

# Theory of polarized neutron scattering in the loop-ordered phase of cuprates

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(Received 27 March 2012; published 16 July 2012)

The collective modes observed in the loop-current ordered state in underdoped cuprates by polarized neutron scattering require that the ground state is a linear combination in each unit cell of the four basis states that are the possible classical magnetic moment configurations in each unit cell. The direction of such moments is in the  $c$  axis of the crystals. The basis states are connected by both time reversal as well as spatial rotations about the center of the unit cells. Several new features arise in the theory of polarized neutron scattering cross section in this situation that appear not to have been encountered before. An important consequence of these is that a finite component transverse to the classical magnetic moment directions is detected in the experiments. We show that this transverse component is of purely quantum-mechanical origin and that its direction in the plane normal to the  $c$  axis is not detectable, even in principle, in experiments, at least in the quantum-mechanical model we have adopted. We estimate the direction of the “tilt” in the moment, i.e., the ratio of the transverse component to the  $c$ -axis component, using parameters of the ground state obtained by fitting to the observed dispersion of the collective modes in the ordered state. We can obtain reasonable agreement with experiments but only by introducing a parameter for which only an approximate magnitude can be estimated. Approximate calculations of the form factors are also provided.

DOI: [10.1103/PhysRevB.86.035124](https://doi.org/10.1103/PhysRevB.86.035124)

PACS number(s): 74.72.-h

## I. INTRODUCTION

Polarized elastic neutron scattering experiments<sup>1,2</sup> and dichroic ARPES<sup>3</sup> have revealed that the pseudogap phase of the cuprates have a long-range magnetic order that breaks time-reversal symmetry without breaking translational symmetry of the lattice. It is a  $\mathbf{Q} = 0$  staggered order with zero net moment in each unit cell. Its geometric arrangement is consistent with the order of a pair of oppositely directed fluxes due to current loops formed in the O-Cu-O links in each unit cell.<sup>4</sup> Classically such an order has four possible domains as shown in Fig. 1. These domains are specified by the directions  $(\pm 1, \pm 1)$  that the order parameter  $\Omega$  makes with respect to the  $x$  and  $y$  axes of the crystal. The order parameter is an *anapole*<sup>5,6</sup> given by

$$\Omega = \int_{\text{cell}} d\mathbf{r} [\mathbf{L}(\mathbf{r}) \times \mathbf{r}], \quad (1)$$

where  $\mathbf{L}(\mathbf{r})$  is the magnetic moment in the unit cell at the point  $\mathbf{r}$ . Such an order, for any of the four possible domains, has orbital magnetic moments  $\mathbf{L}$  pointed in directions along or opposite the  $c$  axis of the crystals. However, polarization analysis of the neutron scattering<sup>1</sup> has shown that this is not true. The direction of the moments, interpreted according to the classic theory of polarized neutron scattering,<sup>7,8</sup> makes a large angle with respect to the  $c$  axis;<sup>9</sup> the direction along the plane is not revealed due to the multidomain nature of the crystals and/or the multidomain nature of the order *or* as we will show here due to its quantum-mechanical nature.

Polarized inelastic scattering was also discovered<sup>10,11</sup> two branches of weakly dispersive collective modes in the same temperature region as the magnetic order and with an intensity as a function of temperature compatible with it. Such collective modes can only be understood as quantum fluctuations of the observed order, just as is true for the one branch of collective modes in the transverse field Ising model.<sup>12</sup> In the paper preceding this,<sup>13</sup> hitherto referred to as I, we have introduced a quantum-mechanical model for the observed order and

calculated the simplest quantum-mechanical ground state of the model as well as the collective modes. The ground state is a product over the unit cells of a sum over the four classical configurations in each unit cell, depicted in Fig. 1 and given with a *particular choice of phases* by

$$|G\rangle = \prod_i \left[ \cos^2 \frac{\theta}{2} |1, 1\rangle_i + \cos \frac{\theta}{2} \sin \frac{\theta}{2} (|1, -1\rangle_i + |-1, 1\rangle_i) + \sin^2 \frac{\theta}{2} |-1, -1\rangle_i \right]. \quad (2)$$

$\theta$  is a parameter that has been determined by fitting the calculated collective mode dispersions to the experiments.  $|\pm 1, \pm 1\rangle_i$  refer to the four configurations in a unit cell  $i$ . As discussed in detail in I, and will be summarized below, one can make unitary transformations consistent with the symmetry of the problem, which introduce other operators in the Hamiltonian, and give a corresponding ground state wave function, which, in general, is a linear combination of the basis states with complex coefficients. We show in this paper that polarized neutron scattering from such a ground state requires a quantum-mechanical description of scattering of neutron of the quantum magnetic moments, whereas the traditional method considers the problem as a quantum-mechanical scattering of neutron from a classical magnetic field due to the ordered magnetic moments, and in some cases, their zero-point fluctuations, which only cause Debye-Waller-like corrections in amplitudes. (The general expressions for polarized neutron scattering in terms of the magnetic structure factor are still, of course, valid. The issue is the approximations in which the magnetic structure factor is calculated.) We show that in this situation, the observed “tilting” of the moments can be explained as a purely quantum phenomenon. One can only deduce by neutron scattering, or by any other experiment, the component of the magnetic moment along the  $c$  axis of the crystal and that perpendicular to it but not the two orthogonal

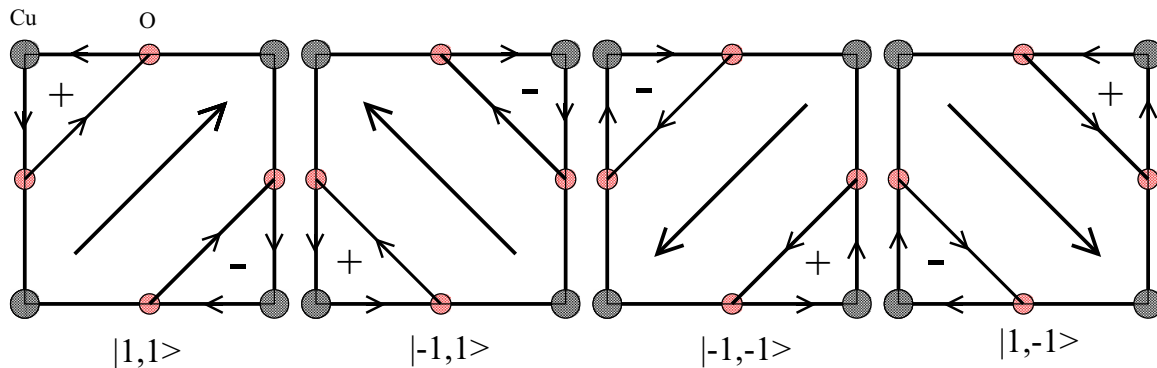


FIG. 1. (Color online) The four possible “classical” domains of the loop-ordered state are shown. In the classical ordered phase, one of these configurations is found in every unit cell. In the quantum case, each unit-cell has an admixture of these four configurations.

components of the latter. We compare various aspects of the experiment with our calculations. Aspects of the symmetry of the observations all appear to be well reproduced. The quantitative magnitude of the “tilt” and its variation with the Bragg vector can only be reproduced by introducing a free parameter, which can only be estimated approximately. We also discuss the other explanations for the tilt, which are correct in principle. We find that if they were a major contributor, there would introduce other features in neutron scattering which are ruled out by the experiments.

The basis states in Eq. (2) may be taken to be the eigenstates of the orbital magnetic moment operator  $\mathbf{L}_3$ , with the three-axis identified with the  $c$  axis of the crystal. An important aspect of the problem is to specify the kinetic energy term that mixes the four basis states in a cell  $i$  to give Eq. (2). This is important because there is obviously no orbital moment vectors pointing in the plane at the four locations indicated in the Fig. 1 because current flow only in the planes is assumed. We will show that an operator with the right commutation rules for an angular momentum exists in the problem but its physical basis is a fluctuating current loop between the four oxygen atoms around a Cu atom in each unit cell. Such an operator occurs naturally in the microscopic theory of loop currents in the cuprates<sup>16</sup> and leads among other things to the marginal Fermi liquid<sup>14,15</sup> in the normal state in the quantum-critical regime.

This paper is organized as follows. In the next section, we summarize the quantum Ashkin-Teller model introduced in I and cast it in the basis of local angular momentum operators, which are more useful to discuss neutron scattering. We will also review the transformation properties of these operators to show that, given the quantum Ashkin-Teller model, the direction of the tilt in the  $x$ - $y$  plane cannot be determined. In the following section, we discuss neutron scattering and its polarization dependence and show that besides the usual matrix element for polarized neutron scattering, there exists also another matrix element due to the finite extent of the current loops. In calculating the neutron scattering intensity, we first consider the moments as point objects at the four sites and subsequently improve the calculation by considering the finite extent of the current loops. This also allows us to estimate the form factors or the momentum dependence of the scattering at the Bragg vectors. In our conclusions, we discuss also alternate ways of obtaining the tilts and show that they are not consistent with the qualitative features of the experiments.

