Scattering Operator for Elastic and Inelastic Resonant X-Ray Scattering

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We show that, in the fast collision approximation, the scattering operator for resonant x-ray scattering can be expressed in terms of simple spin-orbital moment operators $M^{(k)}(\mathbf{l},\mathbf{s})$ of the valence shell involved in the resonance. This theory is applicable to the analysis of a broad range of resonant x-ray elastic and inelastic scattering and absorption experiments involving rare earth, actinide, and transition elements.

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From magnetic structure determination to critical scattering, resonant x-ray magnetic scattering has become a powerful probe of magnetism complementary to magnetic neutron scattering [1–3]. But important questions remain, which we address in this Letter: how is resonant x-ray magnetic scattering related to the atomic spin and orbital moments, and what are the essential differences between neutron and resonant x-ray magnetic scattering?

The neutron magnetic scattering operator f_n is proportional to the Fourier transform of the magnetic moment density, $f_n \propto \mu_n\{\hat{\boldsymbol{\kappa}} \times [\mathbf{L}(\boldsymbol{\kappa}) + 2\mathbf{S}(\kappa)] \times \hat{\boldsymbol{\kappa}}\}$, and neutron scattering studies have been the chief means for magnetic structure and excitation spectra determination in magnetic materials [4]. Also the *nonresonant* x-ray magnetic scattering operator has the simple form $f_m \propto \mathbf{L}(\kappa)\cdot\mathbf{A} + \mathbf{S}(\kappa)\cdot\mathbf{B}$, again linear in $\mathbf{L}(\kappa)$ and $\mathbf{S}(\kappa)$, allowing similar magnetic structure information to be obtained as from neutron scattering [5], although f_m is quite small, typically $\approx 0.01 r_0$, in comparison to $f_n \approx r_0$ for neutron scattering.

Near absorption edges, however, very large resonant enhancements to magnetic sensitive x-ray scattering occur, with amplitudes ranging from $0.1r_0$ to $100r_0$ [1,2]. This strongly enhanced "magnetic" x-ray scattering is actually electric multipole resonance scattering with the magnetic sensitivity arising from the effects of exchange and spin-orbit correlation [2]. It is not at all obvious that the resonant scattering operator F_{EL} is simply related to the atomic orbital and spin moments, as is the case for neutron and nonresonant x-ray magnetic scattering. However, we show that for the important case of "quasielastic" scattering, if the "fast collision approximation" can be made, then indeed $F_{EL} \propto \sum_{k=0}^{2L} T_{EL}^{(k)}(\mathbf{e}_f^*, \mathbf{k}_f; \mathbf{e}_0, \mathbf{k}_0)\cdot M_{EL}^{(k)}(\mathbf{l},\mathbf{s})$, where the $M_{EL}^{(k)}(\mathbf{l},\mathbf{s})$ are kth rank spin-orbital moments of the valence shell involved in the resonance. The odd-order moments are odd under time reversal T and hence purely magnetic, while the even-order moments are even under T, and include the charge multipole moments (giving nonmagnetic Templeton effects). Coherent resonant x-ray scattering then determines correlations between these moments, and gives important information, not obtainable from neutron and nonresonant x-ray magnetic scattering.

Recently, Thole *et al.* [6] and Carra *et al.* [7] have given elegant theoretical discussions of x-ray circular dichroism near the absorption edges in transition metals and rare earths. Here we extend these considerations to treat elastic and inelastic resonant x-ray scattering.

