

Anisotropy in two-dimensional arrays of collinear in-plane rotated identical particles with arbitrary charge or polarization distribution

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As the size and separation between nanometric objects arranged on a two-dimensional lattice become progressively smaller, the influence of interparticle coupling increases to the point that it may dominate the system's collective behavior. In this paper, a simple method to calculate isotropic and anisotropic interaction energies of charged or polarized particles in two-dimensional arrays is developed, where anisotropy refers to changes in energy upon in-plane rotation. The calculations are performed in the framework of a multipole expansion in spherical coordinates. The role of the array symmetry with respect to the order of the expansion is deduced from the symmetry properties of the interaction. The interaction energy is calculated exactly to infinite distance by means of lattice sums; thus, no cut-off radius to nearest neighbors is introduced. Several lattice symmetries, rectangular, quadratic, and hexagonal, up to multifold rotationally symmetric quasicrystals are investigated, and the influence of local disorder is discussed.

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I. INTRODUCTION

In recent years we have witnessed the emergence of the fields of nanoscience and nanotechnology, driven by the quest for properties derived from reduced dimensionality and confinement effects. Anisotropies are a typical example of a property that must be expected to change substantially when reducing the material's dimensions from bulk to the nanometer scale.¹ The existence of energetically preferred directions is intimately linked to the spatial arrangement of the interacting atoms within the material's crystalline structure, and it is obviously dependent on the nearly infinite periodicity in macroscopic samples. The onset of superparamagnetic behavior in magnetic nanoparticles below a certain size limit is an illustrative case.² For the magnetization of an isolated particle to switch direction, all the atomic magnetic moments must be rotated in space. Hence, the total anisotropy barrier can be estimated by counting the number of atoms in the particle and multiplying it by the atomic anisotropy energy. Upon reduction of the particle size, the number of atoms in it diminishes and so does the particle's anisotropy energy; when this barrier becomes comparable or smaller than the thermal energy $k_B T$, thermal fluctuations cause the magnetization to flip spontaneously. Under these conditions, the interactions between adjacent particles in an array, which for the magnetic case are almost negligible for separations on the order of 100 nm, may become dominant and define the stable magnetic state of the array on the 10 nm scale.³

If we restrict ourselves to the two-dimensional (2D) case, the well-known Mermin-Wagner theorem⁴ rules out the existence of long-range order at any finite temperature in isotropic systems. Nevertheless, order can appear in 2D arrays if the particle-particle interactions are anisotropic. It becomes therefore crucial for the successful design and performance

of any given system of nanometric objects, either molecules,^{5,6} spinor condensates, or magnetic particles,⁷⁻⁹ to be able to understand and quantify their interaction energy, and the dependence of this latter with the lattice symmetry.

The purpose of this paper is to present a theoretical study of the interaction and in-plane anisotropy in 2D arrays of charged or polarized objects. The results can be easily compared with experiment.¹⁰ In this work the term *anisotropy* is restricted to changes in self-energy if the charged or polarized particles are rotated coherently around the surface normal of the 2D array (instead of the particle also the polarization may rotate). An analytical method is developed based on multipole expansion that greatly simplifies the calculation and provides a deeper insight into the systems' behavior. The simplification makes use of the fact that it is possible to separate the particle-particle interaction from the summation over the lattice.¹¹ Hence, the calculated energy is exact and no cutoff radius for the computation of the interaction is introduced, although for quadrupole-quadrupole and higher order terms the total energy might be approximated by considering only a few neighbors.¹² However, to calculate the interaction energy of one particle with all the others, it is sufficient to calculate one nearest-neighbor interaction and correct it by a lattice dependent factor. The lattice dependent factor is an *Ewald-type* summation¹³ and depends on the type of nearest-neighbor interaction.

In a general picture the method uses two branches of mathematics: lattice sums as a part of number theory¹⁴ and symmetry as a part of group theory.¹⁵ Both areas, lattice sums¹³ and symmetry considerations¹⁶ are well established in physics and chemistry. Although the use of spherical harmonic functions allows a very general and mathematical view on symmetry, symmetry breaking, and anisotropy, the goal is to use existing methods as a tool to understand the

behavior of real systems. Nevertheless, symmetry plays an important role and reveals several important practical consequences such as the dependence of coupling strength and the range of interparticle coupling on the arrangement symmetry.

The following calculations allow the determination of the multipole moments of interacting particles in systems that exhibit anisotropy. In several cases this also enables the calculation of the isotropic energy. Finally, the knowledge of all terms contributing significantly to the particle-particle interaction (as derived from the collinear state) allows further theoretical investigation, e.g., the simulation of noncollinear states by Monte Carlo methods.

This paper is organized as follows: After an introduction to the basics of the multipolar interaction in Sec. II, the general method used for the calculation of the energy and anisotropy is presented in Sec. III. We then treat the different high-order multipole interactions in Sec. IV. Some cases of particular interest, namely those of the lattices with sixfold (Sec. V) and higher order symmetry (Sec. VI), are considered. In Sec. VII, an example calculation of the anisotropy in an array of disks is carried out to demonstrate our calculation method. Finally, the main findings and implications derived from this work are discussed in Sec. VIII.