## II. LOOP-CURRENT MAGNETIC ORDER

In I, we have fully described the symmetries of the quantum Ashkin-Teller model with which the collective modes of the ordered loop current states are described and compared with experiments. To calculate neutron scattering, we will proceed in two steps. First, we will stay with the abstract representation given in I. To reproduce only the correct symmetry of the magnetic order, the orbital moments have been represented as point objects located in the centroid of the triangular loops of Fig. 1. The locations are labeled by  $\mathbf{R}_{i,a} = \mathbf{R}_i^0 + \mathbf{R}_a$ ,  $a = 1, \dots, 4$ . Here,  $i$  denote the lattice sites,  $\mathbf{R}_i^0$  is the position of the center of the unit cell and  $\mathbf{R}_a$  is the relative position of each local moments in the unit cell. We take  $\mathbf{R}_1 = (r_0, r_0)$ ,  $\mathbf{R}_2 = (-r_0, r_0)$ ,  $\mathbf{R}_3 = (-r_0, -r_0)$ , and  $\mathbf{R}_4 = (r_0, -r_0)$  with a value  $r_0$  smaller than  $1/2$  the lattice constant. The four loop current states are labeled by the eigenvalues of  $\sigma_z$  and  $\tau_z$  of the classical Ashkin-Teller (AT) model. At the classical level, for state  $|1,1\rangle$  there is a magnetic moment perpendicular to the copper oxygen plane pointing up located at  $\mathbf{R}_1$  and another pointing down at  $\mathbf{R}_3$ . Also there are zero moments at  $\mathbf{R}_2$  and  $\mathbf{R}_4$ . All the other three loop current states can be obtained by sequentially rotating  $|1,1\rangle$  by  $\pi/2$  and will be denoted by  $|-1,1\rangle$ ,  $|-1,-1\rangle$ , and  $|1,-1\rangle$ . This labeling is also consistent with the direction of the anapole vector  $\Omega$ . The four states  $(\pm 1, \pm 1)$  are, of course, globally orthogonal. We assume that this is also true of the four local states in any unit cell  $(\pm 1, \pm 1)_i$ , as also each of them between different cells. This is no different than, say, what is done with respect to the local moments formed from the collective degrees of freedom of fermions in itinerant antiferromagnets or ferromagnets for regions of frequency and momenta where their wavefunction do not overlap much the incoherent fermion excitations.

This is adequate to get the symmetries of the neutron scattering intensity for different momentum transfer  $\mathbf{Q}$  and different measured initial and final neutron polarizations. But it is not adequate to give the form factor and relative intensities at different  $\mathbf{Q}$  and polarizations. Calculating such information is a very formidable task. In a second step, we will, however, attempt this in an approximate way by introduce the wave functions responsible for generating the orbital moments as well as the representation of the kinetic energy in terms of current operators. Besides quantitative verisimilitude, this affords some insight into the interesting new physics in the kinetic energy terms.

The Hamiltonian derived in I to calculate the collective modes was written in the space basis of the states  $(\pm 1, \pm 1)$ , and equivalently in the direct product basis with four-dimensional vectors. The transformation from one to the other is

$$|1, 1\rangle_i \equiv |1000\rangle_i, \quad |1, -1\rangle \equiv |0100\rangle_i, \quad \text{etc.} \quad (3)$$

The classical Ashkin-Teller model in this basis is given by

$$H_{\text{AT}} = - \sum_{(i,j)} (J_1 S_i^3 S_j^3 + J_2 T_i^3 T_j^3 + J_4 K_i^{33} K_j^{33}). \quad (4)$$

The quantum terms causing a transition between the four states, which are rotated with respect to each other in the direction of  $\Omega$  by  $\pm\pi/2$ , are given in the same choice of gauge as Eq. (2) by

$$H_Q = \sum_i t(S^1 + T^1) + t'K^{11}, \quad (5)$$

where  $S^i$ ,  $T^i$ , and  $K^{ii}$  are matrices in SU(4) space, specified in I, where their commutation rules are also given. The Hamiltonian  $H_{\text{AT}} + H_Q$  was used to derive the collective modes in I and to get the ground-state wave function (2). The terms  $K_i^{11}$  which causes rotation by  $\pm\pi$ , are unimportant for our purposes here because they cause change in angular momentum by two and therefore do not couple to neutrons, which can change angular momentum only by one in the weak scattering limit.

For calculating neutron scattering, it is more convenient to define a basis set given in terms of the orbital moment operators at the four locations in a cell. Since the local moments are generated by orbital loop current they should be considered in the representation for spin 1. The three components of the effective moment will be denoted by  $\mathbf{L} = (L^1, L^2, L^3)$ . Normally, one would represent  $\mathbf{L}$  by the spin-1 representation of SU(2), i.e., by a three-dimensional representation, with eigenvalues say of  $\pm 1, 0$ . But we have four states per unit cell in the loop current model. As explained in Appendix B, the three-dimensional representation is inadequate to the present case and a four-dimensional representation of the spin-1 states must be used. This representation is given by

$$L^1 = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \quad L^2 = \frac{1}{2} \begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}, \quad (6)$$

$$L^3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

This representation is equivalent to a representation in the basis of two independent set of spin-1/2 operators. This is quite natural to use for the quantum Ashkin-Teller model. We will verify that they satisfy the SU(2) algebra  $[L^i, L^j] = i\epsilon^{ijk}L^k$ . This is a reducible representation with two (orthogonal)  $L_3 = 0$  states that we denote as  $|0^1\rangle$  and  $|0^2\rangle$ . The loop current basis states in each unit cell in this representation have the following

bases in each unit cell:

$$|1, 1\rangle = (|1\rangle_{\mathbf{R}_1}, |0^1\rangle_{\mathbf{R}_2}, |-1\rangle_{\mathbf{R}_3}, -|0^2\rangle_{\mathbf{R}_4}), \quad (7)$$

$$|-1, 1\rangle = (|0^1\rangle_{\mathbf{R}_1}, |-1\rangle_{\mathbf{R}_2}, -|0^2\rangle_{\mathbf{R}_3}, |1\rangle_{\mathbf{R}_4}), \quad (8)$$

$$|-1, -1\rangle = (|-1\rangle_{\mathbf{R}_1}, |0^2\rangle_{\mathbf{R}_2}, |1\rangle_{\mathbf{R}_3}, -|0^1\rangle_{\mathbf{R}_4}), \quad (9)$$

$$|1, -1\rangle = (|0^2\rangle_{\mathbf{R}_1}, |1\rangle_{\mathbf{R}_2}, -|0^1\rangle_{\mathbf{R}_3}, |-1\rangle_{\mathbf{R}_4}). \quad (10)$$

Here,  $|i\rangle_{\mathbf{R}_j}$  stands for the eigenvector of  $L_3$  with eigenvalue  $i = \pm 1$  or 0 at location  $j = 1, \dots, 4$  in a unit cell. The phase factors  $\pm 1$  in front of the states  $|0\rangle_{\mathbf{R}_j}$  are picked so that the states in the left of Eq. (7) have zero net moment in a cell.

While, since it has a classical analog, it is perfectly clear what  $L_{i,s}^3$  physically means, the same cannot be said of  $L_{i,s}^1$  and  $L_{i,s}^2$ . Obviously, these are not proportional to angular momentum operators at the sites  $(i,s)$ , since the currents are required to flow only in the plane. We shall show that there exist operators that have off-diagonal matrix elements in the basis  $(\pm 1, \pm 1)$ , so that using Eq. (7), we shall find (in general complex) matrix elements between the eigenstates with eigenvalues  $\pm 1$  and 0 of the operator  $L_{i,s}^3$ . We shall define  $L_{i,s}^1$  and  $L_{i,s}^2$  through such matrix elements.

#### A. Allowed unitary transformations on the quantum Ashkin-Teller model

The unitary transformations described in I are equivalent to rotations in  $L$  space, as we will explicitly show below. Apart from the crystalline  $z$  axis that defines the direction of the moments of the classical problem there is nothing in the Hamiltonian derived in I for the problem which involves the crystalline  $x$  and  $y$  axis (except that they be orthogonal to the  $z$  axis). Therefore the direction 3 of  $L^3$  may be identified as the  $z$  axis leaving the choice of the 1 and 2 axis with respect to the  $x$  and  $y$  crystalline-axes undetermined. This situation is similar to the traverse field Ising model in which the transverse field is self-generated. One can then choose it to be in any direction normal to the Ising axis with identical experimental results. (Only if the transverse field is an externally applied field, can one find in experiments that the direction of the moments is tilted from the Ising axis towards the external field axis.)

We have shown in I that the classical Ashkin-Teller model has a continuous symmetry  $U(1)_{S^3} \times U(1)_{T^3} \times U(1)_{K^{33}}$ , which is the rotation around operators  $S^3$ ,  $T^3$ , and  $K^{33}$ . The rotation matrix is given by

$$U(\theta) = e^{i\theta_1 S^3/2} e^{i\theta_2 T^3/2} e^{i\theta_3 K^{33}/2}. \quad (11)$$

The classical AT model is invariant under this transformation. It has been shown that the quantum terms introduced depend on the transformation  $U$ . At the same time, this transformation changes the wave functions. For a general wave function  $|\psi\rangle = a|1, 1\rangle + b|1, -1\rangle + c|-1, 1\rangle + d|-1, -1\rangle$  with four complex coefficients  $a, b, c$ , and  $d$ , we have

$$|U\psi\rangle = ae^{i\phi_1}|1, 1\rangle + be^{i\phi_2}|1, -1\rangle + ce^{i\phi_3}|-1, 1\rangle + de^{i\phi_4}|-1, -1\rangle \quad (12)$$

with  $\phi_1 = \frac{\theta_1 + \theta_2 + \theta_3}{2}$ ,  $\phi_2 = \frac{\theta_1 - \theta_2 - \theta_3}{2}$ ,  $\phi_3 = \frac{-\theta_1 + \theta_2 - \theta_3}{2}$ , and  $\phi_4 = \frac{-\theta_1 - \theta_2 + \theta_3}{2}$ . Thus  $U$  puts different phase factors on each of the

four classical states with the sum of all phase factors restricted to zero.