Near resonance the pure electric multipole scattering amplitude is given by [2]

$$f = \langle\psi_f \mid F_{EL} \mid \psi_0\rangle = 4\pi\lambda_0 \sum_{M',M} [\mathbf{e}_f^* \cdot \mathbf{Y}_{LM'}^{(e)}(\hat{\mathbf{k}}_f)][\mathbf{Y}_{LM}^{(e)*}(\hat{\mathbf{k}}_0)\cdot\mathbf{e}_0]\langle\psi_f \mid F_{LM';LM}^{(e)}(\omega) \mid \psi_0\rangle, \tag{1}$$

$$\langle\psi_f \mid F_{LM';LM}^{(e)}(\omega) \mid \psi_0\rangle = \sum_I \frac{1}{2\lambda_{IO}}\left[\frac{\langle\psi_f \mid J_{LM'}^{(e)\dagger} \mid I\rangle\langle I \mid J_{LM}^{(e)} \mid \psi_0\rangle}{E_I - E_0 - \hbar\omega - i\Gamma/2}\right], \tag{2}$$

to a very good approximation, and the current operator is given by

$$J_{LM}^{(e)} = \sum \langle nl_2 m_2 m_s \mid -\frac{4\pi i^L k^L}{(2L+1)!!}\sqrt{\frac{L+1}{L}} Q_{LM} \mid n_c j_1 l_1 m_1 m_s\rangle C_{l_1 m_1;\frac{1}{2}m_s}^{j_1 m_j} \hat{a}_{m_2 m_s}^\dagger \hat{b}_{j_1 m_j}, \tag{3}$$

where $Q_{LM} = er^L Y_{LM}$ is the usual electric multipole moment operator, $\hat{a}$ and $\hat{a}^\dagger$ are annihilation and creation operators for an (nl_2) electron in the valence shell, the operators $\hat{b}$ and $\hat{b}^\dagger$ for an $(n_c l_1 j_1)$ electron in the core shell. $\mid I\rangle = \mid (nl_2)^{+1}(n_c l_1 j_1)^{-1}\psi_0\rangle$ is the excited state with an electron excited to the partially filled valence shell (nl_2) leaving a hole in the core shell $(n_c l_1 j_1)$. Γ is the width of the excited state. Here we restrict our attention to "quasielastic" scattering, where the final state $\mid \psi_f\rangle$ corresponds to the same configuration as the initial state $\mid \psi_0\rangle$, i.e., all core levels filled and the same number of valence shell electrons as initially, but not necessarily the same state, e.g., $\mid (nl_2)^\nu L, S, J, M\rangle \rightarrow \mid (nl_2)^\nu L', S', J', M'\rangle$ transitions may occur, where ν is the number of electrons in the (nl_2) valence shell.

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F_{EL}, Eq. (1) can be expressed in terms of spherical tensors,

$$F_{EL} = 4\pi\lambda\!\!\!^{-}_0 \sum_{k=0}^{2L} \sum_{q=-k}^{k} T_q^{(k)*}(\mathbf{e}_f^*, \hat{\mathbf{k}}_f; \mathbf{e}_0, \hat{\mathbf{k}}_0)_{EL} F_q^{(k)}(\omega)_{EL}, \tag{4}$$

$$T_q^{(k)*}(\mathbf{e}_f^*, \hat{\mathbf{k}}_f; \mathbf{e}_0, \hat{\mathbf{k}}_0)_{EL} = \sqrt{\frac{2k+1}{2L+1}} \sum_{M',M} C^{LM}_{LM';kq} [\mathbf{e}_f^* \cdot \mathbf{Y}^{(e)}_{LM'}(\hat{\mathbf{k}}_f)][\mathbf{Y}^{(e)*}_{LM}(\hat{\mathbf{k}}_0) \cdot \mathbf{e}_0], \tag{5}$$

$$F_q^{(k)}(\omega)_{EL} = \sqrt{\frac{2k+1}{2L+1}} \sum_{M,M'} C^{LM}_{LM';kq} F^{(e)}_{LM';LM}(\omega). \tag{6}$$