II. PROPERTIES OF THE MULTIPOLAR INTERACTION

It is well known that the interaction energy of a system of collinear dipoles, arranged on a periodic lattice, is in general anisotropic: The preferential directions of minimal energy are defined by the symmetry of the unit cell. In the following, this angle-dependent energy contribution, which is due to the stray field interaction of the dipoles, will be called interaction-induced anisotropy. For instance, for a rectangular lattice the preferred direction is parallel to the short edge of the unit cell, since the interacting objects are more closely spaced along that direction and their corresponding interaction is stronger. Starting with the dipoles aligned along this axis, the energy increases when they are rotated coherently toward the long edge. It is also known that for square and hexagonal lattices the dipolar interaction energy is isotropic in the above sense. Nevertheless, it will be shown below that higher order moments are anisotropic also on these lattices and that their order and symmetry determine the nonzero anisotropy constants. There may appear metastable or ground states whose anisotropy reflects the underlying lattice symmetry, as for instance in the fourfold case.¹⁷ However the collinear state, which is considered in the following, does not necessarily represent the ground state of the system; hence, in an experiment it has to be established by additional forces.

The potential of any charge distribution $\rho(\vec{r})$ —electric or magnetic¹⁸—that is confined to a finite volume V can be written in terms of a multipole expansion. The first term in the series, assuming zero net charge,¹⁹ is the dipolar one, followed by the higher order moments. The procedure of expanding a Coulomb-type potential to approximate the potential can be applied in a similar way to calculate the interaction of two, nonoverlapping charge distributions. The details of a particular expansion depend on the choice of the coordinate system. In the following, spherical coordinates

will be used— $\vec{r}=(r, \theta, \varphi)$ —taking advantage of the well-known symmetry properties of the spherical harmonic functions $Y_{lm}(\theta, \varphi)$.²⁰ The definition for the multipole moments reads

$$Q_{lm} = \sqrt{\frac{4\pi}{2l+1}} \int_V d\vec{r} \rho(\vec{r}) Y_{lm}(\theta, \varphi) r^l. \quad (1)$$

Further details about the expansion of the interaction energy are given elsewhere.²¹

The interaction of two charge distributions A and B with multipole moments Q^A and Q^B is calculated via the interaction tensor T .^{22,23} If the two charge distributions are separated by the distance vector \vec{R}_{AB} the interaction energy reads

$$E_{AB} = \sum_{l_A l_B m_A m_B} T_{l_A l_B m_A m_B}(\vec{R}_{AB}) \frac{Q_{l_A m_A}^A Q_{l_B m_B}^B}{4\pi\epsilon_0}, \quad (2)$$

where

$$T_{l_A l_B m_A m_B} \propto Y_{l_A + l_B, -(m_A + m_B)}(\theta_{AB}, \varphi_{AB}). \quad (3)$$

In case of magnetic interaction, ϵ_0 has to be replaced by μ_0 . To simplify the formulas, the term $(4\pi\epsilon_0)^{-1}$ will be omitted in the following, i.e., the energy is given in units of this factor.

As mentioned before, only 2D arrays are treated. The natural choice for the z axis is the direction perpendicular to the 2D plane. Hence, one has $\theta_{AB} \equiv \pi/2$. The spherical harmonic functions further simplify and only the dependence on φ_{AB} remains. Therefore, it is possible to write T as

$$T_{l_A l_B m_A m_B}(\vec{R}_{AB}) = t_{l_A l_B m_A m_B} \frac{e^{-i(m_A + m_B)\varphi_{AB}}}{R_{AB}^{l_A + l_B + 1}}, \quad (4)$$

where $t_{l_A l_B m_A m_B}$ is a real number given by

$$t_{l_B l_A m_B m_A} = \frac{(-1)^{l_B} 2^{l_A + l_B}}{\pi} \cos \pi \frac{l_A + l_B + m_A + m_B}{2} \times \frac{\Gamma\left(\frac{l_A + l_B + m_A + m_B + 1}{2}\right)}{\sqrt{\Gamma(l_A + m_A + 1)\Gamma(l_B + m_B + 1)}} \times \frac{\Gamma\left(\frac{l_A + l_B - m_A - m_B + 1}{2}\right)}{\sqrt{\Gamma(l_A - m_A + 1)\Gamma(l_B - m_B + 1)}}. \quad (5)$$

It follows from Eq. (5) and from the properties of the spherical harmonics that

$$T_{l_A l_B m_A m_B}(\vec{R}_{AB}) = (-1)^{m_A + m_B} T_{l_A l_B -m_A -m_B}^*(\vec{R}_{AB}),$$

$$T_{l_A l_B m_A m_B}(\vec{R}_{AB}) = (-1)^{l_A + l_B} T_{l_B l_A m_B m_A}(\vec{R}_{AB}),$$

$$T_{llm_A m_B}(\vec{R}_{AB}) = T_{llm_B m_A}(\vec{R}_{AB}),$$

$$0 = T_{l_A l_B 00}(\vec{R}_{AB})|_{l_A + l_B \text{ odd}, \theta_{AB} = \pi/2}. \quad (6)$$

The anisotropy is determined by calculating the interaction energy for different orientations of the multipole moments. In spherical coordinates a moment is rotated by applying the Wigner D -function such that

$$Q_{ln}^{\text{new}} = \sum_m D_{nm}^l(\alpha, \beta, \gamma) Q_{lm}^{\text{old}}, \quad (7)$$

where the Wigner D -function is defined as

$$D_{nm}^l(\alpha, \beta, \gamma) = e^{-i(m\alpha+n\gamma)} d_{nm}^l(\beta). \quad (8)$$

An angular position is defined by the Euler angles α , β , and γ . The first and the last represent rotations around the z axis and result only in a phase factor, as the spherical harmonics are eigenfunctions with respect to this operation. The term $d_{nm}^l(\beta)$ handles the rotation around the y axis.²⁰ Although this rotation is required in general, e.g., to turn the axial multipoles of linear molecules into the plane, it is not part of the anisotropy calculation, as only in-plane rotations will be considered in the following. Hence, a single rotation around the z axis by the angle γ is sufficient.

