Scattering of slow neutrons and magnetic properties of transition metals and alloys

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It is shown that many phenomena studied by scattering of slow neutrons in ferromagnetic transition metals and their alloys can be described in a unified manner on the basis of the Hubbard model and its generalizations. Consideration is given to some new possibilities of neutron spectroscopy opened up by the commissioning of powerful pulsed sources such as the IBR-2 pulsed reactor.

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INTRODUCTION

Fifty years ago, the authors of the then most complete monograph on magnetism characterized the situation in the physics of magnetic phenomena as follows: "Even recently questions relating to magnetism appeared to be exceptionally unfavorable for theoretical investigations. This was due to the circumstance that the investigators had concentrated mainly on ferromagnetic phenomena, since these played and still play a very important part in technology. But the theoretical treatment of ferromagnetism presents such great difficulties that this field is at present one of the most obscure in the whole of physics."[1]

During the fifty years which have elapsed, the physics of magnetic phenomena has been transformed into a very extensive branch of modern physical science.[2] To a large degree, the progress in the study of the structural and dynamical properties of magnetic substances is due to the achievements of magnetic neutron-diffraction studies.[3,4] The unique possibilities of the method of thermal neutron scattering make it possible to obtain information about the magnetic and crystal structure, the distribution of magnetic moments, the spectrum of magnetic excitations, critical fluctuations, and so forth. To interpret the data, it is necessary to take into account the electron–electron and electron–nucleus interactions in the system and the Pauli principle. Thus, magnetism can be described properly only in the framework of a quantum statistical theory of the condensed state.

Because of the presence of an incomplete inner *nd* or *nf* shell, all free atoms of the transition elements are strongly magnetic by virtue of Hund's rules. When a crystal is formed, the atomic shells are rearranged and for a clear understanding of the properties of the crystal it is necessary to know the wave functions and energies of the former valence electrons. The calculations of the energy levels of electrons in a crystal is very complicated[5,6]; speaking qualitatively, one needs to know how much the atomic wave functions of the valence electrons are changed—how much they are delocalized—when the crystal is formed.

In the theory of magnetism, the method of model Hamiltonians has proved to be very effective. Without exaggeration, one can say that the great successes in the physics of magnetic phenomena are to a considerable extent due to the use of some very simple and schematic model representations for the "theoretical interpretation of ferromagnetism." At the present time, there are essentially three of these models used in the quantum theory of magnetism.

Historically, the first was Heisenberg's model of localized spins (and its limiting case, the Ising model[7]); then followed the model of a ferromagnetic Fermi liquid[2] and the Hubbard model.[8]

The Heinsenberg model[2-4,9] is based on the assumption that the wave functions of magnetically active electrons in a crystal differ little from the atomic orbitals. It is assumed that this model applies basically to substances in which the ground-state energy is separated by a gap of finite width from the energy of excited current states, i.e., it applies to semiconductors and insulators. The model also applies well to a number of magnetic rare-earth elements, since the incomplete *f* shells have small effective radii (for many rare-earth *f* metals, indirect exchange through conduction electrons plays an important part in establishing the magnetic order).

The model of collectivized electrons,[1,10] or the model of a ferromagnetic Fermi liquid, applies to metals in which the system of former valence electrons forms a mobile Fermi liquid over the entire volume of the crystal. (Sometimes, for *d* metals, in which the incomplete *d* shells do not have such small effective radii as the *f* shells, so that there is an appreciable overlapping of the nearest neighbors, one speaks of a mixture of the two Fermi liquids of the *f* and *d* electrons.)

The narrow-band model, or Hubbard model,[8,11] is in a certain sense an intermediate model and was originally proposed for the description of 3*d* metals. At the present time, the Hubbard model and its generalizations are used to describe the magnetic properties of pure 3*d* metals and their alloys, chalcogenides of transition and rare-earth metals, actinides, and others.

Thus, all three models give different answers to the question of the extent to which the wave functions of the former valence electrons are changed in the crystal. These models (or combinations of them) make it possible to describe many phenomena and obtain qualitatively, and frequently quantitatively, correct results. Sometimes (not always) very complicated and laborious calculations of the electron band structure yield virtu-

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ally nothing new compared with the results obtained on the basis of these schematic and rough models.

However, despite the successes achieved in understanding the physics of magnetic phenomena, the difficulties of exact calculation of the electron band structure and the performing of all the necessary experiments means that, except for the rare-earth elements, we still cannot say with complete confidence which of the microscopic models (or combinations of them) gives the most adequate approximation to the real situation in a particular substance. It is for this reason that the determination of the true mechanism behind the occurrence of a magnetically ordered state is currently regarded as problem number one in the theory of magnetism.

A precise understanding of the physical processes leading to the occurrence of ferromagnetism is particularly important when we turn to the theoretical description of alloys of ferromagnetic transition metals. Alloys of magnetic metals are widely used in technology, so that their theoretical study has great practical importance.

In the present review, we show that the investigation of the spectrum of magnetic excitations of pure transition metals and their alloys is of great interest for refining our theoretical model representations of the nature of the magnetic state in these substances. The most direct and convenient method of experimental study of the spectrum of magnetic excitations is the method of inelastic scattering of thermal neutrons. In this connection, we discuss some new possibilities of the method of neutron spectroscopy opened up by the commissioning of powerful pulsed neutron sources such as the IBR-2 pulsed reactor. In particular, we consider the possibility of direct measurement of Stoner excitations in ferromagnetic transition metals. The direct measurement of Stoner excitations in a wide range of momentum and energy transfers is of great importance for determining the degree of localization or delocalization of the magnetically active electrons in ferromagnetic transition metals. We show that the Hubbard model makes it possible to describe from a unified point of view a very large number of phenomena relating to the magnetic behavior of pure ferromagnetic transition metals and their alloys.

1. HUBBARD MODEL

In recent years, the Hubbard model[8,11,12] has come to be used rather widely in the description of the magnetic and electric properties of transition metals and their alloys. In the present paper, we shall show that the excitation spectrum of the Hubbard model and some of its simple modifications is of considerable interest from the point of view of application of the method of neutron scattering. We shall first discuss pure $3d$ metals, and, more concretely, nickel, iron, and cobalt. It is assumed[13] that the original energy spectrum of the system is a broad sp band, in which a system of five narrow intersecting d bands (Fig. 1) is embedded. In the Hubbard model, an attempt is made to take into

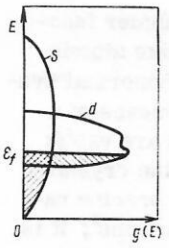

FIG. 1. Band structure of a ferromagnetic transition metal.

account the entire complex of unusual properties of $3d$ metals. In particular, it is known experimentally that the spin-wave scattering of slow neutrons[3,4] in these substances can be described on the basis of the Heisenberg model. It has also been found that the distributions of the charge density in ferromagnetic metals are close to the atomic distributions.[2-4] On the other hand, the mean atomic magnetic moments differ appreciably from the atomic values and are fractional. That the d electrons make an appreciable contribution to the low-temperature specific heat $c_{el}=\pi^3/3g(\varepsilon_f)T=\gamma T$ is indicated by the fact that the coefficient γ in transition metals is greater than in normal metals. Strong collectivization of the d electrons is also indicated by estimates of the binding energy and investigation of the Fermi surfaces.

In the Hubbard model,[8,11,12] these aspects of the behavior of the system can be described by assuming that the d electrons form a band but are subject to strong Coulomb repulsion at one lattice site.

We consider the system of d electrons, whose Hamiltonian has the usual form[4]

$$H=\sum_i\left[\frac{1}{2m}\mathbf{p}_i^2+v(\mathbf{r}_i)\right]+1/2\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}=h+V. \tag{1}$$

We go over to the second-quantization representation, introducing field operators $\Psi_\sigma(\mathbf{r})$ and $\Psi_\sigma^+(\mathbf{r})$. In this representation, the Hamiltonian (1) takes the form

$$H=\sum_\sigma\int d^3r\Psi_\sigma^+(\mathbf{r})\,h\Psi_\sigma(\mathbf{r})$$
$$+1/2\sum_{\sigma\sigma'}\int\int d^3r\,d^3r'\Psi_\sigma^+(\mathbf{r}')\,\Psi_{\sigma'}^+(\mathbf{r})\,V\Psi_{\sigma'}(\mathbf{r}')\,\Psi_\sigma(\mathbf{r}). \tag{2}$$

The eigenfunctions of the unperturbed Hamiltonian h form a complete orthonormal system of functions, called Bloch functions, $\{\varphi_{kn\sigma}(\mathbf{r})\}$. The index n characterizes a particular given band. Expanding the field operators in terms of the operators $a_{kn\sigma}^+$ and $a_{kn\sigma}$ for the Bloch states $\varphi_{kn\sigma}$,

$$\Psi_\sigma^+(\mathbf{r})=\sum_{kn}\varphi_{kn\sigma}^*(\mathbf{r})\,a_{kn\sigma}^+, \tag{3}$$

we rewrite the Hamiltonian (2) in the form

$$H=\sum_{kn\sigma}\varepsilon_n(\mathbf{k})\,a_{kn\sigma}^+a_{kn\sigma}$$
$$+1/2\sum_{kk'q}\sum_{\substack{mn\\pf}}\sum_{\sigma\sigma'}V_{nm,\,pf}(\mathbf{k},\mathbf{k}',\mathbf{q})\,a_{kn\sigma}^+a_{k+q\,p\sigma'}^+a_{k+qm\sigma}a_{k'f\sigma}. \tag{4}$$

Here

$$V_{nm,\,pf}(\mathbf{k},\mathbf{k}',\mathbf{q})=\langle\varphi_{kn\sigma}(r)\,\varphi_{k+qp\sigma'}(r')|V(\mathbf{r}-\mathbf{r}')|\varphi_{k+qm\sigma'}\varphi_{k'f\sigma}\rangle. \tag{5}$$

The eigenfunctions $\varphi_{kn\sigma}(\mathbf{r})$ of the unperturbed Hamiltonian can be expanded in a Fourier series:

$$\varphi_{kn\sigma}(\mathbf{r})=N^{-1/2}\sum_i\phi_{n\sigma}(\mathbf{r}-\mathbf{R}_i)\exp(i\mathbf{k}\mathbf{R}_i). \tag{6}$$

The functions $\phi_{n\sigma}$, which are known as Wannier functions, are localized in space and behave like atomic wave functions; they form a complete orthonormal system of functions obtained from $\varphi_{kn\sigma}(\mathbf{r})$ by means of a unitary transformation whose coefficients are $\exp(i\mathbf{k}\cdot\mathbf{R}_i)$. We denote the number of atoms in the crystal by N. It is rather difficult to analyze the precise nature of the localization of the Wannier functions[5]; it is, however, clear that at large distances the Wannier functions are small. In actual calculations it is assumed that the Bloch functions corresponding to wave vector k in band n can be calculated by one of the known methods, for example, the $X\alpha$ method.[6]

We now express the Hamiltonian (2) in the second-quantization representation in the Wannier basis:

$$H=\sum_{ij}\sum_{mm'\sigma} t_{ij}^{mm'} a_{im\sigma}^{+} a_{jm'\sigma}$$
$$+1/2\sum_{ijkl}\sum_{\substack{mn\\m'n'}}\sum_{\sigma\sigma'}\left\langle im\sigma, jn\sigma'\left|\frac{1}{r}\right|km'\sigma,\ ln'\sigma'\right\rangle a_{im\sigma}^{+}a_{jn\sigma'}^{+}a_{ln'\sigma'}a_{km'\sigma}; \tag{7}$$

$$t_{ij}^{mm'}=\int d^3r\,\phi_m^*(\mathbf{r}-\mathbf{R}_i)\,h(\mathbf{r})\,\phi_{m'}(\mathbf{r}-\mathbf{R}_j); \tag{8}$$

$$\left\langle im\sigma,\ jn\sigma'\left|\frac{1}{r}\right|km'\sigma,\ ln'\sigma\right\rangle$$
$$=e^2\int\frac{\phi_m^*(\mathbf{r}-\mathbf{R}_i)\,\phi_n^*(\mathbf{r}'-\mathbf{R}_l)\,\phi_{m'}(\mathbf{r}-\mathbf{R}_k)\,\phi(\mathbf{r}'-\mathbf{R}_e)\,d^3rd^3r'}{|\mathbf{r}-\mathbf{r}'|}. \tag{9}$$

The matrix element $t_{ij}^{mm'}$ describes hops of an electron from atom to atom for different orbital states; the higher the transition frequency, the more strongly collectivized are the electrons, i.e., the width of the bands is smaller, the more strongly the electrons are bound.

For simplicity, we restrict ourselves in this section to one band. It is also convenient to represent the Hamiltonian (7) in the form

$$H=\sum_{ij\sigma}t_{ij}a_{i\sigma}^{+}a_{j\sigma}+U/2\sum_{i\sigma}n_{i\sigma}n_{i-\sigma}$$
$$+1/2\sum_{ij}{}'\sum_{\sigma\sigma'}\left\langle ij\left|\frac{1}{r}\right|ij\right\rangle n_{i\sigma}n_{j\sigma'}-1/2\sum_{ij}{}'\sum_{\sigma\sigma'}J_{ij}a_{i\sigma}^{+}a_{i\sigma'}a_{j\sigma'}^{+}a_{j\sigma}$$
$$+\sum_{ij}{}'\sum_{\sigma\sigma'}\left\langle ii\left|\frac{1}{r}\right|jj\right\rangle a_{i\sigma}^{+}a_{i\sigma'}a_{j\sigma'}^{+}a_{j\sigma}. \tag{10}$$

Here, we have introduced the notation

$$U=e^2\int|\phi(\mathbf{r}-\mathbf{R}_i)|^2\,|\mathbf{r}-\mathbf{r}'|^{-1}\,|\phi(\mathbf{r}'-\mathbf{R}_i)|^2\,d^3rd^3r';$$
$$J_{ij}=e^2\int\phi^*(\mathbf{r}-\mathbf{R}_i)\,\phi(\mathbf{r}-\mathbf{R}_j)|\mathbf{r}-\mathbf{r}'|^{-1}\phi^*(\mathbf{r}'-\mathbf{R}_j)\,\phi(\mathbf{r}'-\mathbf{R}_i)\,d^3rd^3r',$$

where J_{ij} is the direct exchange integral, and U is the integral of the intra-atomic Coulomb correlation of the electrons with opposite spins. From the point of view of magnetism, the third term in (10) is of no interest, since it is proportional to $A_{ij}n_in_j$. The last term in (10) describes transitions of antiparallel spin pairs; we shall not consider these effects here. Estimates show[4] that for many transition metals and their compounds the largest integral in (10) is U. On the basis of this, Hubbard[8] proposed the model

$$H=\sum_{ij\sigma}t_{ij}a_{i\sigma}^{+}a_{j\sigma}+\frac{U}{2}\sum_{i\sigma}n_{i\sigma}n_{i-\sigma}. \tag{11}$$

The repulsion of the electrons at one center represented by U does not decrease when the atoms are diluted.

Thus, the Hubbard model contains the possibility of transition from a simple band scheme to a Heitler–London-type description. One can therefore expect that the most interesting effects—the transition from an ordinary metal for $|t_{ij}|\gg U$ (described by a band scheme) to a dielectric with strong correlation of Heitler–London type for $|t_{ij}|\ll U$, and also the various magnetic properties—must already be contained in the Hamiltonian (11). The possibility of construction interpolation solutions—which interpolate from the atomic to the band limit and describe the collapse of the gap in the spectrum of single-particle states—was proved in Refs. 14–17.

In the case of a single electron per atom ($n=1$) and a strong interaction ($U\gg|t_{ij}|$) one can show[11] in second-order perturbation theory that the effective Hamiltonian $H_{\text{eff}}=H(U)[E_0-H(t_{ij})]^{-1}H(U)$ reduces to the antiferromagnetic Heisenberg Hamiltonian:

$$H_{\text{eff}}=\frac{1}{2}\sum_{ij}{}'|t_{ij}|^2/U\{\sigma_i\sigma_j-1\}.$$

Thus, the ground state of the system for strong correlation and half-filled band is most probably antiferromagnetic.

The Hubbard Hamiltonian is rotationally invariant. This means that under the action of the operator of spin rotation $R=\exp\{-\frac{1}{2}i\varphi\sum_j\sigma_j\hat{\mathbf{k}}\}$ $(R^+R=RR^+=1)$, where φ is the angle of rotation around the unit vector $\hat{\mathbf{k}}$, the relation $H'=RHR^+$ holds. Here, $\sigma_{ix}=(a_{i\uparrow}^{+}a_{i\downarrow}+a_{i\downarrow}^{+}a_{i\uparrow})$, $\sigma_{iy}=-i(a_{i\uparrow}^{+}a_{i\downarrow}-a_{i\downarrow}^{+}a_{i\uparrow})$, and $\sigma_{iz}=(n_{i\uparrow}-n_{i\downarrow})$. One can also show that the Hubbard Hamiltonian is invariant under the time reversal T $(T^*T=TT^*=1)$: $H'=THT^*$. Time reversal for a crystal leads to fulfillment of the important equation $\varepsilon(\mathbf{k})=\varepsilon(-\mathbf{k})$ irrespective of the spatial symmetry of the system. The rotational invariance of the Hamiltonian also leads to important physical consequences of a general nature, which we now discuss.