One should note the special case  $\theta_1 = \theta_2 = 0$ , when this unitary transformation is simply a rotation of  $\mathbf{S}$  and equivalently of  $\mathbf{L}$  in the  $x$ - $y$  plane:

$$UL^1U^\dagger = \cos \theta_3 L^1 - \sin \theta_3 L^2, \quad (13)$$

$$UL^2U^\dagger = \sin \theta_3 L^1 + \cos \theta_3 L^2. \quad (14)$$

So, given the quantum Ashkin-Teller model, the direction of the moments perpendicular to the  $z$  axis is undeterminable.

We now show more generally that  $\mathbf{L}_i$  have the properties of angular momentum operators. As already discussed in Ref. 13, by making use of Eq. (7), etc., one can express the local spin operator  $\mathbf{L}$  in terms of the Ashkin-Teller model operators of  $S^i, T^i$  (defined in Ref. 13) as follows:

$$\begin{aligned} L_{\mathbf{R}_1}^x &= L_{\mathbf{R}_2}^x = \frac{1}{2}(S^1 + T^1), & L_{\mathbf{R}_3}^x &= L_{\mathbf{R}_4}^x = -\frac{1}{2}(S^1 + T^1), \\ L_{\mathbf{R}_1}^y &= L_{\mathbf{R}_3}^y = \frac{1}{2}(S^2 + T^2), & L_{\mathbf{R}_2}^y &= L_{\mathbf{R}_4}^y = \frac{1}{2}(S^2 - T^2), \\ L_{\mathbf{R}_1}^z &= -L_{\mathbf{R}_3}^z = \frac{1}{2}(S^3 + T^3), & L_{\mathbf{R}_2}^z &= -L_{\mathbf{R}_4}^z = \frac{1}{2}(S^3 - T^3). \end{aligned}$$

Using the commutation relations given for  $S^i$  and  $T^i$  in I, it is easy to verify that the  $\mathbf{L}$  satisfy the SU(2) algebra (up to an overall minus sign). Therefore  $\mathbf{L}$  can be regard as an angular momentum operators.

### III. POLARIZED NEUTRON SCATTERING

The neutron scattering Hamiltonian is

$$H_{\text{int}} = \int d\mathbf{r} \mathbf{B}(\mathbf{r}) \cdot \sigma(\mathbf{r}). \quad (15)$$

$\sigma(\mathbf{r})$  is the spin of the neutron at point  $(\mathbf{r})$  in the crystal where the magnetic field *operator* is  $\mathbf{B}(\mathbf{r})$ . The source of the magnetic field are the magnetic moment *operators* due to spin or in our case orbital moments  $\mathbf{L}(\mathbf{R}_i^0 + \mathbf{R}_a)$  at locations  $(\mathbf{R}_i^0 + \mathbf{R}_a)$ . One can Fourier transform Eq. (15) and rewrite it in terms of the magnetic moments  $\mathbf{L}$  at the momentum transfer  $\mathbf{Q}$  as<sup>7,8</sup>

$$\sum_a e^{i\mathbf{Q}\cdot\mathbf{R}_a} F_a(\mathbf{Q}) \mathbf{L}_{a,\perp}(\mathbf{Q}) \cdot \sigma(\mathbf{Q}). \quad (16)$$

Here,  $\mathbf{L}_{a,\perp}(\mathbf{Q}) = \mathbf{L}_a - (\mathbf{L}_a \cdot \hat{\mathbf{Q}})\hat{\mathbf{Q}}$  is the component of  $\mathbf{L}_a$  perpendicular to  $\hat{\mathbf{Q}}$  and  $F_a(\mathbf{Q})$  is the form factor.

It is important to discuss how the directions of the Pauli matrices  $\sigma$  are fixed in the usual situation in which the directions of  $\mathbf{L}$  are known with respect to the crystalline axes and the difference in the present case. The quantization axis of the neutron spin is fixed externally to the sample by applying a (small) magnetic field in a specific direction, with respect, say to the momentum transfer direction  $\hat{\mathbf{Q}}$  of the neutron. This fixes  $\sigma_3$  with respect to the crystalline axes and the experiment is done with various choices of direction  $i = 3$  with respect to  $\hat{\mathbf{Q}}$ . The other directions 1 and 2 are then fixed through knowing the direction of  $\mathbf{L}$  with respect to the crystalline directions and the use of the dot product in Eq. (15). In effect,  $\mathbf{B}$  can be treated classically in such situations.

This is to be contrasted with the present situation in which the basis vectors of the ground state  $(\pm 1, \pm 1)$  specify only

the direction of the orbital moment, up or down (or zero) as being along the normal to the Cu-O planes denoted here by the  $z$  axis. Taking matrix elements of  $\mathbf{B}$  in the ground state (2) leads to off-diagonal terms in these basis vectors. As noted this cannot be specified as a magnetic field operator generated by magnetic moments in specific directions with respect to the crystalline axes; all that can be said is that the off-diagonal matrix elements are matrix elements of a magnetization operator orthogonal to the direction  $\hat{\mathbf{z}}$  with which the basis vector are specified. A purely real ground-state wave function means that only matrix elements of  $S^1$  and  $T^1$  generate the off-diagonal elements and so only  $\mathbf{L}_\perp^1(\mathbf{Q})$  enters in Eq. (16). Correspondingly, only  $\sigma_1$  appears in Eq. (16). There is no way to fix 1 with respect to the crystalline axes. If, however, one used a more general choice of the wave function so that it is complex,  $\mathbf{L}_\perp(\mathbf{Q})$  are determined by matrix elements of  $S^1, T^1$  as well as  $S^2, T^2$  and, correspondingly,  $\sigma_2$  enters in the calculation. The final answer for the spin-flip cross sections of the neutrons cannot (and does not) depend on the choice of the wave function, nor can the directions 1 and 2 be determined with respect to the crystalline axes.

The difference in our case from the traditional case arises from the fact that  $\mathbf{L}$  does not come physically from an atomic orbital moment where the three different components of the orbital angular momentum can be defined with respect to the crystalline axes. Rather, in our case, only the  $z$  component is defined in the basis; the mixing in the ground state of the basis is due to a transverse field operator as discussed above. The physical basis for the transverse field will be specified below.

Our purpose is to interpret experiments that deduce everything from measuring (functions of) the matrix elements of  $\sigma(\mathbf{Q})$  through three different choices of the quantization axis 3 with respect to the  $\mathbf{Q}$ . From Eq. (16), it follows that when the polarization of the neutron, i.e., the direction 3 of  $\sigma$  is chosen parallel to  $\mathbf{Q}$ , there is only spin-flip scattering, while for any other choice there is both spin-flip and spin-non-flip scattering. We have identified  $L^3$  as proportional to  $L_z$ . As explained, we have a freedom of choice of rotating the 1 and 2 directions of the neutron  $\sigma$  by any arbitrary angle about its chosen axis 3. It thus follows that for any choice of  $\mathbf{Q}$  and the neutron polarization, one can never determine  $\mathbf{L}_x$  and  $\mathbf{L}_y$ . One can only determine  $\mathbf{L}_z$  and the component of  $\mathbf{L}$  perpendicular to it, which we will call  $\mathbf{L}_\perp$ . Having shown this, we can do the calculation in the simplest choice in which the wave function is real and only the operators  $S^1, T^1$ , and  $K^{33}$  appear in the Hamiltonian.

The situation may be contrasted with the case when the direction of order of the system is fixed by, for example, crystalline anisotropy as in the anisotropic Heisenberg model. The order parameter  $\langle \mathbf{M} \rangle$  is then fixed with respect to the crystalline axes and may be regarded as a classical source for a classical  $\mathbf{B}(\mathbf{r})$  in Eq. (17). The magnitudes of two of the components of  $\langle \mathbf{M}_x, \mathbf{M}_y, \mathbf{M}_z \rangle$  can then be determined by measuring the neutron scattering cross-sections by polarizing the neutron beam in two different directions with respect to a momentum transfer  $\mathbf{Q}$  and using Eq. (16). One can then change  $\mathbf{Q}$  and repeat the measurement to determine all the three directions of  $\langle \mathbf{M} \rangle$  for simple magnetic order (or measure at other  $\mathbf{Q}$  for more complex order.) If one has an Ising model in a external transverse field, the direction of  $\mathbf{M}$  is similarly fixed.

The problem discussed above is different also from problems of scattering neutrons in the quantum Heisenberg antiferromagnets, where the kinetic energy terms in the Hamiltonian are quadratic operators in the spins, as opposed to the present case where they are linear. In such cases, quantum mechanics only induces a reduction in the ordered spin moment without changing its orientation through a Debye-Waller factor due to zero-point spin fluctuations while transferring weight to an incoherent background.

#### IV. MATRIX ELEMENTS FOR NEUTRON SCATTERING

We shall show here that there are two kinds of matrix elements in scattering of neutrons due to the linear combination in the ground state (2). This can be seen most clearly from the rotational and time-reversal properties of the basis states written in the form of Eq. (6). The basis states are connected through what we might call the time-reversal part of the dipole Hamiltonian, which involve  $L^+\sigma^- + L^-\sigma^+$ . This is the usual scattering. But as already mentioned, the basis states also go to each other under successive  $\pi/2$  and  $\pi$  rotations in real space through the axis normal to the plane at the center of a cell. We show here that the dipole interaction (17) has a finite projection to such rotation operators also. We will call these matrix elements of the “rotational” kind. The matrix elements from a given initial and a given final basis states for both kinds must be summed and then squared to get the scattering cross section.