III. ANISOTROPY

We define anisotropy as the change in energy if the multipole moments are rotated coherently within the plane of their arrangement. Because the parallel alignment is not necessarily the ground state, this might require additional forces (see also Appendix C), e.g., a homogeneous field in the case of dipoles on a square lattice.²⁴ The only angle-dependent factor in Eq. (4) is the argument of the exponential function. Let us assume a lattice with rotational symmetry C_n . The simple lattices, which will be treated here, have $n=2$ (rectangular), $n=4$ (square), or $n=6$ (hexagonal). For all these cases it is possible to combine those lattice points with the same distance R_{AB} but different angles φ_{AB} in one sum. The interaction energy is then proportional to this sum as

$$E \propto \sum_{k=0}^{n-1} e^{-iM\varphi_k} = \sum_{k=0}^{n-1} e^{-iM(2\pi k/n)} = n \delta_{0, M \bmod(n)}. \quad (9)$$

The Kronecker- δ in this formula is easily understood: The energy is only nonzero if $M=0$ or M is a multiple of n , since in these cases the exponent is an integer multiple of $2\pi i$ and each summand equals one. For all other cases it is possible to apply the rule for geometric series

$$\sum_{k=0}^{n-1} (e^{2\pi i(M/n)})^k = \frac{(e^{2\pi i(M/n)})^n - 1}{e^{2\pi i(M/n)} - 1} = 0, \quad (10)$$

as it is assured that the denominator is not zero. For the interaction energy we have $M=m_A+m_B$ and consequently it is necessary that $m_A+m_B=0$ or m_A+m_B is a multiple of n . In general the angles φ_k may have an offset φ_0 . This offset results in a phase factor $\exp(-iM\varphi_0)$, but does not change the fact that the sum in case of $M \bmod(n)=0$ is vanishing. Furthermore, for large distances there might be more than n points with the same distance, but due to symmetry the number must be a multiple of n , which allows to apply the above-mentioned steps several times, i.e., one has to construct sev-

eral sums of the type of Eq. (9). The sums might differ by a phase factor, but—as mentioned before—this does not change the fact that the sums with $M \bmod(n)=0$ are zero.

Consider, e.g., a dipole with $|m_{A,B}|_{\text{max}}=1$ and $|m_A+m_B| \leq 2$. Obviously, if $n > 2$, only terms with $m_A+m_B=0$ can contribute to the energy. In Eq. (8) the angle dependence of in-plane rotations, i.e., around the z axis, is accounted for by a factor $e^{iM\gamma}$. As the multipole moments are assumed to rotate coherently, there will be two factors corresponding to the two interacting multipole moments Q^A and Q^B : $e^{im_A\gamma}$ and $e^{im_B\gamma}$. Combining them into a single term gives $e^{i(m_A+m_B)\gamma}$. On a rectangular lattice, where $n=2$, the prefactor due to the lattice summation is only nonzero if $m_A+m_B=0$ or $|m_A+m_B|=2$. If $m_A+m_B=0$ then $e^{i0\gamma}=1$ is independent of the angle, which is equivalent to a zero anisotropy. The terms with $|m_A+m_B|=2$ result in an anisotropic contribution, which is proportional to $\cos 2\gamma$. The dipole case will be treated in more detail below.

A. Conclusions from symmetry

Considering the lattice symmetry the following three general conclusions can be drawn: (i) Any system of multipole moments of (pure) order l has isotropic behavior on a lattice with rotational symmetry C_n as long as $n > 2l$. (ii) If the anisotropy is described by a series of cosine functions of the form $E=c_k \cos k\gamma$, only k with $k \leq 2l$ can appear. (iii) On a lattice with rotational symmetry C_n only k with $k \bmod(n)=0$ are allowed, including $k=0$.

The main simplification is, hence, the fact that only a few multipole components can contribute to the anisotropy energy. This is a consequence of symmetry—and the underlying symmetry of the multipole moments is that of the spherical harmonic functions. Therefore, the problem can be alternatively formulated as that of finding the spherical harmonic functions that adopt the symmetry of the underlying lattice, i.e., the rotational group C_n (or even D_n). This approach leads to the concepts of symmetry adapted functions,²⁵ or in other words, one tries to find the basis functions to the irreducible representations of the rotational group,¹⁵ which is beyond the needs of this work.

B. General sum formulas

To calculate the overall energy, the interaction of all multipole moments with each other has to be considered. The most general form for the interaction energy is Eq. (2). Nevertheless, this expression can be simplified, based on the previous considerations and the well-known property $Q_{lm} = (-1)^m Q_{l-m}^*$ of multipole moments, as well as on the properties listed in Eqs. (6). It is possible to separate the energy into an isotropic E_{iso} and an anisotropic term $E_{\text{ani}}(\gamma)$; each one of them can be divided into two sums, where the first one satisfies $l_A=l_B$, while for the second one combinations of different orders as $l_A > l_B$ appear. The sum for E_{iso} , utilizing $c+c^*=2 \text{Re}(c)$, $c \in \mathbb{C}$, reads