2. GENERALIZED SUSCEPTIBILITY AND SPIN WAVES

In accordance with linear-response theory,[18] one can introduce a generalized spin susceptibility $X(\mathbf{q},\omega)$. If the external magnetic field is sufficiently weak, the magnetization due to it is determined by

$$M(\mathbf{r},t)=\int d^3r'dt'X(\mathbf{r}-\mathbf{r}',\ t-t')\,H(\mathbf{r}',\ t'). \tag{12}$$

After Fourier transformation, we obtain $M(\mathbf{q},\omega)=X(\mathbf{q},\omega)\times H(\mathbf{q},\omega)$. Here, $X(\mathbf{q},\omega)$ describes the response of the system to the external magnetic field $H(\mathbf{r},t)=H(\mathbf{q},\omega)\exp[i(\mathbf{qr}-\omega t)]$. If the field is real, the magnetization is

$$M(\mathbf{r},t)=H(\mathbf{q},\omega)\,\mathrm{Re}\{X(\mathbf{q},\omega)\exp[i(\mathbf{qr}-\omega t)]\}. \tag{13}$$

The frequency dependence of the susceptibility is determined by the retarded commutator

$$X(\mathbf{r}-\mathbf{r}',\omega)=\frac{i}{\hbar}\int_{-\infty}^{t}dt\exp(i\omega t)\langle[M(\mathbf{r},t),M(\mathbf{r},0)]\rangle. \tag{14}$$

For free electrons, the static spin susceptibility (Pauli susceptibility) is

$$X_p=2\mu_B^2D(\varepsilon_f),$$

where $\mu_B=e\hbar/(2mc)$ is the Bohr magneton, and $D(\varepsilon_f)$

is the density of states at the Fermi level.

The generalized spin susceptibility for a system of interacting electrons is determined by the expression

$$X^{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega) = (g\mu_B)^2 \frac{i}{\hbar} \int_{-\infty}^{t} dt \exp(i\omega t) \langle [S^\alpha(\mathbf{r}, t), S^\beta(\mathbf{r}', 0)] \rangle. \quad (15)$$

For the Hubbard Hamiltonian (11) in the Hartree–Fock approximation $n_{i\uparrow}n_{i\downarrow} \langle n_{i\uparrow} \rangle n_{i\downarrow} + n_{i\uparrow} \langle n_{i\downarrow} \rangle$ we obtain for the energies of the electrons in the magnetic field

$$E_{k\uparrow} = \varepsilon_k + U\langle n_\downarrow \rangle - (g\mu_B/2) H;$$
$$E_{k\downarrow} = \varepsilon_k + U\langle n_\uparrow \rangle + (g\mu_B/2) H.$$

The calculation of the static susceptibility (15) for $T = 0$ in this case is elementary:

$$X = (g^2\mu_B^2/2) D(\varepsilon_f)/[1 - UD(\varepsilon_f)]. \quad (16)$$

This result was first obtained by Stoner. The quantity $S = [1 - UD(\varepsilon_f)]^{-1}$ has become known as the *Stoner enhancement*. The criterion for the occurrence of Stoner magnetism has the form $UD(\varepsilon_f) > 1$ and is related to the occurrence of a singularity of the susceptibility. The occurrence of a singularity of the susceptibility (15) as $q, \omega \to 0$ was analyzed in a most general case by Edwards and Fisher.[19] Since the total spin for the Hubbard model is an integral of the motion ($[\sum_i S_i^z, H] = 0$), the operators $S^\pm = S^x \pm iS^y$ change the total z component by ± 1. At the same time, the operator $\sum_i S_i^-$ also commutes with the Hamiltonian. Edwards and Fisher showed that due to the rotational invariance of the Hubbard model the generalized transverse spin susceptibility $X^{+-}(\mathbf{q}, \omega)$ has a spin-wave pole of the form

$$\hbar\Omega_q = Dq^2 + O(q^4);$$
$$Dq^2 = \frac{1}{2\langle S^z \rangle} \{\hbar q \langle [J_{\mathbf{q}}^-, S_{-\mathbf{q}}^+]_- \rangle - \hbar^2 q^2 \lim_{\omega \to 0} \lim_{q \to 0} X_J\}. \quad (17)$$

Here

$$\left.\begin{aligned} X_J &= \frac{i}{\hbar} \int_{-\infty}^{t} dt \exp(i\omega t) \langle [J_{\mathbf{q}}^-(t), J_{-\mathbf{q}}^+] \rangle; \\ \hbar q J_{\mathbf{q}}^- &= [S^-(\mathbf{q}), H]. \end{aligned}\right\} \quad (18)$$

In the limit $\omega \to 0, q/\omega \to 0$, the expression (17) is an exact formula and is valid for any metallic or nonmetallic ferromagnet or nonferromagnet in a static magnetic field. In the general case, D is determined by the band structure of the crystal. For a simple cubic lattice, the random-phase approximation gives the following result[4] for the Hubbard model:

$$D = \frac{U}{6\Delta} \sum_k \{\nabla_k^2 \varepsilon_k\} (n_{k\uparrow} + n_{k\downarrow}) + \frac{U}{3\Delta^2} N^{-1} \sum_k \{\nabla_k \varepsilon_k\}^2 (n_{k\uparrow} - n_{k\downarrow}). \quad (19)$$

Here, $\varepsilon_k = \sum_{ij} t_{ij} \exp\{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)\}$ is the band energy, and $\Delta = U/N[\sum_p (n_{p\downarrow} - n_{p\uparrow})]$ is the band splitting. The generalized susceptibility $X^{+-}(q, \omega)$ satisfies the important sum rule

$$\int_{-\infty}^{\infty} \operatorname{Im} X^{+-}(q, \omega)\, d\omega = \frac{\pi}{\hbar} (n_\downarrow - n_\uparrow) = -\frac{2\pi}{\hbar} \langle S^z \rangle. \quad (20)$$

The exact formula of Edwards and Fisher[19] for the susceptibility

$$X = -\frac{2\langle S^z \rangle}{\hbar\omega} + \frac{q^2}{\omega^2} \left\{ X_J - \frac{1}{\hbar q} \langle [J_{\mathbf{q}}^-, S^+(-\mathbf{q})] \rangle \right\} \quad (21)$$

shows that for $q = 0$ we have only the first term in (21), which corresponds to a pole of spin-wave type. Thus, the sum rule (20) is satisfied. Clearly, for small q the contribution of the spin-wave pole must predominate. This circumstance is very important for analyzing the scattering of slow neutrons. Thus, the presence of the spin-wave pole in the spectrum of magnetic excitations of the system is a consequence of the rotational invariance of the Hamiltonian.

In their early paper of Ref. 20, 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 collectivized electrons.[21] Therefore, the study of, for example, the temperature dependence of the mean moment in Ni and Fe in the framework of low-temperature spin-wave theory does not, as a rule, give any indications in favor of a particular model. Various methods have been proposed (see, for example, Ref. 22) to test the band theory of magnetism. An interesting result was obtained by Foner *et al.*[21] by means of the Mössbauer effect. On the basis of a prediction of Wohlfarth,[23] they investigated the behavior of Fe and Ni in very strong magnetic fields (higher than technical saturation) at $T = 4.2$ °K. In this region, the contribution of the spin waves is almost completely suppressed. They found that $X_{HF} = \partial M/\partial H > 0$, whereas for the model of localized spins under the same conditions one must have $X_{HF} = 0$. This is an important argument in favor of the band model of magnetism. However, to interpret the experiment in Ref. 21 the simplest Stoner model (16) was used, so that the conclusions are only qualitative in nature.

From our point of view,[24,25] the clearest difference between the models is manifested in the spectrum of magnetic excitations. The collectivized model has a more complicated spectrum than the model of localized spins. This spectrum has great interest from the point of view of application of the method of scattering of slow neutrons, which is unique for the direct study of the magnetic dynamics of magnetically ordered substances.

3. THEORY OF NEUTRON SCATTERING IN TRANSITION METALS

Among the experimental methods used in solid-state physics, neutron methods occupy a quite unique position. Scattering of slow neutrons makes it possible to determine the crystal structure, the position of the atomic magnetic moments, the distribution of unpaired electrons, the frequency spectra, and the dispersion curves of the various elementary excitations. In this section, we consider the scattering of slow neutrons by magnetic excitations of a transition metal.

It is well known[3,4] that the cross section of inelastic neutron scattering can be expressed in terms of the imaginary part of the generalized spin susceptibility $X^{\alpha\beta}(\mathbf{q}, \omega)$. The transverse spin susceptibility is defined by

$$X^{+-}(\mathbf{q}, \omega) = (g\mu_B)^2 \int_{-\infty}^{\infty} \ll S^+(\mathbf{q}, t)\, S^-(-\mathbf{q}) \gg \exp(i\omega t)\, dt, \quad (22)$$

where

$$\ll A(t),\ B\gg = -\frac{i}{\hbar}\Theta(t)\langle[A(t),\ B]\rangle$$

is the two-time retarded thermal Green's function.[18] The spin operators in (22) can be expressed by means of the second-quantization operators in the q representation[4]:

$$S^+(\mathbf{q}) = F(\mathbf{q})\sum_k S_k^+(\mathbf{q}) = F(\mathbf{q})\sum_k a_{k+q,\uparrow}^+ a_{k\downarrow};$$

$$S^-(\mathbf{q}) = F(\mathbf{q})\sum_k S_k^-(q) = F(\mathbf{q})\sum_k a_{k\downarrow}^+ a_{k+q,\uparrow};$$

$$F(\mathbf{q}) = \int d^3r \exp(i\mathbf{qr})|\phi(\mathbf{r})|^2.$$

Then the cross section for inelastic scattering of neutrons by the transverse spin components can be written in the form

$$\frac{d^2\sigma}{d\Omega\, dE} = \left(\frac{\gamma e^2}{m_e c^2}\right)^2 \frac{k}{k_0}|F(\mathbf{q})|^2 \frac{1}{4}\{1+(\tilde{\mathbf{q}}\mathbf{m})^2\}\frac{N}{(g\mu_B)^2\pi} \times \frac{1}{1-\exp(-\hbar\beta\omega)}\{\mathrm{Im}\,X^{+-}(\mathbf{q},\ \omega) - \mathrm{Im}\,X^{+-}(-\mathbf{q},\ -\omega)\}. \quad (23)$$

Since the structure of the generalized spin susceptibility 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 experiments can be used to gauge the adequacy of the microscopic models. However, to judge reliably the applicability of a particular model, it is necessary to measure the susceptibility at all points of the Fourier space and for all temperatures, which is not always permitted by the existing experimental techniques. The calculation of the spin susceptibility $X^{+-}(\mathbf{q}, \omega)$ for the Hubbard model (11) in the random-phase approximation[4,26] leads to the result

$$X^{+-}(\mathbf{q},\ \omega) = \frac{X_0^{+-}(\mathbf{q},\ \omega)}{1-U/(g\mu_B)^2 X_0^{+-}(\mathbf{q},\ \omega)}, \quad (24)$$

where

$$X_0^{+-}(\mathbf{q},\ \omega) = (g\mu_B)^2 N^{-1}\sum_k \frac{n_{k\downarrow}-n_{k+q,\uparrow}}{E(\mathbf{k}+\mathbf{q},\uparrow)-E(\mathbf{k}\downarrow)+\hbar\omega}; \quad (25)$$

$$n_{k\sigma} = \langle n_{k\sigma}\rangle = \{\exp[\beta(E(\mathbf{k}\sigma)-\varepsilon_f)]+1\}^{-1}; \quad E(\mathbf{k}\sigma) = \varepsilon_k + \frac{U}{N}\sum_p n_{p\sigma}.$$

Equation (24) is the dynamical generalization of Stoner's result (16) for $T \neq 0$.

The poles of the total susceptibility (24) are given by the equation

$$1 = \frac{U}{N}\mathrm{Re}\sum_k \frac{n_{k\downarrow}-n_{k+q,\uparrow}}{\hbar\omega-\varepsilon_{k+q}+\varepsilon_k-\Delta}. \quad (26)$$

From Eq. (26) in the limit $\mathbf{q}, \omega \to 0$, $|\mathbf{q}|/\omega \to 0$ there follows an expression for the spin-wave pole $\hbar\Omega_q = Dq^2$ of the form (19). Among the poles of the susceptibility (24) there are poles of the Hartree–Fock susceptibility (25):

$$\mathrm{Im}\,X_0^{+-}(\mathbf{q},\ \omega) = \pi(g\mu_B)^2 N^{-1}\sum_k (n_{k+q,\uparrow}-n_{k\downarrow})\delta(\hbar\omega-\varepsilon_{k+q}+\varepsilon_k-\Delta). \quad (27)$$

The excitations determined by the dispersion law

$$\hbar\omega_q = \varepsilon_{k+q}-\varepsilon_k+\Delta, \quad (28)$$

are usually called *Stoner excitations*. In contrast to the spin-wave excitations, the spin flip is determined here by the single-particle motion rather than the collective motion of the system (Fig. 2). The excitation spectrum determined by Eq. (26) is shown schematically in Fig. 3.

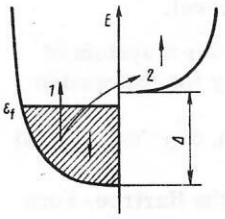

FIG. 2. Excitations in the collectivized model. The excitations of types 1 and 2 arise without and with spin flip.

Far from the point of intersection of the Stoner and spin-wave spectrum, we can approximately separate the contributions to the scattering cross section from these two types of excitation. For this, we represent $\mathrm{Im}X^{+-}(\mathbf{q}, \omega)$ in the form

$$\mathrm{Im}\,X^{+-}(\mathbf{q},\ \omega) = \mathrm{Im}\,X_0^{+-}\{[1-U/(g\mu_B)^2\,\mathrm{Re}\,X_0^{+-}]^2 + [U/(g\mu_B)^2\,X_0^{+-}]^2\}^{-1}. \quad (29)$$

Since $\mathrm{Im}X_0^{+-}(\mathbf{q}, \omega) = 0$ when (q, ω) does not belong to the region in which the Stoner excitations are defined, it follows from (29) that

$$\frac{U}{(g\mu_B)^2}\mathrm{Im}\,X^{+-}(\mathbf{q},\ \omega) = -\pi\delta\{1-U/(g\mu_B)^2\,\mathrm{Re}\,X_0^{+-}(\mathbf{q},\ \omega)\}. \quad (30)$$

Since

$$1-U/(g\mu_B)^2\,\mathrm{Re}\,X_0^{+-}(\mathbf{q},\ \omega) \approx (\hbar\Omega(\mathbf{Q})+\hbar\omega)\frac{1}{\Delta},$$

we obtain from (30)

$$\mathrm{Im}\,X^{+-}(\mathbf{q},\ \omega) = -\pi(g\mu_B)^2\frac{\Delta}{U}\delta(\hbar\omega+\hbar\Omega(\mathbf{Q})), \quad (31)$$

where $\pm\mathbf{Q} = \mathbf{q}-\boldsymbol{\tau}$; $\boldsymbol{\tau}$ is a wave vector of the reciprocal lattice. Using (29)–(31), we obtain from (23) the cross section for spin-wave scattering of slow neutrons:

$$\left(\frac{d^2\sigma}{d\Omega\, dE}\right)_{s.w.} = \frac{k}{k_0}\frac{(2\pi)^3}{v_0}\left(\frac{\gamma e^2}{m_e c^2}\right)^2|F(q)|^2\frac{1}{4}\{1+(\tilde{\mathbf{q}}\mathbf{m})\}\langle S^z\rangle \times \sum_{\mathbf{Q}}\sum_{\boldsymbol{\tau}}\{n(\Omega(\mathbf{Q}))\,\delta(\hbar\omega+\hbar\Omega(\mathbf{Q}))\,\delta(\mathbf{Q}+\mathbf{q}-\boldsymbol{\tau}) + [n(\Omega(\mathbf{Q}))+1]\,\delta(\hbar\omega-\hbar\Omega(\mathbf{Q}))\,\delta(\mathbf{q}-\mathbf{Q}-\boldsymbol{\tau})\}, \quad (32)$$

where

$$\langle S^z\rangle = \frac{N\Delta}{U}; \quad n(\Omega) = [\exp(\beta\hbar\Omega)-1]^{-1}.$$

The scattering cross section (32) is identical to the cross section for scattering by spin waves in the Heisenberg model calculated in the random-phase approximation (see, for example, Ref. 4).

However, for the Hubbard model (11), as follows from Eqs. (27) and (29) in the energy range in which an electron can overcome the energy barrier associa-

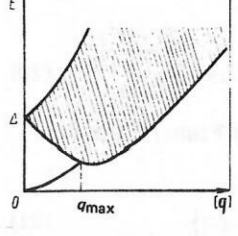

FIG. 3. Spectrum of spin-wave and Stoner excitations in the single-band Hubbard model.

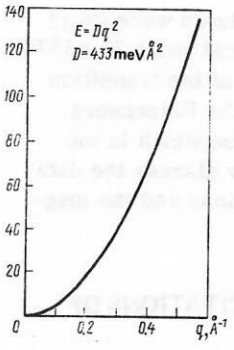

FIG. 4. Dispersion law of spin waves in Ni.[99]

ted with spin flip in the effective field, one must observe scattering of the neutrons by the Stoner modes[3]:

$$\left(\frac{d^2\sigma}{d\Omega\, dE}\right)_{\text{s.p.}} = \left(\frac{\gamma e^2}{m_e c^2}\right)^2 \frac{k}{k_0}\frac{1}{4}|F(q)|^2\{1+(\tilde{\mathbf{q}}\mathbf{m})^2\} \times \sum_{\sigma\neq\sigma'}\sum_{\mathbf{k}} n_{\mathbf{k}\sigma}(1-n_{\mathbf{k}+\mathbf{q}\sigma'})\,\delta(E(\mathbf{k}+\mathbf{q}\sigma')-E(\mathbf{k}\sigma-\hbar\omega)). \quad (33)$$

Thus, the inelastic neutron scattering occurs in this case on account of excitation of the transitions $|\mathbf{k}\sigma\rangle \to |\mathbf{k}+\mathbf{q}\sigma'\rangle$. The ferromagnetic transition metals have well-defined peaks of inelastic scattering by spin waves. For many metals the dispersion law Dq^2 has been measured with high accuracy. Figure 4 shows the results of neutron measurements for Ni. The cross section for scattering (33) by Stoner excitations has a very different nature from the cross section for scattering by spin waves. In accordance with (33), the Stoner scattering must lead to broad diffuse peaks of low intensity. Since such excitations do not arise in the Heisenberg model, their direct detection by means of inelastic neutron scattering would be a very important argument in favor of the Hubbard model. This is all the more important in that there are many indirect data supporting their existence. We shall discuss these data in the following sections.

4. MAGNETIC PROPERTIES OF NICKEL, IRON, AND COBALT

We now discuss briefly the results of some experimental and theoretical investigations into ferromagnetic transition metals, namely, Ni, Fe, and Co. A general review of the problem from different points of view is well presented in Refs. 27–30.