A great simplification for the structure of the operator $F_q^{(k)}(\omega)$ occurs for the important cases where either the width Γ or the deviation $\Delta\omega = E_I - E_0 - \hbar\omega$ from resonance is large compared to the splitting Δ of the excited state configuration. Then E_I can be replaced by $\overline{E}_I$ in Eq. (2), and the energy denominator taken outside the summation. In this case the $F_q^{(k)}(\omega)$'s factor into a single scalar resonance factor R [Eq. (8)] and multipole moment operators $M_q^{(k)}$ which are simple single-particle operators summed over the valence electrons [see Eq. (16)]. This is a "fast collision" approximation: When the core electron is initially injected into an empty orbital of the valence shell, then generally it and the core hole exert torques on each other and the other valence electrons, causing changes in the state of these electrons. The rate at which these changes take place, however, is determined by ΔE_I, and to a good approximation they can be neglected if $\Delta E_I T$ is small, where $T = \mid \Delta\omega - i\Gamma/2 \mid^{-1}$ measures the collision duration.

Making the fast collision approximation,

$$F^{(e)}_{LM';LM}(\omega) = R(l_1 j_1; L; l_2) S_{LM';LM}(l_1 j_1; l_2), \tag{7}$$

where the dimensionless "reduced resonance scattering amplitude" $R(l_1 j_1; L; l_2)$ is

$$R(l_1 j_1; L; l_2) = K(l_1 L l_2) \mid \langle R_{nl_2}(r) \mid r^L \mid R_{n_c l_1 j_1}(r) \rangle \mid^2 / [E_I - E_0 - \hbar\omega - i\Gamma/2] \,, \tag{8}$$

$$K(l_1 L l_2) = (e^2/\lambda\!\!\!^{-2L+1}) \{(2l_1+1)(2L+1)(L+1)/[L(2l_2+1)]\} [C^{l_2 0}_{l_1 0; L0}/(2L+1)!!]^2,$$

and

$$\langle \psi_f \mid S_{LM';LM}(l_1 j_1; l_2) \mid \psi_0 \rangle = \sum_{\text{all } m,m'} \langle \psi_f \mid \hat{b}^\dagger_{j_1 m'_j} \hat{a}_{m'_2 m'_s} \hat{a}^\dagger_{m_2 m_s} \hat{b}_{j_1 m_j} \mid \psi_0 \rangle [C^{j_1 m'_j}_{l_1 m'_1; \frac{1}{2} m'_s} C^{j_1 m_j}_{l_1 m_1; \frac{1}{2} m_s} C^{l_2 m'_2}_{l_1 m'_1; LM'} C^{l_2 m_2}_{l_1 m_1; LM}] \,. \tag{9}$$

Since the core states are filled in the initial and final states, $\langle \psi_f \mid \hat{b}^\dagger_{j_1 m'_j} \hat{a}_{m'_2 m'_s} \hat{a}^\dagger_{m_2 m_s} \hat{b}_{j_1 m_j} \mid \psi_0 \rangle = \delta_{m'_j m_j} \langle \psi_f \mid \times \hat{a}_{m'_2 m'_s} \hat{a}^\dagger_{m_2 m_s} \mid \psi_0 \rangle$. The operators $\hat{a}^\dagger_{m_2 m_s} \hat{a}_{m'_2 m'_s}$ can be expressed by Judd's spin-orbit double tensor operators $W^{(\kappa,l)}_{\mu m}$ [8]. We define double tensor operators for "hole" multipole moments

$$\overline{W}^{(\kappa,l)}_{\mu m} = \sqrt{\frac{(2\kappa+1)(2l+1)}{2(2l_2+1)}} \sum_{m_2 m_s m'_2 m'_s} (-\hat{a}_{m'_2 m'_s} \hat{a}^\dagger_{m_2 m_s}) C^{\frac{1}{2} m_s}_{\frac{1}{2} m'_s; \kappa\mu} C^{l_2 m_2}_{l_2 m'_2; lm} \tag{10}$$

$[\overline{W}^{(\kappa,l)}_{\mu m} = W^{(\kappa,l)}_{\mu m} - \sqrt{2(2l_2+1)}\delta_{\kappa,0}\delta_{l,0}]$. The operators $\overline{W}^{(\kappa,l)}_{\mu m} \propto \sum_{i \in l_2} [s^{(\kappa)}_\mu V^{(l)}_m(\mathbf{l})]_i$, where $V^{(l)}(l_i)$ is the lth rank spherical tensor of $\mathbf{l}_i$, which is defined $V^{(n)}_m(\mathbf{l}) = C^{nm}_{1\mu;n-1,m-\mu} l_\mu V^{(n-1)}_{m-\mu}(\mathbf{l})$, and $V^{(1)}_\mu(\mathbf{l}) = l_\mu$.

