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Electronic energy spectra in antiferromagnetic media with broken reciprocity

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Electronic energy spectra $\varepsilon(\mathbf{q})$ of antiferromagnetically ordered media may display nonreciprocity; that is, the energies corresponding to Bloch states with wave numbers $\mathbf{q}$ and $-\mathbf{q}$ may be different. In this paper a simple Kronig-Penney model, which includes a staggered microscopic magnetic and electric fields of the proper symmetry, is employed to estimate the magnitude of nonreciprocity effects in systems such as antiferromagnetically ordered crystals as well as periodical layered structures. [S0163-1829(97)06318-2]

I. INTRODUCTION

In common crystals, the spectra $\varepsilon(\mathbf{q})$ of all elementary excitations, such as photonic, phononic, electronic, and magnetic, possess the fundamental property of being symmetric with respect to the sign of the Bloch wave vector $\mathbf{q}$. For a nondegenerate band structure this property, referred to as the *reciprocity* principle, reads

$$\varepsilon(\mathbf{q})=\varepsilon(-\mathbf{q}), \tag{1}$$

for all $\mathbf{q}$.

The reciprocity principle is a direct consequence of the time reversal and/or space inversion symmetry. Indeed, $\mathbf{q}$ changes sign both under the space inversion operation I and under time reversal R, whereas ε is a scalar. If neither space inversion nor time reversal operations are present in the macroscopic symmetry group of a crystal, the reciprocity principle may not apply, and instead of Eq. (1) we may get

$$\varepsilon(\mathbf{q})\neq\varepsilon(-\mathbf{q}). \tag{2}$$

Relation (1) may still apply to isolated points of accidental degeneracy or to some special directions of the wave vector $\mathbf{q}$ for which $\mathbf{q}$ and $-\mathbf{q}$ are related by a symmetry operation(s) other than the missing I and R. Recall that the absence of time-reversal symmetry implies the existence of a spontaneous long-range magnetic order in the crystal, and/or that the system is placed in an external magnetic field. In this study we restrict ourself to the former circumstance.

Generally, from symmetry considerations, nonreciprocity (see Fig. 1) occurs when none of the symmetry operations g, belonging to the macroscopic symmetry group G of the crystal, transform $\mathbf{q}$ to $-\mathbf{q}$, i.e.,

$$T(g)\mathbf{q}\neq-\mathbf{q} \quad \text{for all} \quad g\in G, \tag{3}$$

where $T(g)$ is the transformation corresponding to the symmetry operation g of the macroscopic (point) symmetry group G of the crystal.

Indeed, if at least one of the symmetry operations from G transforms $\mathbf{q}$ to $-\mathbf{q}$, then $\varepsilon(\mathbf{q})=\varepsilon(-\mathbf{q})$. If such transformation cannot be achieved by any of the symmetry operations, then there would be no symmetry reasons for the equality $\varepsilon(\mathbf{q})=\varepsilon(-\mathbf{q})$ to apply for this particular direction of the wave vector $\mathbf{q}$.

Along with Eq. (3) we consider the stronger condition

$$\sum_{g\in G} T(g)\mathbf{q}\neq 0, \tag{4}$$

which will be referred to as the condition for *strong nonreciprocity* (this term refers not to the magnitude of the effect but to its symmetry). The stronger condition Eq. (4), suggests that there is at least one direction $\mathbf{n}$ of the wave vector $\mathbf{q}$ for which

$$T(g)\mathbf{q}=\mathbf{q} \quad \text{for any} \quad g\in G, \quad \text{and} \quad \mathbf{q}\|\mathbf{n}, \tag{5}$$

The key difference between conditions (3) and (4) is that the weaker one, Eq. (3), still allows the point $\mathbf{q}=0$ of the Brillouin zone to possess a higher symmetry than that of any

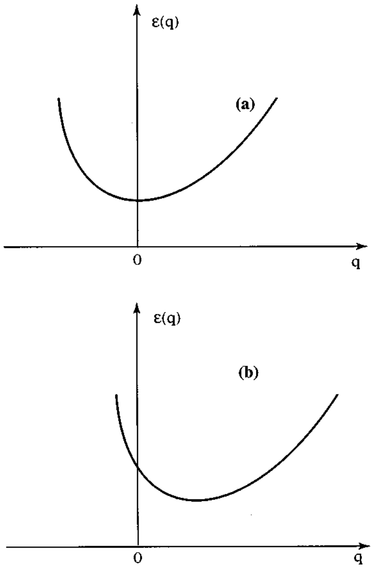

FIG. 1. Schematic examples of nondegenerate asymmetric spectra: (a) the case of weak nonreciprocity; (b) the case of strong nonreciprocity.