Since the local loop current is actually an extended object, the neighboring loop currents although orthogonal have a finite matrix element through the spatial dependence of the dipole interactions Hamiltonian:

$$H_{\text{int}}(\mathbf{R}) = \frac{\boldsymbol{\sigma} \cdot \mathbf{L} - 3(\boldsymbol{\sigma} \cdot (\widehat{\mathbf{r}} - \widehat{\mathbf{R}}))(\mathbf{L} \cdot (\widehat{\mathbf{r}} - \widehat{\mathbf{R}}))}{|\mathbf{r} - \mathbf{R}|^3} \\ = -\boldsymbol{\sigma} \cdot \nabla_{\mathbf{r}} \times \left[ \mathbf{L} \times \nabla_{\mathbf{r}} \frac{1}{|\mathbf{r} - \mathbf{R}|} \right]. \quad (17)$$

Here,  $(\widehat{\mathbf{r}} - \widehat{\mathbf{R}})$  is the unit vector along  $(\mathbf{r} - \mathbf{R})$ .  $\mathbf{r}$  and  $\mathbf{R}$  are the position vector of neutrons and local moments, respectively.

Let  $|\psi_a\rangle$  denote one of the four loop current state  $|\pm 1, \pm 1\rangle$  and  $|\psi_a, \mathbf{R}_i\rangle$  denote the local moment state of  $\psi_a$  located at  $\mathbf{R}_i$ . This local moment state can be written as the direct product of the coordinate part and a “moment” part as  $|\psi_a, \mathbf{R}_i\rangle = |\phi(\mathbf{R} - \mathbf{R}_i)\rangle |\psi_a, \mathbf{R}_i\rangle_s$ . Here, the moment part  $|\psi_a, \mathbf{R}_i\rangle_s$  are the four possible states  $|\pm 1\rangle$  and  $|0^{1,2}\rangle$ . The coordinate part  $\phi(\mathbf{R} - \mathbf{R}_i)$  describes the spatial wave-function of the magnetic moment centering around  $\mathbf{R}_i$ . For orbital moments,  $\phi$  may be taken to be the real part of the wave function, while  $\psi$  may be taken to be a phase varying around the loop for the loop currents. For  $\phi(\mathbf{R} - \mathbf{R}_i) = \delta(\mathbf{R} - \mathbf{R}_i)$ , there are only the usual matrix elements of the dipole interaction between the basis states of Eq. (2) because

$$\int d^3 R \phi(\mathbf{R} - \mathbf{R}_i) H_{\text{int}}(\mathbf{R}) \phi(\mathbf{R} - \mathbf{R}_j) \\ = \int d^3 R \delta(\mathbf{R} - \mathbf{R}_i) H_{\text{int}}(\mathbf{R}) \delta(\mathbf{R} - \mathbf{R}_j) \propto \delta_{ij}. \quad (18)$$

We will call the matrix elements of the dipole interactions for  $(i = j)$  the matrix elements of the “spin” kind.

But for finite size  $\phi$ 's, the above matrix element is, in general, not zero. The detailed form of this function  $\phi(\mathbf{R})$  is not very important to us. Here, we also assume that the distribution function satisfies the orthogonal relations as  $\int d^3 R \phi(\mathbf{R} - \mathbf{R}_i) \phi(\mathbf{R} - \mathbf{R}_j) = \delta_{ij}$ .

Then such matrix element are

$$\langle \psi_a, \mathbf{R}_i | H_{\text{int}}(\mathbf{R}) | \psi_b, \mathbf{R}_j \rangle \\ = - \int d^3 R \phi(\mathbf{R} - \mathbf{R}_i) \boldsymbol{\sigma} \cdot \mathbf{B} \phi(\mathbf{R} - \mathbf{R}_j), \\ \mathbf{B} = \nabla_{\mathbf{r}} \times \left[ \mathbf{L}_{ij} \times \nabla_{\mathbf{r}} \frac{1}{|\mathbf{r} - \mathbf{R}|} \right].$$

Here,  $\mathbf{L}_{ij} = \langle \psi_a, \mathbf{R}_i | \mathbf{L} | \psi_b, \mathbf{R}_j \rangle_s$ . We will call them matrix elements of the “rotational kind.”

##### A. Matrix element of the “spin” kind

The ground-state expectations of  $\mathbf{L}_i$  using Eq. (7) are

$$\langle \mathbf{L}_i(\mathbf{R}_1) \rangle = (\sin \theta, \cos \theta), \quad (19)$$

$$\langle \mathbf{L}_i(\mathbf{R}_2) \rangle = (\sin \theta, 0), \quad (20)$$

$$\langle \mathbf{L}_i(\mathbf{R}_3) \rangle = (-\sin \theta, -\cos \theta), \quad (21)$$

$$\langle \mathbf{L}_i(\mathbf{R}_4) \rangle = (-\sin \theta, 0), \quad (22)$$

where now the two components refer to the “directions”  $\hat{t}$  and  $\hat{z}$ , respectively.

The calculation in Eq. (19) is only for one unit cell. The magnetization in the lattice just repeats the same result in each unit cell,

$$\mathbf{L}(\mathbf{Q}) = \sum_{\mathbf{R}_{ia}} \mathbf{L}(\mathbf{R}_{ia}) e^{-i\mathbf{Q} \cdot \mathbf{R}_{ia}},$$

and the magnetization is given by

$$L_t(\mathbf{Q}) = \sum_n \sin \theta (e^{-i\mathbf{Q} \cdot \mathbf{R}_1} + e^{-i\mathbf{Q} \cdot \mathbf{R}_2} - e^{-i\mathbf{Q} \cdot \mathbf{R}_3} - e^{-i\mathbf{Q} \cdot \mathbf{R}_4}) \\ \times \delta(\mathbf{Q} - \boldsymbol{\tau}_n), \quad (23)$$

$$L_z(\mathbf{Q}) = \sum_n \cos \theta (e^{-i\mathbf{Q} \cdot \mathbf{R}_1} - e^{-i\mathbf{Q} \cdot \mathbf{R}_3}) \delta(\mathbf{Q} - \boldsymbol{\tau}_n). \quad (24)$$

Here,  $\boldsymbol{\tau}_n$  is the reciprocal lattice vector of the lattice. Suppose the unit vector of transfer momentum is  $\hat{\mathbf{q}}$ , then the scattering intensity is

$$I(\mathbf{Q}) \propto |\langle \mathbf{L}_{\perp}(\mathbf{Q}) \rangle|^2. \quad (25)$$

Since we treat the orbital current loop as a pointlike spin, the scattering amplitude is a constant as a function of  $\mathbf{Q}$ . So, this calculation is not designed to give the structure factor correctly.

Suppose this is the only contribution to scattering. Then at any  $\mathbf{Q} = (a^*, 0, 0)$ , barring multiple Cu-O layers per unit cell (which we will have to consider for  $\text{YBa}_2\text{Cu}_2\text{O}_{6+\delta}$ ) the tilt angle would be determined by

$$\frac{|L_t|}{|L_z|} \approx \frac{2 \sin \theta \cdot 2 \sin(Qr_0)}{\cos \theta \cdot 2 \sin(Qr_0)}.$$

For the fitted parameters from calculation of the collective modes in I, we have  $\sin \theta = -0.26$ , so the tilt angle is only about  $28^\circ$ .

### B. Matrix elements of ‘rotational’ kind

We now consider the second kind of scattering starting from Eq. (19). We can make use of the fact  $\frac{1}{r} = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi}{q^2}$  to transform the above result to momentum space:

$$\langle \psi_a, \mathbf{R}_i | H_{\text{int}}(\mathbf{R}_1) | \psi_b, \mathbf{R}_j \rangle = \boldsymbol{\sigma} \cdot \int d^3Q e^{i\mathbf{Q}\cdot\mathbf{r}} \hat{\mathbf{Q}} \times (\mathbf{L}_{ij} \times \hat{\mathbf{Q}}) S^{ij}(\mathbf{Q}) \quad (26)$$

$$\text{with } S_{ij}(\mathbf{Q}) = \int d^3R \phi(\mathbf{R} - \mathbf{R}_i) \phi(\mathbf{R} - \mathbf{R}_j) e^{-i\mathbf{Q}\cdot\mathbf{R}}.$$

Now we can expand the exponential factor and the leading nonzero term is

$$S_{ij}(\mathbf{q}) \approx -i \int d^3R \phi(\mathbf{R} - \mathbf{R}_i) \phi(\mathbf{R} - \mathbf{R}_j) (\mathbf{Q} \cdot \mathbf{R}). \quad (27)$$

To be specific, we consider  $S_{12}(\mathbf{q})$  first. For simplicity, we assume that the distribution is isotropic  $\phi(\mathbf{R}) = \phi(|\mathbf{R}|)$ . Since  $\mathbf{R}_1 = (r_0, r_0)$  and  $\mathbf{R}_2 = (-r_0, r_0)$ , then it is easy to see that  $\phi(|\mathbf{R} - \mathbf{R}_1|) \phi(|\mathbf{R} - \mathbf{R}_2|)$  is even function about  $R_x$  and  $R_z$ . Thus we have

$$S_{12}(\mathbf{Q}) \approx -iq_y \int d^3R \phi(\mathbf{R} - \mathbf{R}_1) \phi(\mathbf{R} - \mathbf{R}_2) R_y = -iQ_y C, \quad (28)$$

$$S_{23}(\mathbf{Q}) \approx -iq_x \int d^3R \phi(\mathbf{R} - \mathbf{R}_2) \phi(\mathbf{R} - \mathbf{R}_3) R_x = iQ_x C, \quad (29)$$

$$S_{34}(\mathbf{Q}) \approx -iq_x \int d^3R \phi(\mathbf{R} - \mathbf{R}_3) \phi(\mathbf{R} - \mathbf{R}_4) R_y = iQ_y C, \quad (30)$$

$$S_{41}(\mathbf{Q}) \approx -iq_x \int d^3R \phi(\mathbf{R} - \mathbf{R}_4) \phi(\mathbf{R} - \mathbf{R}_1) R_x = -iQ_x C, \quad (31)$$

where  $C = \int d^3R \phi(|\mathbf{R} - \mathbf{R}_1|) \phi(|\mathbf{R} - \mathbf{R}_2|) R_y$ . We see that  $C$  is of  $O(r_0)$ . We will find the coefficient only by fitting to the data.

