It is clear that some of the parameters describing the transition to the magnetically ordered state do depend on the detailed nature of the forces between the microscopic magnetic moments. The strength of the interaction will be reflected in the critical temperature which is high if the aligning forces are strong and low if they are weak. In quantum theory of magnetism, the method of model Hamiltonians has proved to be very effective. Without exaggeration, one can say that the great advances in the physics of magnetic phenomena are to a considerable extent due to the use of very simplified and schematic model representations for the theoretical interpretation.

3.1. *Heisenberg model*

The Heisenberg model is based on the assumption that the wave functions of magnetically active electrons in crystals differ little from the atomic orbitals. The physical picture can be represented by a model in which the localized magnetic moments originating from ions with incomplete shells interact through a short-range interaction. Individual spin moments form a regular lattice. The model of a system of spins on a lattice is termed the Heisenberg ferromagnet[22] and establishes the origin of the coupling constant as the exchange energy. The Heisenberg ferromagnet in a magnetic field H is described by the Hamiltonian

$$H = -\sum_{ij} J(i–j)\mathbf{S}_i \cdot \mathbf{S}_j - g\mu_{\mathrm{B}} H \sum_i S_i^z \,. \tag{1}$$

The coupling coefficient $J(i–j)$ is the measure of the exchange interaction between spins at the lattice sites i and j and is defined usually to have the property $J(i–j = 0) = 0$. This constraint means that only the inter-exchange interactions

are taken into account. The coupling, in principle, can be of a more general type (non-Heisenberg terms). For crystal lattices in which every ion is at the centre of symmetry, the exchange parameter has the property

$$J(i–j) = J(j–i)\,.$$

We can rewrite then the Hamiltonian (1) as

$$H = -\sum_{ij} J(i–j)(S_i^z S_j^z + S_i^+ S_j^-)\,. \tag{2}$$

Here $S^\pm = S^x \pm iS^y$ are the raising and lowering spin angular momentum operators. The complete set of spin commutation relations is

$$[S_i^+, S_j^-]_- = 2S_i^z\delta_{ij}; \qquad [S_i^+, S_i^-]_+ = 2S(S+1) - 2(S_i^z)^2;$$
$$[S_i^\mp, S_j^z]_- = \pm S_i^\mp \delta_{ij}; \qquad S_i^z = S(S+1) - (S_i^z)^2 - S_i^- S_i^+;$$
$$(S_i^+)^{2S+1} = 0, \qquad (S_i^-)^{2S+1} = 0\,.$$

We omit the term of interaction of the spin with an external magnetic field for the brevity of notation. The statistical mechanical problem involving this Hamiltonian was not exactly solved, but many approximate solutions were obtained.

To proceed further, it is important to note that for the isotropic Heisenberg model, the total z-component of spin $S_{\text{tot}}^z = \sum_i S_i^z$ is a constant of motion, i.e.

$$[H, S_{\text{tot}}^z] = 0\,. \tag{3}$$

There are cases when the total spin is not a constant of motion, as, for instance, for the Heisenberg model with the dipole terms added.

Let us define the eigenstate $|\psi_0\rangle$ so that $S_i^+|\psi_0\rangle = 0$ for all lattice sites $\mathbf{R}_i$. It is clear that $|\psi_0\rangle$ is a state in which all the spins are fully aligned and for which $S_i^z|\psi_0\rangle = S|\psi_0\rangle$. We also have

$$J_{\mathbf{k}} = \sum_i e^{(i\mathbf{k}\cdot\mathbf{R}_i)} J(i) = J_{-\mathbf{k}}\,,$$

where the reciprocal vectors $\mathbf{k}$ are defined by cyclic boundary conditions. Then we obtain

$$H|\psi_0\rangle = -\sum_{ij} J(i–j)S^2 = -NS^2 J_0\,.$$

Here N is the total number of ions in the crystal. So, for the isotropic Heisenberg ferromagnet, the ground state $|\psi_0\rangle$ has an energy $-NS^2J_0$.

The state $|\psi_0\rangle$ corresponds to a total spin NS.

Let us consider now the first excited state. This state can be constructed by creating one unit of spin deviation in the system. As a result, the total spin is $NS-1$. The state

$$|\psi_k\rangle = \frac{1}{\sqrt{2SN}} \sum_j e^{(i\mathbf{k}\cdot\mathbf{R}_j)} S_j^- |\psi_0\rangle$$

is an eigenstate of H which corresponds to a single magnon of the energy

$$E(q) = 2S(J_0 - J_q)\,. \tag{4}$$

Note that the role of translational symmetry, i.e. the regular lattice of spins, is essential, since the state $|\psi_k\rangle$ is constructed from the fully aligned state by decreasing the spin at each site and summing over all spins with the phase factor $e^{i\mathbf{k}\cdot\mathbf{R}_j}$ (we consider the 3-dimensional case only). It is easy to verify that

$$\langle\psi_k|S^z_{\rm tot}|\psi_k\rangle = NS - 1\,.$$

The above consideration was possible because we knew the exact ground state of the Hamiltonian. There are many models where this is not the case. For example, we do not know the exact ground state of a Heisenberg ferromagnet with dipolar forces and the ground state of the Heisenberg antiferromagnet.

3.2. *Itinerant electron model*

E. Stoner has proposed an alternative, phenomenological band model of magnetism of the transition metals in which the bands for electrons of different spins are shifted in energy in a way that is favorable to ferromagnetism. The band shift effect is a consequence of strong intra-atomic correlations. The itinerant-electron picture is the alternative conceptual picture for magnetism.[23,24] It must be noted that the problem of antiferromagnetism is a much more complicated subject.[25] The antiferromagnetic state is characterized by a spatially changing component of magnetization which varies in such a way that the net magnetization of the system is zero. The concept of antiferromagnetism of localized spins, which is based on the Heisenberg model and two-sublattice Néel ground state, is relatively well founded contrary to the antiferromagnetism of delocalized or itinerant electrons. In relation to the duality of localized and itinerant electronic states, G. Wannier showed the importance of the description of the electronic states which reconcile the band and local (cell) concept as a matter of principle.

3.3. *Hubbard model*

There are big difficulties in the description of the complicated problem of magnetism in a metal with the d band electrons which are really neither "local" nor "itinerant" in a full sense. The Hubbard model[12] is in a certain sense an intermediate model (the narrow-band model) and takes into account the specific features of transition metals and their compounds by assuming that the d electrons form a band, but are subject to a strong Coulomb repulsion at one lattice site. The Hubbard Hamiltonian is of the form[26,27]

$$H = \sum_{ij\sigma} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}\,. \tag{5}$$

It includes the intra-atomic Coulomb repulsion U and the one-electron hopping energy t_{ij}. The electron correlation forces electrons to localize in the atomic orbitals

which are modelled here by a complete and orthogonal set of the Wannier wave functions $[\phi(\mathbf{r}-\mathbf{R}_j)]$. On the other hand, the kinetic energy is reduced when electrons are delocalized. The band energy of Bloch electrons $\epsilon_{\mathbf{k}}$ is defined as follows:

$$t_{ij} = N^{-1} \sum_k \epsilon_k^d e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \tag{6}$$

where N is the number of lattice sites. This conceptually simple model is mathematically very complicated.[26,27] The Pauli exclusion principle which does not allow two electrons of common spin to be at the same site, plays a crucial role. It can be shown, that under transformation RHR^+, where R is the spin rotation operator

$$R = \bigotimes_j \exp\left(\frac{1}{2} i\phi \boldsymbol{\sigma}_j \cdot \mathbf{n}\right) \tag{7}$$

the Hubbard Hamiltonian is invariant under spin rotation, i.e. $RHR^+ = H$. Here ϕ is the angle of rotation around the unitary axis $\mathbf{n}$ and $\boldsymbol{\sigma}$ is the Pauli spin vector; symbol $\bigotimes_j$ indicates a tensor product over all site subspaces. The summation over j extends to all sites.