other point in its vicinity. In this case, any nondegenerate branch of a spectrum $\varepsilon(\mathbf{q})$ would have a vanishing vector derivative, $\boldsymbol{\nu}(\mathbf{q})\equiv\partial\varepsilon/(\mathbf{q})/\hbar\partial\mathbf{q}$, at the Brillouin zone (BZ) center, as shown schematically in Fig. 1(a); i.e., the group velocity $\boldsymbol{\nu}(\mathbf{q})$ of the corresponding $\mathbf{q}=0$ excitation vanishes. This is a direct consequence of the fact that the vectors $\boldsymbol{\nu}(\mathbf{q})$ and $\mathbf{q}$ transform in the same way under any time-space operations g from the magnetic symmetry group G.

On the other hand, the stronger condition (4) or, equivalently, Eq. (5), suggests that the group-velocity $\boldsymbol{\nu}(\mathbf{q})$ may be finite at the center of the Brillouin zone [see Fig. 1(b)]. The corresponding direction of $\boldsymbol{\nu}(0)$ will be parallel to the vector $\mathbf{n}$, which, according to Eq. (5) is invariant under all transformations of the group G.

Conditions (4) or (5) for strong nonreciprocity may be met in magnetically ordered materials with some special magnetic symmetry. Such materials may display an asymmetric *linear magnetoelectric effect*. Indeed, by definition, the linear magnetoelectric effect$^{1-9}$ is characterized by a nonzero cross-magnetoelectric susceptibility tensor, $\boldsymbol{\alpha}=\partial\mathbf{P}/\partial\mathbf{H}$, where $\mathbf{P}$ and $\mathbf{M}$ are the electric and magnetic polarizations of the material. From the definition of the tensor $\boldsymbol{\alpha}$ we get

$$\boldsymbol{\alpha}_{yz}-\boldsymbol{\alpha}_{zy}\propto E_yH_z-E_zH_y\propto q_x\,, \tag{6}$$

where the symbol $\propto$ indicates equivalence of the transformation properties. Using Eq. (5), with $\mathbf{n}\|\mathbf{x}$, we observe that from symmetry considerations the necessary and sufficient condition for a spectrum to display strong nonreciprocity is the existence of an *asymmetrical* linear magnetoelectric susceptibility tensor, i.e., $\boldsymbol{\alpha}\neq\boldsymbol{\alpha}^T$, where the superscript T denotes the transposition operation.

It is important to note, however, that the physical origins of the magnetoelectric effect and nonreciprocity of the spectra of various elementary excitations are generally different; the sole known exception is provided by the long-wave electromagnetic spectrum for which the linear magnetoelectric susceptibility underlies the possible occurrence of nonreciprocal behavior.[5] For instance, in conducting media the conventional magnetoelectric effect does not exist by definition; instead, there may exist a kinetic magnetoelectric effect as predicted in Ref. 10, while the electronic spectrum may display significant nonreciprocity.

Nonreciprocity [Eq. (2)] was predicted first theoretically for the electromagnetic spectrum in magnetoelectric crystals (see Ref. 5 and references therein). An extensive symmetry analysis of the electromagnetic and acoustic spectral nonreciprocity has been presented in Ref. 11. However, in these studies only the low-frequency hydrodynamic limit has been discussed. The nonreciprocity property (2) pertaining to electronic spectra has been discussed in the context of systems with *toroidal current ordering*,[12] as well as for a model system with an alternate magnetic-field distribution with a one-dimensional (1D) periodicity.[13]

In this study we focus on characteristic qualitative features of the band structure of a ''nonreciprocal material.'' To this aim, we consider a simple microscopic model which adequately reflects the space-time symmetry of the crystal and is solvable throughout the BZ. We restrict ourselves in this study to the most interesting case of strong nonreciprocity.