$$\begin{aligned}
 E_{\text{iso}} = & \sum'_{R_{AB}} \left[\sum_l \left(T_{ll00} Q_{l0}^2 + 2 \sum_{m=1}^l (-1)^m T_{llm-m} |Q_{lm}|^2 \right) \right. \\
 & + 2 \sum_{l_A > l_B} \left(T_{l_A l_B 00} Q_{l_A 0} Q_{l_B 0} + \sum_{m=1}^{l_B} \text{Re}(T_{l_A l_B m-m} Q_{l_A m} Q_{l_B -m}) \right. \\
 & \left. \left. \times [1 + (-1)^{l_A + l_B}] \right) \right], \quad (11)
 \end{aligned}$$

where an *accent* over the sum denotes that $|\vec{R}_{AB}|=0$ is omitted. As $m_A = -m_B$, it is possible to replace T by t , because the exponential factor is equal to 1. Keep in mind that if, apart from rotations around the z axes, other rotations are allowed, E_{iso} is not constant. The last factor of Eq. (11) [taking also into account the last of Eqs. (6)] is an important feature, which arises from the lattice symmetry: If multipole moments have a parallel alignment on a lattice with symmetry C_n and $n \geq 2$, there is no energy contribution due to the interaction of moments with different parity. In other words, the sum over l_A, l_B with $l_A > l_B$ is nonvanishing and contributes to the energy only if

$$l_A + l_B = 2z, \quad z \in \mathbb{N}_0, \quad (12)$$

i.e., either both are even or both are odd. Hence, there is no dipole-quadrupole, no quadrupole-octopole interaction, and so on. The same factor appears in the anisotropic sum, which then has the form

$$\begin{aligned}
 E_{\text{ani}}(\gamma) = & \sum'_{R_{AB}} \left\{ \sum_l \left(\sum_{\substack{m > 0 \\ n|2m}} 2 \text{Re}(T_{llmm} Q_{lm}^2) \right) \right. \\
 & + 4 \sum_{\substack{m_A > |m_B| \\ n|m_A + m_B}} \text{Re}(T_{llm_A m_B} Q_{l m_A} Q_{l m_B}) \\
 & \left. + 4 \sum_{\substack{l_A > l_B \\ l_A + l_B = 2z}} \sum_{\substack{m_A + m_B > 0 \\ n|m_A + m_B}} [\text{Re}(T_{l_A l_B m_A m_B} Q_{l_A m_A} Q_{l_B m_B})] \right\}, \quad (13)
 \end{aligned}$$

where, with $z \in \mathbb{N}_0$, the last summation already incorporates the symmetry property of Eq. (12), as well as all other possible simplifications. These sums can easily be evaluated in any computer algebra system (see, e.g., Ref. 26) or even by hand.

IV. ANISOTROPIES OF LOW ORDER MOMENTS ON LOW SYMMETRY LATTICES

In the following some higher order multipole moments as well as the known results for the dipole, as part of the more general dipole-octopole interaction, will be treated.

A. Anisotropies of quadrupoles on a rectangular lattice

In contrast to dipoles, quadrupoles can behave anisotropically on square lattices, but are isotropic on hexagonal ones. The general rectangular lattice with edge lengths (a, b) in-

cludes the square in the limit $a=b$. The energy can be separated into three terms, the isotropic part E_{iso} , a twofold part $E_2(\gamma)$ and a fourfold part $E_4(\gamma)$. Furthermore, introducing $Q_{lm} = \kappa_{lm} e^{i\psi_{lm}}$, $(\kappa_{lm}, \psi_{lm}) \in \mathbb{R}$ (clearly, $Q_{l0} = \kappa_{l0}$) and simplifying, these three terms read

$$\begin{aligned}
 E_{\text{iso}} = & \sum'_{R_{AB}} \frac{1}{R_{AB}^5} (t_{2200} \kappa_{20}^2 - 2t_{221-1} \kappa_{21}^2 + 2t_{222-2} \kappa_{22}^2) \\
 = & \sum'_{R_{AB}} \frac{1}{R_{AB}^5} \left(\frac{9}{4} \kappa_{20}^2 - 3 \kappa_{21}^2 + \frac{3}{4} \kappa_{22}^2 \right), \quad (14)
 \end{aligned}$$

$$\begin{aligned}
 E_2(\gamma) = & \sum'_{R_{AB}} \left[2t_{2211} \kappa_{21}^2 \text{Re} \left(\frac{e^{i2(\psi_{21}-\varphi)}}{R_{AB}^5} \right) \right. \\
 & \left. + 4t_{2220} \kappa_{20} \kappa_{22} \text{Re} \left(\frac{e^{i(\psi_{22}-2\varphi)}}{R_{AB}^5} \right) \right] \\
 = & -5 \kappa_{21}^2 \text{Re} \left(e^{2i\psi_{21}} \sum'_{R_{AB}} \frac{e^{-2i\varphi}}{R_{AB}^5} \right) \\
 & - 5 \sqrt{\frac{3}{2}} Q_{20} \kappa_{22} \text{Re} \left(e^{i\psi_{22}} \sum'_{R_{AB}} \frac{e^{-2i\varphi}}{R_{AB}^5} \right), \quad (15)
 \end{aligned}$$

and

$$\begin{aligned}
 E_4(\gamma) = & \sum'_{R_{AB}} \left\{ 2t_{2222} \kappa_{22}^2 \text{Re} \left[\frac{e^{i2(\psi_{22}-\varphi)}}{R_{AB}^5} \right] \right\} \\
 = & \frac{35}{4} \kappa_{22}^2 \text{Re} \left(e^{2i\psi_{22}} \sum'_{R_{AB}} \frac{e^{-4i\varphi}}{R_{AB}^5} \right). \quad (16)
 \end{aligned}$$