The equivalent expression for the Hubbard model that manifests the property of rotational invariance explicitly can be obtained with the aid of the transformation

$$\mathbf{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} a_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} a_{j\sigma'} \,. \tag{8}$$

Then the second term in (5) takes the following form

$$n_{i\uparrow} n_{i\downarrow} = \frac{n_i}{2} - \frac{2}{3}\mathbf{S}_i^2 \,.$$

As a result we get

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i \left(\frac{n_i^2}{4} - \frac{1}{3}\mathbf{S}_i^2\right) . \tag{9}$$

The total z-component S_{tot}^z commutes with Hubbard Hamiltonian and the relation (3) is valid.

3.4. *Multi-band models: Model with s–d hybridization*

The Hubbard model is the single-band model. It is necessary, in principle, to take into account the multi-band structure, orbital degeneracy, interatomic effects and electron-phonon interaction. The band structure calculations and the experimental studies showed that for noble, transition and rare-earth metals the multi-band effects are essential. An important generalization of the single-band Hubbard model is the so-called model with s–d hybridization.[28,29] For transition d metals, investigation of the energy band structure reveals that s–d hybridization processes play an important part. Thus, among the other generalizations of the Hubbard model that correspond more closely to the real situation in transition metals, the model

with s–d hybridization serves as an important tool for analyzing of the multi-band effects. The system is described by a narrow d-like band, a broad s-like band and a s–d mixing term coupling the two former terms. The model Hamiltonian reads

$$H = H_d + H_s + H_{s\text{-}d}\,. \tag{10}$$

The Hamiltonian H_d of tight-binding electrons is the Hubbard model (5).

$$H_s = \sum_{k\sigma} \epsilon_k^s c_{k\sigma}^\dagger c_{k\sigma} \tag{11}$$

is the Hamiltonian of a broad s-like band of electrons.

$$H_{s-d} = \sum_{k\sigma} V_k (c_{k\sigma}^\dagger a_{k\sigma} + a_{k\sigma}^\dagger c_{k\sigma}) \tag{12}$$

is the interaction term which represents a mixture of the d-band and s-band electrons. The model Hamiltonian (10) can be interpreted also in terms of a series of Anderson impurities placed regularly in each site (the so-called periodic Anderson model). The model (10) is rotationally invariant also.

3.5. *Spin-fermion model*

Many magnetic and electronic properties of rare-earth metals and compounds (e.g. magnetic semiconductors) can be interpreted in terms of a combined spin-fermion model[30,31] that includes the interacting localized spin and itinerant charge subsystems. The concept of the $s(d)$–f model plays an important role in the quantum theory of magnetism, especially the generalized d–f model, which describes the localized $4f(5f)$-spins interacting with d-like tight-binding itinerant electrons and takes into consideration the electron–electron interaction. The total Hamiltonian of the model is given by

$$H = H_d + H_{d-f}\,. \tag{13}$$

The Hamiltonian H_d of tight-binding electrons is the Hubbard model (5). The term H_{d-f} describes the interaction of the total $4f(5f)$-spins with the spin density of the itinerant electrons

$$H_{d-f} = \sum_i J\boldsymbol{\sigma}_i \cdot \mathbf{S}_i = -JN^{-1/2} \sum_{kq} \sum_\sigma [S_{-q}^{-\sigma} a_{k\sigma}^\dagger a_{k+q-\sigma} + z_\sigma S_{-q}^z a_{k\sigma}^\dagger a_{k+q\sigma}] \tag{14}$$

where sign factor z_σ is given by

$$z_\sigma = (+,-), \qquad \sigma = (\uparrow,\downarrow)$$

and

$$S_{-q}^{-\sigma} = \begin{cases} S_{-q}^- & \sigma = + \\ S_{-q}^+ & \sigma = - \end{cases}.$$

In general the indirect exchange integral J strongly depends on the wave vectors $J(\mathbf{k};\mathbf{k}+\mathbf{q})$ having its maximum value at $\mathbf{k} = \mathbf{q} = 0$. We omit this dependence

for the sake of brevity of notation. To describe the magnetic semiconductors the Heisenberg interaction term (1) should be added[32,33] (the resulting model is called the modified Zener model). These model Hamiltonians (and their simple modifications and combinations) are the most commonly used models in quantum theory of magnetism. In our previous paper,[16] where the detailed analysis of the neutron scattering experiments on magnetic transition metals and their alloys and compounds was made, it was concluded that at the level of low-energy hydrodynamic excitations one cannot distinguish between the models. The reason for that is the spin-rotation symmetry. In terms of Refs. 3 and 8, the spin waves (collective waves of the order parameter) are in a quantum protectorate precisely in this sense. I will argue below the latter statement more explicitly.

4. Symmetry and Physics of Magnetism

In many-body interacting systems, the symmetry is important in classifying different phases and understanding the phase transitions between them.[4,5] To implement the QP idea it is necessary to establish the symmetry properties and corresponding conservation laws of the microscopic models of magnetism. The Goldstone theorem states that, in a system with broken continuous symmetry (i.e. a system such that the ground state is not invariant under the operations of a continuous unitary group whose generators commute with the Hamiltonian), there exists a collective mode with frequency vanishing as the momentum goes to zero. For many-particle systems on a lattice, this statement needs a proper adaptation. In the above form, the Goldstone theorem is true only if the condensed and normal phases have the same translational properties. When translational symmetry is also broken, the Goldstone mode appears at zero frequency but at nonzero momentum, e.g. a crystal and a helical spin-density-wave (SDW) ordering. As has been noted, this present paper is an attempt to explain the physical implications involved in the concept of QP for quantum theory of magnetism. All the three models considered above, the Heisenberg, the Hubbard, and the spin-fermion model, are spin rotationally invariant, $RHR^{+} = H$. The spontaneous magnetization of the spin or fermion system on a lattice that possesses the spin rotational invariance, indicate on a broken symmetry effect, i.e. that the physical ground state is not an eigenstate of the time-independent generators of symmetry transformations on the original Hamiltonian of the system. As a consequence, there must exist an excitation mode, that is an analog of the Goldstone mode for the continuous case (referred to as "massless" particles). It was shown that both the models, the Heisenberg model and the band or itinerant electron model of a solid, are capable of describing the theory of spin waves for ferromagnetic insulators and metals.[16] In their paper,[34] Herring and Kittel showed that in simple approximations the spin waves can be described equally well in the framework of the model of localized spins or the model of itinerant electrons. Therefore the study of, for example, the temperature dependence of the average moment in magnetic transition metals in the framework of low-temperature

spin-wave theory does not, as a rule, give any indications in favor of a particular model. Moreover, the itinerant electron model (as well as the localized spin model) is capable of accounting for the exchange stiffness determining the properties of the transition region, known as the Bloch wall, which separates adjacent ferromagnetic domains with different directions of magnetization. The spin-wave stiffness constant D is defined so that the energy of a spin wave with a small wave vector $\mathbf{q}$ is $E \sim Dq^2$. To characterize the dynamic behavior of the magnetic systems in terms of the quantum many-body theory, the generalized spin susceptibility (GSS) is a very useful tool.[35] The GSS is defined by

$$\chi(\mathbf{q},\omega) = \int dt \langle\langle S^-_{\mathbf{q}}(t), S^+_{-\mathbf{q}}\rangle\rangle e^{-i\omega t}\,. \tag{15}$$