$S_{LM';LM}$ can now be expressed in terms of $\overline{W}^{(\kappa,l)}_{\mu m}$, and, utilizing the theorems of Yutsis, Levinson, and Vanagas [9] to evaluate the Clebsch-Gordan sums,

$$\begin{aligned} S_{LM';LM}(l_1 j_\pm; l_2) &= \sum_k \left(-\frac{j_\pm + \frac{1}{2}}{2l_1+1} c_k \overline{W}^{(0,k)}_q \pm \sum_{l=|k-1|,\neq k}^{k+1} d_{kl} \overline{W}^{(1,l)k}_q \right) C^{LM}_{LM';kq} \\ &\equiv \sum_{k,q} M^{(k)}_q(l_1 j_\pm; L; l_2) C^{LM}_{LM';kq}, \end{aligned} \tag{11}$$

where $\overline{W}^{(1,l)k}_q$ is the spin-orbit coupled tensor operator, $\overline{W}^{(1,l)k}_q = \sum_{\mu,m} C^{kq}_{1\mu;lm} \overline{W}^{(1,l)}_{\mu,m}$, and

$$c_k = (-1)^k \sqrt{\frac{2(2l+1)}{2L+1}} (2l_2+1) \begin{Bmatrix} L & l_2 & l_1 \\ l_2 & L & k \end{Bmatrix}, \quad d_{kl} = \sqrt{\frac{l_1(l_1+1)2(2l+1)}{(2l_1+1)(2L+1)}} (2l_2+1)\sqrt{2k+1} \begin{Bmatrix} l_1 & l_1 & 1 \\ l_2 & l_2 & l \\ L & L & k \end{Bmatrix}. \tag{12}$$

Now $F_q^{(k)}(\omega)_{EL}$, Eq. (6), becomes

$$F_q^{(k)}(\omega)_{EL} = R(l_1 j_\pm; L; l_2)\sqrt{\frac{2L+1}{2k+1}} M_q^{(k)}(l_1 j_\pm; L; l_2) \ . \tag{13}$$

Substituting from Eq. (13) into Eq. (4), we finally obtain

$$F_{EL} = 4\pi \lambda\!\!\!^{-}_0 R(l_1 j_1; L; l_2) \sum_{k=0}^{2L} \sum_{q=-k}^{k} \sqrt{\frac{2L+1}{2k+1}} T_{q\ EL}^{(k)*} M_q^{(k)}(l_1 j_1; L; l_2) \ . \tag{14}$$

For the important case of $E1$ resonant scattering,

$$\begin{aligned} F_{E1}(\mathbf{e}_f^*, \hat{\mathbf{k}}_f; \mathbf{e}_0, \hat{\mathbf{k}}_0) = \tfrac{3}{2}\lambda\!\!\!^{-}_0 R(l_1 j_1; 1; l_2)[(\mathbf{e}_f^* \cdot \mathbf{e}_0) M^{(0)}(l_1 j_1; 1; l_2) - (i/\sqrt{2})(\mathbf{e}_f^* \times \mathbf{e}_0) M^{(1)}(l_1 j_1; 1; l_2) \\ - \sqrt{\tfrac{3}{5}} V^{(2)}(\mathbf{e}_f^* \otimes \mathbf{e}_0) M^{(2)}(l_1 j_1; 1; l_2)]. \end{aligned} \tag{15}$$