II. ELECTRON ENERGY SPECTRUM OF A RHOMBIC ANTIFERROMAGNET CRYSTAL WITH STRONG NONRECIPROCITY

Consider the single-electron Schrödinger equation

$$\left\{\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\,\mathbf{A}(\mathbf{r})\right)^2+eV(\mathbf{r})\right\}\psi(\mathbf{r})=\varepsilon\,\psi(\mathbf{r}), \tag{7}$$

where the scalar potential $V(\mathbf{r})$ and the vector potential $\mathbf{A}(\mathbf{r})$ are 3D-periodic functions, i.e.,

$$V(\mathbf{r})=V(\mathbf{r}+\mathbf{a});\quad \mathbf{A}(\mathbf{r})=\mathbf{A}(\mathbf{r}+\mathbf{a}). \tag{8}$$

Here $\mathbf{a}$ is a lattice vector, $\mathbf{a}=N_x\mathbf{a}_x+N_y\mathbf{a}_y+N_z\mathbf{a}_z$, where $(\mathbf{a}_x,\mathbf{a}_y,\mathbf{a}_z)$ are the primitive lattice translations, and (N_x,N_y,N_z) are integers.

The spatially varying electric and magnetic fields in the lattice are defined by the standard relations

$$\mathbf{E}(\mathbf{r})=-\nabla V(\mathbf{r})=\mathbf{E}(\mathbf{r}+\mathbf{a}),\quad \mathbf{H}(r)=\nabla\times\mathbf{A}(\mathbf{r})=\mathbf{H}(\mathbf{r}+\mathbf{a}). \tag{9}$$

The necessary condition for constructing the lattice scalar and vector potentials, $V(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$, such that they would reflect adequately the actual space-time magnetic symmetry of a magnetoelectric crystal with strong nonreciprocity, is that the space distributions of $\mathbf{A}(\mathbf{r})$ and $V(\mathbf{r})$ be consistent with the key symmetry condition (4).

The translational periodicity requirement Eq. (8) implies the absence of macroscopic (space averaged) electric and magnetic fields, i.e.,

$$\langle\mathbf{E}(\mathbf{r})\rangle=\langle\mathbf{H}(\mathbf{r})\rangle=0, \tag{10}$$

where $\langle\cdots\rangle$ denotes spatial averaging.

The conditions on the electric and magnetic fields in the lattice expressed in Eq. (8) or, equivalently, Eq. (10), are of key importance since otherwise Bloch's theorem would not apply to the Hamiltonian (7) and the corresponding electron energy spectrum would display the complicated features that occur in the presence of external uniform electric and/or magnetic fields (for a recent review see Ref. 14 and references therein). Physically, these conditions mean that the medium is neither a ferromagnet nor a ferroelectric, and no external fields are applied. For methodological reasons, we consider only models where the existence of the macroscopic electric and magnetic polarizations can be ruled out for symmetry reasons alone. In other words, the relations given in Eq. (10) should be imposed by the magnetic symmetry group G of the spatial distributions of $\mathbf{A}(\mathbf{r})$ and $V(\mathbf{r})$.

In light of the above assumptions and requirements, we assume that both the scalar and vector potentials can be represented as a superposition of three separable contributions, depending each on a single coordinate x, y, or z. Let us consider field distributions which vary only along the y coordinate. From Eqs. (8) and (9) we obtain

$$\mathbf{E}(y)=\mathbf{E}(y+a_y)\|\mathbf{y},\quad \mathbf{H}(y)=\mathbf{H}(y+a_y)\perp\mathbf{y}. \tag{11}$$

More specifically, we choose

$$\mathbf{E}(y)\|\mathbf{y},\quad \mathbf{H}(y)\|\mathbf{z}. \tag{12}$$

The following functional forms of $H_z(y)$ and $E_y(y)$ comply with both symmetry conditions (5) and (8).

$$H_z(y)=\sum_N g(y-Na), \quad g(y)=-g(-y), \tag{13}$$

$$E_y(y)=\sum_N f(y-Na), \quad f(y)=-f(-y). \tag{14}$$

Indeed, the time-space symmetry of the above microscopic field distributions belongs to the magnetic symmetry class

$$D_{2h}(C_{2V})\equiv\frac{m_x'}{2_x}\frac{m_y}{2_y'}\frac{m_z}{2_x'}\equiv m'mm, \tag{15}$$

satisfying the key requirement [Eq. (4), or, equivalently, Eq. (5)] for strong nonreciprocity with $\mathbf{n}\|\mathbf{x}$, as well as the additional symmetry conditions which lead to the absence of macroscopic electric and magnetic polarizations [i.e., relations (8) or (10)]. In Eq. (15) we have employed standard notation,[2] i.e., $g'\equiv gR$, where R is the time-reversal operation.