For the Hubbard model $S^-_i = a^+_{i\downarrow}a_{i\uparrow}$. This GSS satisfies the important sum rule

$$\int \mathrm{Im}\ \chi(\mathbf{q},\omega)d\omega = \pi(n_\downarrow - n_\uparrow) = -2\pi\langle S^z\rangle\,. \tag{16}$$

It is possible to check that[16]

$$\chi(\mathbf{q},\omega) = -\frac{2\langle S^z\rangle}{\omega} + \frac{q^2}{\omega^2}\left\{\Psi(\mathbf{q},\omega) - \frac{1}{q}\langle[Q^-_{\mathbf{q}}, S^+_{-\mathbf{q}}]\rangle\right\}\,. \tag{17}$$

Here the following notation was used for $\mathbf{q}Q^-_{\mathbf{q}} = [S^-_{\mathbf{q}}, H]$ and $\Psi(\mathbf{q},\omega) = \langle\langle Q^-_{\mathbf{q}}|Q^+_{-\mathbf{q}}\rangle\rangle_\omega$. It is clear from (17) that for $\mathbf{q} = 0$ the GSS (15) contains only the first term corresponding to the spin-wave pole for $\mathbf{q} = 0$ which exhausts the sum rule (16). For small $\mathbf{q}$, due to the continuation principle, the GSS $\chi(\mathbf{q},\omega)$ must be dominated by the spin wave pole with the energy

$$\omega = D\mathbf{q}^2 = \frac{1}{2\langle S^z\rangle}\{\mathbf{q}\langle[Q^-_{\mathbf{q}}, S^+_{-\mathbf{q}}]\rangle - \mathbf{q}^2 \lim_{\omega\to 0}\lim_{\mathbf{q}\to 0}\Psi(\mathbf{q},\omega)\}\,. \tag{18}$$

This result is the direct consequence of the spin rotational invariance and is valid for all the three models considered above.

5. Spin Quasiparticle Dynamics

In this section, to make the discussion more concrete and to illustrate the nature of spin excitations in the above described models, let us consider the generalized spin susceptibility (GSS), which measures the response of "magnetic" degrees of freedom to an external perturbation.[35] The GSS is expressed in terms of the double-time thermal GF of spin variables,[22,12] that is defined as

$$\begin{aligned}\chi(\mathbf{q};t-t') &= \langle\langle S^+_{\mathbf{q}}(t), S^-_{-\mathbf{q}}(t')\rangle\rangle \\ &= -i\theta(t-t')\langle[S^+_{\mathbf{q}}(t), S^-_{-\mathbf{q}}(t')]_-\rangle \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-i\omega t}\chi(\mathbf{q},\omega)\,.\end{aligned} \tag{19}$$

The poles of the GSS determine the energy spectra of the excitations in the system. The explicit expressions for the poles are strongly dependent on the model used for the system and the character of approximations.[16,35]

The next step in description of the spin quasiparticle dynamics is to write down the equation of motion for the GF. Our attention is focused on the spin dynamics of the models. To describe self-consistently the spin dynamics of the models one should take into account the full algebra of relevant operators of the suitable "spin modes", which are appropriate for the case.

5.1. *Spin dynamics of the Hubbard model*

Theoretical calculations of the GSS in transition $3d$ metals have been largely based on the single-band Hubbard Hamiltonian.[35] The GSS for this case reads

$$\chi(\mathbf{q},\omega) = \langle\langle \sigma^+_{\mathbf{q}} | \sigma^-_{-\mathbf{q}} \rangle\rangle_\omega \,. \tag{20}$$

Here

$$\sigma^+_{\mathbf{k}} = \sum_{\mathbf{p}} a^\dagger_{\mathbf{k}\uparrow} a_{\mathbf{k}+\mathbf{p}\downarrow}, \qquad \sigma^-_{\mathbf{k}} = \sum_{\mathbf{p}} a^\dagger_{\mathbf{k}\downarrow} a_{\mathbf{k}+\mathbf{p}\uparrow} \,.$$

The result of the RPA calculation[35] has the following form

$$\chi(\mathbf{q},\omega) = \langle\langle \sigma^+_{\mathbf{q}} | \sigma^-_{-\mathbf{q}} \rangle\rangle_\omega = \frac{\chi^0(\mathbf{q},\omega)}{1 - U\chi^0(\mathbf{q},\omega)} \tag{21}$$

where

$$\chi^0(\mathbf{q},\omega) = N^{-1} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}\uparrow} - n_{\mathbf{k}+\mathbf{q}\downarrow}}{\omega + \epsilon^d_{\mathbf{k}+\mathbf{q}} - \epsilon^d_{\mathbf{k}} - \Delta} \tag{22}$$

$$\Delta = \frac{U}{N} \sum_{\mathbf{k}} (n_{\mathbf{k}\downarrow} - n_{\mathbf{k}\uparrow}) \,. \tag{23}$$

The excitation spectrum of the Hubbard model determined by the poles of susceptibility (22) is shown schematically in Fig. 1. The experimental data for three typical magnetic material are listed in Table 1. Note, that typically $q_{\max} \leq 0.75\mathbf{k}_{\mathrm{F}}$.

Table 1. Experimental data for transition metals.

Element	T_{c}	$D\,\mathrm{meV}\cdot A^2$	μ_{B}	$\Delta\,\mathrm{eV}$	$q_{\max}$
Fe	1043 K	280	2.177	—	—
Co	1403 K	510	1.707	0.91	—
Ni	631 K	433	0.583	0.5 ± 0.1	0.8 A^{-1}
MnSi	30 K	52	0.4	—	—

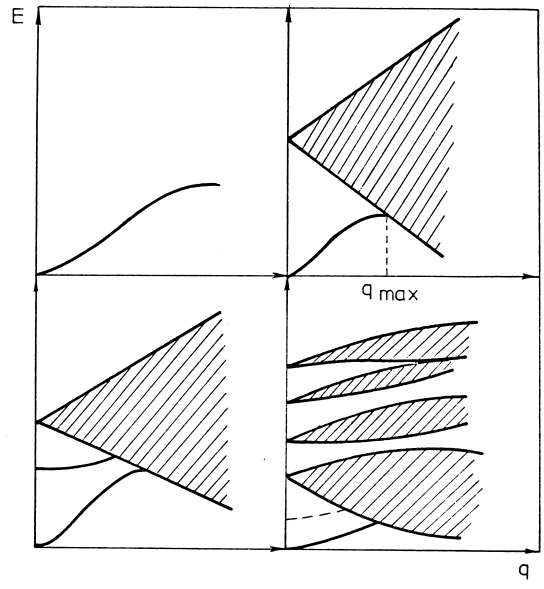

Fig. 1. Schematic form of the excitation spectra of the four microscopic models of magnetism: (a) upper-left, the Heisenberg model; (b) upper-right, the Hubbard model; (c) down-left, the modified Zener (spin-fermion) model; (d) down-right, the multiband Hubbard model.