From the definition of $\overline{W}^{(\kappa,l)k}$, the operators $M^{(k)}(l_1 j_1; 1; l_2)$ are

$$\begin{aligned} M^{(0)}(l_1 j_\pm; 1; l_2) &= \frac{j_\pm + \frac{1}{2}}{2l_1+1} \alpha_0 N_h(l_2) \mp \gamma_0 \sum_{i \in l_2} (\mathbf{s}_i \cdot \mathbf{l}_i), \\ M^{(1)}(l_1 j_\pm; 1; l_2) &= \frac{j_\pm + \frac{1}{2}}{2l_1+1} \alpha_1 \mathbf{L}(l_2) \pm \beta_1 \mathbf{S}(l_2) \pm \gamma_1 \sum_{i \in l_2} \left(\mathbf{s}_i - \frac{3\{\mathbf{s}_i \cdot \mathbf{l}_i, \mathbf{l}_i\}_+}{2l_2(l_2+1)} \right), \\ M^{(2)}(l_1 j_\pm; 1; l_2) &= -\frac{j_\pm + \frac{1}{2}}{2l_1+1} \alpha_2 \sum_{i \in l_2} V^{(2)}(\mathbf{l}_i) \pm \beta_2 \sum_{i \in l_2} V^{(2)}(\mathbf{s}_i \otimes \mathbf{l}_i) \pm \gamma_2 \sum_{i \in l_2} V^{(2)}[\mathbf{s}_i \otimes V^{(3)}(\mathbf{l}_i)]. \end{aligned} \tag{16}$$

Here $V_q^{(k)}(T^{(\kappa)} \otimes U^{(p)}) \equiv \sum_{\mu,\nu} C^{kq}_{\kappa\mu;p\nu} T_\mu^{(\kappa)} U_\nu^{(p)}$. The coefficients α, β, and γ are given in Table I. The operator sums are over the $(nl_2)^\nu$ electrons in the valence shell.

Using the Wigner-Eckart theorem, $\frac{1}{l(l+1)} V_q^{(2)}(\mathbf{l}) = \eta V_q^{(2)}(\hat{\mathbf{r}})$, and $\mathbf{s} - \frac{3\{\mathbf{s}\cdot\mathbf{l},\mathbf{l}\}_+}{2l(l+1)} = \eta[\mathbf{s} - 3(\mathbf{s}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}]$, where $\eta = -\frac{(2l+3)(2l-1)}{2l(l+1)}$.

For $E2$ transitions $M^{(0)}$, $M^{(1)}$, and $M^{(2)}$ will be given again by Eq. (16) except for different coefficients (α, β, and γ), and in addition F_{E2} [see Eq. (14)] will have $M^{(3)}$ (octupole) and $M^{(4)}$ (hexadecapole) moment operator contributions [10].

Equation (14) relates the scattering operators F_{EL} to the spin-orbit multipole moment operators $M_q^{(k)}$, and thus provides a means to determine the valence shell properties through resonant scattering, and, via the optical theorem, absorption. Because of their different angular dependences, the various moment contributions $M_q^{(k)}$ to the scattering and absorption processes can be selected experimentally.

These fast collision results should be rather good for resonant scattering at the L_2, L_3 edges in the rare earths and actinides, as well as for the M_4, M_5 edges in the actinides, for which $\Delta \lesssim \Gamma$ and the splitting is not resolved (for example, for the rare earth L_2, L_3 transitions to the $4f$ shell, the splitting $\Delta \approx$1–5 eV, while $\Gamma \gtrsim 5$ eV). However, for the M_4, M_5 transitions in the rare earths, $\Delta \gtrsim \Gamma$ and the multiplet structure can be resolved. The higher-order contributions can be included with multiplet calculations of the type performed by Thole *et al.* [11], but these higher-order corrections will have a more complex operator form. The simplicity of the fast collision approximation can be regained by tuning off resonance so that $\Delta \ll \Delta\omega$. Even off resonance, the M_4, M_5 scattering amplitudes will be appreciable because they are $\approx$(10–100)r_0 at resonance.