Nickel. This is the metal most fully investigated. The Curie point is $T_C(\text{Ni}) = 631\,^\circ\text{K}$.[2] The mean atomic magnetic moment for the ferromagnetic state of the crystal, expressed in Bohr magnetons, is $\mu(\text{Ni}) = 0.583$ (data for room temperature).[31] Mott was one of the first to suggest that the observed fractional magnetic moments arise because the Fermi energy lies within the $3d$ band. At the same time, the Fermi energy must lie at levels in Ni, Fe, and Co such that the number of holes in the $3d$ band can be 0.6 in Ni, 1.7 in Co, and 2.2 in Fe; this explains the experimental values of the magnetic moment. What can information about the mean atomic magnetic moments tell us about the problem in which we are interested, namely, are the electrons localized or collectivized? The mean atomic magnetic moment is a static characteristic. Its theoretical calculation ensures a good test for the wave functions of the electrons in a metal.[32,33] The degree of localization (or collectivization) of magnetically active electrons can be characterized only on the basis of the contributions made to the mean moment by the electrons near the bottom or top of the band. However, this is inadequate to decide in favor of a particular microscopic model (see the Introduction).

The temperature dependences of the electron specific heat for ferromagnetic metals were calculated for the first time by Stoner[34] on the basis of the band model in the effective-field approximation and for parabolic density-of-states curve. This calculation was perfected by Hunt,[35] and subsequently by Shimizu and Terao[36] for nickel and iron. The low-temperature magnetic specific heat of nickel was also calculated by Thompson.[37] It was shown that in the low-temperature region the spin-wave specific heat calculated in the approximation of noninteracting spin waves does not agree entirely satisfactorily with the experimental data. The agreement can be improved[38] by the choice of the density of states of nickel on the basis of detailed theoretical calculations of the band structure.[39-42] However, the calculations of Ref. 36, made on the basis of Stoner's model for nickel and iron, agree best with the experiments. In this model there exist only Stoner excitations, which were not taken into account in Thompson's calculation in Refs. 37 and 38. In the opinion of Shimizu and Terao,[36] the contribution from both the spin-wave and the Stoner excitations must be taken into account in the calculation if the magnetic electron specific heat is to be correctly explained.

In recent years, a rather substantial number of theoretical calculations have been made of the band structure of ferromagnetic nickel.[39-54] On the basis of these calculations, it has been possible to explain satisfactorily the ferromagnetic anisotropy energies of nickel and iron,[55] the internal fields in nickel and iron and the isomer shift of iron,[48] the spin-wave energies of iron, cobalt, and nickel,[52] the spectroscopic splitting factor and the magnetomechanical ratio of nickel and iron,[56] and numerous other characteristics. Our understanding of the energy band structure of Ni, Fe, and Co has been made more precise by study of the x-ray spectra,[57] measurement of the spin polarization of electrons tunneling from ferromagnets,[58-60] and photoemission investigations.[61-64] The experimental study of photoemission electrons makes it possible, in particular, to determine the band splitting Δ. For Ni, the best estimate based on all the experimental and theoretical investigations is $\Delta \approx 0.5 \pm 0.1$ eV. However, the photoemission experiments do not permit establishment of the contribution of the various types of excitation. Indirect evidence for the existence of Stoner excitations is also provided by investigation of the de Haas–van Alphen effect in transition $3d$ metals.[65,66] It was noted in Ref. 67 that exact description of Raman scattering of light in transition metals requires allowance for the additional scattering by Stoner excitations. At small momenta and zero temperature, the intensity of light scattering by magnons is greater than by Stoner excitations. However, the contribution to the scattering intensity from the magnons and from the Stoner excita-

tions depends differently on the specific band structure of the metal.[68]

Iron. The Curie point is $T_C(\mathrm{Fe}) = 1043\,^\circ\mathrm{K}$.[2] The mean atomic magnetic moment for the ferromagnetic state is $\mu(\mathrm{Fe}) = 2.177$.[31] Investigation of the temperature dependence of the electron specific heat of iron[36] indicates an important contribution from Stoner excitations. Calculations of the energy band structure of iron[69-73] have deepened our understanding of its magnetic properties. Study of the Fermi surface of iron[74-77] and nickel,[74] the spin–orbit coupling, and the optical conductivity of iron[77] shows that the model of collectivized electrons applies very well. Investigations into the temperature dependence of the exchange splitting in iron[65] by means of the de Haas–van Alphen effect give indications of an important contribution from Stoner excitations.

Nevertheless, an agreed opinion on why iron is magnetic still does not exist. In Ref. 78, the following question is posed: Should the magnetic properties of iron be described on the basis of the notion of localized moments or on the basis of a band description as in the Stoner model? In Ref. 78, studied hyperfine fields in the alloys FeSi and FeMn were studied. The available information on the state of the magnetically active electrons in Fe obtained from measurement of the hyperfine fields was analyzed in the review of Ref. 79. It is demonstrated convincingly in Refs. 78 and 79 that the electrons in Fe partly retain a localized nature, so that the simple Stoner model is invalid. The Hubbard model, which takes into account both aspects of the electron behavior—collectivized and localized—gives a much more adequate description of the real situation in the metal; in this model, the collectivized and localized aspects of the electron behavior have a complementary nature.

Cobalt. The Curie point is $T_C(\mathrm{Co}) = 1403\,^\circ\mathrm{K}$.[2] The mean atomic magnetic moment is $\mu(\mathrm{Co}) = 1.707$.[31] The electron energy band structure of cobalt was calculated in Refs. 80–83. On the basis of these calculations, a simple interpretation was given of the photoelectron measurements in nickel and cobalt,[84] and also an interpretation of the measurements of the hyperfine fields.[85] Investigations of the low-temperature electron specific heat made it possible to determine the coefficient γ.[86] The exchange splitting in cobalt is greater than in nickel: $\Delta(\mathrm{Co}) = 0.91$ eV.[80] At the same time, it is indicative that the ratio of the effective Coulomb interaction U to the width of the d band is approximately the same for all three metals Fe, Ni, and Co: $U/w \approx 0.14$–0.16.

In Ref. 87, the band model was used to calculate the Curie point of Co. The energy band structure, the wave functions, and the density of states were found from first principles. The theoretical value $T_C \approx 1370 \pm 200\,^\circ\mathrm{K}$ was obtained. An estimate of the transition temperature for Co on the basis of the Heisenberg model of localized spins gives a value which is too high, namely, $T_C \approx 1870\,^\circ\mathrm{K}$. We now discuss the data on the spectrum of magnetic excitations and the magnetization.

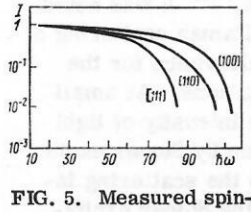

FIG. 5. Measured spin-wave intensity in Ni at room temperature along three symmetric directions.[99]

5. SPECTRUM OF MAGNETIC EXCITATIONS OF Ni, Fe, AND Co

Very important information about the state of magnetically active electrons is obtained by investigating the spectrum of magnetic excitations. The most interesting investigations (from the point of view of comparison of the localized model and the band model) were made by means of neutron scattering.

The scattering of neutrons in Ni has been investigated in detail in a number of theoretical and experimental studies.[88-101] The early neutron investigations into the spectrum of magnetic excitations in Ni are reviewed in Refs. 95, 100, and 101; the later results are discussed in the review of Ref. 30.

Thermal neutron scattering enables one to measure directly the scattering law $S(q, \omega)$ in a wide range of energy, $\hbar\omega$, and momentum, q, transfers:

$$q = k_0 - k = (m/\hbar)(v_0 - v);\ m/\hbar = 0.3956\ \text{Å}^{-1} \cdot \text{cm}^{-1} \cdot \text{msec},$$
$$\hbar\omega = (\hbar^2/2m)(k_0^2 - k^2) = (1/2)\, m\,(v_0^2 - v^2);\ \hbar^2/2m = 2.072\ \text{meV} \cdot \text{Å}^{-2}.$$

In principle, one can investigate the region of q values in the interval 0.1–10 Å^{-1} and energies $\hbar\omega$ in the interval 10–10^3 meV.

In the study of neutron scattering in transition metals, one can in a first approximation ignore the contribution of the orbital angular momentum.[102] For Ni the calculation shows[96] that at large momentum and energy transfers the importance of the orbital contribution increases. The ferromagnetic metals have well-defined peaks of inelastic scattering by spin waves. For Ni, Fe, and Co, the dispersion law

$$\hbar\omega = Dq^2(1 - \beta q^2 + \gamma q^4) \tag{34}$$

has been measured with high accuracy. The results of the neutron measurements for Ni are shown in Fig. 4. In a number of papers[103-106] the spectrum of spin-wave excitations measured by means of neutron scattering has been interpreted on the basis of the Heisenberg model. The experiments were made on nickel[104] and iron.[104-106] However, subsequent investigations of the spin-wave spectrum in iron[107-111] and cobalt (Refs. 90, 100, 112, and 115) showed that the collectivized model corresponds more closely to reality. The decisive argument in favor of the collectivized model was an indirect indication of the existence of Stoner excitations.

It was found[99] that in nickel the spin-wave intensity of neutron scattering along the direction [110] decreases slowly with increasing energy and at $E \approx 100$ meV decreases abruptly by more than an order of magnitude. This sudden decrease in the intensity was explained by

the intersection of the spin-wave spectrum with the Stoner continuum. The energy at which the decrease in the intensity occurred was different for the three principal symmetric directions (80 meV for the direction [111] and 110 meV for the direction [100]) (Fig. 5).

Calculations of the generalized susceptibility $X^{+-}(q,\omega)$ and its poles on the basis of calculations of the energy band structure of nickel[98] with allowance for the dependence of the band spin splitting on the quasimomentum and many-band effects showed that along the direction [111] the region of Stoner excitations lies lower than along the other two directions (Fig. 6), which agrees with the experiment. A similar behavior of the spin-wave intensity is observed in iron[109] with the difference that the energies of the abrupt decrease are $E \approx 90$ meV for the direction [100], $E \approx 95$ meV for [110], and $E \approx 100$ meV for [111].

Detailed neutron measurements of the temperature dependence of the spectrum of magnetic excitations were made for both nickel[95,96] and iron.[110] It was expected that the Stoner continuum would be shifted by a change in the temperature, since the band splitting Δ, which is proportional to the magnetization, must change. The measurements in nickel[99] along the direction [111] showed that the point of intersection of the spin-wave spectrum and the Stoner spectrum hardly changes in the temperature range from 4.2 to 715 °K (Fig. 7). Moreover, the spin-wave spectrum in this temperature range also changes only slightly. The coefficient of stiffness D in the dispersion law $\hbar\omega = Dq^2$ decreases from 555 meV · Å^2 at 4.2 °K to 280 meV · Å^2 at $T_C = 631$ °K; with further increase in the temperature to 715 °K, the coefficient D hardly changed.

These results were obtained by means of a triaxial spectrometer. The technique of small-angle scattering[107] gives the different value $D = 125$ meV · Å^2 at $T = T_C$. However, despite these discrepancies the condition $D(T) \to D_0$ is satisfied as $T \to T_C$. A similar temperature dependence is observed for iron.[110] For the measurements, ^{60}Ni and (^{54}Fe + Si) crystals were used. The isotopes ^{60}Ni and ^{54}Fe have very small nuclear scattering amplitudes compared with the normal isotopes. At the same time, the phonon scattering is in this case less, and the incoherent nuclear scattering makes a small contribution.

Thus, one can say that the experiments on inelastic neutron scattering in transition metals give important

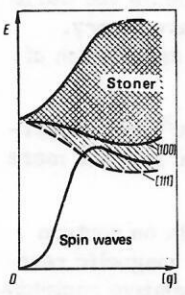

FIG. 6. Results of theoretical calculation of the excitation spectrum for Ni (Ref. 98) in the direction [111].

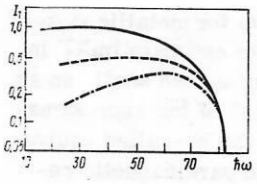

FIG. 7. Temperature dependence of the spin-wave intensity in Ni.[99]

indirect indications of the existence of Stoner excitations. Detailed theoretical calculations[98] confirm this conclusion.

What are the prospects of direct investigation of the Stoner excitations? An important consequence of the calculations made in Ref. 98 is the assertion that at large momentum transfers the spin-wave scattering cross section is only two or three times greater than the Stoner scattering cross section (Fig. 8). One can give a very simple qualitative interpretation of this circumstance,[24,25] which is based on the results of the theoretical calculation of Thompson.[116] Thompson considered the Hubbard model, took the sum rule (20),

$$\int_{-\infty}^{\infty} \operatorname{Im} X^{+-}(q,\omega) = (2\pi/\hbar)(n_\downarrow - n_\uparrow),$$

and used the random-phase approximation to calculate the susceptibility and the effective-mass approximation, By a numerical calculation he showed that

$$\int_{-\infty}^{\infty} d\omega \operatorname{Im} X_0^{+-}(q = 0.9q_{\max},\ \omega) = \frac{2\pi}{\hbar}\frac{\Delta}{U} - \int_{-\infty}^{\infty} d\omega \operatorname{Im} X_{\text{s.w.}}^{+-}(q = 0.9q_{\max},\ \omega) = \frac{2\pi}{\hbar}\frac{\Delta}{U}\left(1 - \frac{1}{2}\right) = \frac{2\pi}{\hbar}\frac{\Delta}{2U}. \quad (35)$$

He found that for a strong ferromagnet ($\Delta > \varepsilon_f$, which corresponds to Ni) the free susceptibility is

$$\operatorname{Im} X_0^{+-}(q,\omega) = \begin{cases} 0, & |y| > 1; \\ \frac{3}{4}\pi\frac{\Delta}{U\delta E}(1-y^2), & |y| < 1, \end{cases}$$

where $y = (\Delta' - \omega)/\delta E$, $\Delta' = \Delta + \hbar^2 q^2/2m^*$, and $\delta E = \hbar^2 q k_f/m^*$; m^* is the effective electron mass. Thus, the width of the diffuse peak, which is determined by $\operatorname{Im} X_0^{+-}(q,\omega)$, will be $\delta E = (q/k_f)\varepsilon_f$.

Let us estimate δE. Following Ref. 117, we assume that $q_{\max} \lesssim 0.75 k_f$. Then for $q = 0.9q_{\max}$ we find that δE

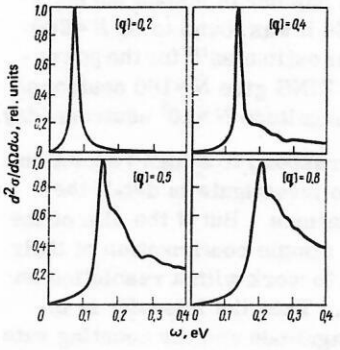

FIG. 8. Theoretical calculation of the total scattering cross section in Ni as a function of the quasimomentum.[98]

$\approx 0.67\varepsilon_f$. The exact calculations of ε_f for metallic nickel[50] show that $\varepsilon_f = 7.6$ eV. However, to estimate $\mathrm{Im}X_0^{+-}$ in framework of Thompson's calculation, we shall, so as not to violate the "self-consistency" of the approximations, use the estimates of ε_f for the so-called equivalent free electron gas model in the paramagnetic region.[95] In the framework of this model, which corresponds to the approximations of Ref. 116, $\varepsilon_f = 0.4$ eV. Thus, the width of the diffuse Stoner peak is $\delta E = 0.67\varepsilon_f = 0.67 \times 0.4 = 0.27$ eV. The width of the spin-wave peak at $q = 0.9q_{max}$ can be taken to be 0.1 eV (Refs. 94, 95, 99, and 100). Since in accordance with (35) the areas of the two peaks are equal for $q = 0.9q_{max}$, the amplitude of the Stoner peak will be approximately three times less than that of the spin-wave peak. Thus, our qualitative estimates agree with the exact numerical calculations (Fig. 8) of Ref. 98.

The measurements of the spectrum of magnetic excitations in nickel[99] and iron[109,110] were made using stationary reactors by means of a triaxial crystal spectrometer. The band splitting Δ of Ni, Fe, and Co has the smallest value $\Delta \approx 0.5$ eV for Ni. Therefore, to measure the Stoner excitations in Ni it is necessary to have a flux of neutrons with energy in the range 0.1–1 eV. We recall that the point at which the spin-wave spectrum along the direction [111] terminates corresponds to an energy 80 meV, so that the range of energy transfers of interest to use lies in the interval 0.08–0.5 eV.

It is clear that the ordinary technique is not well suited to measure excitations of such high energy even in the presence of a hot source. A very promising method is the time-of-flight method. The pulsed neutron sources have the necessary power to ensure sufficient luminosity, and the narrow pulse makes it possible to work with good resolution and a low background level. According to the estimates of Ref. 118, the flux of neutrons expected at distance 30 m from the IBR-2 pulsed reactor for $E_0 = 0.5$ eV and $\Delta E_0 = 0.0045$ eV, pulse time $\tau = 3$ μsec, and moderator measuring 20 × 20 cm, can be assumed to be

$$J = 2.5 \times 10^4 \text{ neutrons} \cdot \text{cm}^{-1} \cdot \text{sec}^{-2}.$$

In Ref. 24, estimates were made of the counting rate of the facility in the case of scattering of such a flux of slow neutrons by Stoner excitations. The estimates discussed above for the Stoner scattering cross section were used. The expected number of counts during a measurement time of $t = 24$ h was found to be $N \approx 200$ –250 neutrons/day. Similar estimates[119] for the powerful pulsed neutron source ZING give $N \approx 160$ neutrons/day. Thus, in order of magnitude $N \approx 10^2$ neutrons/day.

These upper bounds correspond to a high resolution, which makes it possible to investigate in detail the properties of Stoner excitations. But if the aim of the experiment is merely the simple confirmation of their existence, it is sufficient to work with a resolution an order of magnitude lower. Then the intensity is increased by an order of magnitude and the counting rate is raised.