5.2. *Spin dynamics of the spin-fermion model*

When the goal is to describe self-consistently the quasiparticle dynamics of two interacting subsystems the situation is more complicated. For the spin-fermion model (14) the relevant algebra of operators should be described by the "spinor" $\binom{\mathbf{S}_i}{\boldsymbol{\sigma}_i}$ ("relevant degrees of freedom").[31] Once this has been done, one should introduce the generalized matrix spin susceptibility of the form

$$\begin{pmatrix} \langle\langle S^+_{\mathbf{k}} | S^-_{-\mathbf{k}} \rangle\rangle & \langle\langle S^+_{\mathbf{k}} | \sigma^-_{-\mathbf{k}} \rangle\rangle \\ \langle\langle \sigma^+_{\mathbf{k}} | S^-_{-\mathbf{k}} \rangle\rangle & \langle\langle \sigma^+_{\mathbf{k}} | \sigma^-_{-\mathbf{k}} \rangle\rangle \end{pmatrix} = \hat{\chi}(\mathbf{k}, \omega)\,. \tag{24}$$

The spectrum of quasiparticle excitations without damping follows from the poles of the generalized mean-field susceptibility.

Let us write down explicitly the first matrix element χ_0^{11}

$$\langle\langle S^+_{\mathbf{q}} | S^-_{-\mathbf{q}} \rangle\rangle^0 = \frac{2JN^{-1/2}\langle S^z_0 \rangle}{\omega - JN^{-1}(n_\uparrow - n_\downarrow) + 2J^2 N^{-1/2}\langle S^z_0 \rangle (1 - U\chi_0^{df})^{-1}\chi_0^{df}} \tag{25}$$

where

$$\chi_0^{df}(\mathbf{k}, \omega) = N^{-1}\sum_{\mathbf{p}} \frac{(n_{\mathbf{p}+\mathbf{k}\downarrow} - n_{\mathbf{p}\uparrow})}{\omega_{\mathbf{p},\mathbf{k}}}\,, \tag{26}$$

$$\begin{aligned} \omega_{\mathbf{p},\mathbf{k}} &= (\omega + \epsilon^d_{\mathbf{p}} - \epsilon^d_{\mathbf{p}+\mathbf{k}} - \Delta)\,, \\ \Delta &= 2JN^{-1/2}\langle S^z_0 \rangle - UN^{-1}(n_\uparrow - n_\downarrow)\,. \end{aligned} \tag{27}$$

This result can be considered as reasonable approximation for description of the dynamics of localized spins in heavy rare-earth metals like Gd. (cf. Ref. 30).

The magnetic excitation spectrum that follows from the GF (24) consists of three branches — the acoustic spin wave, the optic spin wave and the Stoner continuum.[31] In the hydrodynamic limit, $\mathbf{q} \to 0$, $\omega \to 0$ the GF (24) can be written as

$$\langle\langle S^+_{\mathbf{q}} | S^-_{-\mathbf{q}} \rangle\rangle^0 = \frac{2N^{-1/2}\langle \tilde{S}^z_0 \rangle}{\omega - E(\mathbf{q})} \tag{28}$$

where the acoustic spin wave energies are given by

$$E(\mathbf{q}) = Dq^2 = \left[\frac{1}{2}\sum_{\mathbf{k}}(n_{\mathbf{k}\uparrow} + n_{\mathbf{k}\downarrow})\left(\mathbf{q}\frac{\partial}{\partial \mathbf{k}}\right)^2 \epsilon^d_{\mathbf{k}} + (2\Delta)^{-1} \right.$$
$$\left. \times \sum_{\mathbf{k}}(n_{\mathbf{k}\uparrow} - n_{\mathbf{k}\downarrow})\left(\mathbf{q}\frac{\partial}{\partial \mathbf{k}}\epsilon^d_{\mathbf{k}}\right)^2\right] \Big/ [2N^{1/2}\langle S^z_0\rangle + (n_\uparrow - n_\downarrow)] \tag{29}$$

and

$$\langle \tilde{S}^z_0 \rangle = \langle S^z_0 \rangle \left[1 + \frac{(n_\uparrow - n_\downarrow)}{2N^{3/2}\langle S^z_0\rangle}\right]^{-1} . \tag{30}$$

In GMF approximation the density of itinerant electrons (and the band splitting Δ) can be evaluated by solving the equation

$$n_\sigma = \sum_{\mathbf{k}} \langle a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}\rangle = \sum_{\mathbf{k}} \{\exp[\beta(\epsilon^d_{\mathbf{k}} + UN^{-1}n_{-\sigma} - JN^{-1/2}\langle S^z_0\rangle - \epsilon_{\mathrm{F}})] + 1\}^{-1} . \tag{31}$$

Hence, the stiffness constant D can be expressed by the parameters of the Hamiltonian (13).

The spectrum of the Stoner excitations is given by[31]

$$E^{\mathrm{St}}(q) = \epsilon^d_{\mathbf{k}+\mathbf{q}} - \epsilon^d_{\mathbf{k}} + \Delta . \tag{32}$$

If we consider the optical spin wave branch then by direct calculation one can easily show that

$$E_{\mathrm{opt}}(q) = E^0_{\mathrm{opt}} + D\left(\frac{UE_{\mathrm{opt}}}{J\Delta - 1}\right) q^2 ,$$
$$E^0_{\mathrm{opt}} = J(n_\uparrow - n_\downarrow) + 2J\langle S^z_0\rangle . \tag{33}$$

From Eq. (33) one also finds the GF of itinerant spin density in the generalized mean field approximation

$$\langle\langle \sigma^+_{\mathbf{k}} | \sigma^-_{-\mathbf{k}} \rangle\rangle^0_\omega = \chi^{df}_0(\mathbf{k},\omega) \Big/ \left\{1 - \left[U - \frac{2J^2\langle S^z_0\rangle}{\omega - J(n_\uparrow - n_\downarrow)}\right]\chi^{df}_0(\mathbf{k},\omega)\right\} . \tag{34}$$

5.3. *Spin dynamics of the multi-band model*

Now let us calculate the GSS for the Hamiltonian (10). In general, one should introduce the generalized matrix spin susceptibility of the form

$$\begin{pmatrix} \langle\langle \sigma^-_{\mathbf{q}} | \sigma^+_{-\mathbf{q}} \rangle\rangle & \langle\langle \sigma^-_{\mathbf{q}} | s^-_{-\mathbf{q}} \rangle\rangle \\ \langle\langle s^+_{\mathbf{q}} | \sigma^-_{-\mathbf{q}} \rangle\rangle & \langle\langle s^-_{\mathbf{q}} | s^+_{-\mathbf{q}} \rangle\rangle \end{pmatrix} = \hat{\chi}(\mathbf{q}, \omega)\,. \tag{35}$$