Any functional form for $f(y)$ and $g(y)$ is acceptable, provided that the magnetic symmetry of the corresponding field distributions is not higher[15] than that given in Eq. (15). In this context it is important to remember that the resulting symmetry group is defined as the intersection of those of the electric and magnetic components taken separately. Clearly, the electric component itself never possesses the proper symmetry because it is always invariant under the time-reversal operation. At the same time, the magnetic component by itself can provide the proper symmetry. It would be interesting to consider both situations: (i) when the microscopic magnetic field yields the effect by itself, and (ii) when only a combination of the two fields possesses the proper symmetry. Indeed, both of the above situations may be realized in magnetically ordered systems; most of the known magnetoelectric crystals fall into the second category, for which the electric component of the microscopic field does not affect the resulting macroscopic symmetry of the system.

The one-dimensionally periodic fields given in Eqs. (13) and (14) should be complemented by the two additional microscopic electric components

$$E_y=\sum_N f_x(x-Na_x), \quad E_z=\sum_N f_z(z-Na_z);$$

$$\text{with } f(y)=-f(-y), \tag{16}$$

which altogether represent a three-dimensional periodic lattice. The contributions given in Eq. (16) give rise to a complete 3D electronic band structure, while not affecting the resulting macroscopic time-space symmetry of the system. These components of the microscopic field will be treated perturbatively.

The field configuration described by Eqs. (13)–(16) is not just the simplest one which complies with the symmetry requirements Eqs. (5) and (10), it is also qualitatively similar to those existing in some actual crystals exhibiting the linear magnetoelectric effect (see, for instance, Ref. 16). Furthermore, a magnetic-field distribution with the above symmetry can be realized in some periodic layered superstructures (see Ref. 11, and references therein).

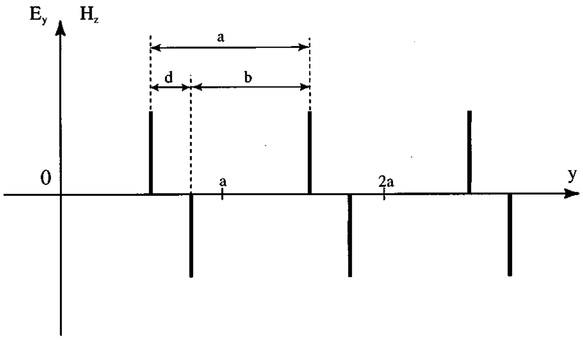

FIG. 2. A Kronig-Penney-type distribution of the microscopic electric and magnetic fields, $E_y(y)$ and $H_z(y)$, respectively, which is expected to exhibit nonreciprocity of the spectrum for $\mathbf{q}\|\mathbf{x}$. If $b\neq d\equiv a-b$, the microscopic magnetic field alone provides the required magnetic point symmetry of $D_{2h}(C_{2V})\equiv(m_x'/2_x)(m_y/2_y')/(m_z/2_x')\equiv m'mm$.

III. ELECTRON ENERGY SPECTRUM FOR A THREE-DIMENSIONAL MODEL OF THE KRONIG-PENNEY TYPE

The field pattern of the Kronig-Penney type which is consistent with Eqs. (13) and (14) and, consequently, with the symmetry conditions for strong nonreciprocity, has the following functional form:

$$H\equiv H_z=\frac{1}{2}H_0a\sum_N\left\{\delta\left(y-\frac{b}{2}-Na\right)-\delta\left(y+\frac{b}{2}-Na\right)\right\}, \tag{17}$$

$$E\equiv E_y=\frac{1}{2}E_0a\sum_N\left\{\delta\left(y-\frac{b}{2}-Na\right)-\delta\left(y+\frac{b}{2}-Na\right)\right\}. \tag{18}$$

It is displayed schematically in Fig. 2, where $a=b+d$ is the magnetic lattice period in the y direction. If for this particular field distribution we take $b=d$, then both the electric and magnetic components are needed in order to obtain the proper $D_{2h}(C_{2\nu})\equiv m'mm$ magnetic symmetry; otherwise, i.e., when $b\neq d$, the magnetic component alone insures the existence of strong nonreciprocity with the characteristic direction $\mathbf{n}\|\mathbf{x}$. The quantities H_0 and E_0 have a simple physical meaning; they equal the mean absolute values of the corresponding microscopic fields

$$H_0=\langle|\mathbf{H}(\mathbf{r})|\rangle; \quad E_0=\langle|\mathbf{E}(\mathbf{r})|\rangle. \tag{19}$$