With the facilities currently available, the direct measurement of Stoner excitations in Ni, Fe, and Co is rather difficult because of the large band splitting. Therefore, the experimentalists try to find band ferromagnets with a small value of Δ. In Ref. 120, the intermetallic compound MnSi, which is a weak band ferromagnet, was chosen to investigate magnetic excitations. A ferromagnetic state is induced in MnSi by an external magnetic field with intensity higher than 6 kOe. The neutron scattering experiment was done by means of a triaxial crystal spectrometer.

In a magnetic field of 10 kOe at 5 °K, well-defined spin-wave excitations were observed below 2.5 meV. The dispersion law was found in the form $\hbar\omega_q(\text{meV}) = 0.13 + 52q^2(\text{Å}^2)$ for the direction [100]. Above 3 meV, appreciable broadening of the spin-wave peak was observed, and this was attributed to intersection of the Stoner continuum. Thus, the stiffness coefficient in MnSi is an order of magnitude lower than in nickel. The band splitting could not be determined; only the energy at the intersection of the Stoner continuum was found. For the direction [100], this energy is 2.6 meV.

The scattering of neutrons in Fe_3Al (Ref. 121) also gives indirect confirmation of the existence of Stoner excitations. For the direction [111], the energy at the intersection of the Stoner continuum is about 12 meV. In the intermetallic compound Pd_3Fe (Ref. 122), the dispersion curve of the magnons in the direction [001] intersects the Stoner continuum at $E \approx 40$ meV.

Thus, investigations into the spectrum of magnetic excitations of ferromagnetic transition metals and some of their compounds provide very weighty arguments for the existence of Stoner excitations, and the development of the experimental techniques could lead to their direct observation.

6. CONTRIBUTION OF SPIN WAVES AND STONER EXCITATIONS TO THE MAGNETIZATION

The study of the temperature dependence of the magnetization is of great interest from the point of view of comparing the localized model and the collectivized model. Unfortunately, sufficient clarity has not yet been achieved in this question.

Wohlfarth[27] analyzed the magnetic, thermal, and magnetoelastic properties of strong and weak band ferromagnets on the basis of simple thermodynamic considerations. In his opinion, the properties of strong band ferromagnets, in particular, Ni, can be given a fairly satisfactory description below the Curie point on the basis of the simple spin-wave theory. Stoner excitations are important in the description of weak ferromagnets.

The more detailed analysis of Shimizu[28] and, in particular, Riedi[123] shows that the situation is much more complicated than follows from Ref. 27.

Riedi[123] analyzed the experimental data on neutron scattering, magnetization, and nuclear magnetic resonance and attempted to determine the relative contribution of the spin waves and the Stoner excitations to the temperature dependence of the magnetization $M(T)$.

Now in fact the temperature dependence of the magnetization depends strongly on the model used for the description. For a simple cubic Heisenberg ferromagnet, the temperature dependence of the magnetization in the spin-wave approximation has the form

$$\Delta M_{\text{s.w.}} = M(0) - M(T) \sim F(3/2T)\,(g\mu_B/M(0))\left(\frac{kT}{4\pi D(T)}\right)^{3/2} - O(T^{5/2}) = aT^{3/2}(1+bT+\ldots). \quad (36)$$

The first coefficients a of the term $T^{3/2}$ for Ni and Fe were found in Ref. 124. In a band ferromagnet, there are in addition to the spin waves the Stoner excitations, which also contribute to the thermodynamic behavior. Therefore, in the general case, the temperature dependence $\Delta M(T)$ must be determined by the contributions of the spin waves and the Stoner excitations, and also the contribution due to their interaction.

In a certain range of parameter values of the system, $\Delta M(T)$ can be represented approximately as a superposition of these two contributions:

$$\Delta M(T) \sim \Delta M_{\text{s.w.}} + \Delta M_{\text{s.p.}}. \quad (37)$$

The temperature dependence $\Delta M_{\text{s.p.}}(T)$ is different for weak and strong ferromagnets (see Ref. 123):

$$\Delta M_{\text{s.p.}}(T) = \begin{cases} \sigma_{00}\,[2I(T)/n]\exp(-\Delta/kT) & \text{— for strong ferromagnet,} \\ \sigma_{00}AT^2 & \text{— for weak ferromagnet.} \end{cases} \quad (38)$$

The more accurate calculation of Herring[125] with allowance for the interaction of the spin waves and the single-particle excitations gives for a weak ferromagnet the expression

$$\Delta M_{\text{s.p.}}(T) = AT^2 - CT^{5/2}. \quad (39)$$

Thus, investigation of the temperature dependence of the magnetization can in principle give important arguments in support of one or the other model. However, the problem is complicated by the fact that for reliable conclusions the measurements must be very accurate, since $\Delta M(T)$ is very small in the low-temperature region.

In recent years, detailed theoretical and experimental investigations have been made into the temperature dependence of the magnetization of Ni (Refs. 124, 126–130) and Fe (Refs. 124, 128, 131–134). Analysis of the data on neutron scattering, the magnetization, and nuclear magnetic resonance shows that Ni and Fe behave differently. The low-temperature magnetization of Fe is well described by

$$\Delta M(T) = B_0 T^{3/2}, \quad (40)$$

where B_0 is a constant (in agreement with the spin-wave theory).

As follows from (36), using inelastic scattering of neutrons to measure the spin-wave stiffness D, one can find the coefficient B_0. For Fe, all the three values of B_0 obtained by means of inelastic neutron scattering, measurements of the magnetization, and nuclear magnetic resonance, agree well with one another.

At higher temperatures, the coefficient B in (40) depends on the temperature. For the Hubbard model, calculation of the coefficient of spin-wave stiffness in the Hartree–Fock approximation leads to the temperature dependence[4]

$$D(T) = D_0 - D_1T^2 - D_2T^{5/2}. \quad (41)$$

The contribution $D(T)$ proportional to T^2 arises from the allowance for the electron–magnon interaction. Using the technique of small-angle scattering, Stringfellow[107] measured $D(T)$ for Ni and Fe. It was found that $D_1 = 0$ for Ni. For Fe, $D_1 \neq 0$ in the low-temperature region, and the dependence of D on T^2 is important. Thus, the temperature dependence of the spin-wave stiffness for Ni has the form

$$D = D_0 - D_1T^{5/2}. \quad (42)$$

According to Aldred,[129] the best values of D for Ni are $D(T = 4.2\,^\circ\text{K}) = 555$ meV·Å^2 and $D(T = 295\,^\circ\text{K}) = 455$ meV·Å^2. Using these data obtained by means of neutron scattering, one can determine the coefficient B in the temperature dependence (40) of the magnetization.

It was found that the value of B for Ni obtained from measurements of the magnetization and nuclear magnetic resonance is approximately 30–40% lower than the value given by the neutron experiments. Aldred[129] has suggested that this pronounced difference in the behavior of Ni and Fe can be explained by the circumstance that the low-temperature behavior of Fe is satisfactorily described by the spin-wave picture but that for Ni it is necessary to take into account the contribution from the Stoner excitations. Therefore, Aldred considered the additional Stoner contribution to the magnetization of Ni:

$$\Delta M_{\text{s.p.}}(T) = \Delta M(T) - \Delta M(T)_{\text{s.w.}}. \quad (43)$$

He attempted to describe the measured temperature dependence $\Delta M(T)$ on the basis of the expression (38). Unfortunately, the accuracy of the measurements of Ref. 129 did not make it possible to choose between the alternatives in (38). Neither dependence $\Delta M_{\text{s.p.}}$ lies entirely satisfactorily on the experimental curve, although the dependence AT^2 is still a better approximation to it.

Riedi[130] determined the contribution $\Delta M_{\text{s.p.}}$ for Ni by means of nuclear magnetic resonance. His result is

$$\Delta M_{\text{s.p.}} = 1{,}68\cdot10^{-6}T^{3/2} + 3{,}22\cdot10^{-7}T^2. \quad (44)$$

He showed that the term proportional to T^2 does not depend on $D(T)$ in the entire region of experimental values of the spin-wave stiffness. Riedi therefore assumes[123,130] that the T^2 dependence in (44) can be attributed to the contribution of the Stoner excitations. His analysis shows that the expression (39) agrees less well with the experiment than the simple dependent T^2.

There is no doubt that the results of Refs. 123–134 are very important, though they are not entirely unambiguous. It follows from (44) that $\Delta/k \neq 0$ is very small, since Ni is a strong ferromagnet.[135] Measurements of the magnetization give $\Delta/k = 162\,^\circ\text{K}$.[130] Riedi assumes that this value must be at least an order of magnitude smaller to explain the observed discrepancy with the neutron data.

Thus, additional very accurate experiments are need-

ed to draw a final conclusion about the contributions of the Stoner and spin-wave excitations. It is, however, clear that the spin-wave description alone is inadequate for Ni. It is unreasonable to hope that an accuracy in the measurements of the temperature dependence of the magnetization sufficient for unambiguous conclusions will be achieved, since the two contributions enter additively. It is for this reason that we believe scattering of slow neutrons to be the only method that can give reliable and direct information about the Stoner excitations.[136]

7. SOME GENERALIZATIONS OF THE HUBBARD MODEL

In discussing the experimental data on the scattering of slow neutrons in ferromagnets, it is necessary to bear in mind the approximate nature of the theoretical predictions discussed above. Hitherto, we have been considering the excitation spectrum of the single-band Hubbard model. In a real metal, however, the situation may be more complicated. Even for a two-band model the picture of inelastic neutron scattering is modified qualitatively and quantitatively; the Stoner scattering cross section can then be appreciable for not too large $q < q_{max}$ as well.

The spectrum of the magnetic excitations of the two-band Hubbard model[137] is shown in Fig. 9. In contrast to the single-band model, there are four quasi-Stoner continua associated with transitions within a band and between bands, and also a branch of optical spin waves and the so-called interband spin-wave branch. Thus, the model of collectivized electrons has a very rich excitation spectrum in the "optical" region.

1. An important generalization of the single-band Hubbard model is the Hubbard model with $s-d$ hybridization, which describes direct scattering of the electrons of the s and d bands[138]:

$$H=\sum_{ij\sigma} t_{ij}d^{+}_{i\sigma}d_{j\sigma}+\frac{U}{2}\sum_{i\sigma} n_{i\sigma}n_{i-\sigma}$$
$$+\sum_{k} E(k)\,a^{+}_{k\sigma}a_{k\sigma}+\sum_{ik\sigma}(V_{ik}d^{+}_{i\sigma}a_{k\sigma}+\text{h.c.}). \qquad (45)$$

The existence of a broad band of s electrons is also taken into account implicitly in the ordinary single-band Hubbard model in realistic estimates of the Coulomb-repulsion parameter. Since the hopping rate of d electrons from atom to atom is appreciably lower than the characteristic velocity of the conduction electrons, the latter can be effectively correlated with the d electrons and screen their fields. For transition $3d$ metals, investigation of the energy band structure reveals that $s-d$ hybridization processes play an important part. Ziman[139] showed that for noble and transition metals in the framework of the Korringa–Kohn–Rostoker method the d band is effectively a resonance in the broad sp band. This permits the assumption that the broadening of the atomic d levels may derive from the $s-d$ hybridization, competing with the direct overlapping of the wave functions of the d electrons. This point of view was confirmed in Refs. 140–143. Subsequently, direct calculations on the basis of interpolation schemes[144] showed that the overlap integrals of the wave functions of the d electrons can be smaller than the overlap integrals of the wave functions of the s and d electrons, although the difference is not too large.

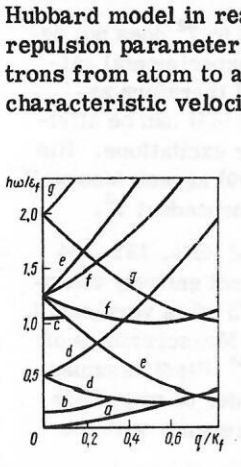

FIG. 9. Excitation spectrum of the two-band Hubbard model as calculated in Ref. 137.

Thus, among the other generalizations of the Hubbard model that correspond more closely to the real situation in pure transition models, the model with $s-d$ hybridization occupies one of the principal positions. The single-particle properties of the variants of this model were investigated in Refs. 145–148. The spin-wave pole of the generalized susceptibility for the model (45) was calculated in Ref. 149 in the atomic limit for the d electrons and for very strong $s-d$ hybridization. However, these approximations are quite invalid for real transition metals. A detailed theory of the scattering of slow neutrons for the Hubbard model with $s-d$ hybridization is given in Ref. 150; the calculation is a direct generalization of that of Izyuama, Kim, and Kubo.[26] They showed that for the single-band Hubbard model, ignoring the overlapping of the wave functions at different sites, one can express the generalized transverse spin susceptibility $X^{+-}(q,\omega)$ of the system in terms of the Hartree–Fock susceptibility $X_0^{+-}(q,\omega)$ in the form (24).

The Hartree–Fock susceptibility of the system (45) can be calculated by means of a simple (u,v) transformation of the linearized Hamiltonian

$$H^{HF}=\sum_{k\sigma}\tilde{E}_{\sigma}(k)\,d^{+}_{k\sigma}d_{k\sigma}+\sum_{k\sigma}\varepsilon_k a^{+}_{k\sigma}a_{k\sigma}+\sum_{k\sigma}(V_k a^{+}_{k\sigma}d_{k\sigma}+\text{h.c.}) \qquad (46)$$

to the form

$$H^{HF}=\sum_{k\sigma}\{\omega_{1k\sigma}\alpha^{+}_{k\sigma}\alpha_{k\sigma}+\omega_{2k\sigma}\beta^{+}_{k\sigma}\beta_{k\sigma}\}. \qquad (47)$$

Here

$$\omega^{1}_{2k\sigma}=\frac{1}{2}\{(\tilde{E}_{\sigma}(k)+\varepsilon_k)\pm\sqrt{(\tilde{E}_{\sigma}(k)-\varepsilon_k)^2+4|V_k|^2}; \qquad (48)$$
$$\tilde{E}_{\sigma}(k)=E(k)+\frac{U}{N}\sum_{p} n_{p\sigma}.$$

The expression for the imaginary part of the Hartree–Fock susceptibility can be expressed in the form[150]

$$\operatorname{Im}X^{HF}(q,\omega)=-\pi(g\mu_B)^2\frac{1}{N}\sum_{k}\{u^{\alpha}_{k+q\downarrow}u^{\alpha}_{k\uparrow}(n^{\alpha}_{k\uparrow}-n^{\alpha}_{k+q\downarrow})$$
$$\times\delta(\hbar\omega+\omega_{1k+q\downarrow}-\omega_{2k\uparrow})$$
$$+v^{\beta}_{k+q\downarrow}v^{\beta}_{k\uparrow}(n^{\beta}_{k\uparrow}-n^{\beta}_{k+q\downarrow})\,\delta(\hbar\omega+\omega_{2k+q\downarrow}-\omega_{2k\uparrow})$$
$$+u^{\alpha}_{k+q\downarrow}v^{\beta}_{k\uparrow}(n^{\beta}_{k\uparrow}-n^{\alpha}_{k+q\downarrow})\,\delta(\hbar\omega+\omega_{1k+q\downarrow}-\omega_{2k\uparrow})$$
$$+v^{\alpha}_{k+q\downarrow}u^{\alpha}_{k\uparrow}(n^{\alpha}_{k\uparrow}-n^{\beta}_{k+q\downarrow})\,\delta(\hbar\omega+\omega_{1k+q\downarrow}-\omega_{2k\uparrow})\}. \qquad (49)$$

Thus, the Stoner cross section for scattering of slow neutrons

$$\left(\frac{d^2\sigma}{d\Omega\, dE}\right)_{s.p.} = \left(\frac{\gamma e^2}{m_e c^2}\right)^2 \frac{1}{4} |F(q)|^2 \frac{k'}{k} (1+\tilde{q}_z^2) \frac{N}{\pi (g\mu_B)^2}$$
$$\times \{(n(\omega)+1)\, \mathrm{Im}\, X^{HF}(-q, \omega) + n(-\omega)\, \mathrm{Im}\, X^{HF}(q, \omega)\} \qquad (50)$$

will describe scattering by the four quasi-Stoner continua.

To calculate the generalized spin susceptibility from the transverse spin components for the model (45), it is necessary to calculate the two-time Green's function $\langle\langle \Theta_k(q) = d^+_{k+q\downarrow} d_{k\uparrow} | B\rangle\rangle_\omega$. The chain of equations for the Green's functions can be reduced to a closed system of four equations by means of the following random-phase approximation:

$$[\Theta_k(q),\ H_d] \approx (E(k) - E(k+q))\, \Theta_k(q)$$
$$+ \Delta\Theta_k(q) - \frac{U}{N} \sum_p (n_{k+q\downarrow} - n_{k\uparrow})\, \Theta_p(q);$$
$$[d^+_{k+q\downarrow} a_{k\uparrow},\ H_d] \approx -E(k+q)\, d^+_{k+q\downarrow} a_{k\uparrow} - \frac{U}{N} \sum_p n_{p\uparrow} d^+_{k+q\downarrow} a_{k\uparrow}$$
$$+ \frac{U}{N} \langle d^+_{k\uparrow} a_{k\uparrow}\rangle \sum_p d^+_{p+q\downarrow} d_{p\uparrow}.$$

As a result, the expression for the transverse spin susceptibility $X^{-+}(q, \omega)$ can be written in a form analogous to (24):

$$X^{-+}(q, \omega) = X^{HF}(q, \omega)\{1 - U/(g\mu_B)^2 X^{HF}(q, \omega)\}^{-1}. \qquad (51)$$

Here, the susceptibility in the Hartree–Fock approximation $X^{HF}(q, \omega)$ has a very complicated form (see Ref. 150) and in the limit $V_{jk} \to 0$ goes over into the usual expression (25). Since the Hamiltonian (45) remains rotationally invariant, it follows from Edward's general theory (17) that the susceptibility (51) must have a spin-wave pole. The existence of a spin-wave pole of the susceptibility $X^{-+}(q, \omega)$ is shown in Ref. 150. At the same time, we have

$$\mathrm{Im}\, X^{-+}(q \to 0,\ \omega \to 0) \sim -\pi (g\mu_B)^2 b/U \delta(\hbar\omega - \hbar\Omega_q), \qquad (52)$$

where b is a constant determined numerically. The cross section of inelastic neutron scattering by the spin waves can be expressed in this case in exactly the same way as (32).