Here

$$s^+_{\mathbf{k}} = \sum_{\mathbf{q}} c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}+\mathbf{q}\downarrow}, \qquad s^-_{\mathbf{k}} = \sum_{\mathbf{q}} c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}+\mathbf{q}\uparrow}\,.$$

Let us consider for brevity the calculation of the Green function $\langle\langle \sigma^-_{\mathbf{q}} | \sigma^+_{-\mathbf{q}} \rangle\rangle$. According to Ref. 35, the object now is to calculate the Green function $\langle\langle \theta_{\mathbf{k}}(\mathbf{q}) = a^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega$. In the random phase approximation (RPA), the equations of motion for the relevant Green functions are reduced to the closed form

$$\begin{aligned}
&(\omega + \epsilon^d_\uparrow(\mathbf{k}+\mathbf{q}) - \epsilon^d_\downarrow(\mathbf{k}))\langle\langle \theta_{\mathbf{k}}(\mathbf{q}) | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega \\
&\quad = (n_{\mathbf{k}+\mathbf{q}\downarrow} - n_{\mathbf{k}\uparrow}) A(\mathbf{q}, \omega) - V_{\mathbf{k}+\mathbf{q}} \langle\langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega \\
&\qquad + V_{\mathbf{k}} \langle\langle a^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega\,,
\end{aligned} \tag{36}$$

$$\begin{aligned}
&(\omega - \epsilon^d_\downarrow(\mathbf{k}) + \epsilon^s_{\mathbf{k}+\mathbf{q}}) \langle\langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega \\
&\quad = \langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}+\mathbf{q}\downarrow} \rangle A(\mathbf{q}, \omega) + V_{\mathbf{k}} \langle\langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega - V_{\mathbf{k}+\mathbf{q}} \langle\langle \theta_{\mathbf{k}}(\mathbf{q}) | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega\,,
\end{aligned} \tag{37}$$

$$\begin{aligned}
&(\omega - \epsilon^d_\uparrow(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}}) \langle\langle a^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} | \sigma^+_{-q} \rangle\rangle_\omega \\
&\quad = \langle a^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} \rangle A(\mathbf{q}, \omega) + V_{\mathbf{k}} \langle\langle a^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega - V_{\mathbf{k}+\mathbf{q}} \langle\langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega\,,
\end{aligned} \tag{38}$$

$$\begin{aligned}
&(\omega + \epsilon^s_{\mathbf{k}+\mathbf{q}} - \epsilon^s_{\mathbf{k}}) \langle\langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega \\
&\quad = +V_{\mathbf{k}} \langle\langle c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega - V_{\mathbf{k}+\mathbf{q}} \langle\langle a^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega\,.
\end{aligned} \tag{39}$$

Here the following definitions were introduced

$$\begin{aligned}
\epsilon^d_\sigma(\mathbf{k}) &= \epsilon^d_{\mathbf{k}} + \frac{U}{N} \sum_{\mathbf{p}} \langle a^\dagger_{\mathbf{p}\sigma} a_{\mathbf{p}\sigma} \rangle\,, \\
A(\mathbf{q}, \omega) &= 1 - \frac{U}{N} \langle\langle \sigma^-_{\mathbf{q}} | \sigma^+_{-\mathbf{q}} \rangle\rangle_\omega\,.
\end{aligned} \tag{40}$$

To truncate the hierarchy of Green functions equations (36)–(39) the RPA linearization was used

$$\begin{aligned}
[\theta_{\mathbf{k}}(\mathbf{q}), H_d]_- \sim\ & (\epsilon^d_{\mathbf{k}} - \epsilon^d_{\mathbf{k}+\mathbf{q}}) \theta_{\mathbf{k}}(\mathbf{q}) + \Delta\theta_{\mathbf{k}}(\mathbf{q}) \\
& - \frac{U}{N} \sum_{\mathbf{p}} (\langle a^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} a_{\mathbf{k}+\mathbf{q}\downarrow} \rangle - \langle a^\dagger_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} \rangle) \theta_{\mathbf{p}}(\mathbf{q})\,,
\end{aligned}$$

$$[a^{\dagger}_{\mathbf{k}+\mathbf{q}\downarrow}c_{k\uparrow}, H_d]_- \sim -\epsilon^d_{\mathbf{k}+\mathbf{q}}a^{\dagger}_{\mathbf{k}+\mathbf{q}\downarrow}c_{\mathbf{k}\uparrow} - \frac{U}{N}\sum_{\mathbf{p}} n_{\mathbf{p}\uparrow}\langle a^{\dagger}_{\mathbf{k}+\mathbf{q}\downarrow}c_{\mathbf{k}\uparrow}\rangle + \frac{U}{N}\langle a^{\dagger}_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}\rangle \sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}a_{\mathbf{p}\uparrow}\,. \quad (41)$$

Now, we will use these equations to determine the spin susceptibility of d-electron subsystem in the random phase approximation. It can be shown that

$$\chi(\mathbf{q},\omega) = \langle\langle\sigma^-_{\mathbf{q}}|\sigma^+_{-\mathbf{q}}\rangle\rangle_\omega = \frac{\chi^{\mathrm{MF}}(\mathbf{q},\omega)}{1 - U\chi^{\mathrm{MF}}(\mathbf{q},\omega)}\,. \quad (42)$$

We introduced here the notation $\chi^{\mathrm{MF}}(\mathbf{q},\omega)$ for the mean field susceptibility to distinguish it from the $\chi^0(\mathbf{q},\omega)$ (22).

The expression for the $\chi^{\mathrm{MF}}(\mathbf{q},\omega)$ is of the form

$$\begin{aligned}\chi^{\mathrm{MF}}(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}}\{(n_{\mathbf{k}+\mathbf{q}\downarrow} - n_{\mathbf{k}\uparrow})[-|V_{\mathbf{k}}|^2((\omega + \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}+\mathbf{q}})\\ + (\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}})) + (\omega + \epsilon^s_{\mathbf{k}+\mathbf{q}} - \epsilon^s_{\mathbf{k}})(\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}})\\ \times(\omega - \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}+\mathbf{q}})] - (\omega + \epsilon^s_{\mathbf{k}+\mathbf{q}} - \epsilon^s_{\mathbf{k}})[V_{\mathbf{k}}\langle a^{\dagger}_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}\rangle\\ \times(\omega - \epsilon^d_{\downarrow}(\mathbf{k}) - \epsilon^s_{\mathbf{k}+\mathbf{q}}) + V_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k}+\mathbf{q}\downarrow}a_{\mathbf{k}+\mathbf{q}\downarrow}\rangle(\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}})]\}R^{-1}\,,\end{aligned} \quad (43)$$

where

$$\begin{aligned}R = \{-|V_{\mathbf{k}}|^2((\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^d_{\downarrow}(\mathbf{k}))(\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}})\\ + (\omega - \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}+\mathbf{q}})(\omega + \epsilon^s_{\mathbf{k}+\mathbf{q}} - \epsilon^s_{\mathbf{k}})\\ + (\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^d_{\downarrow}(\mathbf{k}))(\omega - \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}+\mathbf{q}})\\ + (\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}})(\omega + \epsilon^s_{\mathbf{k}+\mathbf{q}} - \epsilon^s_{\mathbf{k}})) + (\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q})\\ - \epsilon^d_{\downarrow}(\mathbf{k}))(\omega - \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}+\mathbf{q}})(\omega + \epsilon^d_{\uparrow}(\mathbf{k}+\mathbf{q}) - \epsilon^s_{\mathbf{k}})(\omega + \epsilon^s_{\mathbf{k}+\mathbf{q}} - \epsilon^s_{\mathbf{k}})\}\,.\end{aligned} \quad (44)$$

Note, that if $V_{\mathbf{k}} = 0$ then, $\chi^{\mathrm{MF}}(\mathbf{q},\omega)$ is reduced precisely to $\chi^0(\mathbf{q},\omega)$ (22).

