

# Exact many-body sum rule for the magneto-optical spectrum of solids

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Using a many-body formulation we show that the integral over the imaginary part of the off-diagonal optical conductivity gives—at zero temperature—exactly the many-electron center of mass angular momentum in the volume, i.e.,  $\int_0^\infty \text{Im}[\sigma_{xy}(\omega)] d\omega \propto \langle (\mathbf{R} \times \mathbf{P})_z \rangle$ , with  $\mathbf{R}$  the center of mass coordinate and  $\mathbf{P}$  the total relativistic momentum. At elevated temperatures the sum rule is no longer exactly fulfilled, but the temperature-related correction is estimated to be very small. In a single-particle description the sum rule leads to the total orbital moment in the volume plus an additional term.

## I. INTRODUCTION

In recent years x-ray magneto-optical (MO) spectroscopies, like x-ray magnetic circular dichroism (XMCD),<sup>1,2</sup> x-ray magnetic scattering,<sup>3</sup> the x-ray Faraday<sup>4</sup> or Kerr effect,<sup>5</sup> have become available as valuable tools to investigate magnetic properties of solids. The usefulness of XMCD in particular has been much increased by the XMCD sum rules, which allow one to obtain the spin or orbital moment of an atom from an energy integral over a finite XMCD spectrum.<sup>6,7</sup> Together with the sum rules, XMCD is such a powerful tool because it can provide element-specific information on an atom in a solid. A drawback of the sum rules, however, is that these have been derived for atoms. When the ‘‘atomic’’ sum rules are applied to XMCD spectra measured for solids, this implies that the extended valence band of a transition metal element in that solid is approximated simply by atomic states. Furthermore, the nonspherical potential of an atom in the solid is approximated by the spherical potential of an isolated atom. In addition, there are a number of other, less important approximations involved. In spite of this, the atomic sum rules have given reasonable values for the spin and orbital moments of various materials.<sup>8,9</sup>

In optics there exist also exact sum rules, such as, e.g., the so-called  $f$  sum rule, which relates the total number of electrons in the volume to an integral over the absorptive part of the diagonal optical conductivity. The  $f$  sum rule is valid for solids as well as atoms. Naturally, the question arises if, similarly, MO sum rules exist that would be valid for solids. Recently, one of the present authors has given a sum rule for the absorptive part of the off-diagonal optical conductivity, for which the energy integral gives the total orbital moment within the volume, but there was a second term, which was estimated to be small.<sup>10</sup> That derivation was, however, based on an independent-particle expression for the optical conductivity tensor. A better and more appropriate approach would obviously be to use a many-particle formulation.

In the following we present the derivation of a MO sum rule that is valid for solids, starting from a many-body formulation. We obtain thereby a fundamental relationship between the MO conductivity spectrum and the many-electron

center of mass (CM) angular momentum, which is exactly valid at zero temperature. The correction term for elevated temperatures will be shown to be negligible. The CM angular momentum is, however, not equal to the total many-electron orbital moment. Within a single-particle formulation it can be shown that the CM angular momentum leads to the total orbital moment plus a supplementary term, in accordance with the previous single-particle investigation.<sup>10</sup> The importance of the many-electron MO sum rule is, first, that it is exact, and may therefore serve as the appropriate starting point for making various controllable approximations, e.g., for deriving sum rules for atoms in a finite frequency range. Second, as we shall show, the  $f$  sum rule and the MO sum rule can be formulated in a unified manner as a bilinear product of  $\mathbf{R}$  and  $\mathbf{P}$ .