Note that this new term is also proportional to  $\mathbf{L}_\perp(\mathbf{Q})$ , just as the traditional matrix elements for polarized neutron scattering. But the momentum dependence is different from the classical neutron diffraction expression. We can repeat this calculation at all possible neighboring local moments and find similar expressions. Recall that the four states are collections of four local spin-1 states. The ground state is superposition of the four states, thus it is also a collections of four local spin-1 states. To compute the total neutron scattering amplitude, we need to evaluate the matrix elements of  $\mathbf{L}$  between all the neighboring local spin-1 states of the ground state. The four local spin-1 states of the ground state is given by (here we only write the spin part)

$$\begin{aligned} |G, \mathbf{R}_1\rangle_s &= c^2|1\rangle + sc|0^1\rangle + sc|0^2\rangle + s^2|-1\rangle, \\ |G, \mathbf{R}_2\rangle_s &= sc|1\rangle + c^2|0^1\rangle + s^2|0^2\rangle + sc|-1\rangle, \\ |G, \mathbf{R}_3\rangle_s &= s^2|1\rangle - sc|0^1\rangle - sc|0^2\rangle + c^2|-1\rangle, \\ |G, \mathbf{R}_4\rangle_s &= sc|1\rangle - s^2|0^1\rangle - c^2|0^2\rangle + sc|-1\rangle. \end{aligned}$$

Here,  $c = \cos\theta$  and  $s = \sin\theta$ . Then it is straightforward to find the following matrix elements for  $\mathbf{L}$ :

$$\begin{aligned} \langle G, \mathbf{R}_1 | \mathbf{L} | G, \mathbf{R}_2 \rangle_s &= \left[ \frac{(1 + \sin^2\theta)}{4}, -\frac{i}{2} \cos\theta, \frac{\sin(2\theta)}{4} \right], \\ \langle G, \mathbf{R}_2 | \mathbf{L} | G, \mathbf{R}_3 \rangle_s &= \left[ \frac{1}{2} \cos^2\theta, -\frac{i}{2} \cos\theta, -\frac{1}{4} \sin(2\theta) \right], \\ \langle G, \mathbf{R}_3 | \mathbf{L} | G, \mathbf{R}_4 \rangle_s &= -\left[ \frac{(1 + \sin^2\theta)}{4}, \frac{i}{2} \cos\theta, \frac{\sin(2\theta)}{4} \right], \\ \langle G, \mathbf{R}_4 | \mathbf{L} | G, \mathbf{R}_1 \rangle_s &= \left[ -\frac{1}{2} \cos^2\theta, -\frac{i}{2} \cos\theta, \frac{1}{4} \sin(2\theta) \right]. \end{aligned}$$

Other matrix elements are the complex conjugate of the above equations. If we put all the terms together, one can see that the imaginary part cancel out and only the real part contributes. We find the scattering amplitude in the momentum space as

$$\langle G | H_{\text{int}}(\mathbf{R}) | G \rangle = 2 \sum_{(ij)} \boldsymbol{\sigma} \cdot \hat{\mathbf{Q}} \times (\mathbf{L}_{ij} \times \hat{\mathbf{Q}}) S_{ij}(\mathbf{Q}) \quad (32)$$

with index pair  $(i, j) = (1, 2), (2, 3), (3, 4), (4, 1)$  and  $\mathbf{L}_{ij} = \text{Re}\langle G, \mathbf{R}_i | \mathbf{L} | G, \mathbf{R}_j \rangle_s$ . Putting all the above results together, we find

$$\begin{aligned} \langle G | H_{\text{int}}(\mathbf{R}) | G \rangle &= -4iQ_y C \boldsymbol{\sigma} \cdot \hat{\mathbf{Q}} \times (\mathbf{L}_{12} \times \hat{\mathbf{Q}}) \\ &\quad - 4iQ_x C \boldsymbol{\sigma} \cdot \hat{\mathbf{Q}} \times (\mathbf{L}_{41} \times \hat{\mathbf{Q}}). \end{aligned} \quad (33)$$

Again, we can consider the transfer momentum  $\mathbf{Q} = (a^*, 0, 0)$ . The scattering amplitude is

$$\langle G | H_{\text{int}}(\mathbf{R}) | G \rangle = -4iQ_x C \boldsymbol{\sigma} \cdot \hat{\mathbf{Q}} \times (\mathbf{L}_{41} \times \hat{\mathbf{Q}}), \quad (34)$$

which can be rewritten as

$$\langle G | H_{\text{int}}(\mathbf{R}) | G \rangle = \boldsymbol{\sigma} \cdot \hat{\mathbf{Q}} \times [\mathbf{L}_{\text{eff}} \times \hat{\mathbf{Q}}], \quad (35)$$

$$\mathbf{L}_{\text{eff}} = 4iQ_x C \left[ \frac{1}{2} \cos^2\theta, -\frac{1}{4} \sin(2\theta) \right]. \quad (36)$$

### C. Total matrix element

The form in Eq. (35), has the same structure as the matrix element of the ‘spin kind’ Eq. (25). We can combine them together to find the total magnetization as

$$\mathbf{L}_{\text{tot}} = \mathbf{L}_0 + \mathbf{L}_{\text{eff}}, \quad \mathbf{L}_0 = 2i \sin(Q_x r_0) (2 \sin\theta, \cos\theta), \quad (37)$$

$$\mathbf{L}_{\text{eff}} = 4iQ_x C \left[ \frac{1}{2} \cos^2\theta, -\frac{1}{4} \sin(2\theta) \right],$$

where the two components again refer to  $t$  and  $z$ , respectively. Here,  $\mathbf{L}_0$  is the magnetization form the ‘spin-type’ contribution.

The parameter  $r_0$  specifies the location of the moments. For the ground state determined from the collective modes, we have  $\sin\theta = -0.26$ . If we assume that  $Q_x C \approx -0.5 \sin(Q_x r_0)$ , then we find that for transfer momentum  $\mathbf{Q} = (a^*, 0, 0)$ , the tilted angle is about  $50^\circ$ . The experimental results are  $55 \pm 7^\circ$  and  $35 \pm 7^\circ$ , respectively,<sup>1</sup> for YBaCuO<sub>6.6</sub>. But most of the data available for the collective modes from which the angle  $\theta$  is deduced is in Hg1201 with a  $T_c \approx 61$  K, which from the general phenomenology has properties close to those in YBaCuO<sub>6.6</sub>. Collective modes have also been found in YBaCuO<sub>6.6</sub><sup>11</sup> at similar frequencies but detailed information about the dispersion of the two branches of collective modes is unavailable. The tilt in Hg1201 at  $(1, 0, 1)$  is deduced to be<sup>9</sup>

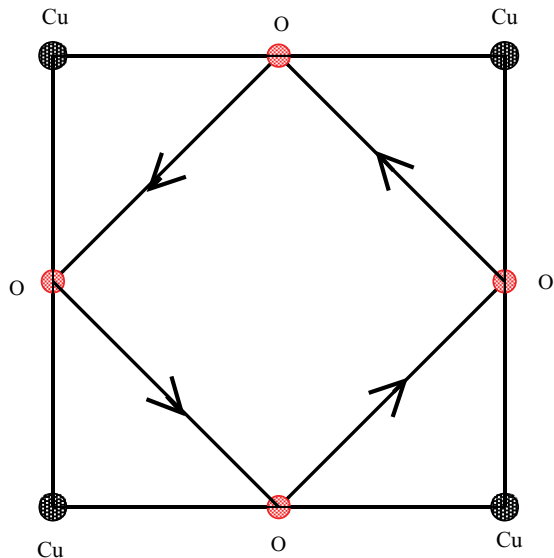


FIG. 2. (Color online) Current pattern of the rotation operator in Eq. (38).

$45 \pm 20$  within the estimates provided here. We can claim that with  $C = O(r_0)$ , we get the correct trend and the magnitudes of the tilt in agreement with experiment within the stated error bars. It should be stated that a simplified model is used to calculate the collective modes and the ground state from which  $\theta$  is determined. It could easily be  $\pm 10^\circ$  from that deduced.