The spectrum of quasiparticle excitations corresponds to the poles of the spin susceptibility (22); it corresponds to the spin-wave modes and to the Stoner-like spin-flip modes. Let us discuss first the question about the existence of a spin-wave pole among the set of poles of the susceptibility (42). If we set $\mathbf{q} = 0$ in (43) the secular equation for poles becomes

$$\begin{aligned}1 = \frac{U}{N}\sum_{\mathbf{k}}\{(n_{\mathbf{k}\downarrow} - n_{\mathbf{k}\uparrow})[-|V_{\mathbf{k}}|^2(2\omega - \Delta) + \omega(\omega + \epsilon^d_{\uparrow}(k) - \epsilon^s_{\mathbf{k}})\\ \times(\omega - \epsilon^d_{\downarrow}(k) + \epsilon^s_{\mathbf{k}})] - \omega[V_{\mathbf{k}}\langle a^{\dagger}_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}\rangle(\omega - \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}})\\ + V_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k}\downarrow}a_{\mathbf{k}\downarrow}\rangle(\omega + \epsilon^d_{\uparrow}(\mathbf{k}) - \epsilon^s_{\mathbf{k}})]\}(-|V_{\mathbf{k}}|^2(2\omega + \Delta)^2\\ + \omega(\omega - \epsilon^d_{\downarrow}(\mathbf{k}) + \epsilon^s_{\mathbf{k}})(\omega + \epsilon^d_{\uparrow}(\mathbf{k}) - \epsilon^s_{\mathbf{k}})(\omega + \epsilon^s_{\mathbf{k}} - \epsilon^s_{\mathbf{k}}))^{-1}\end{aligned} \quad (45)$$

which is satisfied if $\omega = 0$. It follows from general considerations of Sec. 4 that when the wave length of a spin wave is very long (hydrodynamic limit), its energy $E(\mathbf{q})$ must be related to the wave number $\mathbf{q}$ by $E(\mathbf{q}) = D\mathbf{q}^2$. Thus the solution for the equation

$$1 = U_{\chi}^{\mathrm{MF}}(\mathbf{q}, \omega) \tag{46}$$

exists which has the property $\lim_{\mathbf{q}\to 0} E(\mathbf{q}) = 0$ and this solution corresponds to a spin-wave excitation in the multiband model with s–d hybridization (42). Thus we derived a formula (42) for the dynamic spin susceptibility $\chi(\mathbf{q}, \omega)$ in RPA and shown, that it can be calculated in terms of the mean field spin susceptibility $\chi^{\mathrm{MF}}(\mathbf{q}, \omega)$ by analogy with the single-band Hubbard model.

Let us consider the poles of the $\chi^{\mathrm{MF}}(\mathbf{q}, \omega)$. It is instructive to remark that the Hamiltonian (10) can be rewritten in the mean field approximation as

$$H^{\mathrm{MF}} = \sum_{\mathbf{k}\sigma} \epsilon_{\sigma}^{d}(\mathbf{k}) a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}^{s} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} (c_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + a_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}) \,. \tag{47}$$

The Hamiltonian (46) can be diagonalized by the Bogoliubov (u, v)-transformation

$$a_{\mathbf{k}\sigma} = u_{\mathbf{k}\sigma} \alpha_{\mathbf{k}\sigma} + v_{\mathbf{k}\sigma} \beta_{\mathbf{k}\sigma}, \qquad c_{\mathbf{k}\sigma} = u_{\mathbf{k}\sigma} \beta_{\mathbf{k}\sigma} - v_{\mathbf{k}\sigma} \alpha_{\mathbf{k}\sigma} \,. \tag{48}$$

The result of diagonalization is

$$H^{\mathrm{MF}} = \sum_{\mathbf{k}\sigma} (\omega_{1\mathbf{k}\sigma} \alpha_{\mathbf{k}\sigma}^{\dagger} \alpha_{\mathbf{k}\sigma} + \omega_{2\mathbf{k}\sigma} \beta_{\mathbf{k}\sigma}^{\dagger} \beta_{\mathbf{k}\sigma}) \tag{49}$$

where

$$\omega_{-\mathbf{k}\sigma}^{+} = 1/2[(\epsilon_{\sigma}^{d}(\mathbf{k}) + \epsilon_{\mathbf{k}}^{s}) \pm \sqrt{(\epsilon_{\sigma}^{d}(\mathbf{k}) - \epsilon_{\mathbf{k}}^{s})^2 + 4|V_{\mathbf{k}}|^2}] \tag{50}$$

$$\begin{cases} u_{\mathbf{k}\sigma}^2 \\ v_{k\sigma}^2 \end{cases} = \left[1 \pm \frac{(\omega_{2\mathbf{k}\sigma}^{1} - \epsilon_{\sigma}^{d}(\mathbf{k}))^2}{V_{\mathbf{k}}^2} \right]^{-1} \tag{51}$$

Then we find

$$\begin{aligned} \chi^{\mathrm{MF}}(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \Bigg\{ & u_{\mathbf{k}+\mathbf{q}\downarrow}^2 u_{\mathbf{k}\uparrow}^2 \frac{(n_{\mathbf{k}\uparrow}^{\alpha} - n_{\mathbf{k}+\mathbf{q}\downarrow}^{\alpha})}{(\omega + \omega_{1\mathbf{k}+\mathbf{q}\downarrow} - \omega_{1\mathbf{k}\uparrow})} \\ & + v_{\mathbf{k}+\mathbf{q}\downarrow}^2 v_{\mathbf{k}\uparrow}^2 \frac{(n_{\mathbf{k}\uparrow}^{\beta} - n_{\mathbf{k}+\mathbf{q}\downarrow}^{\beta})}{(\omega + \omega_{2\mathbf{k}+\mathbf{q}\downarrow} - \omega_{2\mathbf{k}\uparrow})} + u_{\mathbf{k}+\mathbf{q}\downarrow}^2 v_{\mathbf{k}\uparrow}^2 \frac{(n_{\mathbf{k}\uparrow}^{\beta} - n_{\mathbf{k}+\mathbf{q}\downarrow}^{\alpha})}{(\omega + \omega_{1\mathbf{k}+\mathbf{q}\downarrow} - \omega_{2\mathbf{k}\uparrow})} \\ & + v_{\mathbf{k}+\mathbf{q}\downarrow}^2 u_{\mathbf{k}\uparrow}^2 \frac{(n_{\mathbf{k}\uparrow}^{\alpha} - n_{\mathbf{k}+\mathbf{q}\downarrow}^{\beta})}{(\omega + \omega_{2\mathbf{k}+\mathbf{q}\downarrow} - \omega_{1\mathbf{k}\uparrow})} \Bigg\} . \end{aligned} \tag{52}$$

The present consideration shows that for the correlated model with s–d hybridization the spectrum of spin quasiparticle excitations is modified in comparison with the single-band Hubbard model.