## II. DERIVATION

### A. Many-body formulation

Our derivation starts from the Kubo linear-response formula for the components  $\sigma_{\mu\nu}$  of the optical conductivity tensor. A useful, short notation for  $\sigma_{\mu\nu}(\omega)$  is (see, e.g., Refs. 11,12)

$$\sigma_{\mu\nu}(\omega) = -\frac{i\hbar}{V} \sum_{\kappa\kappa'} \frac{1}{Z} \left( \frac{e^{-\beta E_\kappa} - e^{-\beta E_{\kappa'}}}{E_\kappa - E_{\kappa'}} \right) \frac{J_{\kappa\kappa'}^\mu J_{\kappa'\kappa}^\nu}{\hbar \omega^+ - (E_{\kappa'} - E_\kappa)}, \quad (1)$$

where  $\kappa$  and  $E_\kappa$  denote the many-electron state and its energy,  $J_{\kappa\kappa'}^\nu$  is the matrix element of the current operator,  $\beta = (k_B T)^{-1}$ ,  $V$  is the unit cell volume, and  $Z$  is the partition function, i.e.,  $\text{Tr}[\exp(-\beta H)]$ . The many-particle current operator is given by

$$\mathbf{J} \equiv -\frac{e}{m} \mathbf{P} = -\frac{e}{m} \sum_n^N \mathbf{\Pi}_n, \quad (2)$$

where  $n$  labels the  $N$  electrons present in the volume,  $\mathbf{P}$  is the total momentum, and  $\mathbf{\Pi}$  is the one-particle momentum operator. In the nonrelativistic approximation, one has for the one-particle momentum operator simply  $\mathbf{\Pi} = \mathbf{p} = -i\hbar \nabla$ . We

assume here that there is no external magnetic field, but that there is an internal magnetic field that is due to the spin polarization of the electrons. It is known that for magneto-optics a relativistic formulation is required, since MO effects only occur when spin polarization and spin-orbit coupling are present simultaneously.<sup>13,14</sup> It is imperative that these effects are present in the energies and electron wave functions, but the relativistic contribution to the momentum operator is not important. In a relativistic description one has  $\mathbf{\Pi} = mc\boldsymbol{\alpha}$ , where  $\boldsymbol{\alpha}$  is the standard  $4 \times 4$  Dirac matrix. The difference between the two ways of writing the one-particle momentum operators is in effect very small, since it can be shown that  $mc\boldsymbol{\alpha} = \mathbf{p} + O(1/c^2)$ .<sup>15</sup>

From Eq. (2) it can be recognized that for  $\mu \neq \nu$  the absorptive part of  $\sigma_{\mu\nu}$  equals the imaginary part of  $\sigma_{\mu\nu}$ , which we shall denote by  $\sigma_{\mu\nu}^{(2)}$ . It can be rewritten as

$$\sigma_{\mu\nu}^{(2)}(\omega) = -\frac{\pi e^2 \hbar}{m^2 V} \sum_{\kappa \kappa'} \frac{1}{Z} \left( \frac{e^{-\beta E_\kappa} - e^{-\beta E_{\kappa'}}}{E_\kappa - E_{\kappa'}} \right) \times \text{Im}(P_{\kappa\kappa'}^\mu P_{\kappa'\kappa}^\nu) \delta(\hbar\omega - (E_{\kappa'} - E_\kappa)). \quad (3)$$

To bring this expression into a form that is more convenient for our present purpose, we make use of the equality

$$\mathbf{P} = \frac{im}{\hbar} [H, \mathbf{R}], \quad (4)$$

which leads to

$$\langle\langle \kappa | R^\mu | \kappa' \rangle\rangle (E_\kappa - E_{\kappa'}) = \frac{\hbar}{im} \langle\langle \kappa | P^\mu | \kappa' \rangle\rangle. \quad (5)$$

Here  $\mathbf{R} \equiv \sum_n \mathbf{r}_n$  is  $N$  times the center of mass coordinate of the electrons in the volume, and  $\langle\langle \dots \rangle\rangle$  denotes the Hilbert space integration. For the imaginary part of the conductivity one obtains

$$\sigma_{\mu\nu}^{(2)}(\omega) = -\frac{\pi e^2}{mV} \sum_{\kappa \kappa'} \frac{1}{Z} (e^{-\beta E_\kappa} - e^{-\beta E_{\kappa'}}) \times \text{Re}(R_{\kappa\kappa'}^\mu P_{\kappa'\kappa}^\nu) \delta(\hbar\omega - (E_{\kappa'} - E_\kappa)). \quad (6)$$