2. In the band model of magnetism, as in the localized model, great interest attaches to explicit allowance for the electron–phonon interaction. Because of this interaction, there is inelastic transfer of energy from the system of magnetic electrons to the lattice vibrations; for the detailed description of neutron scattering, this circumstance is important.[151]

The electron–phonon interaction is determined by the cjange in the potentials $v(\mathbf{R})$ of the ions of the lattice when allowance is made for their thermal vibrations:

$$H_{e-ph} = \sum_{l r_i} \{v(\mathbf{R}_l - \mathbf{r}_i) - \langle v(\mathbf{R}_l - \mathbf{r}_i)\rangle_{ph}\}, \qquad (53)$$

where $\mathbf{R}_l = \mathbf{l} + \mathbf{u}_l$ are the coordinates of the ions, $\mathbf{l}$ are the equilibrium positions, $\mathbf{u}_l$ are the thermal displacements, and $\mathbf{r}_i$ are the coordinates of the electrons. In Ref. 151, the Bloch functions are determined using the potential $v(\mathbf{l} - \mathbf{r}) = \langle v(\mathbf{R} - \mathbf{r})\rangle_{ph}$ of the ions averaged over the lattice vibrations:

$$\left\{-\frac{1}{2m_0}\frac{\partial^2}{\partial \mathbf{r}^2} + \sum_l \tilde{v}(\mathbf{l} - \mathbf{r})\right\} \varphi_{\mathbf{k}}(\mathbf{r}) = \varepsilon_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{r}). \qquad (54)$$

This definition differs from the usual one [see (1)–(3)] and makes it possible to take into account elastic electron–phonon scattering processes. In the second-quantization representation, the Hamiltonian of the single-band Hubbard model with allowance for the electron–phonon interaction can be written in the form[151]

$$H = H_e + H_{ph} + H_{e-ph}; \qquad (55)$$
$$H_{ph} = \sum_q \omega_q b^+_q b_q; \qquad (55a)$$
$$H_{e-ph} = \sum_{pq} V_{p,\ p+q} a^+_{p\sigma} a_{p+q\sigma} \frac{1}{N}$$
$$\times \sum_l \exp(i\mathbf{q}\mathbf{l}) (\exp(i\mathbf{q}\mathbf{u}_l) - \langle \exp(i\mathbf{q}\mathbf{u}_l)\rangle). \qquad (55b)$$

Here, H_e is the single-band Hubbard Hamiltonian (11). $v = U/N$ is the energy of the Coulomb correlation at one site, $V = V_0 N$ is the volume of the system, and b^+_q and b_q are the operators of creation and annihilation of phonons with quasimomentum q, polarization j, and energy ω_{qj}; $q = (\mathbf{q}, j)$. The matrix element of the electron–ion interaction has the form

$$V_{p,\ p+q} = v(q) \int d^3r \varphi^*_{\mathbf{p}}(\mathbf{r}) \exp(-i\mathbf{q}\mathbf{r})\, \varphi_{\mathbf{p}+\mathbf{q}}(\mathbf{r}) = v(q) F(q,\ p+q) \approx V_q,$$

where $v(q) = 1/V_0 \int d^3r \exp(-i\mathbf{q}\mathbf{r}) v(\mathbf{r})$ is the Fourier transform of the electron–ion potential. The potential $v(\mathbf{R}_l - \mathbf{r})$ is the effective (screened by the conduction electrons) interaction potential of the magnetic electrons and ions.

For a system with the Hamiltonian (55), Plakida and Smirnov[151] calculated the cross-section of magnetovibration scattering with allowance for single-phonon transitions:

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{mv} = \sigma_{mv}(k) \frac{k'}{k} \left\{\exp[-2W(q)] \frac{(2\pi)^3}{MV_0} \sum_{\tau pj} \frac{(\mathbf{q}\mathbf{e}_{pj})^2}{2\omega_{pj}}\right.$$
$$\left. \times \left[n(\omega_{pj}) + \frac{1}{2} \pm \frac{1}{2}\right] \delta(\mathbf{q} \pm \mathbf{p} - 2\pi\tau)\, \delta(\omega \pm \omega_{pj}). \qquad (56)\right.$$

Here

$$\sigma_{mv}(k) = (\gamma r_0)^2 (1 - e_z^2) \frac{1}{4} |F(k)|^2 |V_q|^2 \frac{1}{4} \left[\frac{1/N(\pi_\uparrow - \pi_\downarrow)}{1 - v^2 \pi_\uparrow \pi_\downarrow}\right]^2 \qquad (57)$$

is the effective cross section of magnetovibration scattering. It can be seen that the scattering cross section (56) has the form of the usual single-phonon nuclear scattering. However, the effective cross section (57) contains not only the usual factors for elastic magnetic scattering $[(1 - e_z^2)|F(k)|^2]$ and the square of the magnetization $(n_\uparrow - n_\downarrow)^2 \sim (\pi_\uparrow - \pi_\downarrow)^2$ as in the model of localized spins, but also the square $|V_q|^2$ of the matrix element of the electron–phonon interaction, which permits estimation of this quantity by means of magnetovibration scattering of neutrons in metals.

The electron–phonon interaction in the Hubbard model was also considered in Refs. 152–156. Morkowski[153] calculated the magnon relaxation time due to interaction with the phonons in the second order of perturbation theory. Using the method of two-time thermal Green's functions, George[154] obtained an expression for the renormalized spin-wave stiffness in the random-phase approximation. In Ref. 156, Yamada calculated the magnon relaxation time and the renormalization of the spin-wave stiffness by means of the Matsubara Green's functions in the random-phase approximation. It is important that, in contrast to the other calculations,[154,155] Yamada's calculation[156] gives an expression

for $\delta D \sim T^4$ which agrees with the phenomenological result of Ref. 152. Yamada[156] also estimated these quantities numerically for Ni and Fe.

3. From the point of view of scattering of slow neutrons, great interest attaches to the spectrum of magnetic excitations of the so-called Zener model.[157] The Hamiltonian of this model can be written in the form

$$H=\sum_{ij\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} - 2J \sum_{i} \sigma_i \mathbf{S}_i, \tag{58}$$

where $\sigma_i^{+}=a_{i\uparrow}^{+}a_{i\downarrow}$, $\sigma_i^{-}=a_{i\downarrow}^{+}a_{i\uparrow}$, and $\sigma_i^{z}=1/2(a_{i\uparrow}^{+}a_{i\uparrow}-a_{i\downarrow}^{+}a_{i\downarrow})$ are the spin operators of the collectivized electrons, and $\mathbf{S}_i$ is the operator of the localized spin at site i corresponding to Hund's rule. We rewrite the Hamiltonian (58) in the k representation:

$$H=\sum_{k\sigma} \varepsilon_k a_{k\sigma}^{+} a_{k\sigma} + UN^{-1} \sum_{kk'q} a_{k+q\uparrow}^{+} a_{k\uparrow} a_{k'-q\downarrow}^{+} a_{k'\downarrow}$$
$$- JN^{-1/2} \sum_{kq} [a_{k+q\uparrow}^{+} a_{k\downarrow} S_q^{-} + a_{k+q\downarrow}^{+} a_{k\uparrow} S_q^{+} + (a_{k+q\uparrow}^{+} a_{k\uparrow} - a_{k+q\downarrow}^{+} a_{k\downarrow}) S_q^{z}]. \tag{59}$$

The generalized transverse spin susceptibility of the system with the Hamiltonian (59)

$$\chi^{+-}(q,\omega)=\int_{-\infty}^{\infty} \ll \sigma_q^{+}(t),\ \sigma_{-q}^{-} \gg \exp(i\omega t)\, dt \tag{60}$$

can be calculated in the random-phase approximation, as for the ordinary Hubbard model (11). The obtained result is[157]

$$\chi^{+-}(q,\omega)=\chi_0(q,\omega)/\{1-[U-2J^2\langle S^z\rangle/(\omega-Jnx)]\,\chi_0(q,\omega)\}, \tag{61}$$

where

$$\chi_0(q,\omega)=-N^{-1}\sum_k \frac{n_{k+q\uparrow}-n_{k\downarrow}}{\omega-(\varepsilon_k-\varepsilon_{k+q})-\Delta} \tag{62}$$

is the susceptibility of the collectivized electrons in the Hartree–Fock approximation; $\Delta=Unx+2J\langle S^z\rangle$; $nx=N^{-1}\sum_k(n_{k\uparrow}-n_{k\downarrow})$. The transverse susceptibility for the localized spins can be found similarly:

$$\ll S^{+}(q)|S^{-}(-q)\gg_{\omega}=2\langle S^z\rangle/\{\omega-Jnx$$
$$+2J^2\langle S^z\rangle\chi_0(q,\omega)[1-U\chi_0(q,\omega)]^{-1}\}. \tag{63}$$

For $q,\ \omega \to 0$ we find the spectrum of the spin-wave excitations of the system; it is determined by the poles of the susceptibility (61) and (63):

$$\left.\begin{aligned} \hbar\omega_{ac}&=Dq^2 && \text{– for the acoustical branch,}\\ \hbar\omega_{0p}&=E_{0p}+D(UE_{0p}/J\Delta-1)\,q^2 && \text{– for the optical branch.}\end{aligned}\right\} \tag{64}$$

Here, $E_{0p}=Jnx+2J\langle S^z\rangle$. Physically, this result corresponds to the circumstance that the system contains the inequivalent spin subsystems of the collectivized and localized spins. Besides these two types of excitation, there is the continuum of Stoner excitations

$$\hbar\omega_{\mathbf{q}}=(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}})+\Delta, \tag{65}$$

which is determined by the poles of the susceptibility (62). The spectrum of magnetic excitations of the Zener model is shown schematically in Fig. 10. Thus, in contrast to the single-band Hubbard model (11), the spectrum of the Zener model contains an additional branch of optical spin waves. The presence of this optical spin wave is due to the circumstance that the system consists of two subsystems, as for the two-band Hubbard model.[137,158] To see this more clearly, we set $U=0$ in the Hamiltonian (59). We then arrive at the

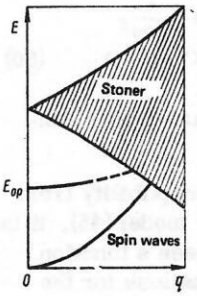

FIG. 10. Schematic form of the excitation spectrum of the modified Zener model.[157]

Hamiltonian of the $s-d$ model:

$$H=\sum_{k\sigma}\varepsilon_k a_{k\sigma}^{+}a_{k\sigma} - JN^{-1}\sum_{kqi}\exp(-i\mathbf{q}\mathbf{R}_i)$$
$$\times[a_{k+q\uparrow}^{+}a_{k\downarrow}S_i^{-}+a_{k+q\downarrow}^{+}a_{k\uparrow}S_i^{+}+(a_{k+q\uparrow}^{+}a_{k\uparrow}-a_{k+q\downarrow}^{+}a_{k\downarrow})S_i^{z}]. \tag{66}$$

The Hamiltonian (66) is widely used to describe the $s-d$ exchange interaction between an impurity spin and the spins of the conduction electrons in nonmagnetic metals (see Ref. 159 and the literature quoted there).

Let us consider the calculation of the Green's functions $\langle\langle S^{-}(\mathbf{q})\,|\,S^{+}(-\mathbf{q})\rangle\rangle_{\omega}$. For the imaginary part of the susceptibility in the random-phase approximation, we obtain[25]

$$-\frac{1}{\pi}\operatorname{Im}\chi^{-+}(\mathbf{q},\omega)=2S\delta(\omega-\omega_{ac}(\mathbf{q}))+nx\delta(\omega-\omega_{0p}(\mathbf{q}))$$
$$+(2S+nx)\frac{v_0}{(2\pi)^3}\int_{<\varepsilon_f} d^3q\,[\delta(\omega-\varepsilon_{k+q\downarrow}-\varepsilon_{k\uparrow})-\delta(\omega-\varepsilon_{k\downarrow}+\varepsilon_{k-q\uparrow})]. \tag{67}$$

In the approximation of the effective mass $\varepsilon_k=k^2/2m^*$ as $q\to 0$ we find that

$$\left.\begin{aligned} \omega_{ac}(q)&=D_1q^2;\quad D_1=\frac{n[1-(2/3)\,\varepsilon_f(x/JS)]}{2m^*(2S+nx)};\\ \omega_{0p}(q)&=J(2S+nx)+D_2q^2;\quad D_2=\frac{S[1+(4/3)\,\varepsilon_f/(Jn)]}{m^*x(2S+nx)}.\end{aligned}\right\} \tag{68}$$

Thus, the Hubbard model admits many generalizations, which makes it possible to take into account numerous physically important interactions in a real transition metal. This is particularly important when one is comparing experimental data on inelastic neutron scattering in a metal with results of theoretical calculations. As follows from our discussion, the detailed investigation of the spectrum of magnetic excitations in the optical and acoustical ranges is of very great interest from the point of view of comparing the localized model and the band model of magnetism. It is also important to emphasize that these two approaches, the localized and the band, do not contradict each other. They are, rather, "complementary" aspects of the quantum statistical description of the state of magnetically active electrons in a real metal. The acoustic part of the spectrum of the magnetic excitations is a reflection of a certain localization of the spins, while the optical part reflects their delocalization. This deep "complementarity" is well reflected by the Zener model (58), which is one of the most interesting models of magnetism. The diversity of the models reflects the diversity of the aspects of the magnetic behavior of real magnets of interest to us.

8. ALLOYS OF MAGNETIC TRANSITION METALS

In recent years, the electron structure and various physical properties of alloys of transition metals have been intensively studied. For the study of the magnetic properties of alloys of transition metals, scattering of slow neutrons has proved to be very helpful. Investigation of the elastic and inelastic scattering of slow neutrons in alloys yields unique information about the magnetic moments and form factors, and also the change in the spin-wave stiffness.

It should be noted that neutron investigations into the distribution of the magnetic moment in magnetic alloys and the change in the spin-wave stiffness stimulated to a large degree the development of modern methods for calculating the electron structure of disordered alloys; these methods are extremely helpful for the solution of many problems in solid-state physics. They include the coherent potential method,[160] which is now well known.

The Hubbard model was very helpful for describing many electron and magnetic properties of alloys of transition metals and is successfully used in many studies. To describe disordered alloys by means of the Hubbard model, one introduces random parameters, and therefore speaks of the Hubbard model with random parameters.

We now turn to its description. It is assumed that the interaction of the electrons in a binary disordered alloy A_cB_{1-c} of two magnetic components is described by the model Hamiltonian

$$H=\sum_{ij\sigma} t_{ij}a_{i\sigma}^{+}a_{j\sigma}+\sum_{i\sigma}\varepsilon_i n_{i\sigma}+\sum_i U_i n_{i\sigma}n_{i-\sigma}. \tag{69}$$

Here, as in (11), $a_{i\sigma}$ and $a_{i\sigma}^{+}$ are the operators of annihilation and creation of Wannier electrons at site i with spin σ. It is assumed that the hopping integrals t_{ij} are the same for both species of atoms A and B, i.e., $t_{ij}^{AA}=t_{ij}^{BB}=t_{ij}$; the band structure of the pure components A and B in the absence of Coulomb interaction is the same. In (69), ε_i and U_i are the single-particle potential and the intra-atomic Coulomb interaction, respectively:

$$\varepsilon_i=\begin{cases}\varepsilon_i^A, & i\in A;\\ \varepsilon_i^B, & i\in B;\end{cases}\qquad U_i=\begin{cases}U_i^A, & i\in A;\\ U_i^B, & i\in B.\end{cases} \tag{70}$$

For a disordered alloy, ε_i and U_i take random values depending on the atom, of species A or B, which occupies the site.

The Hamiltonian (69) has been investigated by many people in different limiting cases. If it is assumed that one of the components of the alloy (for example, B) consists of nonmagnetic atoms, then one can set $U^B=0$. This case corresponds to Wolff's model.[161,162] If we set $\varepsilon_i^A=\varepsilon_i^B$ in (69), we obtain the model Hamiltonian used by a number of authors[163,164] for the theoretical description of the Pd–Ni alloy. The case when $U_i^A=U_i^B$ was considered by Fulde and Luther[165] to analyze the scattering of paramagnons by impurities; Yamada and Shimizu[166] calculated the spin-wave spectrum. Moriya[167] investigated the electron structure near a magnetic impurity ($U_i^A\neq 0$) in a nonmagnetic matrix ($U_i^B\neq 0$) and calculated numerous physical characteristics of the impurity system. The interaction between impurities was considered in Ref. 168. All the studies of Refs. 161–168 were restricted to the approximation of a strongly dilute alloy.

The coherent-potential method[160] makes it possible to consider an alloy with finite impurity concentration. One can identify two theoretical directions which use the coherent-potential method to describe disordered alloys.

The first was initiated in Ref. 169. This gives a theoretical interpretation of the concentration dependence of the mean magnetization, the atomic moments of the components, and the electron specific heat for the alloy Ni_cFe_{1-c}. The papers of Refs. 170–174 are in the same direction.

The approach of Hasegawa and Kanamori[169] is based on the use of the Hartree–Fock approximation for describing the intra-atomic Coulomb correlation. In this case, the Hamiltonian (69) is written in the form[169]

$$H=\sum_{ij\sigma} t_{ij}a_{i\sigma}^{+}a_{j\sigma}+\sum_{i\sigma}E_{i\sigma}a_{i\sigma}^{+}a_{i\sigma}, \tag{71}$$

where

$$E_{i\sigma}=\varepsilon_i+U_i\langle n_{i-\sigma}\rangle. \tag{71a}$$

Thus, the disorder, which is described in the framework of the coherent-potential approximation, is characterized by the two parameters $E_{A\sigma}$ and $E_{B\sigma}$. The mean population numbers $\langle n_{i-\sigma}\rangle$ in (71a), which are different for the different components of the alloy ($\langle n_{i-\sigma}\rangle = n_{A\sigma}$ or $n_{B\sigma}$, $i\in A$ or B), must be determined in a self-consistent manner. This last circumstance has the consequence that not every unit cell is electrically neutral and transfer of a finite charge may take place.