It only remains to evaluate the sum

$$\text{Re} \left(\sum'_{R_{AB}} \frac{e^{-ui\varphi}}{R_{AB}^5} \right) = \sum'_{R_{AB}} \frac{\cos u\varphi}{R_{AB}^5} = \sum'_{R_{AB}} \frac{\cos u \tan^{-1} \frac{y}{x}}{R_{AB}^5}, \quad (17)$$

where $u=(0,2,4)$, and the exponential is expanded to sine and cosine. The sum over the sine function vanishes as the considered lattices have inversion symmetry. The cosine and arc tangent can be expanded, eventually giving sums of the form $S(\vec{r}, u, v, w)$, $\vec{r}=(a, b)$ (see Appendix A); in detail

$$\sum'_{R_{AB}} \frac{1}{R_{AB}^5} = S\left(\vec{r}, \frac{5}{2}\right),$$

$$\sum'_{R_{AB}} \frac{\cos 2\varphi}{R_{AB}^5} = \underbrace{S\left(\vec{r}, \frac{7}{2}, 2, 0\right) - S\left(\vec{r}, \frac{7}{2}, 0, 2\right)}_{=0 \text{ if } a=b},$$

$$\begin{aligned}
 \sum'_{R_{AB}} \frac{\cos 4\varphi}{R_{AB}^5} = & S\left(\vec{r}, \frac{9}{2}, 4, 0\right) - 6S\left(\vec{r}, \frac{9}{2}, 2, 2\right) + S\left(\vec{r}, \frac{9}{2}, 0, 4\right) \\
 = & S\left(\vec{r}, \frac{5}{2}\right) - 8S\left(\vec{r}, \frac{9}{2}, 2, 2\right). \quad (18)
 \end{aligned}$$

Of course, the second sum vanishes for $a=b$. The sums $S(\vec{r}, u)$ for different $a/b, b=1$ are shown in Fig. 1. The

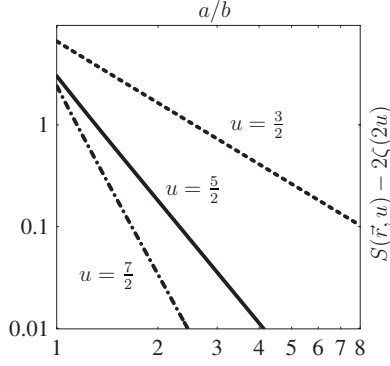


FIG. 1. Evaluated sum $S(\vec{r}, u)$ for $u = \frac{3}{2}$ (---), $u = \frac{5}{2}$ (—), and $u = \frac{7}{2}$ (-·-) as a function of a/b , where the sum is scaled to hold $b = 1$. To emphasize the behavior when approaching a linear chain—large a —the constant term $2\zeta(2u)$ is subtracted from each sum.

slowly converging sums for the anisotropic terms are plotted in Fig. 2.

As an example, let us consider a quadrupole that has only $Q_{20} = 1$ and rotate it in-plane by $\beta = \pi/2$ plus an arbitrary angle γ_0 within the plane. The in-plane axial multipole has the form $\kappa_{22} = \kappa_{2-2} = \sqrt{3}/8$, $\kappa_{21} = \kappa_{2-1} = 0$, and $\kappa_{20} = -1/2$, with $Q_{2m} = \kappa_{2m} \exp(-im\gamma_0)$, and the energy on a lattice with $a = 2b$ is thus

$$E(\gamma) \approx 1.092 - 3.685 \cos[2(\gamma + \gamma_0)] + 6.860 \cos[4(\gamma + \gamma_0)]. \quad (19)$$

Obviously, a common phase in the multipole moments only gives a phase in the energy function. In case of a general moment with different γ_{lm} the cosine functions may have different phase factors.

B. Dipole-octopole interaction on a rectangular lattice

Due to Eq. (12), the next higher order correction to the dipole-dipole interaction is introduced by an octopole. As the interaction can be separated into contributions of the same

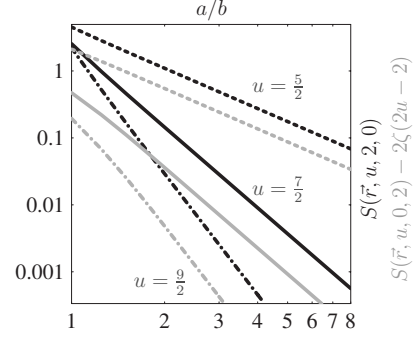


FIG. 2. Evaluated sum $S(\vec{r}, u, 2, 0)$ (black) and $S(\vec{r}, u, 0, 2)$ (gray) for $u = \frac{5}{2}$ (---), $u = \frac{7}{2}$ (—), and $u = \frac{9}{2}$ (-·-) as a function of a/b , where the sum is scaled to hold $b = 1$. While $S(\vec{r}, u, 2, 0)$ goes to zero with increasing a , $S(\vec{r}, u, 0, 2)$ approaches $2\zeta(2u-2)$. To show the convergence, this constant term has been subtracted. It is then obvious from the slope that both types of sums converge in the same way, i.e., $\propto a^{3-2u}$.