6. Quasiparticle Excitation Spectra and Neutron Scattering

The investigation of the spectrum of magnetic excitations of transition and rare-earth metals and their compounds is of great interest for refining our theoretical model representations about the nature of magnetism. Experiments that probe the quasi-particle states could shed new light on the fundamental aspects of the physics of magnetism. The most direct and convenient method of experimental study of the spectrum of magnetic excitations is the method of inelastic scattering of thermal neutrons. It is known experimentally that the spin wave scattering of slow neutrons in transition metals and compounds can be described on the basis of the Heisenberg model. On the other hand, the mean magnetic moments of the ions in solids differ appreciably from the atomic values and are often fractional. The main statement of the present consideration is that the excitation spectrum of the Hubbard model and some of its modifications is of considerable interest from the point of view of the choice of the relevant microscopic model. Let us consider the neutron scattering cross section which is proportional to the imaginary part of the GSS[35]

$$\frac{d^2\sigma}{d\Omega d\omega} = \left(\frac{\gamma e^2}{m_e c^2}\right)^2 |F(\mathbf{q})|^2 \left(\frac{-1}{2}\right) \frac{\mathbf{k}'}{\mathbf{k}} (1 + \tilde{q}_z^2) \times [(N(\omega) + 1) \operatorname{Im} \chi(-\mathbf{q}, \omega) + N(-\omega) \operatorname{Im} \chi(\mathbf{q}, \omega)] . \tag{53}$$

Here $N(E(\mathbf{k}))$ is the Bose distribution function $N(E(\mathbf{k})) = [\exp(E(\mathbf{k})\beta) - 1]^{-1}$. To calculate the cross section (53), we obtain from (42) the imaginary part of the susceptibility, namely

$$\operatorname{Im} \chi(\mathbf{q}, \omega) = \frac{\operatorname{Im} \chi^{\mathrm{MF}}(\mathbf{q}, \omega)}{[1 - U \operatorname{Re} \chi^{\mathrm{MF}}(\mathbf{q}, \omega)]^2 + [U \operatorname{Im} \chi^{\mathrm{MF}}(\mathbf{q}, \omega)]^2} . \tag{54}$$

The spin wave pole occurs where $\operatorname{Im} \chi^{\mathrm{MF}}(\mathbf{q}, \omega)$ tends to zero.[35] In this case, we can in (54) take the limit $\operatorname{Im} \chi^{\mathrm{MF}}(\mathbf{q}, \omega) \to 0$ so that

$$U \operatorname{Im} \chi(\mathbf{q}, \omega) \sim -\pi \delta[1 - U \operatorname{Re} \chi^{\mathrm{MF}}(\mathbf{q}, \omega)] \tag{55}$$

but

$$1 - U \operatorname{Re} \chi^{\mathrm{MF}}(\mathbf{q} \to 0, \omega \to 0) \sim b^{-1}(\omega - E(\mathbf{q})) \tag{56}$$

and thus

$$\operatorname{Im} \chi(\mathbf{q} \to 0, \omega \to 0) \sim -\pi \frac{b}{U} \delta(\omega - E(\mathbf{q})) . \tag{57}$$

Here b is a certain constant, which can be numerically calculated and $E(\mathbf{q})$ is the acoustic spin wave pole $E(\mathbf{q} \to 0) = 0$.

Turning now to the calculation of the cross section (53), we obtain the following result

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \left(\frac{\gamma e^2}{m_e c^2}\right)^2 |F(\mathbf{q})|^2 \left(\frac{1}{4}\right) \frac{\mathbf{k}'}{\mathbf{k}} (1 + \tilde{q}_z^2) N \frac{b}{U} \times \sum_{\mathbf{p}} [N(E(\mathbf{p}))\delta(\omega + E(\mathbf{p})) + (N(E(\mathbf{p})) + 1)\delta(\omega - E(\mathbf{p}))] . \tag{58}$$

According to formula (58), the cross section for the acoustic spin wave scattering will be identical for the Heisenberg and Hubbard (single-band and multiband) model. So, at the level of low-energy, hydrodynamic excitations one cannot distinguish between the models. However, for the Hubbard model, the poles of the GSS will contain, in addition to acoustic spin-wave pole, the continuum of the Stoner excitations $E^{\mathrm{St}}(\mathbf{q}) = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{q}} + \Delta$, as is shown on Fig. 1. The spectra of the spin-fermion model and multiorbital (multi-band) Hubbard model are shown for comparison.

The cross section (58) does not include the contribution arising from the scattering by Stoner excitations, i.e. that determined by $\chi^{\mathrm{MF}}(\mathbf{q},\omega)$. It was shown in paper[16] that in a single-band Hubbard model of transition metal in the limit when the wave vector of the elementary excitations goes to zero, the acoustic spin-wave mode dominates the inelastic neutron scattering, and the contribution to the cross section due to Stoner-mode scattering goes to zero. It was shown that the Stoner-mode scattering intensity does not become comparable to the spin-wave scattering intensity until $\mathbf{q} = 0.9\mathbf{q}_{\max}$ (see Fig. 1). Here $\mathbf{q}_{\max}$ is the value of $\mathbf{q}$ when the spin wave enters the continuum. For large values of $\mathbf{q}$ and ω the energy gap Δ for spin flipping Stoner excitations may be overcome. In this case

$$\operatorname{Im}\chi(\mathbf{q},\omega) \sim \operatorname{Im}\chi^{\mathrm{MF}}(\mathbf{q},\omega)\,. \tag{59}$$

From (52) we obtain for $\operatorname{Im}\chi^{\mathrm{MF}}(\mathbf{q},\omega)$ the result

$$\begin{aligned}\operatorname{Im}\chi^{\mathrm{MF}}(\mathbf{q},\omega) = -\frac{\pi}{N}\sum_{\mathbf{k}}\{&u^2_{\mathbf{k}+\mathbf{q}\downarrow}u^2_{\mathbf{k}\uparrow}(n^{\alpha}_{\mathbf{k}\uparrow} - n^{\alpha}_{\mathbf{k}+\mathbf{q}\downarrow})\delta(\omega + \omega_{1\mathbf{k}+\mathbf{q}\downarrow} - \omega_{1\mathbf{k}\uparrow})\\ &+ v^2_{\mathbf{k}+\mathbf{q}\downarrow}v^2_{\mathbf{k}\uparrow}(n^{\beta}_{\mathbf{k}\uparrow} - n^{\beta}_{\mathbf{k}+\mathbf{q}\downarrow})\delta(\omega + \omega_{2\mathbf{k}+\mathbf{q}\downarrow} - \omega_{2\mathbf{k}\uparrow})\\ &+ u^2_{\mathbf{k}+\mathbf{q}\downarrow}v^2_{\mathbf{k}\uparrow}(n^{\beta}_{\mathbf{k}\uparrow} - n^{\alpha}_{\mathbf{k}+\mathbf{q}\downarrow})\delta(\omega + \omega_{1\mathbf{k}+\mathbf{q}\downarrow} - \omega_{2\mathbf{k}\uparrow})\\ &+ v^2_{\mathbf{k}+\mathbf{q}\downarrow}u^2_{\mathbf{k}\uparrow}(n^{\alpha}_{\mathbf{k}\uparrow} - n^{\beta}_{\mathbf{k}+\mathbf{q}\downarrow})\delta(\omega + \omega_{2\mathbf{k}+\mathbf{q}\downarrow} - \omega_{1\mathbf{k}\uparrow})\}\,.\end{aligned} \tag{60}$$