For the single-article Hamiltonian (71), one can use the standard scheme of the coherent-potential method, which we describe here, using the notation of Ref. 160. In the coherent-potential approximation, one considers a single-electron Hamiltonian of the form

$$H=W+D=W+\sum_n D_n. \tag{72}$$

Here, W is the periodic part, and D is the sum of random contributions, each associated with one site. The single-electron properties of the alloy are calculated as ensemble averages over all possible configurations of the atoms in the lattice. Usually, one considers the single-electron Green's function $G(z)$ averaged in this manner:

$$\langle G(z)\rangle=\langle(z-D-W)^{-1}\rangle\equiv(z-W-\Sigma)^{-1}. \tag{73}$$

We define the T matrix for a given configuration of the alloy by means of the equation

$$G=\langle G\rangle+\langle G\rangle T\langle G\rangle. \tag{74}$$

Then the functional equation for determining the unknown operator Σ will be given by the condition

$$\langle T[\Sigma]\rangle=0. \tag{75}$$

Equation (75) is a self-consistent definition of the op-

erator Σ.

Assuming that

$$D-\Sigma=\sum_n (D_n-\Sigma_n)=\sum_n V_n, \tag{76}$$

one can introduce the local scattering operator

$$T_n=V_n(1-\langle G\rangle V_n)^{-1}. \tag{77}$$

By means of the operator T_n, the effective medium characterized by the operator Σ is replaced by scattering by the real atom at the given site n. In the coherent-potential method, the general self-consistency condition (75) is replaced by its single-site approximation

$$\langle T_n[\Sigma]\rangle=0. \tag{78}$$

Thus, in this approach the impurity is assumed to be in an effective medium whose Green's function is chosen to make the T matrix of scattering by the impurity vanish on the average. We ignore scattering by pairs of atoms and larger clusters. The coherent-potential method is exact in the atomic limit, when hopes of electrons from site to site are very improbable. The comparison of the virtual-crystal approximation, the average T-matrix approximation, and the coherent-potential approximation made in Ref. 175 showed that the third is no worse an approximation than the first.

In the coherent-potential method, the averaged Green's function $\langle G(E)\rangle$ of the disordered system is obtained from the Green's function for an ideal lattice by replacing the energy by a complex quantity. The analytic properties of quantities calculated in the single-site approximation of the coherent potential are nontrivial; the Green's function $\langle G(z)\rangle$ is analytic everywhere except the lines of the cuts corresponding to the impurity band and the band of the matrix.

It is important that in the coherent-potential method the effect of electron scattering due to the disorder is described by a complex quantity, namely, the coherent potential. From the point of view of quantum mechanics, there is nothing unusual about this. We recall that for multiple scattering of a wave by an arbitrary ensemble of scatterers one introduces an ensemble-averaged wave function, and the potential in the Schrödinger equation becomes complex.[176] The imaginary part of the potential describes absorption due to scattering.

The main characteristic of the excitation spectrum of the system is the density of states $D(\varepsilon)$ per unit energy. It is determined by the imaginary part of the Green's function $\langle G(z)\rangle=G^{CPA}$. On the basis of the single-particle density of states one can give a good description by means of the coherent-potential method of the behavior of the asphericity parameter γ for alloys of Ni, Fe, and Co.[177]

This parameter is an important characteristic which can be measured experimentally by means of the scattering of slow neutrons and it is defined by

$$\gamma=\mu_{e_g}/\mu, \tag{79}$$

where μ_{e_g} is the magnetic moment determined by electrons in states of e_g type, and μ is the total spin magnetic moment.

The neutron-scattering experiments show that the measured values of γ fit very closely onto a straight line when plotted against μ for virtually all alloys of Ni, Fe, and Co, i.e.,

$$\gamma=a+b\mu. \tag{80}$$

It is only for pure Ni that this does not hold; γ_{Ni} is significantly smaller than the value which follows from (80). A possible reason for this deviation for pure Ni could be the influence of electron correlation or the particular single-particle behavior of the system. In Ref. 177, only the single-particle properties of the system in the approach (71) of Hasegawa and Kanamori were considered, and it was shown that the influence of correlations is not very important for calculation as the asphericity parameter. As in Ref. 169, the concentration range $0\leq c\leq 0.5$ of the $Ni_{1-c}Fe_c$ alloy was considered. Using the coherent-potential method, Hasegawa and Kanamori calculated the magnetic moment μ and the local moments μ(Ni) and μ(Fe). Their results agree well with the experiments. It must, however, be noted that they used not the real density of states but a strongly idealized function and that the problem was solved using many free parameters.

In Ref. 177, the real theoretical density of states[51,178] was used for the first time to calculate the parameter γ. For the exact calculation of γ, it is necessary to take into account separately the e_g and t_{2g} states. It is very difficult to obtain such separate densities of states because of their strong hybridization. In Ref. 177, use was made of the circumstance that at points and on lines of high symmetry, where there is no hybridization, the wave functions can be identified with e_g and t_{2g} states. It was assumed that quantitatively the behavior of the wave functions is not strongly changed on the transition to other points. The employed theoretical density of states consists of six sub-bands, two of which are associated with s electrons, while the remaining four at the points and lines of high symmetry have the behavior of the density of states of electrons in the t_{2g} and e_g states. One can therefore propose an approximate separation of the density of states into components for the t_{2g} and e_g electrons.

In the coherent-potential method, the expression for the density of states in the alloy $Ni_{1-c}Fe_c$ has the form

$$D_i^{CPA}(\varepsilon)=-\frac{z_i}{\pi}\operatorname{Im}G_i^{CPA}(\varepsilon), \tag{81}$$

where

$$G_i^{CPA}=\frac{1}{z_i}\int d\varepsilon'\frac{D_i^{Ni}(\varepsilon')}{\varepsilon-\Sigma_i-\varepsilon'}; \tag{82}$$

Σ_i is the coherent potential defined by

$$\Sigma_i=x\Delta+\Sigma_i(\Delta-\Sigma_i)G_i^{CPA}(\varepsilon); \tag{83}$$

Δ describes the shift between the atomic levels of Fe and Ni. In Ref. 169, this parameter depends very strongly on the spin ($\Delta_\uparrow/\Delta_\downarrow=5.6$) and on the concentration. In Ref. 177, in contrast, it was assumed that Δ is virtually independent of these quantities in order to take into account systematically the single-particle properties of the model. The problem could be solved

without the use of free parameters. The density of states $D_i^{CPA}(\varepsilon)$ and the local densities $D_i^{loc.Ni}(\varepsilon)$ and $D_i^{loc.Fe}(\varepsilon)$ were calculated for $i=t_{2g}$ and different concentrations. The parameter γ obtained on the basis of these results for $D_i^{CPA}(\varepsilon)$ is shown in Fig. 11. The agreement with experiment is good.

It is interesting to note that the results for the values of μ, μ(Ni), and μ(Fe) calculated in Ref. 177 were less good than in the work of Hasegawa and Kanamori. A possible reason for this could be the influence of correlations on the value of μ, for whose description additional free parameters were used in Ref. 169. At the same time, as can be seen from Fig. 11, the behavior of the asphericity parameter can already be well explained on the basis of a single-article density of states with optimal approximation to the real density. For a further discussion of the Hasegawa–Kanamori approach, see Ref. 179.

A different direction in the description of disordered alloys by means of the Hamiltonian (69) was developed in Refs. 180 and 181; specifically, the alloy Pd–Ni was considered in Ref. 180. The difference between these two approaches was analyzed by Fukuyama.[162,174] He showed that in the approach of Harris and Zuckermann[180] the main attention is concentrated on the dynamical effects of the Coulomb interaction, and the spatial variation of the potential is ignored. Therefore, single-article quantities such as the local density of states are spatially homogeneous, except for the possible existence of virtually bound states. The scheme is self-consistent if the equality $\varepsilon_{A\sigma}=\varepsilon_{B\sigma}$ holds in Eq. (69); in this case, one can, in contrast to (71), take into account some processes of electron–hole scattering of higher order.

The difference between the Hasegawa–Kanamori approach[169,173,179] and the Harris–Zuckermann approach[180] is most clearly manifested in the treatment of collective effects, especially in the calculation of the spin susceptibility. This is due to the circumstance that in the construction of the theory of the electron and magnetic properties of the disordered alloys described by the Hamiltonian (69) it is necessary to take into account the random distribution of the atoms of the components on the lattice and the influence of the Coulomb correlation of the electrons on the electron structure and the physical properties. As we have seen above, the single-particle characteristics of an alloy (for example, the asphericity parameter γ) depend weakly on the correlation effects, but for the collective properties correct allowance for the correlations is more important.

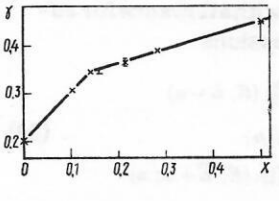

FIG. 11. Dependence of the asphericity parameter γ on the concentration x (the crosses are the theoretical values and the error-bar symbols indicate the experimental values).[177]

9. SPIN WAVES AND THEIR STABILITY IN DISORDERED FERROMAGNETIC METALLIC ALLOYS

In recent years, great interest has been shown in the study of inelastic scattering of slow neutrons in disordered magnetic metallic alloys.[182-192] There is a large body of experimental data on the variation of the spin-wave stiffness D of alloys as a function of the concentration.

The early calculations of the spin-wave energies in alloys in the framework of the band model were based on the rigid-band approximation (Refs. 42 and 193–195). In this approach, the alloy is described as a pure metal with appropriately chosen density of electrons and band splitting. Essentially, the theory of Yamada and Shimizu[166] is in this direction. In 1973, Hill and Edwards[196] obtained an approximate expression for the spin-wave stiffness D of an alloy in terms of the single-electron Green's functions.

For the Hubbard model with random parameters (69), the spin-wave stiffness was calculated by Fukuyama[172,174] and by Riedinger and Nauciel-Bloch.[197,198] The electron–electron interaction was taken into account in the Hartree–Fock approximation, and the disorder in the coherent-potential approximation (CPA). Edwards and Hill[199] gave a much simpler and elegant derivation of the expression for the spin-wave stiffness in the CPA–RPA approximation using the general expressions (17) and (18). The decoupling scheme in the RPA is given in Ref. 200.

The results of neutron measurements of the spin-wave stiffness of strongly ferromagnetic alloys based on Ni are given in Refs. 184–192, and the results are interpreted in detail by means of the band model. In particular, in Ref. 191 inelastic neutron scattering was used to measure the coefficient of spin stiffness of the alloy $Ni_{1-c}Co_c$ for the concentrations $c=0.21$ and 0.5 (at room temperature) and for concentration $c=0.05$ (at $T=4.2$ and 293 °K). The measurements were made by means of a triaxial spectrometer. It was found that the stiffness coefficient decreases slowly with increasing Co concentration, and for $c=0.05$ the value of D depends rather weakly on the temperature. Between the values $c=0.21$ and $c=0.5$ the value of D hardly changes. The theoretical interpretation of these results is given first on the basis of the simplest model of a rigid band, and the correlation is described in the Hartree–Fock approximation. In this approximation, D was calculated for the three alloys NiCo, NiFe, and NiMn. The best agreement with experiment is observed for the first alloy; the worst, for the last. This is probably due to the increased difference between the valences of the alloy's components. One then uses the RPA–CPA approximation. The agreement with experiment as compared with the rigid-band model is improved—slightly for the alloy NiCo and more appreciably for NiFe and NiMn. Nevertheless, it is noted by the authors that the RPA–CPA approximation gives an

unsatisfactory explanation of the behavior of the stiffness coefficient in the alloy $Ni_{1-c}Fe_c$ for $c=0.5$.

Thus, the further improvement in the theory must be based on a more accurate allowance for the interelectron correlations. The point is that the Hartree–Fock approximation strongly overestimates the correlation effects and the tendency of the system to form a magnetically ordered state. More accurate allowance for the correlations must weaken the tendency of the system to magnetic ordering and thus reduce the spin-wave rigidity. This idea was realized in Ref. 201.

To take into account the effects of electron correlation in the calculation of D, Kolley and Kolley[202] developed a scheme which goes beyond the framework of the RPA and is based on the coherent ladder approximation (CLA),[203,204] i.e., on a self-consistent combination of the coherent-potential approximation and the local ladder approximation[205] in the particle–particle channel. It is convenient to use such a T-matrix approximation for strong short-range interactions and low carrier density, so that it can be applied to Ni, Pd, and Pt. If the energy-dependent T matrix is replaced by an effective interaction of Kanamori type,[206] as is done, for example, in the calculation of the paramagnetic susceptibility[207] and magnetostriction,[208] we again arrive at the theory of spin waves in a RPA–CPA framework.

The theory of interelectron correlation in the local ladder approximation in disordered alloys developed in Refs. 202–204 proved very helpful for the investigation of spin waves and their stability in both pure metals[209] and in disordered ferromagnetic metallic alloys.[201,210] In the framework of this approach, and following Ref. 201, we calculate here D for the single-band Hubbard model with random parameters at zero temperature. We have determined the correlation effects preserving the energy dependence of the T matrix.

We rewrite the Hubbard Hamiltonian with random parameters (69) in the form

$$H^{\{\nu\}}=\sum_{k\sigma}\varepsilon_k n_{k\sigma}+\sum_{i\sigma}\varepsilon_i^{\nu}n_{i\sigma}+\sum_i U_i^{\nu}n_{i\uparrow}n_{i\downarrow}, \tag{84}$$

where $n_{k\sigma}$ and $n_{i\sigma}$ are the population-number operators for the Bloch and Wannier states, respectively, with spin σ, and ε_k is the band energy, which is assumed to be independent of the given configuration $\{\nu\}$ of the alloy. The single-particle potential ε_i^{ν} and the bare interatomic Coulomb interaction U_i^{ν} take random values ε^{ν} and U^{ν} ($\nu=A, B$) depending on whether the site is occupied by atom A or B. We have the multiple index $\{\nu\}=\{\nu_1, \ldots \nu_i, \ldots, \nu_N\}$, where $\nu_i=A, B$ describes the configuration of the alloy as a whole.

The spin-wave energy $\omega_q=Dq^2$ for cubic crystals can be determined from the pole of the transverse spin susceptibility $\chi^{+-}(q, \omega)$, which leads to the following expression for the stiffness coefficient:

$$D=-\frac{1}{2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c}\lim_{\omega\to 0}\lim_{q\to 0}\left[\frac{\omega^2}{q^2}\left(\chi^{+-}(q,\ \omega)+\frac{2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c}{\omega}\right)\right], \tag{85}$$

where $2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c=(n_\uparrow-n_\downarrow)$ is the magnetization per site (n_σ is the mean number of electrons per site); $\langle\cdots\rangle^{\{\nu\}}$ is the mean value with respect to the ground state for the given configuration $\{\nu\}$; and $\langle\cdots\rangle_c$ is the mean over the configurations. In Refs. 196, 199, and 200, the following formula was used for alloys:

$$D=\frac{1}{2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c}\left[\lim_{q\to 0}\frac{1}{q^2}\langle\langle[S_q^+,\ qJ_{-q}^-]\rangle^{\{\nu\}}\rangle_c-\lim_{\omega\to 0}\lim_{q\to 0}\chi_J^{+-}(q,\omega)\right], \tag{86}$$

which is expressed in terms of the response function $\chi_J^{+-}(q, \omega)$ for the spin current by analogy with (17).

For the Hubbard model with random parameters (84), the Fourier transforms of the operator of the transverse spin density S_q^+ [or $S_{-q}^-=(S_q^+)^+$] and the current operator J_q^+ [or $J_{-q}^-=(J_q^+)^+$], which here do not depend on the random parameters, have the form

$$\left.\begin{aligned}S_q^+&=\frac{1}{\sqrt{N}}\sum_k a_{k\uparrow}^+a_{k+q\downarrow};\\ qJ_q^+&=\frac{1}{\sqrt{N}}\sum_k(\varepsilon_{k+q}-\varepsilon_k)a_{k\uparrow}^+a_{k+q\downarrow},\end{aligned}\right\} \tag{87}$$

where $a_{k\sigma}^+$ and $a_{k\sigma}$ are the operators of creation and annihilation of an electron in the state $|k\sigma\rangle$, and N is the number of lattice sites.