order l plus a combination of terms of different orders with $l_A \neq l_B$, the following example contains, naturally, the results for the pure dipole as well as the pure octopolar terms. The isotropic terms are

$$E_{\text{iso}}^{\text{dd}} = S\left(\vec{r}, \frac{3}{2}\right) (Q_{10}^2 - |Q_{11}|^2), \quad (20)$$

$$E_{\text{iso}}^{\text{oo}} = S\left(\vec{r}, \frac{7}{2}\right) \left(\frac{25}{4} Q_{30}^2 - \frac{75}{8} |Q_{31}|^2 + \frac{15}{4} |Q_{32}|^2 - \frac{5}{8} |Q_{33}|^2 \right), \quad (21)$$

$$E_{\text{iso}}^{\text{do}} = -S\left(\vec{r}, \frac{5}{2}\right) \left[3Q_{10}Q_{30} + 3\sqrt{\frac{3}{2}} \text{Re}(Q_{31}Q_{1-1}) \right]. \quad (22)$$

At this point it becomes obvious that the pair interaction decouples from the lattice sum. The superscripts dd and oo denote the pure dipolar and the pure octopolar terms, while the mixed term is labeled do. The anisotropic terms read

$$E^{\text{dd}}(\gamma) = -3 \underbrace{\left[S\left(\vec{r}, \frac{5}{2}, 2, 0\right) - S\left(\vec{r}, \frac{5}{2}, 0, 2\right) \right]}_{=0 \text{ if } a=b} \text{Re}(Q_{11}^2), \quad (23)$$

$$\begin{aligned} E^{\text{oo}}(\gamma) = & - \underbrace{\left[S\left(\vec{r}, \frac{9}{2}, 2, 0\right) - S\left(\vec{r}, \frac{9}{2}, 0, 2\right) \right]}_{=0 \text{ if } a=b} \left[\left(\frac{105}{8} \text{Re}(Q_{31}^2) + 7\sqrt{\frac{15}{2}} \text{Re}(Q_{32}Q_{30}) + 7\sqrt{\frac{15}{16}} \text{Re}(Q_{33}Q_{3-1}) \right) \right. \\ & + \left[S\left(\vec{r}, \frac{7}{2}\right) - 8S\left(\vec{r}, \frac{11}{2}, 2, 2\right) \right] \left(\frac{63}{4} \text{Re}(Q_{32}^2) + \frac{21}{4} \sqrt{15} \text{Re}(Q_{33}Q_{31}) \right) \\ & \left. - \underbrace{\left[S\left(\vec{r}, \frac{13}{2}, 6, 0\right) - S\left(\vec{r}, \frac{13}{2}, 0, 6\right) \right]}_{=0 \text{ if } a=b} + \underbrace{\left[15S\left(\vec{r}, \frac{13}{2}, 2, 4\right) - 15S\left(\vec{r}, \frac{13}{2}, 4, 2\right) \right]}_{=0 \text{ if } a=b} \right] \frac{231}{8} \text{Re}(Q_{33}^2). \end{aligned} \quad (24)$$

Again it is obvious that the first and the last term in Eq. (24) vanish if $a=b$, as there is no twofold nor sixfold anisotropy on a square lattice. Finally, there is the term due to the anisotropic interaction between dipole and octopole,

$$E^{\text{do}}(\gamma) = \underbrace{\left[S\left(\vec{r}, \frac{7}{2}, 2, 0\right) - S\left(\vec{r}, \frac{7}{2}, 0, 2\right) \right]}_{=0 \text{ if } a=b} \left(5\sqrt{\frac{3}{2}}\text{Re}(Q_{31}Q_{11}) + \sqrt{30}\text{Re}(Q_{32}Q_{10}) + \sqrt{\frac{5}{2}}\text{Re}(Q_{33}Q_{1-1}) \right) - 7 \left[S\left(\vec{r}, \frac{5}{2}, 2, 2\right) - 8S\left(\vec{r}, \frac{9}{2}, 2, 2\right) \right] \sqrt{\frac{5}{2}}\text{Re}(Q_{33}Q_{11}). \quad (25)$$

In case of $a=b=1$ the prefactor of the last term is almost -40 . Therefore, a noticeable fourfold anisotropy should arise even from a small octopole moment, while the twofold anisotropy vanishes again.

V. SIXFOLD SYMMETRY LATTICES

The next higher symmetry corresponds to the hexagonal lattice with $C_n=6$. The summation formulas given in Appendix A cannot be applied to this case. Nevertheless, the hexagonal lattice can be described as a centered rectangular one, and it is therefore possible to generate it by superimposing two identical rectangular lattices that are shifted against each other as shown in Fig. 3. The energy of a moment in it can thus be calculated in terms of two lattice sums, with each site being a member of one rectangular sublattice and in the center of the unit cell of the other. The latter position requires the more general sums given in Ref. 27. For the octopole moment, however, this is not necessary as direct summation is already sufficient. The dipole and quadrupole moments only give a constant contribution, which can be calculated with the help of Eq. (A4). The first sum to be evaluated for the octopole is of the form

$$\sum_{R_{AB}} \frac{\cos 6\varphi}{R_{AB}^7} \approx 5.915, \quad (26)$$

where the next-nearest-neighbor distance is $a=1$ and it is understood that R_{AB} runs over the points of the hexagonal