The spatial distributions of the vector and scalar potentials corresponding to the field pattern given in Eqs. (17) and (18), are

$$A(y)\equiv A_x(y)=\tfrac{1}{2}H_0a\rho(y); \quad V(y)=\tfrac{1}{2}E_0a\Big(\rho(y)+\tfrac{1}{2}\Big), \tag{20}$$

where

$$\rho(y)=\sum_{N}\left\{\Theta\left(y+\frac{b}{2}-Na\right)-\Theta\left(y-\frac{b}{2}-Na\right)\right\}-\frac{1}{2}, \tag{21}$$

with Θ denoting the Heaviside step function. Substituting Eq. (20) into the Schrödinger equation (7) and setting

$$\Psi(\mathbf{r})=\chi(y)\exp i\{q_x x+q_z z\}, \tag{22}$$

we obtain the following equation for the function $\chi(y)$:

$$\frac{\partial^2\chi(y)}{\partial y^2}+\left\{\frac{2m}{\hbar^2}\,\varepsilon(\mathbf{q})-q_z{}^2 -l_H^{-2}\left[\frac{\rho(y)a}{2l_H}-q_x l_H\right]^2-u(y)\right\}\chi(y)=0, \tag{23}$$

where

$$l_H=(\hbar c/eH_0)^{1/2}\quad\text{and}\quad u(y)=2meV(y)/\hbar^2. \tag{24}$$

The quantity l_H is the *magnetic length* which corresponds to the characteristic radius of the first quantum Landau level in a magnetic field of strength H_0.

Equation (23) is of the form of the Kronig-Penney model (see, for example Ref. 18), with the corresponding dispersion relation

$$\cos(aq_y)=\cos(\beta d)\mathrm{ch}(\gamma b)+\frac{\gamma^2-\beta^2}{2\beta\gamma}\sin(\beta d)\mathrm{sh}(\gamma b), \tag{25}$$

where

$$\beta^2=\frac{2m}{\hbar^2}\,\varepsilon(\mathbf{q})-q_z^2-\left(q_x+\frac{a}{4l_H^2}\right)^2,$$

$$\gamma^2=-\frac{2m}{\hbar^2}\,\varepsilon(\mathbf{q})+q_z^2+\left(q_x-\frac{a}{4l_H^2}\right)^2+u_0;\quad u_0=\frac{m}{\hbar^2}\,E_0ea. \tag{26}$$

Equation (25) determines the energy spectrum $\varepsilon(\mathbf{q})$ for the case of the one-dimensional periodic crossed electric and magnetic fields given in Eqs. (17) and (18).

To account for the additional field components given in Eq. (16), which together with those given in Eqs. (17) and (18) yield a three-dimensional crystal structure, we employ perturbation theory. In general, these components of the fields may not be smaller than those given by Eq. (17) or Eq. (18). However the contributions given in Eqs. (17) and (18), being of the proper symmetry, are the ones responsible for the spectral nonreciprocity [exhibited by the dispersion relation given in Eq. (25) for $q_x\neq 0$], while the additional field components Eq. (16) are included in order to create a three-dimensional band structure within the framework of the symmetry imposed by the principal field components given by Eqs. (13) and (14) [or equivalently, Eqs. (17) and (18)]. Consequently, it is sufficient for our purpose here to consider the effect of these additional field components in an approximate manner since they do not introduce new qualitative features.

Let us represent the components (16) of the microscopic electric field, which are periodic in the x and z directions, as a Fourier series [with W representing the corresponding components; see Eq. (16), or Eqs. (17) and (18)]