The integration over the frequency is the next step in the derivation of the sum rule. This leads, for  $\mu \neq \nu$ , to

$$\int_0^\infty \sigma_{\mu\nu}^{(2)}(\omega) d\omega = -\frac{\pi e^2}{mV\hbar} \sum_{\kappa} \sum_{\kappa' > \kappa} \frac{1}{Z} (e^{-\beta E_\kappa} - e^{-\beta E_{\kappa'}}) \times \text{Re}(R_{\kappa\kappa'}^\mu P_{\kappa'\kappa}^\nu). \quad (7)$$

The sum over  $\kappa'$  has become restricted by the positive energy branch, and the term with  $\kappa = \kappa'$  disappears, because, when replacing  $R_{\kappa\kappa'}^\mu$  by  $P_{\kappa\kappa'}^\mu$ , again, it can be shown that the real part is zero. The terms in Eq. (7) can be rearranged as follows:

$$\int_0^\infty \sigma_{\mu\nu}^{(2)}(\omega) d\omega = -\frac{\pi e^2}{mV\hbar} \left( \sum_{\kappa} \sum_{\kappa' \neq \kappa} \frac{e^{-\beta E_\kappa}}{Z} \text{Re}(R_{\kappa\kappa'}^\mu P_{\kappa'\kappa}^\nu) - 2 \sum_{\kappa} \sum_{\kappa' > \kappa} \frac{e^{-\beta E_{\kappa'}}}{Z} \text{Re}(R_{\kappa\kappa'}^\mu P_{\kappa'\kappa}^\nu) \right). \quad (8)$$

To arrive at the MO sum rule we now consider the many-electron CM angular momentum defined by  $\mathbf{K} = \mathbf{R} \times \mathbf{P}$ . The expectation value of its  $z$  component is

$$\langle K_z \rangle = \sum_{\kappa} \frac{e^{-\beta E_\kappa}}{Z} \langle\langle \kappa | R^x P^y - R^y P^x | \kappa \rangle\rangle. \quad (9)$$

Using Eq. (5) and the closure relation for many-particle states, this can be expressed as

$$\langle K_z \rangle = 2 \sum_{\kappa} \sum_{\kappa' \neq \kappa} \frac{e^{-\beta E_\kappa}}{Z} \text{Re}(R_{\kappa\kappa'}^x P_{\kappa'\kappa}^y). \quad (10)$$

Comparison of Eqs. (10) and (8) leads directly to the MO sum rule,

$$\int_0^\infty \sigma_{xy}^{(2)}(\omega) d\omega = -\frac{\pi e^2}{2mV\hbar} \langle\langle (\mathbf{R} \times \mathbf{P})_z \rangle\rangle + \mathcal{R}_{xy}, \quad (11)$$

where the remainder  $\mathcal{R}_{xy}(T)$  is given by

$$\mathcal{R}_{xy}(T) = \frac{2\pi e^2}{mV\hbar} \sum_{\kappa} \sum_{\kappa' > \kappa} \frac{e^{-\beta E_{\kappa'}}}{Z} \text{Re}(R_{\kappa\kappa'}^x P_{\kappa'\kappa}^y). \quad (12)$$

Thus, apart from  $\mathcal{R}_{xy}$ , the integral over the absorptive part of  $\sigma_{xy}(\omega)$  gives the CM angular momentum times a prefactor. The remainder  $\mathcal{R}_{xy}(T)$  can be shown to vanish at zero temperature, since at zero temperature only the ground state is populated. As the sum over  $\kappa'$  in Eq. (12) starts from at least the first excited state,  $\mathcal{R}_{xy}(0) = 0$  due to the thermal population factor. Thus, for  $T = 0$ , we obtain the *exact* sum rule,

$$\int_0^\infty \sigma_{xy}^{(2)}(\omega) d\omega = -\frac{\pi e^2}{2mV\hbar} \langle\langle (\mathbf{R} \times \mathbf{P})_z \rangle\rangle. \quad (13)$$