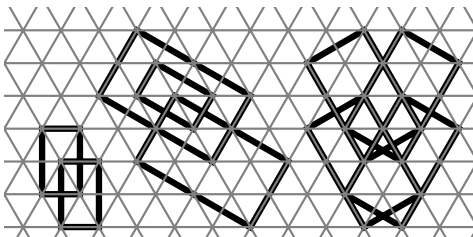


FIG. 3. Representation of the hexagonal, kagome, and honeycomb lattice as a superposition of rectangular ones. The hexagonal lattice (left) can be constructed out of two simple rectangular lattices, while the kagome lattice (center) requires three. To construct the honeycomb lattice (right), four simple rectangular lattices must be combined. The honeycomb lattice, hence, can be understood as the superposition of two hexagonal ones.

lattice. The honeycomb and kagome lattices,^{28,29} which are related to the hexagonal lattice, are also of theoretical and experimental interest. Both of them contain points of sixfold symmetry, although they are not lattice sites. One could say that for the lattice sites the symmetry is locally broken by the addition of a threefold or twofold term, respectively. This can be easily verified by numerical energy calculations, which show that, e.g., for a dipole on the kagome lattice, terms of the form $\cos(2\varphi)$ appear. The twofold symmetry breaking can have three different orientations, separated by an angle $\varphi_0=2\pi/3$. Therefore, taking three different lattice sites, the sum is proportional to $\cos(2\varphi) + \cos[2(\varphi+2\pi/3)] + \cos[2(\varphi+4\pi/3)]$, which is angle independent. Hence, there is on average no twofold anisotropy. As these two lattices can again be represented by a superposition of rectangular ones (see Fig. 3), it is possible to calculate the local anisotropy of a single moment by means of the sums in Ref. 27. As for the hexagonal lattice, the first anisotropic term that does not vanish on average appears for the octopole and can therefore be calculated by direct summation. For the isotropic energy of lower order moments analytical solutions exist (see, e.g., Ref. 30).

VI. LATTICES WITH ROTATIONAL SYMMETRY $C_{n>6}$

The results presented in the previous sections are based only on symmetry considerations, and therefore they hold also for non-Bravais lattices like the above-mentioned honeycomb and kagome lattices. The predictions can be extended also to quasiperiodic systems, provided that a mean symmetry is present in them. This is, for example, the case for the Penrose lattice (see Fig. 4).^{31,32} The technical relevance of quasicrystals might be questionable³³ (in several cases long-range order seems to be antiferromagnetic in quasicrystals,³⁴ if present at all³⁵), but they are used in non-linear optics³⁶ and—by laser interference—can be produced by rather standard lithographic methods. A quasicrystalline light field, e.g., due to interfering laser beams, may also trap dielectric particles on a surface and force them into a nonperiodic structure. In any case, quasicrystals are a good example of systems with higher rotational symmetries. Furthermore, the local symmetry is broken everywhere, although the nearest-neighbor distances and in-plane angles are well defined. This makes quasicrystals also a good template to study disorder in a controlled way. The local disorder leads to

strong fluctuations in the local interaction energy and the angle-dependent energy of a single multipole in the lattice may deviate strongly from the mean value of the complete system. Fortunately, in a very large (infinite) lattice these fluctuations cancel out, in a similar way as described above for the honeycomb lattice. The system will then behave like a lattice with tenfold symmetry, as shown in Table I. Hence, the lowest order on a Penrose lattice with anisotropy (on average) is a fifth-order moment, the dotriacontapole.

Finally, we would like to give one remark on quasicrystals like the Penrose lattice. Although the tiling is not periodic, each region of arbitrary size and shape can be found infinitely often in the lattice. Also, if the tiling is rotated by multiples of 36° , the copy of a rotated region of arbitrary size and shape can be found infinitely often.³⁷ This repetitive behavior in nonperiodic systems is known, e.g., from the irrational number π , in whose sequence of decimals any arbitrarily large sequence of digits will also appear infinitely often. From this point of view the symmetry is somewhat higher than might be expected from the term *nonperiodic*.

VII. EXAMPLE CALCULATION OF THE ANISOTROPY OF HOMOGENEOUS MAGNETIZED DISKS ON A RECTANGULAR LATTICE

As a demonstration of our calculation method, the anisotropy of in-plane magnetized disks on a rectangular lattice will now be computed. The lattice constants in the x and y directions are a and b , respectively. Due to symmetry the disks only have moments with l odd and $|m|=1$. Consequently, there is only a twofold anisotropy. Using the multipole moments calculated with the help of Eq. (B1) and inserting the moments into Eqs. (23)–(25), the angle-dependent energy of a disk of radius R_0 , height h , and volume $V = \pi R_0^2 h$ is

$$\begin{aligned}
 E(\gamma) = \cos 2\gamma \frac{\mu_0 M_S^2 V^2}{4\pi} & \left(\frac{3}{2} \left\{ S \left[\begin{pmatrix} a \\ b \end{pmatrix}, \frac{3}{2} \right] - 2S \left[\begin{pmatrix} a \\ b \end{pmatrix}, \frac{5}{2}, 2, 0 \right] \right\} \right. \\
 & + \frac{105}{384} \left\{ S \left[\begin{pmatrix} a \\ b \end{pmatrix}, \frac{7}{2} \right] - 2S \left[\begin{pmatrix} a \\ b \end{pmatrix}, \frac{9}{2}, 2, 0 \right] \right\} (h^2 - 3R_0^2)^2 \\
 & - \sqrt{\frac{75}{192}} (h^2 - 3R_0^2) \left\{ S \left[\begin{pmatrix} a \\ b \end{pmatrix}, \frac{5}{2} \right] \right. \\
 & \left. \left. - 2S \left[\begin{pmatrix} a \\ b \end{pmatrix}, \frac{7}{2}, 2, 0 \right] \right\} \right). \quad (27)
 \end{aligned}$$

The uniaxial anisotropy energy density is

$$\mathcal{E}(\gamma) = \frac{E(\gamma)}{2V} = K_u \cos 2\gamma \quad (28)$$

as the interaction energies contributing to the sums S originate from two disks each, therefore belonging to twice the volume of a disk.