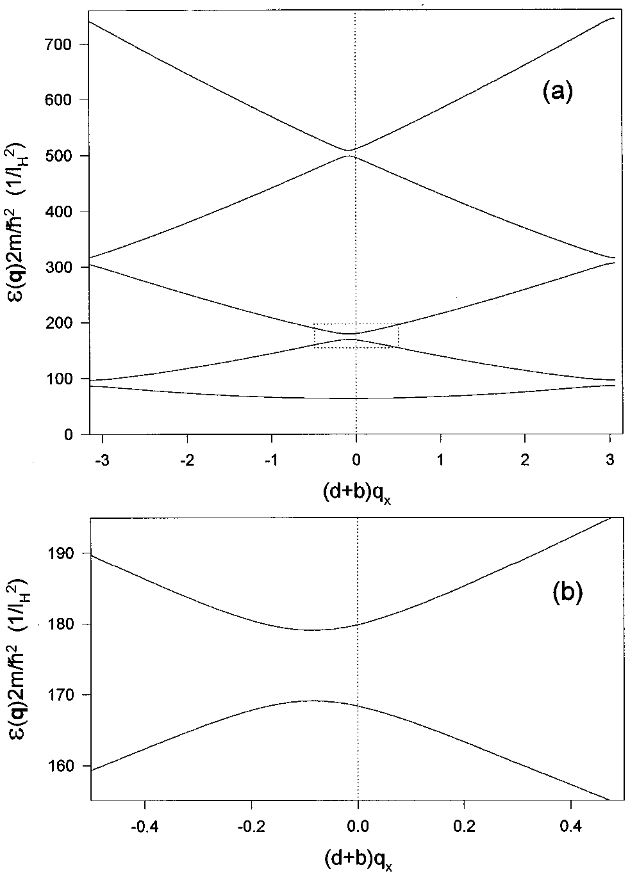

FIG. 3. Normalized energy spectra [$\varepsilon(\mathbf{q})2m/\hbar^2$ in units of l_H^{-2}] vs $(d+b)q_x$, plotted for $u_0=500l_H^{-2}$, $d=b=0.3l_H$, and $|2mW_{\mathbf{K}}/\hbar^2|=5.0l_H^{-2}$ for all $\mathbf{K}$. The region indicated by the dotted box is shown enlarged in (b).

$$W(\mathbf{r})=\sum_{\mathbf{K}}W_{\mathbf{K}}\exp i(\mathbf{K}\cdot\mathbf{r}),\quad \mathbf{K}=\left(\frac{2\pi}{a_x}\,n_x,0,\,\frac{2\pi}{a_z}\,n_z\right), \tag{27}$$

where a_x and a_z are primitive lattice translations in the x and z directions; n_x and n_z are integers. Applying standard perturbation theory we find for the spectrum $\varepsilon(\mathbf{q})$

$$\varepsilon(\mathbf{q})=\frac{1}{2}\,\{\varepsilon_0(\mathbf{q})+\varepsilon_0(\mathbf{q}-\mathbf{K}) \pm\sqrt{(\varepsilon_0(\mathbf{q})-\varepsilon_0(\mathbf{q}-\mathbf{K}))^2+4|W_{\mathbf{K}}|^2}\}, \tag{28}$$

where $\varepsilon_0(\mathbf{q})$ is the dispersion relation in the absence of the periodic electric field (27), given by Eqs. (25) and (26). Analysis of the band structure given by Eq. (28) can be performed numerically.

In accordance with the results of the symmetry considerations given in Secs. I and II, nonreciprocal behavior is expected to occur in our model system if and only if the wave vector $\mathbf{q}$ has a nonzero x component. As examples, we show in Figs. 3 and 4 typical energy spectra for $\mathbf{q}\|\mathbf{x}$. In the case shown in Fig. 3 we choose $b=d$ [see Eqs. (17) and (18), and Eqs. (25) and (28)]. This special case corresponds to a microscopic magnetic field $\mathbf{H}(\mathbf{r})$, with higher symmetry than that required for conditions (4) or (5) to apply. Therefore, for nonreciprocity to exist in this case, both the magnetic and