It should be emphasized that the CM angular momentum  $\mathbf{K}$  is not identical to the total angular momentum of the electrons in the volume, which is defined as  $\mathbf{I} = \sum_n (\mathbf{r}_n \times \mathbf{p}_n)$ . The angular momentum is related to the orbital moment  $M_l$  through  $M_l^z = -\langle I_z \rangle \mu_B / \hbar$ . Therefore, while the MO sum rule is exact, it does not lead to the orbital moment, as one might have wished. Only for one-electron systems does the MO sum rule (13) yield the orbital moment. The CM angular momentum  $\mathbf{K}$  can obviously be written as  $\mathbf{I}$  plus a correction term. To understand, first, what the correction term means and how important it is, and to estimate, second, the importance of  $\mathcal{R}_{xy}$  at elevated temperatures, it is more convenient to adopt a single-particle description. This we shall do in what follows.

## B. Single-particle formulation

To start with, we mention that the quantity that is of physical interest is the angular momentum  $\mathbf{I}_z = \sum_n (\mathbf{r}_n \times \mathbf{p}_n)_z$ , which contains the canonical momentum  $\mathbf{p}$  instead of the relativistic momentum. As already mentioned, the difference between the relativistic  $\mathbf{\Pi}$  and  $\mathbf{p}$  is  $O(1/c^2)$ , which is, in Rydberg units,  $\approx 1 \times 10^{-5}$ . Therefore, in practical applications the difference between the two operators can be neglected. This holds even for uranium compounds.<sup>15</sup>

The expression for  $\langle K_z \rangle$  can be reformulated using second quantization. Introducing the creation and annihilation operators  $a_i^\dagger, a_i$  for single-particle states  $i$ , one obtains for the CM angular momentum

$$\begin{aligned} \langle K_z \rangle &= 2 \sum_{i,j,k,l} \text{Re}(R_{ij}^x P_{kl}^y) \langle a_i^\dagger a_j a_k^\dagger a_l \rangle \\ &= 2 \sum_{i,j} \text{Re}(R_{ii}^x P_{jj}^y) \langle a_i^\dagger a_i a_j^\dagger a_j \rangle \\ &\quad + 2 \sum_{i,j} \text{Re}(R_{ij}^x P_{ji}^y) \langle a_i^\dagger a_j a_j^\dagger a_i \rangle, \end{aligned} \quad (14)$$

where the many-body states are still contained in the expectation values. The first term in Eq. (14) is zero because the real part vanishes, and for the same reason the second term becomes

$$2 \sum_{i \neq j} \text{Re}(R_{ij}^x P_{ji}^y) \langle a_i^\dagger a_i a_j a_j^\dagger \rangle. \quad (15)$$

For  $i \neq j$  the expectation value can be approximated by

$$\begin{aligned} \langle a_i^\dagger a_i a_j a_j^\dagger \rangle &= \langle a_i^\dagger a_i (1 - a_j^\dagger a_j) \rangle \\ &\approx \langle a_i^\dagger a_i \rangle \langle 1 - a_j^\dagger a_j \rangle = f(\epsilon_i) [1 - f(\epsilon_j)]. \end{aligned} \quad (16)$$

Here  $f(\epsilon_i)$  is the Fermi-Dirac distribution function, which follows from  $f(\epsilon_i) = \langle a_i^\dagger a_i \rangle$ . The single-particle expression for  $\langle K_z \rangle$  thus becomes

$$\langle K_z \rangle = 2 \sum_{i>j} \text{Re}(R_{ij}^x P_{ji}^y) [f(\epsilon_i) + f(\epsilon_j) - 2f(\epsilon_i)f(\epsilon_j)]. \quad (17)$$