Now it follows from (60) that $\operatorname{Im}\chi^{\mathrm{MF}}(\mathbf{q},\omega)$ is nonzero only for values of the energies equal to the energies of the Stoner-type excitations

$$\begin{aligned}E^{\mathrm{St}}_1(\mathbf{q}) &= \omega_{1\mathbf{k}\uparrow} - \omega_{1\mathbf{k}+\mathbf{q}\downarrow}\,,\\ E^{\mathrm{St}}_2(\mathbf{q}) &= \omega_{2\mathbf{k}\uparrow} - \omega_{2\mathbf{k}+\mathbf{q}\downarrow}\,,\\ E^{\mathrm{St}}_3(\mathbf{q}) &= \omega_{2\mathbf{k}\uparrow} - \omega_{1\mathbf{k}+\mathbf{q}\downarrow}\,,\\ E^{\mathrm{St}}_4(\mathbf{q}) &= \omega_{1\mathbf{k}\uparrow} - \omega_{2\mathbf{k}+\mathbf{q}\downarrow}\,.\end{aligned} \tag{61}$$

With (60) and (61) we obtain

$$\begin{aligned}\frac{d^2\sigma}{d\Omega d\omega} \sim \left(\frac{\gamma e^2}{m_e c^2}\right)^2 |F(\mathbf{q})|^2 \left(\frac{1}{4}\right)\frac{\mathbf{k}'}{\mathbf{k}}(1+\tilde{q}_z^2)\frac{N}{\pi}\\ \times\left[(N(\omega)+1)\operatorname{Im}\chi^{\mathrm{MF}}(-\mathbf{q},\omega) + N(-\omega)\operatorname{Im}\chi^{\mathrm{MF}}(\mathbf{q},\omega)\right].\end{aligned} \tag{62}$$

Although for the single-band model the Stoner-mode scattering cross section remains relatively small until $\mathbf{q}$ is fairly close to $\mathbf{q}_{\max}$, it can be shown (see Ref. 16) that in the multiband models the Stoner-mode cross section may become reasonably large for much smaller scattering vector.

The essential result of the present consideration is the calculation of the GSS for the model with s–d hybridization which is more realistic for transition metals than the single-band Hubbard model. The present qualitative treatment shows that a two-band picture of inelastic neutron scattering is modified in comparison with the single-band Hubbard model. We have found that the long-wave-length acoustic spin-wave excitations should exist in this model and that in the limit $(\lim_{\omega\to 0}\lim_{\mathbf{q}\to 0})$, the acoustic spin-wave mode dominates the inelastic neutron scattering. The spin-wave part of the cross section is renormalized only quantitatively. The cross section due to Stoner-mode scattering is qualitatively modified because of occuring of the four intersecting Stoner-type sub-bands which may lead to the modification of the spin wave intensity fall off with increasing energy transfer. The intersection point $\mathbf{q}_{\max}$ can be essentially renormalized.

7. Conclusions

In summary, in this article, the logic of an approach to the quantum theory of magnetism based on the idea of the QP was described. There is an important aspect of this consideration, which is seen to be the key principle for the interpretation of the spin quasiparticle dynamics of the microscopic models of magnetism.

To summarize, the usefulness of the QP concept for physics of magnetism derives from the following features. From our point of view, the clearest difference between the models is manifested in the spectrum of magnetic excitations. The model of correlated itinerant electrons and the spin-fermion model have more complicated spectra than the model of localized spins (see Fig. 1). Since the structure of the GSS and the form of its poles are determined by the choice of the model Hamiltonian of the system and the approximations made in its calculation, the results of neutron scattering experiments can be used to judge the adequacy of the microscopic models. However, it should be emphasized that to judge reliably the applicability of a particular model, it is necessary to measure the susceptibility (the cross section) at all points of the reciprocal space and for a wide interval of temperatures, which is not always permitted by the existing experimental techniques. Thus, further development of experimental facilities will provide a base for further refining of the theoretical models and conceptions about the nature of magnetism. In terms of Ref. 3, to judge which of the models is more suitable, it is necessary to escape the QP. This can be done by measurements in the high $(\mathbf{q}, \omega)$ region, where $(\mathbf{q} \sim \mathbf{q}_{\max}, E \sim \Delta)$.

The following statements can now be made as to our analysis and its results. In this paper, we shown that quasiparticle dynamics of magnetic materials can be reasonably understood by using the simplified, but workable models of interacting

spins and electrons on a lattice in the light of the QP concept. The spectrum of magnetic excitations of the Hubbard model reflects the dual behavior of the magnetically active electrons in transition metals and their compounds. The general properties of rotational invariance of the model Hamiltonians show that the presence of a spin-wave acoustic pole in the generalized magnetic susceptibility is a direct consequence of the rotational symmetry of the system. Thus, the acoustic spin-wave branch reflects a certain degree of localization of the relevant electrons; the characteristic quantity D, which determines the spin wave stiffness, can be measured directly in neutron experiments. In contrast, in the simplified Stoner model of band ferromagnetism the acoustic spin-waves do not exist. There is a continuum of single-particle Stoner excitations only. The presence of the Stoner continuum for the spectrum of excitations of the Hubbard model is a manifestation of the delocalization of the magnetic electrons. Since the Stoner excitations do not arise in the Heisenberg model, their direct detection and detailed investigation by means of neutron scattering is one of the most intriguing problems of the fundamental physics of magnetic state. Concerning the QP notion studied in the present paper, an important conclusion is that the inelastic neutron scattering experiments on metallic magnets permit one to make the process of escaping the QP very descriptive. In this consideration, our main emphasis was put on the aspects important from the point of view of quantum theory of magnetism, namely, on the dual character of fundamental "magnetic degrees of freedom". Generally speaking, the fortunate circumstance in this discussion is the fact that besides the very general idea of QP also concrete practical tools are available in the physics of magnetism, and the combination of these two approaches is possible in the neutron scattering experiments (for details see Ref. 16). The approach is very versatile since it uses the symmetry properties in the most ingenious fashion. By this consideration an attempt is made to link phenomenological and quantum theory of magnetism together more firmly, thus giving a better understanding of the latter. Finally, to clarify the concept of QP, we comment on somewhat resembling mathematical structures which are encountered when one tries to implement classical dynamic symmetries in quantum field theory[36]; within these schemes one is trying to fit a classical description of particles endowed with internal structures, like spin. However, these analogies, as well as the elaboration of an adequate mathematical formalism for expression of the concept of QP need further studies. Further work is also necessary for the development of compact criteria appropriate for the QP occurrence in all applications.

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