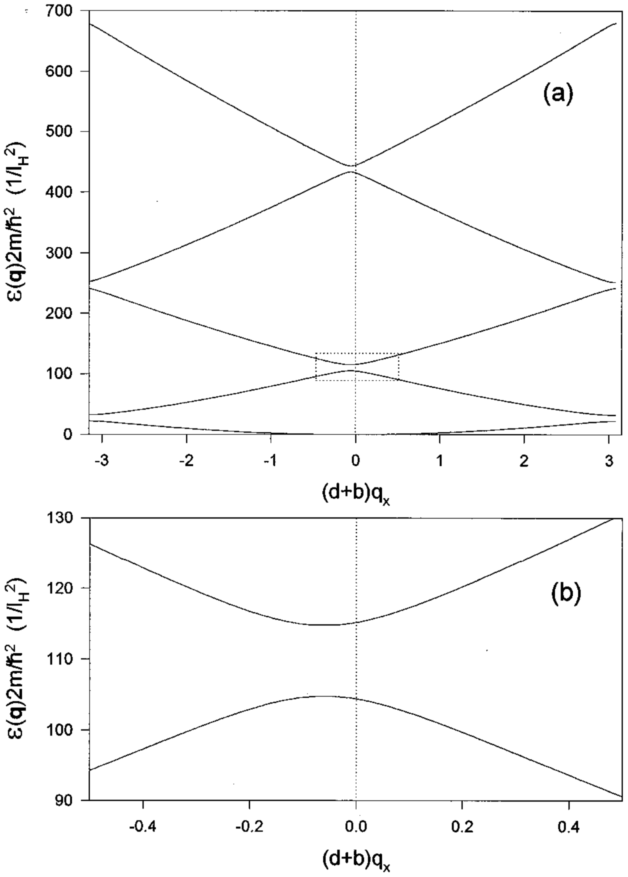

FIG. 4. Normalized energy spectra [$\varepsilon(\mathbf{q})2m/\hbar^2$ in units of $l_H{}^{-2}$] vs $(d+b)q_x$, plotted for $u_0=0$, $d=0.5l_H$, $b=0.1l_H$, and $|2mW_{\mathbf{K}}/\hbar^2=5.0l_H^{-2}$ for all **K**. The region indicated by the dotted box is shown enlarged in (b).

electric components, Eqs. (17) and (18), of the spatially varying fields should be nonzero. The case shown in Fig. 4 corresponds to a system with $b\neq d$. In this situation the magnetic component alone produces the spectral asymmetry portraying strong nonreciprocity.

The most significant features of the spectra shown in Figs. 3 and 4 are:

(1) The values $\pm\pi/a_x$ of the wave vector q_x, which in common crystals represent the BZ boundaries, are no longer special points of the spectrum. While the electron group velocity $v=d\varepsilon/\hbar dq$ vanishes at two values of the wave vector q_x separated by $2\pi/a_x$, these values are not equal to $\pm\pi/a_x$ as is normally the case. Moreover, the corresponding critical values of q_x are not the same for different branches n of the spectrum.

(2) The same is true for the point $\mathbf{q}=0$ of the BZ. The extremal energy for each particular branch n occurs now for some finite wave vector $\mathbf{q}(n)\|\mathbf{x}$, and not at the center of the BZ.

(3) For the case of $\mathbf{q}\perp\mathbf{x}$ the electron energy spectrum appears to be symmetric, i.e.,

$$\varepsilon(\mathbf{q})=\varepsilon(-\mathbf{q}),\quad \text{for } \mathbf{q}\perp\mathbf{x}. \tag{29}$$

This result does not depend on the approximations employed. Indeed, the magnetic symmetry group (15) of the microscopic magnetic- and electric-field distributions (13) and (14) includes the twofold axis 2_x as well as the antireflection $m_x'\equiv R\times m_x$. Either of these operations transfer **q** to $-\mathbf{q}$ for $\mathbf{q}\perp\mathbf{x}$. Thus, there is neither strong nor weak nonreciprocity for wave vector **q** lying in the yz plane.

IV. DISCUSSION AND ESTIMATES OF THE MAGNITUDE OF THE NONRECIPROCITY EFFECT

The magnitude of the nonreciprocity effects may be characterized by the magnitude of the shift $\boldsymbol{\delta}\mathbf{q}$ of the extremal points of the spectrum in **q** space. For instance, a vanishing effect means that the corresponding extrema are situated at the center and at the edges of the regular BZ as should be the case in the absence of magnetic order. In considerations of the magnitude of nonreciprocity effects for the low-lying energy bands it is convenient to introduce a parameter μ defined as

$$\mu\equiv\frac{a_y}{l_H}, \tag{30}$$

where l_H is the magnetic length defined in Eq. (24), and a_y is one of the structural (lattice) periods. The shift $\delta q=\delta q_x$ becomes small when the ratio μ is small. For the sake of specificity, in what follows we will discuss quantitatively the shift of the extremal point which in the absence of the effect would correspond to $\mathbf{q}=0$ and $n=1$.