## V. CALCULATION INCLUDING FORM FACTORS

### A. Real-space representation of the operators ( $S^1 + T^1 + S^2 + T^2$ )

To calculate the neutron scattering including form factors, one needs the wave function that have the orbital moments and the microscopic representation of the operators which lead to the produce the admixed ground-state wave function (2). The approximate space representation of the basis states is relatively straight forward. One may represent them with complex wave functions carrying currents around the indicated loops as in Fig. 1. The subtle issue is in the representation of the operators ( $S_i^1 + T_i^1$ ), which give the linear combination of the classical basis states in the ground state in Eq. (2). They were introduced at a formal level in I simply because such terms are allowed and because they are necessary to calculate the observed collective modes in the loop ordered state. But what is the physical origin of such quantum terms? The physical origin was already derived in connection with calculating the spectra of the collective fluctuations in the quantum-critical regime of the loop ordered phase.<sup>16</sup> A simpler derivation is given in Appendix A. The operator  $S_i^1 + T_i^1$  is given by the current operator schematically shown in Fig. 2 and its Hermitian conjugate that has a current flowing in the opposite direction. In the continuum limit, this is simply the operator proportional to  $\sum_{\text{cells}} \nabla \times \mathbf{j}(\mathbf{r})$ , with  $\mathbf{r}$  measured from the center of each unit cell and with a cutoff at the boundary. We recall from I that the operator ( $S_i^1 + T_i^1$ ) acting on any of the four states ( $\pm 1, \pm 1$ ) in a unit cell admixes the state rotated by  $\pm \pi/2$  to it. This operator corresponds to the collective part

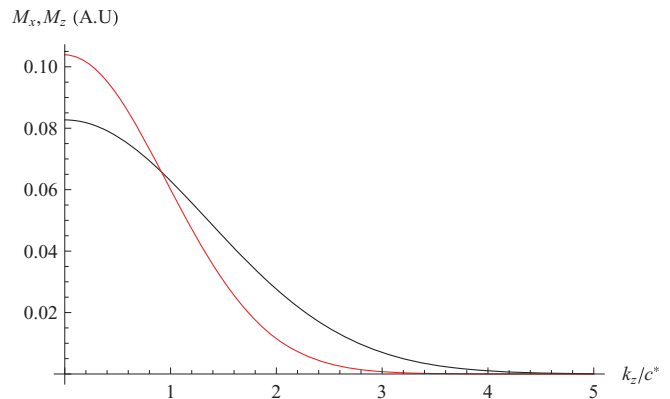


FIG. 3. (Color online)  $M_x$  (black curve) and  $M_z$  (red curve) as a function of  $k_z$ .

of the following fermion operators (see Appendix A):

$$\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} i c_x c_y (p_{x,\mathbf{k}}^\dagger p_{y,\mathbf{k}} - p_{y,\mathbf{k}}^\dagger p_{x,\mathbf{k}}). \quad (38)$$

Here,  $p_{x,\mathbf{k}}$  and  $p_{y,\mathbf{k}}$  are the Fourier transform of the oxygen  $p$ -orbital operators in the  $x$  and  $y$  directions, respectively, around the Cu atom in the unit cell  $i$ . Such an operator is created microscopically through expressing the nearest-neighbor interactions in each unit cell in terms of current operators and combining such current operators to form closed loops within a unit cell. Five different point group symmetries result including that of Eq. (38) sketched in Fig. 2. That this operator admixes the basis states is shown in detail in Appendix A.

Given this, we can calculate the form factor of neutron scattering by further approximations to represent the collective states shown in Figs. 1 and 2. These are described in Appendix A. We now proceed with the comparison with the experiments in evaluation of the neutron scattering using these results.

### B. Results for tilt and form factor

It is easy to see that if we include the form factor effects,  $L_z$  decreases faster than  $L_1$  as  $Q_z$  increases [see Fig. (3)]. (Recall that the subscript 1 in  $L_1$  stands for whatever component of  $\mathbf{L}$  perpendicular to the  $z$  axis is being measured.) We therefore find the tilt angle for  $\mathbf{Q} = (101)$  is larger than  $\mathbf{Q} = (100)$ , qualitatively consistent with the experiments.<sup>1</sup> How the tilt angle depends on the momentum is determined in our calculation by the choice of parameters such as  $r_s$  and  $r_0$ , which is hardly definitive.

For example, as a reasonable guess, we can take  $r_0 = 0.25a$  and  $r_w = 0.175a$ . Here,  $a$  is the lattice constant of  $xy$  plane. The tilted angle is quite sensitive to the current width parameter  $w$ . From experimental data, we know that the intensity of neutron scattering of  $L = 2$  is half of that for  $L = 0$ . For a Gaussian shape dependence of  $Q_z$ , we can deduce that  $w \approx 0.5a$ . The half width of the current is comparable to the radius of the current.

For the above choice of parameters, the intersection of these two circles are  $\mathbf{R}_{1a} = (0.238a, 0.075a)$  and  $\mathbf{R}_{1b} = (0.075a, 0.238a)$ . If we use the approximate form factor of

Eq. (C9), then for transfer momentum  $\mathbf{Q} = \frac{2\pi}{a}(0,1,0)$ , we find that the tiled angle is  $\phi = \arctan(\frac{|L_x|}{|L_z|}) \approx 64^\circ$ .

Since the width  $w = 0.5a$  is not small compared to  $a$ , we can not use the above approximation. Therefore we have to numerically transform Eqs. (C6) and (C4) to momentum space. For  $\mathbf{Q} = \frac{2\pi}{a}(0,1,0)$ , we find that the tiled angle is  $\phi \approx 26^\circ$ . If we also include the “rotation” kind contribution to the moment from Eqs. (C10) and (C11) and choose the parameter  $C = -0.2a$ , we find the total tiled angle is  $\phi \approx 38.5^\circ$ . For YBCO,  $c \approx 3a$ . Therefore for transfer momentum  $\mathbf{Q} = (0, \frac{2\pi}{a}, \frac{2\pi}{c})$ , we find the tiled angle  $\phi \approx 47^\circ$ .

For YBCO, there are two copper-oxygen planes. Suppose the distance between these two layers are  $d$ , then we will have an extra structure factor  $\cos(Q_z \frac{d}{2})$ . This makes the amplitude oscillate with  $Q_z$ .

## VI. CONCLUDING REMARKS

In this paper, we have used the result derived earlier in I that the ground state of the loop-ordered state is a linear combination of the classical basis states. This necessitates a new view of calculating the neutron scattering cross section in which one must consider the flip in the neutron spin due also to the matrix elements of flip operators of the quantum-moments in the ground state. The simplest (mean-field) ground state was considered. This does not include the zero-point deviations due to spin waves. We have calculated these to be a small effect because the collective modes are all at finite energy.

Our method of calculating the neutron scattering cross section may be useful in other quantum problems, for example, the transverse field Ising model, provided the transverse field is not an external field with a specified direction but internally generated. It may also be useful when scattering experiments are done in other loop-ordered states such as the anomalous Hall effect and the topological insulator states.

We have been able to show reasonable consistency of the calculation with the experimental results but a parameter  $C$  was introduced, which we find hard to calculate but can argue only that it should be small compared to 1, as is indeed found. Especially gratifying is that the tilt angle deduced depends on the Bragg vector. This would not happen in the traditional usage in which the neutron spin flips quantum mechanically of a spatially dependent classical magnetic field due to the magnetic order.

It is worthwhile commenting on earlier attempts to understand the tilt. One was based on spin-orbit scattering.<sup>17</sup> This had two difficulties; there is no such term in Hg1201 and the magnitudes do not come out reasonably without giving a scattering at  $(2,0,0)$ , which is not in agreement with elastic experiments. The other idea is that there is a moment on the triangles made through apical oxygens.<sup>18</sup> This is allowed by symmetry.<sup>6</sup> Mean-field calculations do not provide any significant such moment for any reasonable set of parameters. There is a more basic problem with having any significant amplitude for such a contribution. It is that such moments would provide zero contribution of the moment perpendicular to the  $z$  axis for any scattering vector with  $\mathbf{Q}_z = 0$  due to the structure factors in the Cu-O lattices with a plane of reflection in the unit cell perpendicular to the  $z$  axis. As already

mentioned a large tilt has been deduced for  $\mathbf{Q} = (1,0,0)$ .<sup>2</sup> One could introduce currents through the apical oxygens which would produce “tilts” at  $\mathbf{Q} = (1,0,0)$  also. But they are not allowed by symmetry of the currents in the plane but would require additional symmetry breaking. Simultaneous occurrence of two different symmetry breaking would require an unlikely accident.

Our calculations in this paper also have an impact for some other measurements. If the tilt were due to moments in triangles made through apical oxygens as discussed in the previous paragraph, there should be measurable magnetic fields<sup>20</sup> at several sites in the lattice, detectable in NMR experiments. With the quantum origin of tilt fields, the calculations based on a classical magnetic field tilted in specific directions are not valid. Further consequences of the quantum origin of the tilt, for example, in NMR experiments, is well worth further investigation.

## ACKNOWLEDGMENTS

We wish to thank Vivek Aji, Philippe Bourges, Thierry Giamarchi, Martin Greven, Yuan Li, and Yvan Sidis for discussions of the considerations in this paper and the experimental results and Stephen Lovesey for a critical reading of the manuscript. We also thank S. Kivelson and S. Lederer for a discussion of the scattering at  $(1\ 0\ 0)$ .