This expression for  $\langle K_z \rangle$  has to be compared to  $\langle l_z \rangle$  in order to extract the difference between the two quantities. The single-particle equation for  $\langle l_z \rangle$  is

$$\langle l_z \rangle = \sum_i f(\epsilon_i) \langle \langle i | (\mathbf{r} \times \mathbf{p})_z | i \rangle \rangle. \quad (18)$$

Ignoring the tiny difference between  $\mathbf{p}$  and  $\mathbf{\Pi}$ , this can be rewritten as

$$\langle l_z \rangle = 2 \sum_{i>j} \text{Re}(R_{ij}^x P_{ji}^y) [f(\epsilon_i) + f(\epsilon_j)]. \quad (19)$$

We therefore find the following relationship between  $\langle K_z \rangle$  and  $\langle l_z \rangle$ :

$$\langle K_z \rangle = \langle l_z \rangle - 4 \sum_{i>j} \text{Re}(R_{ij}^x P_{ji}^y) f(\epsilon_i) f(\epsilon_j). \quad (20)$$

Relationship (20) shows that  $\langle K_z \rangle$  and  $\langle l_z \rangle$  are closely related, but the additional term does not vanish in general. For  $T=0$  it yields a sum over states  $i, j$  that are both occupied. The immediate consequence of Eq. (20) is that even at  $T=0$  one cannot straightforwardly obtain the orbital moment from an integral over the absorptive part of the off-diagonal conductivity. Only for systems with one electron is the angular momentum without additional term obtained.

At elevated temperatures there exists furthermore in the many-body formulation the term  $\mathcal{R}_{xy}$ .  $\mathcal{R}_{xy}$  can be expressed in a single-particle formulation, which can be done most conveniently by using Eq. (11) together with the single-particle expressions for  $\sigma_{xy}^{(2)}$  and  $\langle (\mathbf{R} \times \mathbf{P})_z \rangle$ . The required single-particle expression for  $\sigma_{xy}(\omega)$  which follows<sup>16</sup> from the many-body expression (1) is

$$\sigma_{xy}(\omega) = -\frac{e^2}{mV} \sum_{ij} [f(\epsilon_i) - f(\epsilon_j)] \frac{R_{ij}^x P_{ji}^y}{\hbar \omega^+ - (\epsilon_j - \epsilon_i)}, \quad (21)$$

which yields for  $\mathcal{R}_{xy}$

$$\mathcal{R}_{xy} = \frac{2\pi e^2}{mV\hbar} \sum_{i>j} \text{Re}(R_{ij}^x P_{ji}^y) f(\epsilon_i) [1 - f(\epsilon_j)]. \quad (22)$$

From this expression it can be seen directly that  $\mathcal{R}_{xy}$  vanishes at  $T=0$ , but also that  $\mathcal{R}_{xy}$  must be small at elevated temperatures. The product  $f(\epsilon_i)[1 - f(\epsilon_j)]$  adopts the form of a sharply peaked function at the Fermi energy  $E_F$ ; therefore the only states that can contribute at elevated temperatures are those very close  $E_F$ , but the states  $i=j$  directly at  $E_F$  are excluded from the sum. Furthermore, taking the steepness of the Fermi-Dirac function into account, and the fact that the whole spectrum of occupied states contributes to  $\langle (\mathbf{R} \times \mathbf{P})_z \rangle$ , it is clear that  $\mathcal{R}_{xy}$  bears no weight against  $\langle (\mathbf{R} \times \mathbf{P})_z \rangle$  even at room temperature. *Consequently, the many-body sum rule (13) is an accurate expression even at elevated temperatures.*