When the microscopic magnetic-field distribution possesses the proper symmetry which allows strong nonreciprocity to exist (i.e., the case of $b\neq d$, see Fig. 4), one can estimate the magnitude of the shift as if it is caused by $\mathbf{H}(\mathbf{r})$ alone. For $\mu\ll 1$ the asymptotic expression for δq_x is

$$\delta q_x\approx\frac{d-b}{4l_H{}^2}. \tag{31}$$

Recall that in accordance with Fig. 2, $a\equiv a_y\equiv b+d$. It is significant that there is no special ''magnetoelectric'' small parameter in our model system other than the amplitude H_0 of the antiferromagnetic microscopic field $\mathbf{H}(\mathbf{r})$ itself. The magnitude of the microscopic electric field does influence the result, but it is not crucial for the very existence of the effect since as discussed above a staggered magnetic field of the proper symmetry by itself can cause nonreciprocal behavior (as is the case here).

Since the internal microscopic magnetic field in common antiferromagnets never exceeds several Tesla, the magnitude of l_H is of the order of 10^{-6} cm or larger. This value exceeds the typical interatomic distance a in crystals by one or two orders of magnitude. Consequently, there is every reason to expect that in common crystalline antiferromagnets nonreciprocity effects of purely ''magnetic'' nature will be small.

Though from the symmetry point of view, the electric component of the microscopic field is not essential for the existence of spectral asymmetry (excluding the special case when $b=d$), it may influence the magnitude of the effect in a significant manner. Taking into account the electric component (18), we obtain the following asymptotic expression for δq_x. When $\mu\ll 1$

$$\delta q_x\sim\frac{a}{4l_H{}^2}\,\varphi(u_0,b,d), \tag{32}$$

where u_0 is given in Eq. (28). This expression is a generalization of Eq. (31) for the case of a nonzero microscopic electric field; $\varphi(u_0,b,d)$ is a dimensionless function. Below, two of the most interesting limiting cases are presented explicitly:

(1) When $u_0 l_H^2 \ll 1$,

$$\varphi(u_0,b,d) \sim \frac{6(d-b)+u_0 b[(d-b)a+2d^2ba^{-1}]}{a(6+u_0ab)}, \tag{33}$$

(2) When $u_0 a^2 \gg 1$,

$$\varphi(u_0,b,d) \sim 1. \tag{34}$$

In any case, when $b \neq d$, $\varphi(u_0,b,d)$ is of the order of magnitude of unity.

The spectral shifts given by Eqs. (31) and (32) may differ, but they are apparently of the same order of magnitude. Therefore, once again we estimate that in common antiferromagnets, within the framework of a spinless approximation the degree of the spectral asymmetry is expected to be rather small, e.g., less than 10^{-2}.

A much stronger magnetic interaction than that of the Zeeman type is known to occur, i.e., the exchange interaction which, in fact, is responsible for the very phenomenon of spontaneous magnetic order. This interaction may also contribute to the spectral asymmetry, but it is not obvious in which cases it may play a significant role. In any case, since accounting for an exchange interaction within the framework of a spinless approximation is unwarranted, we will not consider here its possible contribution to the nonreciprocity.

The estimates (31) and (33) imply that in order to get a relatively strong ''orbital'' nonreciprocity one has to search for magnetically ordered systems in which the corresponding primitive translation a is much greater than a typical interatomic distance. Such circumstance may be found for long-period magnetic structures with periods of $10-10^3$ interatomic distances; examples of such systems include domain structures, both ferro- and antiferromagnetic (a ferromagnetic domain structure can be thought of as a long-period antiferromagnet), as well as certain artificially created layered superlattices with the proper periodicity (examples of such systems are discussed in Ref. 17, and references therein). Under such circumstances, the effects associated with nonreciprocity may be expected to be strong, that is the shift δq_x may be comparable with $2\pi/a$. Finally, it is noteworthy that for the nonreciprocity behavior to be of significance, only one of the three principle translations should meet the condition $\mu < 1$. The above considerations could assist in designing and fabricating materials which could be used for spectroscopic measurements and potential utilization of nonreciprocity effects in solids.

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[1] There exists an extensive literature on the magnetoelectric effect (Refs. 2–9, and references therein), including several proceedings of international conferences. While our investigation does not deal with magnetoelectricity itself, the symmetry aspects of the linear magnetoelectric effect and of nonreciprocity characteristics of excitation spectra are closely related.

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