## APPENDIX A: MICROSCOPIC THEORY OF THE KINETIC ENERGY OPERATOR ( $S^1 + T^1 + S^2 + T^2$ ) FOR THE LOOP CURRENT STATES

The loop current states were derived<sup>4</sup> starting from the basis of the three orbitals  $(d_i, p_{ix}, p_{iy})$  per unit cell. Besides the kinetic energy operator between the neighboring  $d$ ,  $p_x$ , and  $p_y$  orbitals, the model includes local repulsion at each site (the  $U$ 's) and near-neighbor repulsions of charges  $Vn_in_j$ . The on-site repulsions are assumed to serve only to renormalize the remaining terms in the Hamiltonian in the metallic state. A crucial role is played by the operator for nearest neighbor interactions. For spin-diagonal terms in the operator  $n_in_j$ , it may be written as

$$V \sum_{\sigma} n_{i,\sigma} n_{j,\sigma} = V/2(|j_{ij}|^2 - n_i - n_j). \quad (\text{A1})$$

Here,  $j_{ij} = i \sum_{\sigma} c_{i,\sigma}^+ c_{j,\sigma} + \text{H.c.}$  has the operator content of a current. Discarding the one particle terms, a mean-field approximation is made on  $|j_{ij}|^2$ :

$$|j_{ij}|^2 = (r_{ij}^2 + r j_{ij} + r^* j_{ij} + \text{fluctuation operators}). \quad (\text{A2})$$

Here,  $r_{ij}$  is the collective part of  $j_{ij}$ . Now the effective kinetic energy on the link  $(ij)$  is  $t_{ij} + iVr_{ij}/2$ , which gives a complex kinetic energy with a phase  $\approx rV_{ij}/(2t_{ij})$ . Phase differences on links within a unit cell are combined to form closed loops that have invariant fluxes with different point group symmetries. For nonintersecting loops on the Cu-O lattice, there are five and only five such closed loops possible.<sup>16</sup> Two of these, which transform as doubly degenerate vectors  $E_1$ , in the  $(x \pm y)$  directions and their time-reversed partners form the four flux patterns depicted in Fig. 1. Simple mean-field calculations as well as more elaborate calculations<sup>18</sup> show that this is the most



stable allowed symmetry and experiments<sup>1</sup> have shown it to be the realized state in all the underdoped cuprates investigated.

The other current loop that plays a crucial role in our considerations here and in the collective modes of I and played an important role in the calculation of collective fluctuations<sup>16</sup> in the quantum-critical regime is the pattern transforming with the full symmetry of the lattice. It is depicted in Fig. 2. We will show that it has local matrix elements between the states  $(\pm 1, \pm 1)$ . Before we show this, it is important to specify some properties of the basis states  $(\pm 1, \pm 1)$ .

Corresponding to each of the four collective states  $(\pm 1, \pm 1)$ , there are four mean-field kinetic energy Hamiltonians for the fermions:

$$H(\mathbf{k}) = \begin{pmatrix} 0 & it_{pd}S_x & it_{pd}S_y \\ -it_{pd}S_x & 0 & t_{pp}s_x s_y \\ -it_{pd}S_y & t_{pp}s_x s_y & 0 \end{pmatrix} \quad (\text{A3})$$

with  $S_x = \sin(k_x a/2 + \phi_x)$ ,  $S_y = \sin(k_y a/2 + \phi_y)$ ,  $s_x = \sin(k_x a/2)$ , and  $s_y = \sin(k_y a/2)$ . The four different mean-field Hamiltonians correspond to the four different possible order parameters  $(\phi_x, \phi_y) = (\pm\Omega, \pm\Omega)$ , where  $\Omega$  is the magnitude of the order parameter, which is determined variationally. The eigenvalues and eigenstates of the three fermion bands in the zeroth order of  $t_{pp}/t_{pd}$  are given by

$$\begin{aligned} E_1 &= -t_{pd}\sqrt{S_x^2 + S_y^2}, \quad E_2 = 0, \quad E_3 = t_{pd}\sqrt{S_x^2 + S_y^2}, \\ |1, k\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} -i, \frac{S_x}{S_{xy}}, \frac{S_y}{S_{xy}} \end{pmatrix}^T, \quad |2, k\rangle = \begin{pmatrix} 0, -\frac{S_y}{S_{xy}}, \frac{S_x}{S_{xy}} \end{pmatrix}^T, \\ |3, k\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} i, \frac{S_x}{S_{xy}}, \frac{S_y}{S_{xy}} \end{pmatrix}^T \end{aligned}$$

with  $S_{xy} = \sqrt{S_x^2 + S_y^2}$ .

To find the collective operator which rotates among the four states  $(\pm 1, \pm 1)$ , let us first find the operator which rotates among the fermion states of these four collective states. Then the collective operator we are looking for is simply the collective part of such an operator formed from the fermions. Let us use subscript  $a, b, c$ , and  $d$  to label order parameter  $(1, 1)$ ,  $(-1, 1)$ ,  $(-1, -1)$ , and  $(1, -1)$ . Then we can find the exact unitary operators that rotates among the four states such as

$$\begin{aligned} U_{ab} &= |1\rangle_b \langle 1|_a + |2\rangle_b \langle 2|_a + |3\rangle_b \langle 3|_a, \\ U_{bc} &= |1\rangle_c \langle 1|_b + |2\rangle_c \langle 2|_b + |3\rangle_c \langle 3|_b. \end{aligned}$$

The above rotation operators are exact and unique, but they are too complicated to be useful. Since the order parameter  $\Omega$  is small, we only need to make this rotation up to linear order of  $\Omega$ . We also need to impose the requirement that the operator rotating from  $a$  to  $b$  is the same as the operator that rotates from  $b$  to  $c$ .

In finding the operator with the right properties, we are guided by what we know of the operator if we take a continuum of two dimensional states specified by a unit vector in the plane and ask for the operator which rotates such a vector. It is obviously the angular momentum operator in a direction normal to the plane of  $i(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$  or equivalently, the current operator  $\nabla \times \mathbf{j}$  where  $\mathbf{j}$  is proportional to the current operator

in the plane. The equivalent of this operator on the Cu-O lattice is pictorially depicted in Fig. 2.

It is straightforward to calculate that the algebraic representation of the operator (which will be the generator of rotations) in Fig. 2 is given by

$$g_k = ic_x c_y (p_{x,k}^\dagger p_{y,k} - p_{y,k}^\dagger p_{x,k}). \quad (\text{A4})$$

Then the corresponding unitary operator is

$$U = 1 + i\Omega g_k = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\Omega c_x c_y \\ 0 & \Omega c_x c_y & 1 \end{pmatrix}. \quad (\text{A5})$$

We can now check that such an operator makes the  $\pi/2$  rotations that we are looking for up to linear order of  $\Omega$ . It is easy to verify that

$$\begin{aligned} \langle 3, k|_b U|3, k\rangle_a &= 1 + \frac{c_x s_y^2 (s_x s_y s_{xy}^2 - c_x)}{s_{xy}^4} \Omega^2 + O(\Omega^3), \\ \langle 3, k|_c U|3, k\rangle_b &= 1 - \frac{c_y s_x^2 (s_x^2 s_y^2 + c_y + s_y^4)}{s_{xy}^4} \Omega^2 + O(\Omega^3), \\ \langle 3, k|_d U|3, k\rangle_c &= 1 - \frac{c_x s_y^2 (s_x s_y s_{xy}^2 + c_x)}{s_{xy}^4} \Omega^2 + O(\Omega^3), \\ \langle 3, k|_a U|3, k\rangle_d &= 1 + \frac{c_y s_x^2 (s_x^2 s_y^2 - c_y + s_y^4)}{s_{xy}^4} \Omega^2 + O(\Omega^3). \end{aligned}$$

It has already been shown<sup>16</sup> that operator  $g_k$  is also generated by the nearest-neighbor interactions. It then follows that a collective current operator of the same symmetry also exists that serves as a kinetic energy term mixing the collective configurations. In the basis of the collective states  $|\pm 1, \pm 1\rangle$ , this has all the transformation properties and commutation rules of the operator  $(S^1 + T^1 + S^2 + T^2)$ .

## APPENDIX B: NEED FOR A FOUR-DIMENSIONAL REPRESENTATION OF THE OPERATOR S

As discussed the gauge transformation is given by the rotation matrix

$$U(\theta) = e^{i\theta_1 S^3/2} e^{i\theta_2 T^3/2} e^{i\theta_3 K^{33}/2}. \quad (\text{B1})$$

The classical AT model is invariant under this transformation. Under this rotation, the quantum term  $S^1$ ,  $T^1$ , and  $K^{11}$  will be transformed as follows:

$$\begin{aligned} U(\theta)S^1U(\theta)^\dagger &= \cos\theta_3(\cos\theta_1 S^1 - \sin\theta_1 S^2) \\ &\quad - \sin\theta_3(\sin\theta_1 K^{13} + \cos\theta_1 K^{23}), \end{aligned} \quad (\text{B2})$$

$$\begin{aligned} U(\theta)T^1U(\theta)^\dagger &= \cos\theta_3(\cos\theta_2 T^1 - \sin\theta_2 T^2) \\ &\quad - \sin\theta_3(\sin\theta_2 K^{31} + \cos\theta_2 K^{32}), \end{aligned} \quad (\text{B3})$$

$$\begin{aligned} U(\theta)K^{11}U(\theta)^\dagger &= \cos\theta_1 \cos\theta_2 K^{11} + \sin\theta_1 \sin\theta_2 K^{22} \\ &\quad - (\cos\theta_1 \sin\theta_2 K^{12} + \sin\theta_1 \cos\theta_2 K^{21}). \end{aligned} \quad (\text{B4})$$

The quantum terms related by this transformation are equivalent to each other. In the mean time, the mean-field ground state is also transformed to a new form. In the loop current

state basis, the original ground state can be written as  $|G\rangle = (c^2, sc, sc, s^2)^T$ . After the transformation, we have  $|G'\rangle = U(\theta)|G\rangle$ , which is a superposition of the four states with complex number coefficients. Thus after the transformation,  $\langle S^y \rangle$  is nonzero and depends on the gauge parameter  $\theta_{1,2,3}$ .