We now give an important generalization of these results: Some resonant magnetic effects do depend explicitly on the separation of E_I into spin-up and spin-down

TABLE I. Coefficients in Eqs. (16) and (17). Here $6j(k) = \left\{ \begin{matrix} 1 & l_2 & l_1 \\ l_2 & 1 & k \end{matrix} \right\}$, and $9j(l,k) = \left\{ \begin{matrix} l_1 & l_1 & 1 \\ l_2 & l_2 & l \\ 1 & 1 & k \end{matrix} \right\}$.

k	0	1	2
α	$\sqrt{\frac{(2l_2+1)}{3}}6j(0)$	$\sqrt{\frac{3(2l_2+1)}{l_2(l_2+1)}}6j(1)$	$\sqrt{\frac{50(2l_2+1)}{l_2(l_2+1)(2l_2+3)(2l_2-1)}}6j(2)$
$\sqrt{\frac{(2l_1+1)}{l_1(l_1+1)}}\beta$	0	$\sqrt{(2l_2+1)}9j(0,1)$	$\sqrt{\frac{60(2l_2+1)}{l_2(l_2+1)}}9j(1,2)$
$\sqrt{\frac{(2l_1+1)}{l_1(l_1+1)}}\gamma$	$2\sqrt{\frac{(2l_2+1)}{l_2(l_2+1)}}9j(1,0)$	$2\sqrt{\frac{10(2l_2+1)l_2(l_2+1)}{(2l_2+3)(2l_2-1)}}9j(2,1)$	$\frac{280\sqrt{\frac{2}{3}}(2l_2+1)9j(3,2)}{\prod_{n=-3}^{3}(2l_2+1+n)^{\frac{1}{2}}}$

bands, and upon the m_s dependence of the current matrix elements. This is usually true for transitions to d bands, and, in particular, is the case for the first observed resonant magnetic scattering ($2p_{3/2}$ to $5d$ in Ho) [1]. This is not described by the scattering operator as given by Eq. (11).

We assume that there is an exchange splitting Δ between the spin-up and spin-down valence states, $\Delta E_{I0}^{\pm} = \Delta E_{I0} \mp \frac{\Delta}{2}$, and different radial matrix elements to these states, $\langle r^L \rangle^{\pm} = \langle r^L \rangle (1 \pm \delta/2)$. Then for $E1$ transitions, the multipole moments $M^{(k)}_{q(E1)}$ become [10]