The susceptibilities in (85) and (86) can be expressed[202] by means of Eq. (87) in terms of the causal Green's functions at zero temperature as follows:

$$\begin{aligned}&\chi^{+-}(q,\omega)=-\langle\langle S_q^+,\ S_{-q}^-\rangle\rangle_\omega^{\{\nu\}}\rangle_c\\&=\frac{i}{N}\int\frac{dE}{2\pi}\langle\mathrm{tr}\{\Lambda_{0\uparrow\downarrow}^{\{\nu\}}(E, E+\omega;\ q)G_\downarrow^{\{\nu\}}\\&\quad\times(E+\omega)\lambda_0(-q)G_\uparrow^{\{\nu\}}(E)\}\rangle_c;\end{aligned} \tag{88}$$

$$\begin{aligned}&q\chi J^{+-}(q,\omega)=-\langle\langle qJ_q^+,\ qJ_{-q}^-\rangle\rangle_\omega^{\{\nu\}}\rangle_c\\&=-\frac{i}{N}\int\frac{dE}{2\pi}\langle\mathrm{tr}\{\Lambda_{1\uparrow\downarrow}^{\{\nu\}}(E, E+\omega;\ q)G_\downarrow^{\{\nu\}}\\&\quad\times(E+\omega)\lambda_1(-q)G_\uparrow^{\{\nu\}}(E)\}\rangle_c,\end{aligned} \tag{89}$$

where

$$\begin{aligned}&\Lambda_{\alpha ij\uparrow\downarrow}^{\{\nu\}}(E, E+\omega;\ q)\\&=\lambda_{\alpha ij}(q)-\delta_{ij}\int\frac{d\bar{E}}{2\pi}iI_{i\uparrow\downarrow i\downarrow\uparrow}^{\{\nu\}}(E, \bar{E}+\omega;\ \omega)\sum_{mn}G_{im\uparrow}^{\{\nu\}}(\bar{E})\\&\quad\times\Lambda_{\alpha mn\uparrow\downarrow}^{\{\nu\}}(\bar{E}, \bar{E}+\omega;\ q)G_{ni\downarrow}^{\{\nu\}}(\bar{E}+\omega)\quad(\alpha=0, 1);\end{aligned} \tag{90}$$

$$\left.\begin{aligned}&\lambda_{0ij}(q)=\exp(-iqR_i)\delta_{ij};\ \lambda_{1ij}(q)\\&\quad=t_{ij}[\exp(-iqR_i)-\exp(-iqR_j)];\\&t_{ij}=1/N\sum_k\varepsilon_k\exp[ik(R_i-R_j)].\end{aligned}\right\} \tag{91}$$

Here, locality is assumed only for the irreducible particle–hole vertex $I_{i\uparrow i\downarrow i\downarrow i\uparrow}^{\{\nu\}}(E, \bar{E}+\omega;\ \omega)\equiv I_{i\uparrow i\downarrow i\downarrow i\uparrow}^{\{\nu\}}(E, \bar{E}+\omega;\ E+\omega, \bar{E})$, and the trace denotes summation (without the spin) over the single-particle states. It can be seen that the expression (86) is more convenient for calculations than (85), since the Bethe–Salpeter equation (90) for $\alpha=1$ can be solved without making further assumptions about $I_{i\uparrow i\downarrow i\downarrow i\uparrow}^{\{\nu\}}$. The expansion of λ_1 and of the effective current $\Lambda_1^{\{\nu\}}$ with spin flip in (89) and (90) in the first order in q in conjunction with allowance for cubic symmetry leads to the expressions

$$\begin{aligned}&\chi^{+-}(q=0,\omega)=\frac{i}{3N}\int\frac{dE}{2\pi}\langle\mathrm{tr}\{\Lambda_{\uparrow\downarrow}^{\{\nu\}}(E, E+\omega)\\&\quad\times G_\downarrow^{\{\nu\}}(E+\omega)\,\mathbf{j}G_\uparrow^{\{\nu\}}(E)\}\rangle_c;\end{aligned} \tag{92}$$

$$\begin{aligned}&\Lambda_{ij\uparrow\downarrow}^{\{\nu\}}(E, E+\omega)=\mathbf{j}_{ij}-\delta_{ij}\int\frac{d\bar{E}}{2\pi}\,i\,I_{i\uparrow\downarrow i\downarrow\uparrow}^{\{\nu\}}(E, \bar{E}+\omega;\ \omega)\\&\quad\times\sum_{mn}G_{im\uparrow}^{\{\nu\}}(\bar{E})\Lambda_{mn\uparrow\downarrow}^{\{\nu\}}(\bar{E}, \bar{E}+\omega)G_{ni\downarrow}^{\{\nu\}}(\bar{E}+\omega),\end{aligned} \tag{93}$$

where we have introduced the notation $\mathbf{j}_{ij}=-it_{ij}(\mathbf{R}_i-\mathbf{R}_j)$

and

$$\lambda_1(q)=\mathbf{q}\cdot\mathbf{j};\ \ \Lambda^{\{\nu\}}_{1\uparrow\downarrow}(E,\ E+\omega;\ q)=\mathbf{q}\cdot\Lambda^{\{\nu\}}_{1\uparrow\downarrow}(E,\ E+\omega).$$

In the trace, j and $\Lambda_1^{\{\nu\}}$ form a scalar product. Separating the diagonal and nondiagonal parts of $\Lambda_1^{\{\nu\}}$ in (92) and (93), we obtain

$$\chi^{+-}_{\mathbf{j}}(\mathbf{q}=0,\ \omega)$$
$$=\frac{\mathrm{i}}{3N}\int\frac{dE}{2\pi}\,\langle\mathrm{tr}\,\{\mathbf{j}G^{\{\nu\}}_{\downarrow}(E+\omega)\,\mathbf{j}G^{\{\nu\}}_{\uparrow}(E)\}\rangle_c+\tilde{\chi}^{+-}_{\mathbf{j}}(\mathbf{q}=0,\ \omega),\qquad(94)$$

where

$$\tilde{\chi}^{+-}_{\mathbf{j}}(q=0,\ \omega)=\frac{\mathrm{i}}{3N}\int\frac{dE}{2\pi}\Big\langle\sum_i\Lambda_{1ij}(E,\ E+\omega)$$
$$\times\mathrm{K}^{\{\nu\}}_{ii\uparrow}(E+\omega,\ E)\Big\rangle_c,\qquad(95)$$
$$\mathrm{K}^{\{\nu\}}_{ii\uparrow}(E+\omega,\ E)$$
$$=\sum_{mn}G^{\{\nu\}}_{im\downarrow}(E+\omega)\,\mathrm{j}_{mn}G^{\{\nu\}}_{ni\uparrow}(E).\qquad(96)$$

Since the configuration averaging in (95) goes beyond the framework of the CPA, we use an approximation[202] of the type $\langle\Lambda_1^{\{\nu\}}\cdot\mathrm{K}^{\{\nu\}}\rangle_c=\langle\Lambda_1^{\{\nu\}}\rangle\langle\mathrm{K}^{\{\nu\}}\rangle$, so that

$$\mathrm{K}_{\downarrow\uparrow}(E+\omega,\ E)=\langle G^{\{\nu\}}_{\downarrow}(E+\omega)\,\mathrm{j}G^{\{\nu\}}_{\uparrow}(E)\rangle_{cii}$$
$$=\frac{1}{N}\sum_{\mathbf{k}}\mathcal{G}_{\mathbf{k}\downarrow}(E+\omega)\,\mathcal{G}_{\mathbf{k}\uparrow}(E)\,\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}=0\qquad(97)$$

and

$$\tilde{\chi}^{+-}_{\mathbf{j}}(\mathbf{q}=0,\ \omega)=0,$$

i.e., there are no vertex corrections, because of the symmetry under time reversal. Here, $\mathcal{G}_{\mathbf{k}\sigma}$ is the coherent single-particle Green's function with allowance for the electron–electron correlations (see below). Thus, on the basis of the CPA we obtain the expression

$$\chi^{+-}_{\mathbf{j}}(\mathbf{q}=0,\ \omega)=\frac{\mathrm{i}}{3N}\int\frac{dE}{2\pi}\sum_{\mathbf{k}}\mathcal{G}_{\mathbf{k}\downarrow}(E+\omega)\,\mathcal{G}_{\mathbf{k}\uparrow}(E)\,(\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}})^2.\qquad(98)$$

Substituting (98) and the limiting expression

$$\lim_{q\to0}\frac{1}{q^2}\langle\langle[S^+_{\mathbf{q}},\ qJ^-_{-\mathbf{q}}]\rangle^{\{\nu\}}\rangle_c$$
$$=\frac{1}{6N}\sum_{\mathbf{k}\sigma}\langle\langle n_{\mathbf{k}\sigma}\rangle^{\{\nu\}}\rangle_c\,\nabla^2_{\mathbf{k}}\varepsilon_{\mathbf{k}}\qquad(99)$$

in (86) and going over from the causal to the retarded Green's function, we obtain

$$D=\frac{1}{6\pi(n_\uparrow-n_\downarrow)}\,\mathrm{Im}\int_{-\infty}^{\mu}dE\,\frac{1}{N}\sum_{\mathbf{k}}(\mathcal{G}^r_{\mathbf{k}\uparrow}(E)-\mathcal{G}^r_{\mathbf{k}\downarrow}(E))^2\,(\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}),\qquad(100)$$

where μ is the Fermi energy. This expression is formally identical with the one obtained in the RPA–CPA approach[172,196,199] on the basis of the Hartree–Fock approximation.

In the present calculation, however, the CLA scheme[204] is used for the function $\mathcal{G}_{\mathbf{k}\sigma}$. Then the correlation part in terms of the partly averaged causal functions has the form

$$\Sigma^{\nu}_{Ui\sigma}(E)=\int\frac{d\bar{E}}{2\pi\mathrm{i}}\,G^{\nu}_{ii-\sigma}(\bar{E})\,T^{\nu}_i(E+\bar{E}),\ \ (\nu=A,\ B);\qquad(101)$$

$$T^{\nu}_i(E)=\Big[\frac{1}{U^{\nu}_i}+\int\frac{d\bar{E}}{2\pi}\,G^{\nu}_{ii\sigma}(\bar{E})\,G^{\nu}_{ii-\sigma}(E-\bar{E})\Big]^{-1},\qquad(102)$$

where T^{ν}_i is the effective two-particle vertex. The local Green's function $G^{\nu}_{ii\sigma}(z)$, expressed in resolvent form (here, z is the complex energy), is renormalized as follows:

$$G^{\nu}_{ii\sigma}(z)=F_\sigma(z)/\{1-[\tilde{\varepsilon}^{\nu}_{i\sigma}(z)-\Sigma_\sigma(z)]\,F_\sigma(z)\};\qquad(103)$$
$$\tilde{\varepsilon}^{\nu}_{i\sigma}(z)=\varepsilon^{\nu}_i+\Sigma^{\nu}_{Ui\sigma}(z);\qquad(104)$$
$$F_\sigma(z)=\frac{1}{N}\sum_{\mathbf{k}}\mathcal{G}_{\mathbf{k}\sigma}(z);\qquad(105)$$
$$\mathcal{G}_{\mathbf{k}\sigma}(z)=(z-\varepsilon_{\mathbf{k}}-\Sigma_\sigma(z))^{-1};\qquad(106)$$
$$\Sigma_\sigma(z)=c\tilde{\varepsilon}^{A}_{\sigma}(z)+(1-c)\,\tilde{\varepsilon}^{B}_{\sigma}(z)$$
$$-[\tilde{\varepsilon}^{A}_{\sigma}(z)-\Sigma_\sigma(z)]\,F_\sigma(z)\,[\varepsilon^{B}_{\sigma}(z)-\Sigma_\sigma(z)];\qquad(107)$$
$$n=\sum_\sigma n_\sigma=-\frac{1}{\pi}\sum_\sigma\int_{-\infty}^{\mu}dE\,\mathrm{Im}\,F^r_\sigma(E).\qquad(108)$$

Here, Σ_σ is the coherent potential, and n is the mean number of electrons per site. In contrast to the usual CPA, the atomic potential $\tilde{\varepsilon}^{\nu}_{i\sigma}(z)$ [in (107), the index i is omitted] acquires an energy dependence through the mass operator $\Sigma^{\nu}_{Uii}(z)$ on account of the correlations. In the Hartree–Fock approximation, the solution of the systems of equations (103)–(108) simplifies, since instead of (101) and (102) we use the self-energy $\Sigma^{\nu HF}_{Ui\sigma}=U^{\nu}_i n^{\nu}_{i-\sigma}$, where $n^{\nu}_{i\sigma}$ is the mean number of electrons with spin σ at the sites ν:

$$n^{\nu}_{i\sigma}=-\frac{1}{\pi}\int_{-\infty}^{\mu}dE\,\mathrm{Im}\,G^{r\nu}_{ii\sigma}(E).\qquad(109)$$

Using the concrete vertex $I^{\{\nu\}}_{i\,i\,i\,i}(E,\ \bar{E}+\omega;\ \omega)=-T^{\{\nu\}}_i(E+\bar{E}+\omega)$ and the substitution $\nu\to\{\nu\}$, we find from Eqs. (90), (101), and (102) a relation of Ward–Takahashi type:

$$\omega\Lambda^{\{\nu\}}_{0i\uparrow\downarrow}(E,\ E+\omega,\ \mathbf{q})\,\delta_{ij}-\Lambda^{\{\nu\}}_{1ij\uparrow\downarrow}(E,\ E+\omega,\ \mathbf{q})$$
$$=\exp(-\mathrm{i}\mathbf{q}\mathbf{R}_i)\,G^{\{\nu\}-1}_{ij\uparrow}(E+\omega)-G^{\{\nu\}-1}_{ij\uparrow}(E)\exp(-\mathrm{i}\mathbf{q}\mathbf{R}_j),\qquad(110)$$

where

$$(G^{\{\nu\}-1}(E))_{ij\sigma}=(E-\varepsilon^{\nu}_i)\,\delta_{ij}-t_{ij}-\Sigma^{\{\nu\}}_{Ui\sigma}(E)\,\delta_{ij}.\qquad(111)$$

We now consider the question of the stability of the ground state of a ferromagnet with respect to spin-wave excitations. For pure metals, this question is discussed in detail in Ref. 211 in the band model in the Hartree–Fock approximation and in Ref. 209 in the CLA. The condition of stability

$$\hat{D}=D(n_\uparrow-n_\downarrow)>0\qquad(112)$$

for the ground state of the ferromagnet can be obtained from the spectral representation

$$\chi^{+-r}(\mathbf{q},\ \omega)=-\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega'\,\frac{\mathrm{sign}\,\omega'}{\omega-\omega'+\mathrm{i}\varepsilon}\,\hat{I}_{S^+_{\mathbf{q}}S^-_{-\mathbf{q}}}(\omega'),\qquad(113)$$

where the spectral intensity $I_{S^+_{\mathbf{q}}S^-_{-\mathbf{q}}}(\omega)\geq0$ corresponds to the configuration-averaged system. For small q and ω, the magnon pole

$$\chi^{+-r}_{\mathrm{pole}}(\mathbf{q},\ \omega)=(n_\uparrow-n_\downarrow)/(\omega-Dq^2+\mathrm{i}\varepsilon)\qquad(114)$$

can be separated from the Stoner continuum, since the spectral weight of the particle–hole pair excitations tends to zero as $q\to0$. Comparison of (113) and (114) leads to the criterion (112). In the given approximation, the spin-wave damping [instead of $\varepsilon\to0$ in (114)] takes the form

$$\gamma_q=\frac{q^2}{n_\uparrow-n_\downarrow}\,\mathrm{Im}\,\chi^{+-r}(0,\ Dq^2)$$
$$=\frac{Dq^4}{3\pi(n_\uparrow-n_\downarrow)\,N}\sum_{\mathbf{k}}\mathrm{Im}\,\mathcal{G}^r_{\mathbf{k}\uparrow}(\mu)\,\mathrm{Im}\,\mathcal{G}^r_{\mathbf{k}\downarrow}(\mu)\,(\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}})^2,\qquad(115)$$

as in the RPA–CPA approach,[174] though here electron–electron scattering is taken into account.

We now consider the numerical results of the CLA for D and compare them with the experimental data on neutron scattering for the alloys NiFe and NiPd. To make part of the calculation of D in analytic form, we use the simplified expressions[212]

$$\rho_0(E)=\frac{1}{N}\sum_{\mathbf{k}}\delta(E-\varepsilon_{\mathbf{k}})=\frac{2}{\pi w}\left[1-\left(\frac{E}{w}\right)^2\right]^{1/2}\theta(w-|E|); \quad (116)$$

$$\frac{1}{N}\sum_{\mathbf{k}}\delta(E-\varepsilon_{\mathbf{k}})(\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}})^2=\frac{2v_m^2}{\pi w}\left[1-\left(\frac{E}{w}\right)^2\right]^{3/2}\theta(w-|E|), \quad (117)$$

where w is the band half-width, v_m is a quantity of order wa, and a is the lattice parameter. The summation over k in (105) leads with allowance for the unperturbed density of states (116) to the Green's function

$$F_\sigma(z)=(2/w)(\tilde{z}_\sigma-i\sqrt{1-\tilde{z}_\sigma^2}); \quad \tilde{z}_\sigma=[z-\Sigma_\sigma(z)]/w. \quad (118)$$

To make (118) single-valued, we choose the branch of the $\tilde{z}_\sigma$ plane with cut along the real axis from −1 to +1 for which the square root is positive on the upper edge of the cut.

Rewriting (100) in the form

$$D=\frac{1}{6\pi(n_\uparrow-n_\downarrow)}\operatorname{Im}\int_{-\infty}^{\mu}dE\,[\Pi_{\uparrow\uparrow}^{rr}(E,E)+\Pi_{\downarrow\downarrow}^{rr}(E,E)-2\Pi_{\uparrow\downarrow}^{rr}(E,E)], \quad (119)$$

where we have introduced the notation $\Pi_{\sigma\sigma'}^{rr}(E,E)=\Pi_{\sigma\sigma'}(E^+,E^+)$, $E^+=E+i0$ and

$$\Pi_{\sigma\sigma'}(z,z')=\frac{1}{N}\sum_{k}\mathcal{G}_{k\sigma}(z)\mathcal{G}_{k\sigma'}(z')(\nabla_k\varepsilon_k)^2, \quad (120)$$

and then applying the residue theorem with summation over k in (120) with allowance for the approximation (117), we find

$$\Pi_{\sigma\sigma}^{rr}=\frac{2v_m^2}{w^2}\left(3z_\sigma^2-\frac{3}{2}-3iz_\sigma\sqrt{1-z_\sigma^2}\right); \quad z_\sigma=\frac{E^+-\Sigma_\sigma(E^+)}{w}; \quad (121)$$

$$\Pi_{\uparrow\downarrow}^{rr}=\frac{2v_m^2}{w^2}\left(z_\uparrow^2+z_\downarrow^2+z_\uparrow z_\downarrow-\frac{3}{2}+i\frac{(1-z_\uparrow^2)^{3/2}-(1-z_\downarrow^2)^{3/2}}{z_\uparrow-z_\downarrow}\right). \quad (122)$$

Therefore,

$$D=\frac{v_m^2}{3\pi w^2(n_\uparrow-n_\downarrow)}\operatorname{Im}\int_{-\infty}^{\mu}dE\Big[(z_\uparrow-z_\downarrow)^2 - i\sqrt{1-z_\uparrow^2}\left(3z_\uparrow+\frac{2(1-z_\uparrow^2)}{z_\uparrow-z_\downarrow}\right) - i\sqrt{1-z_\downarrow^2}\left(3z_\downarrow-\frac{2(1-z_\downarrow^2)}{z_\uparrow-z_\downarrow}\right)\Big]. \quad (123)$$

The scalar static electrical conductivity σ is calculated in the same approximation as D. As a result, we arrive at the modified Kubo–Greenwood formula

$$\sigma=\frac{e^2N}{6\pi V}\sum_\sigma[\Pi_{\sigma\sigma}^{ra}(\mu)-\operatorname{Re}\Pi_{\sigma\sigma}^{rr}(\mu)]\equiv\sum_\sigma\sigma_\sigma, \quad (124)$$

which contains Green's functions renormalized by allowance for the electron correlations in the framework of the CLA. Here, $\Pi_{\sigma\sigma}^{ra}(\mu)\equiv\Pi_{\sigma\sigma}(\mu^+,\mu^-)$, $\mu^-=\mu-i0$, V is the volume of the system, and e is the unit charge. Introducing (121) and (122) with the substituting $\Pi_{\sigma\sigma}^{ra}=\Pi_{\uparrow\uparrow}^{rr}[z_\uparrow\to\hat{z}_\sigma, z_\downarrow\to\hat{z}_\sigma^*]$ in (124), we obtain the spin-dependent electrical conductivity $[\operatorname{Im}\Sigma_\sigma(\mu^+)<0]$

$$\sigma_\sigma=\hat{\sigma}\pi\Big[\frac{2(\operatorname{Im}\Sigma_\sigma(\mu^+))^2}{w^2}+\frac{w}{\operatorname{Im}\Sigma_\sigma(\mu^+)}\operatorname{Re}\times\Big\{i\sqrt{1-\hat{z}_\sigma^2}\left(i(1-\hat{z}_\sigma^2)+\frac{3}{w}\hat{z}_\sigma\operatorname{Im}\Sigma_\sigma(\mu^+)\right)\Big\}\Big], \quad (125)$$

where

$$\hat{z}_\sigma=[\mu^+-\Sigma_\sigma(\mu^+)]/w; \quad \hat{\sigma}=e^2v_m^2N/(3\pi^2V). \quad (126)$$

The numerical analysis is carried out as follows: first, the parameters w, ε^A, $\varepsilon^B=0$, U^A, U^B, c, n are chosen, and one then solves the self-consistent system of equations (101)–(108) with the Green's function (118). The obtained results are used to find D in accordance with (123).