Since  $\mathbf{M}(\mathbf{q})$  as a physical observable is gauge invariant, it should not depend on the gauge parameter  $\theta_{1,2,3}$ . This gauge dependence should disappear if we make a corresponding unitary transformation on the local spin operator  $S^{1,2,3}$ . But now we meet a immediate difficulty. The transformation  $U(\theta)$  is a  $4 \times 4$  matrix simply given by

$$U(\theta) = \text{diag}\{e^{i\phi_1}, e^{i\phi_2}, e^{i\phi_3}, e^{i\phi_4}\} \quad (\text{B5})$$

with  $\phi_1 = \frac{\theta_1 + \theta_2 + \theta_3}{2}$ ,  $\phi_2 = \frac{\theta_1 - \theta_2 - \theta_3}{2}$ ,  $\phi_3 = \frac{-\theta_1 + \theta_2 - \theta_3}{2}$ , and  $\phi_4 = \frac{-\theta_1 - \theta_2 + \theta_3}{2}$ . Translating this transformation to the basis of local spin-1 state, we find that the corresponding transformation is

$$V(\theta) = \text{diag}\{e^{i\phi_1}, e^{i\phi_2} + e^{i\phi_3}, e^{i\phi_4}\}. \quad (\text{B6})$$

Clearly, one can see that  $V(\theta)$  is not a unitary transformation. Therefore we cannot use  $V(\theta)$  to cancel the gauge dependence.

This difficulty arise because there are four states in the loop current state basis but there are only three states in the local spin-1 state basis. In order to overcome this difficulty, we have introduced a four-dimensional representation of the spin-1 states given in the paper.

### APPENDIX C: APPROXIMATE CALCULATIONS OF FORM FACTOR

We first consider the form factor for the  $L_z$ . Since  $L_z$  only has diagonal matrix elements, we do not need to use the rotation operator yet. The form factor is determined by the current density around the O-Cu-O triangle. To simplify the calculation, we approximate the triangle shape by a circle shape current density and also assume the density is a Gaussian distribution around the circle. Then, the wave function of the local spin states in terms of cylindrical coordinates  $\mathbf{r} = (r \cos \phi, r \sin \phi, z)$  are given by

$$\psi_{a,\pm 1} = \frac{1}{\sqrt{2\pi w}} e^{-\frac{(r-r_s)^2}{4w^2}} e^{-\frac{z^2}{4w^2}} e^{\pm i\phi}, \quad (\text{C1})$$

$$\psi_{a,0} = \frac{1}{\sqrt{2\pi w}} e^{-\frac{(r-r_s)^2}{4w^2}} e^{-\frac{z^2}{4w^2}}. \quad (\text{C2})$$

Here, we assume the radius of the circle is  $r_s$  and centered around  $R_a$  and  $w$  specify the width of these circles. Now we can verify that  $\psi_{a,1}$  gives a torus shape current density:

$$\begin{aligned} \mathbf{j}(\mathbf{r}) &= -\frac{i}{2}(\psi_{a,1}^\dagger \nabla \psi_{a,1} - \psi_{a,1} \nabla \psi_{a,1}^\dagger) \\ &= \frac{1}{2\pi w^2} e^{-\frac{(r-r_0)^2}{2w^2}} e^{-\frac{z^2}{2w^2}} \hat{\phi}. \end{aligned} \quad (\text{C3})$$

Similarly,  $\psi_{\downarrow}$  gives a torus shape current density with opposite direction.  $\psi_0$  is real function, so the current is zero. These three states correspond to  $|\pm 1\rangle$  and  $|0\rangle$  pointlike angular momentum states. If we take  $w \rightarrow \infty$  limit, we find a current circle  $\mathbf{j}(\mathbf{r}) = \delta(r - r_0)\delta(z)\hat{\phi}$ .

We still have  $L_z = \psi^\dagger L_z \psi$ , where  $L_z = -i \frac{\partial}{\partial \phi}$ . The  $\phi$ -dependent part will give the same matrix elements as before. Now, we also have an extra  $r$ - and  $z$ -dependent part as follows:

$$F_{z,a}(\mathbf{r}) = \frac{1}{2\pi w^2} \exp\left[-\frac{(r_a - r_s)^2}{2w^2} - \frac{z^2}{2w^2}\right]. \quad (\text{C4})$$

Here,  $r_a = \sqrt{(x - R_{a,x})^2 + (y - R_{a,y})^2}$  with  $a = 1, 2, 3, 4$ . Then the form factor is the Fourier transformation of the above function. If the current width is narrow, we have

$$\begin{aligned} F(\mathbf{k}) &= \int_{\text{cell}} F(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3 r \approx f(k_r) e^{-\frac{w^2 k_z^2}{2}} e^{-i\mathbf{k}\cdot\mathbf{R}_a} \\ \text{with } f(k_r) &= \frac{1}{\sqrt{2\pi w}} \int_0^\infty e^{-\frac{(r-r_s)^2}{2w^2}} J_0(k_r r) r dr. \end{aligned}$$

Using this result in Eq. (24), we find

$$L_z(\mathbf{k}) = \cos \theta [F_{z,1}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_1} - F_{z,1}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_3}]. \quad (\text{C5})$$

The form factor of  $L_t$  is more complicated, since the rotation operator has its own coordinate dependence. As explained before, the rotation operator is currents flows around the four oxygens in the unit cell. Here, for simplicity, we approximate the current around the oxygens as a big circle with radius  $r_0$  centered at  $\mathbf{R}_t^0$ . We have  $L_t = \psi^\dagger L_t \psi$ . Here,  $L_t$  will annihilate or create the  $e^{i\phi}$  factor. The  $\phi$ -dependent part will give the same matrix elements as before. For the local spin state at  $\mathbf{R}_a$ , we also have an extra  $r$ - and  $z$ -dependent part as follows:

$$\begin{aligned} F_{x,a}(\mathbf{r}) &= \frac{1}{2\pi w^2} \exp\left[-\frac{1}{2w^2}(r - r_0)^2 - \frac{z^2}{2w^2}\right] \\ &\times \exp\left[-\frac{1}{2w^2}(r_a - r_s)^2 - \frac{z^2}{2w^2}\right]. \end{aligned} \quad (\text{C6})$$

Here,  $r = \sqrt{x^2 + y^2}$ . It is easy to transform the  $z$ -dependent part to momentum space. The  $x$ - and  $y$ -dependent part has to be computed by numerics. Including the form factors in Eq. (23), the  $x$  component of moment is

$$\begin{aligned} L_t(\mathbf{k}) &= \sin \theta [F_{x,1}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_1} + F_{x,2}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_2} \\ &- F_{x,3}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_3} - F_{x,4}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_4}]. \end{aligned} \quad (\text{C7})$$

If the current width is quite narrow  $w \ll a$ , here  $a$  is lattice constant of  $xy$  plane, then Eq. (C6) can be approximated by two Gaussian peaks located at  $\mathbf{R}_a^1$  and  $\mathbf{R}_a^2$ , where  $\mathbf{R}_a^1$  and  $\mathbf{R}_a^2$  are the two intersection points of the two circles. Thus we have

$$F_{x,a}(\mathbf{r}) \approx \frac{1}{2\pi w^2} \left[ e^{-\frac{(r-r_0^1)^2}{2w^2}} + e^{-\frac{(r-r_0^2)^2}{2w^2}} \right] e^{-\frac{z^2}{w^2}}. \quad (\text{C8})$$

Transferring to momentum space, we find the form factor as

$$F_{x,a}(\mathbf{k}) = \sqrt{\pi} w e^{-\frac{w^2(k_x^2 + k_y^2)}{2}} (e^{i\mathbf{k}\cdot\mathbf{R}_a^1} + e^{i\mathbf{k}\cdot\mathbf{R}_a^2}) e^{-\frac{w^2 k_z^2}{4}} \quad (\text{C9})$$

with  $a = 1, 2, 3, 4$ .

So far we only considered the “spin” kind contribution to the moments. Similarly, we can also compute the form factor for the “rotation” kind contribution. Follow the same line of arguments, the  $\phi$ -dependent part will give the same matrix elements as before. For the the matrix element  $\langle \psi_a | L_z | \psi_b \rangle$ , there is an extra  $r$ - and  $z$ -dependent part as follows:

$$F_{x,ab}(\mathbf{r}) = \frac{1}{2\pi w^2} \exp\left[-\frac{1}{2w^2}(r-r_0)^2 - \frac{z^2}{2w^2}\right] \\ \times \exp\left[-\frac{1}{4w^2}(r_a-r_s)^2 - \frac{z^2}{4w^2}\right] \\ \times \exp\left[-\frac{1}{4w^2}(r_b-r_s)^2 - \frac{z^2}{4w^2}\right]. \quad (\text{C10})$$

Similarly, or the the matrix element  $\langle \psi_a | L_z | \psi_b \rangle$ , there is an extra  $r$ -and  $z$ -dependent part as follows:

$$F_{z,ab}(\mathbf{r}) = \frac{1}{2\pi w^2} \exp\left[-\frac{1}{4w^2}(r_a-r_s)^2 - \frac{z^2}{4w^2}\right] \\ \times \exp\left[-\frac{1}{4w^2}(r_b-r_s)^2 - \frac{z^2}{4w^2}\right]. \quad (\text{C11})$$

And the form factor is the above function transform to momentum space. Therefore, for transfer momentum  $\mathbf{k} = \frac{2\pi}{a}(0,1,0)$ , we find the effective moment due to the “rotation” kind contribution is

$$\mathbf{L}_{\text{eff}} = -ik_y C [F_{x,12}(\mathbf{k})(1 + \sin^2 \theta), 0, F_{z,12}(\mathbf{k}) \sin 2\theta]. \quad (\text{C12})$$

These results have been used in the paper to calculate the form factor and the tilt angles and compared with experiments.

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