$$
\begin{aligned}
M^{(0)}(l_1 j_{\pm}; 1; l_2) &= \frac{j_{\pm} + \frac{1}{2}}{2l_1 + 1} \alpha_0 [(1 + \overline{\Delta}\delta) N_h(l_2) - 2\epsilon S_z] \mp \gamma_0 \left(\sum_{i \in l_2} (\mathbf{s}_i \cdot \mathbf{l}_i) + \frac{\epsilon}{2} L_z + \frac{\overline{\Delta}\delta}{2} L_z^{(s)} \right), \\
M^{(1)}(l_1 j_{\pm}; 1; l_2) &= \frac{j_{\pm} + \frac{1}{2}}{2l_1 + 1} \alpha_1 [(1 + \overline{\Delta}\delta)\mathbf{L} + \epsilon \mathbf{L}^{(s)}] \pm \beta_1 \left[\mathbf{S} - \left(\frac{\epsilon}{2} N_h - \overline{\Delta}\delta S_z \right) \mathbf{z} \right] \\
&\quad \pm \gamma_1 \sum_{i \in l_2} \left[\left(\mathbf{s} - \frac{3\{\mathbf{s} \cdot \mathbf{l}, \mathbf{l}\}_+}{2l_2(l_2+1)} \right)_i + \frac{\epsilon}{2} \left(\mathbf{z} - \frac{3\{l_z, \mathbf{l}\}_+}{2l_2(l_2+1)} \right)_i + \frac{\overline{\Delta}\delta}{2} \left(\mathbf{z} - \frac{3\{l_z, \mathbf{l}\}_+}{2l_2(l_2+1)} \right)_i^{(s)} \right], \\
M^{(2)}(l_1 j_{\pm}; 1; l_2) &= -\frac{j_{\pm} + \frac{1}{2}}{2l_1 + 1} \alpha_2 \sum_{i \in l_2} [(1 + \overline{\Delta}\delta) V^{(2)}(\mathbf{l}_i) + \epsilon V^{(2)}(\mathbf{l}_i)^{(s)}] \\
&\quad \pm \beta_2 \sum_{i \in l_2} \left([V^{(2)}(\mathbf{s}_i \otimes \mathbf{l}_i) + \frac{\epsilon}{2} V^{(2)}(\mathbf{z} \otimes \mathbf{l}_i) + \frac{\overline{\Delta}\delta}{2} V^{(2)}(\mathbf{z} \otimes \mathbf{l}_i)^{(s)} \right) \\
&\quad \pm \gamma_2 \sum_{1 \in l_2} \left(V^{(2)}[\mathbf{s}_i \otimes V^{(3)}(\mathbf{l}_i)] + \frac{\epsilon}{2} V^{(2)}[\mathbf{z} \otimes V^{(3)}(\mathbf{l}_i)] + \frac{\overline{\Delta}\delta}{2} V^{(2)}[\mathbf{z} \otimes V^{(3)}(\mathbf{l}_i)]^{(s)} \right),
\end{aligned}
\tag{17}
$$

where $\mathbf{z}$ is the unit vector of the local field direction, $O^{(s)} = O(\uparrow) - O(\downarrow)$, and the coefficients α, β, and γ are given in Table I. Here $\overline{\Delta} = \frac{\Delta}{\Gamma(X-1)}$, $X = [\Delta E_{IO} - \hbar\omega]/(\Gamma/2)$, $\epsilon = \delta + \overline{\Delta}$, and $\delta \ll 1$, but $\overline{\Delta}$ is not necessarily small.

Now F_{E1} is obtained by substituting $M_q^{(k)}$ from Eq. (17) into Eq. (15) and replacing R in Eq. (15) by $\overline{R}/(1 - \overline{\Delta}^2)$, where $\overline{R}$ is determined by the mean value of the radial matrix element and the mean value of the energy ΔE_{I0} in the resonance denominator [see Eq. (8)]. This is the form of F_{E1} applicable to the $p \rightarrow d$ resonances in the transition elements, rare earths, and actinides.

For the example of the Ho $2p_{\frac{3}{2}} \rightarrow 5d$ resonance, we have found that the dominant contribution to the linear magnetic term $M^{(1)}$ comes from the difference δ between the spin-up and spin-down radial matrix elements. Inclusion of this contribution, as given by Eq. (17), reverses the sign of $M_0^{(1)}$, and is necessary to obtain agreement with the experimental observations [12].

In summary, we have shown that the scattering amplitude operator F for resonant x-ray scattering can be expressed in terms of simple spin-orbital moment operators $M_{EL}^{(k)}(\mathbf{l}, \mathbf{s})$ of the valence shell involved in the resonance. This holds for the important case of quasielastic scattering in the fast collision approximation. The odd-order moments are purely magnetic, while the even-order moments include the charge multipole moments $\sum_{i \in l_2} Y_q^{(k)}(\hat{\mathbf{r}}_i)$ of the valence shell, as well as magnetic contributions. The simple relation between F and the spin-orbital moments $M^{(k)}(\mathbf{l}, \mathbf{s})$ is of considerable importance for the interpretation of resonant x-ray scattering experiments. Measurements on the Bragg peaks then will determine the thermal expectation values of these moments, while the diffuse scattering may be analyzed to obtain the moment-moment correlations.

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