The transition region between weak and strong ferromagnetism, which depends on the intra-atomic repulsion U^ν (considered here in the Hartree–Fock approximation), is shown in Fig. 12. In particular, the solutions with the parameters $U^A=2$, $U^B=0$ and $U^A=2$, $U^B=2$ were investigated in Ref. 213, but spin waves were not considered. Calculations of the stiffness coefficient D [in units of $d_0=(1/9)wa^2$] in the RPA–CPA scheme (see Fig. 12a) indicate instability of the ferromagnetic state against excitation of spin waves. The partial and total mean magnetizations, $m^\nu=n_\uparrow^\nu-n_\downarrow^\nu$ and $m=n_\uparrow-n_\downarrow$, are shown in Fig. 12d. The bounded region of stable (essentially, saturated) ferromagnetism $D>0$ is shown in Fig. 13b, and $m^\nu>0$ (see Fig. 13a), which is calculated in the Hartree–Fock approximation as a function of the electron density n. The zero of D at the smallest value of n corresponds approximately to a Stoner-type criterion,[204] whereas the other zero indicates a change in the type of the magnetic order.

As can be seen from Fig. 14, there are a large number of neutron data on D for NiFe alloys. As a test, allowance was made for the interelectron correlations, although the given scheme is more convenient for describing the Ni component with 0.6 holes per atom in the d band than the Fe component with high hole density (see, for example, the small value of D at $c=0.4$ in Fig. 14b). The calculations of $D(c)$ on the basis of the CLA are compared in Fig. 14 with the results obtained in the RPA–CPA scheme,[196,198] the rigid-band theory,[109] the approach of Ref. 200, and also the data of Refs. 199, 184, and 185 on inelastic neutron scattering. The stiffness coefficient D for pure Ni is close to

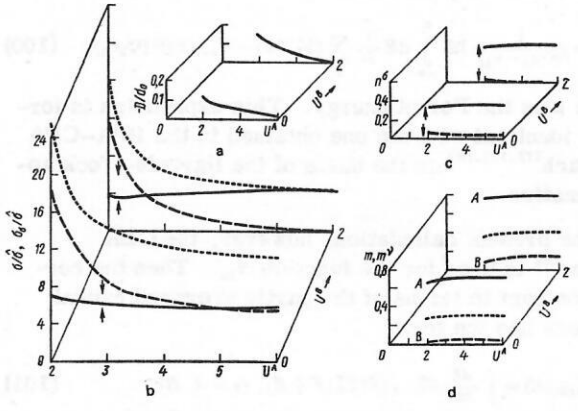

FIG. 12. Dependence of the coefficient of spin-wave stiffness $D<0$ (unstable case) (a), the static electrical conductivity σ_σ and σ (b), the electron density n_σ (c), and the magnetization m^ν and m(d) on U^ν ($\nu=A$, B) in the Hartree—Fock approximation. The values of the parameters are w, ε^A, ε^B, c, $n=1$, −0.8, 0, 0.4, 0.4, respectively.

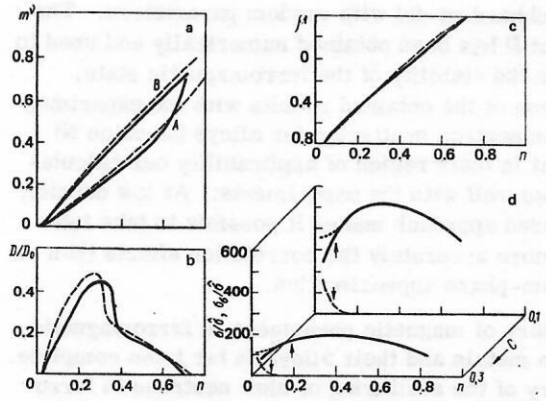

FIG. 13. Dependence of the partial magnetization m^ν (a), the stiffness coefficient D (b), the Fermi energy μ (c), and the electrical conductivity σ_σ and σ (d) on n in the Hartree—Fock approximation. The values of the parameters are w, ε^A, ε^B, U^A, U^B, = 1, 0.2, 0, 4, 3 (a, b, c). The continuous curves correspond to composition $c = 0.1$, the broken curves to $c = 0.3$.

$D_{\mathrm{Ni}} = 555$ meV · Å^2, measured at 4.2 °K.[99]

Calculations for the alloys NiPd were made in the CLA and these results (Fig. 15) are compared with the data of Ref. 214. The parameters for the pure systems were chosen on the basis of Ref. 208. The alloy is formed with $n = cn^{\mathrm{Pd}} + (1-c)n^{\mathrm{Ni}}$ and the different hopping integrals are taken into account through the band width $2w = c(2w)^{\mathrm{Pd}} + (1-c)(2w)^{\mathrm{Ni}}$. Note that in the reduced units U^{Pd}, U^{Ni}, and $\varepsilon^{\mathrm{Pd}} - \varepsilon^{\mathrm{Ni}}$ for all c are reduced to the scale $2w = 1$. The bare U^ν are renormalized self-consistently, and as a result we have the two-particle vertices $T_i^\nu(E + \bar{E})$. In particular, $\Gamma^\nu = T_i^\nu(2\mu)$ and $\Gamma = c\Gamma^A + (1-c)\Gamma^B$ are shown in the reduced units in Fig. 15d.

Thus, the numerical results obtained in the framework of the CLA indicate an influence of electron–electron correlations on the magnon energy in the long-wavelength limit $\omega_q = Dq^2$. Despite the single-band approximation in the Hubbard model with simplified band structure and diagonal disorder, physically reasonable values of D are obtained for the alloys based on Ni. For the energy-dependent two-particle vertices, locality is assumed, which makes it possible to preserve the single-site nature of the CPA. The spin-

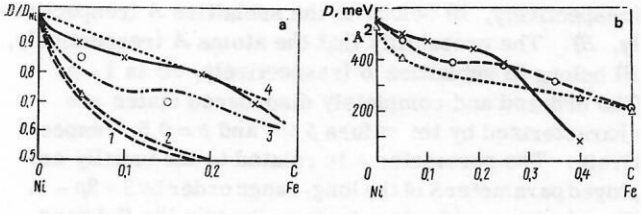

FIG. 14. Dependence of the spin-wave stiffness D in $\mathrm{Fe}_c\mathrm{Ni}_{1-c}$ on the composition. The values of $D(\varkappa)$ were calculated in the coherent ladder approximation for the parameter vaules w, ε^A, ε^B, U^A, U^B, n = 0.5, −0.24, 0, 2.66, 3.4, 0.6, respectively [(b) absolute units: $2w$ = 4.15 eV, α = 4 Å]. a) Calculations: Ref. 196 (1), Ref. 198 (2), Ref. 199 (3), Ref. 200 (4); b) experiments: Ref. 99 (open squares), Ref. 184 (open triangles), and Ref. 185 (open circles).

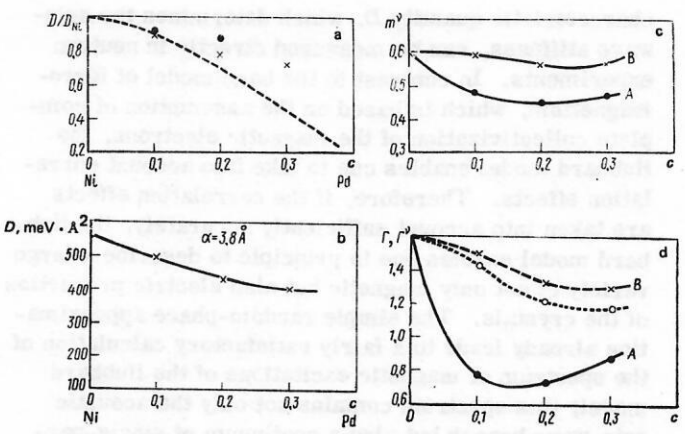

FIG. 15. Dependence of the spin-wave stiffness $D(\varkappa)$ (a), D in absolute units (b), the partial magnetization m^ν (c), and the effective Coulomb interactions Γ^ν and Γ (d) on c in $\mathrm{Pd}_c\mathrm{Ni}_{1-c}$ calculated in the coherent ladder approximation. $(2\omega)^{\mathrm{Pd}}$, $(2w)^{\mathrm{Ni}}$, $\varepsilon^{\mathrm{Pd}} - \varepsilon^{\mathrm{PNi}}$, U^A, U^{Ni} = 6.05, 4.15, 0.3, 9.17, 14.11 eV; $n^{\mathrm{Pd}} = 0.4$, $n^{\mathrm{Ni}} = 0.6$. In Fig. 15a, the broken curve is the calculation of Ref. 214 and the black circles are experimental values (cf. Ref. 214).

wave damping is small, of order q^4. In this sense, the self-consistent method proposed in Refs. 201, 202, and 209 for finding stable ferromagnetism in alloys of transition metals is interesting and promising. The method may also be helpful in investigating the dependence of the spin-wave stiffness of alloys of ferromagnetic transition metals on the degree of ordering of the alloy.

CONCLUSIONS

The investigations of elastic and inelastic scattering of neutrons in magnetic transition metals and their alloys is still, from the fundamental point of view, one of the most interesting directions of magnetic neutron-diffraction studies. Further progress in the theoretical description of the magnetic properties of transition metals and their alloys is intimately related to the experimental investigations, which must give accurate and reliable information about the distribution of the charge and spin densities, the spectrum of magnetic excitations, the exchange couplings, the forces of interatomic coupling, and other physical characteristics of crystals. Magnetic neutron-diffraction studies provide unique experimental data, particularly on the spectrum of magnetic excitations.

In the present paper, we have shown that many phenomena in ferromagnetic transition metals and alloys studied by means of the scattering of slow neutrons can be described from a unified point of view by using the Hubbard model. The spectrum of magnetic excitations of the Hubbard model reflects the dual behavior of the magnetically active d electrons in ferromagnetic transition metals. Investigation into the properties of rotational invariance of the Hubbard Hamiltonian shows that the presence of a spin-wave acoustic pole in the magnetic susceptibility is a direct consequence of the rotational symmetry of the system, as for the Heisenberg model. Thus, the acoustic spin-wave branch reflects a definite degree of localization of the d electrons; the

characteristic quantity D, which determines the spin-wave stiffness, can be measured directly in neutron experiments. In contrast to the band model of ferromagnetism, which is based on the assumption of complete collectivization of the magnetic electrons, the Hubbard model enables one to take into account correlation effects. Therefore, if the correlation effects are taken into account sufficiently accurately, the Hubbard model enables one in principle to describe a large variety of not only magnetic but also electric properties of the crystals. The simple random-phase approximation already leads to a fairly satisfactory calculation of the spectrum of magnetic excitations of the Hubbard model; this spectrum contains not only the acoustic spin-wave branch but also a continuum of single-particle Stoner excitations. The presence of the Stoner continuum is a manifestation of the delocalization of the magnetic electrons.

Since the Stoner excitations do not arise in the Heisenberg model, their detection and detailed investigation by means of neutron scattering is one of the urgent problems of physics of the magnetic state. Moreover, it is to be expected that measurements in the "optical" range will give more interesting results than can be expected on the basis of the single-band Hubbard model, which reflects the basic behavior of the system but is strongly simplified. The Hubbard model admits natural generalizations that enable one to take into account orbital excitation of d levels, $s-d$ hybridization, electron–phonon and electron–magnon interaction, and so forth. We have shown that even the simplest generalizations of the Hubbard model give a much richer spectrum, and, moreover, precisely in the "optical" range. The acoustic spin-wave pole is preserved if the modified Hamiltonian remains rotationally invariant.

The Hubbard model is extremely effective for the theoretical description of the electric and magnetic properties of alloys of transition metals. The introduction of random parameters makes it possible to simulate a disordered alloy of ferromagnetic transition metals. The Hubbard model with random parameters contains as limiting cases the majority of the models of systems with impurities. Use of the coherent-potential approximation makes it possible to calculate numerous physical quantities observed in neutron experiments in a wide range of impurity concentrations. In the calculation of collective characteristics of an alloy such as the spectrum of spin-wave excitations and the static electrical conductivity, it is important to take into account consistently the correlation effects. In the present work, we have shown that the energy of long-wavelength spin waves in alloys of ferromagnetic transition metals can be calculated by using the coherent-potential approximation to describe the disorder in conjunction with general arguments about the rotational invariance of the system. The method of calculation developed by Kolley and Kolley uses the ideas of the microscopic theory of Fermi liquids. The renormalization of the coefficient of spin-wave stiffness due to electron–electron correlations has been calculated self-consistently at zero temperature in the coherent horizontal ladder approximation for the Hubbard model with random parameters. The coefficient D has been obtained numerically and used to determine the stability of the ferromagnetic state. Comparison of the obtained results with the experimental data on neutron scattering for alloys based on Ni shows that in their region of applicability our calculations agree well with the experiments. At low density, the proposed approach makes it possible to take into account more accurately the correlation effects than in the random-phase approximation.

The theory of magnetic phenomena in ferromagnetic transition metals and their alloys is far from complete. The theory of the scattering of slow neutrons in ferromagnetic transition metals based on the random-phase approximation requires a number of refinements.[136,215] In a more accurate approximation,[216] the spectrum $\hbar\omega_q = \varepsilon_{k+q} - \varepsilon_k + \Delta$ of Stoner excitations has the form

$$\hbar\omega_q = \varepsilon_{k+q} - \varepsilon_k + S(k+q).$$

Experimental results must be used to judge the extent to which the random-phase approximation is applicable. At the present time, there are also weighty grounds for believing that a more detailed theory of inelastic neutron scattering in ferromagnetic transition metals must take into account the dependence of the Coulomb correlation on the quasimomentum and the orbital degeneracy.

The further theoretical and experimental study of ferromagnetic alloys of transition metals is of great interest. Recently, scattering of slow neutrons has been used to measure the coefficient of spin-wave stiffness in partly ordered ferromagnetic alloys (Refs. 185, 217, and 218). The recent theoretical studies on partly ordered ferromagnetic alloys[219-224] use many ideas described in the present review; in particular, Ref. 222, which is a development of Ref. 119, develops a theory which permits calculation of the coefficient of spin-wave stiffness as a function of the degree of atomic ordering in ferromagnetic alloys of transition metals of the type $A_{0.5}B_{0.5}$.

It is assumed that the lattice of the alloy can be represented in the form of two interpenetrating sublattices of the components A and B, all the nearest neighbors of the atoms in sublattice A belonging to sublattice B and vice versa. The degree of atomic ordering is characterized by a quantity p, the probability that atoms A (respectively, B) belong to the sublattice A (respectively, B). The probability that the atoms A (respectively, B) belong to sublattice B (respectively, A) is $1-p$. The ordered and completely disordered states are characterized by the values $p=1$ and $p=0.5$, respectively. The parameter p is related to the usually employed parameter S of the long-range order by $S = 2p - 1$. The electron subsystem is described by the Hubbard Hamiltonian (69). The coherent-potential method is used to describe the structural disorder. The standard single-site treatment makes it possible to obtain a system of equations determining the coherent potential, the population numbers, and the effective potential. To calculate the energy of the spin waves, the general equations (17) and (86) are used, as in Ref. 199.

The interelectron correlation is taken into account in the random-phase approximation. The configuration averaging is performed along the lines of Velicky's approach.[212]

For a simple model of an alloy, the coefficient of spin-wave stiffness is calculated numerically as a function of the atomic order parameter p at zero temperature. The choice of the parameter corresponds to the case of the alloy NiFe although the density of states employed is too simplified. This last circumstance hinders direct comparison between the theory and experiment, particularly in view of the fact that the neutron measurements of D as a function of the degree of atomic ordering have been made for Ni_3Fe and Pd_3Fe. Nevertheless, the calculated behavior of D basically corresponds to the experiments, i.e., increase in the degree of disorder leads to a spin-wave "softening" of the system. Further theoretical and experimental study of such systems will be of great interest. The method of inelastic neutron scattering is the only method of verifying theoretical results in this problem.

Further comprehensive theoretical and experimental study of ferromagnetic transition metals and their alloys will deepen our understanding of the nature of magnetism and more precise model theoretical notions and will establish the applicability of approximate data on the magnetic characteristics of such alloys, which is important for applications and understanding of the magnetic and electron properties of this extensive group of materials.

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