### III. DISCUSSION AND CONCLUSIONS

It is instructive to compare the sum rule Eq. (13) to the well-known  $f$  sum rule which gives the total number of electrons in the considered volume (see, e.g., Ref. 17). A general form of the  $f$  sum rule can be derived from the many-body expression (1) for the real part of  $\sigma_{\mu\nu}$ :

$$\int_0^\infty \sigma_{\mu\nu}^{(1)}(\omega) d\omega = -\frac{\pi e^2}{2mV\hbar} \text{Im} \langle [P^\mu, R^\nu] \rangle. \quad (23)$$

In this form the  $f$  sum rule is valid for both  $\mu = \nu$  and  $\mu \neq \nu$ , and also in the relativistic limit. In the nonrelativistic limit the commutator in Eq. (23) reduces to  $-i\hbar N \delta_{\mu\nu}$ , which yields the standard expression for the  $f$  sum rule. With regard to the MO sum rule (13), we note, first, that the prefactor occurring in the MO sum rule is just the same as that of the  $f$  sum rule. Second, both the  $f$  sum rule and the MO sum rule are expressions that contain a bilinear product of  $\mathbf{R}$  and  $\mathbf{P}$ , in one case the commutator and in the other the cross product of  $\mathbf{R}$  and  $\mathbf{P}$ . Thus there apparently exists a unified formulation of both the  $f$  sum rule and the MO sum rule.

In the derivation of the MO sum rule we considered the  $xy$  element of the conductivity tensor and the  $z$  component of the CM angular momentum.  $\sigma_{xy}$  is the only nonzero off-diagonal element in the so-called polar geometry, where the magnetization is parallel to the  $z$  axis and normal to the medium's surface. However, in a more general geometry other off-diagonal elements can be nonzero. For such cases, it is straightforward to generalize Eq. (13) to all components of the CM angular momentum,

$$\varepsilon_{ijk} \int_0^\infty \sigma_{ij}^{(2)}(\omega) d\omega = -\frac{\pi e^2}{2mV\hbar} \langle K_k \rangle, \quad (24)$$

where  $\varepsilon_{ijk}$  is the antisymmetric tensor.

Previously an atomic sum rule applicable to atoms with one electron was proposed.<sup>18,19</sup> This sum rule relates the orbital moment of the one electron to the difference of the oscillator strengths for left- and right-circularly polarized light. If one rewrites the oscillator strengths in terms of the optical conductivity, it can be shown that this atomic sum rule corresponds to the one-electron limit of the MO sum rule (13), as one would expect (except for the volume not accounted for in Refs. 18 and 19).

Comparing the atomic XMCD sum rules<sup>6,7</sup> to the one derived here, we note first that the present sum rule is related only to the orbital-moment sum rule<sup>6</sup> because  $\mu^+ - \mu^- \approx -8\pi\sigma_{xy}^{(2)}/c$  for x-ray frequencies, with  $\mu^\pm$  the x-ray absorption coefficients. One could think of the MO sum rule (13) as being the sum of all atomic orbital-moment sum rules over all edges, but the MO sum rule is not normalized by the total absorption spectrum. Moreover, the MO sum rule is exact and not subject to any of the restrictions of the atomic sum rules that were mentioned in the Introduction. Nevertheless, in spite of the serious approximations that are made when the atomic sum rules are applied to atoms in a solid, the atomic sum rules have as their main advantage that in

principle they provide element-specific information. The many-body sum rule, on the other hand, has as advantage that it is exact and valid for atoms as well as solids. The exact sum rule could therefore be used as a starting point to study or derive approximate sum rule expressions that contain controllable correction terms, e.g., for those contributions that originate from final states which are hybridized valence states instead of pure atomic states. Other approaches to overcoming some of the restrictions of the atomic orbital-moment sum rule have been considered recently.<sup>20,21</sup>

To conclude, we have shown that the spectral integral over the absorptive part of the off-diagonal conductivity gives the many-body CM angular moment of the electrons in a unit cell of a solid. This MO sum rule is exactly valid for  $T=0$ . The temperature-induced correction term can be neglected to a very good approximation. The many-body CM angular moment is equal to the orbital moment plus an additional term, where the latter in general disappears only for one-electron systems.

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