The anisotropy constant as a function of lattice spacing for permalloy disks with radius $R_0=20$ nm and height $h=5$ nm on a rectangular lattice is shown in Fig. 5. Curves considering only dipole-dipole interaction, as well as curves

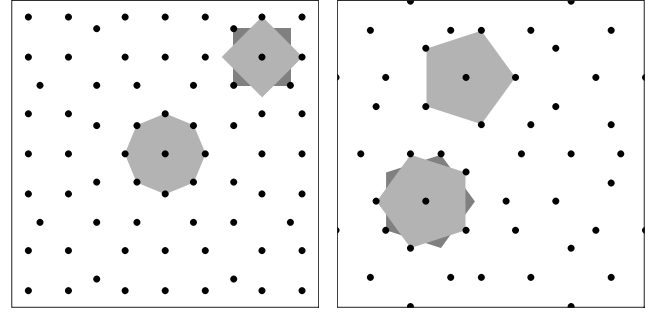


FIG. 4. Sections of the Ammann-Beenker (left) and the Penrose lattice (right). The lattices are scaled in such a way that the edges of the octagon and decagon—the nearest-neighbor distances—have lengths 1.

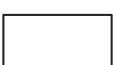



















including octopolar corrections, are presented. For a lattice with $2a=b=200$ nm the anisotropy is still significantly larger than the typical growth-induced anisotropy of a few 100 Jm^{-3} . Compared to experiment,³ the calculated values are somewhat high, as nonuniform magnetization and surface roughness in the disks decrease the surface charge, and therefore the interaction energy.

VIII. DISCUSSION

Besides providing a simple and efficient method to calculate the interaction energies for a system of identical particles with arbitrary charge or polarization distribution, the method described in the previous sections leads to several relevant conclusions. First of all, it is necessary to emphasize that dipolar coupling is frequently taken as a synonym of the more general electrostatic or magnetostatic interactions, neglecting the existence of higher order multipole terms and their associated effects. As discussed above, these multipoles can introduce anisotropy contributions that might play a dominant role in systems that were otherwise expected to behave isotropically, thereby essentially affecting their collective behavior.

Another important outcome of this work is related to the interparticle coupling in two-dimensional arrays. For most practical applications, and most notably for use as discrete magnetic storage media, it is necessary to ensure that the magnetization of any given particle can be controlled and modified independently of that of its neighbors. Simple inspection of Table I reveals that, in order to reduce the (electro-) magnetostatic coupling between adjacent identical objects with arbitrary moments, the rectangular or square arrangements are the least favorable choices. The higher the moments involved, the faster the interaction energy decays with increasing distance and the higher the required symmetry of the lattice to exclude anisotropic energy. As a rule of thumb one can thus conclude that the higher the lattice symmetry, the easier it is to compensate the stray field of surrounding particles. These considerations make, e.g., the Penrose tiling an interesting candidate. Of course, the practical use of these types of arrangements may create other problems, particularly for addressing the individual particles or bits in storage media. Nevertheless, our results emphasize

TABLE I. Typical anisotropy energies for in-plane axial multipole moments, e.g., linear molecules. Each table element depicts a polar plot of the anisotropy energy (scaled by an arbitrary factor to fit into the table) as well as the coefficients c_k for the expansion of the anisotropy in series of cosine functions (see Sec. III A). The anisotropy energy must be divided by twice the volume of one particle to get the anisotropy energy density. A constant energy has been added to shift the minimum to zero. The last two columns give results for the Ammann-Beenker and the Penrose tiling (see Fig. 4), which have eightfold and tenfold symmetry, respectively. These lattices represent so-called quasicrystalline structures and no simple summation of the lattice contribution is possible. The energy of multipole moments placed on these two lattices has been summed up numerically. The orientation of the multipole moments is varied and the energy as a function of the angle is fitted by cosine functions. The fit results are the values given in these columns. Due to the rather short-range interaction the results converge fast with increasing lattice size. The table is given for in-plane linear moments, which have, if oriented in the z direction, $Q_{l0}=1$. The nearest-neighbor distance is one and the energy is in units of $(4\pi\epsilon_0)^{-1}$. Therefore, the given constants c_k can be rescaled considering the scaling behavior in Eqs. (1), (2), and (4).

					
dipole	 $c_2 \approx 2.78$	—	—	—	—
quadrupole	$c_2 \approx -3.69$ $c_4 \approx 6.86$ 	$c_4 \approx 11.1$ 	—	—	—
octopole	$c_2 \approx 8.17$ $c_4 \approx -9.97$ $c_6 \approx 18.2$ 	$c_4 \approx -18.1$ 	$c_6 \approx -53.4$ 	—	—
hexadecapole	$c_2 \approx -21.5$ $c_4 \approx 23.8$ $c_6 \approx -29.4$ $c_8 \approx 55.1$ 	$c_4 \approx 45.3$ $c_8 \approx 114$ 	$c_6 \approx 87.5$ 	$c_8 \approx -21.4$ 	—
dotriacontapole	$c_2 \approx 32.6$ $c_4 \approx -66.0$ $c_6 \approx 74.3$ $c_8 \approx 93.5$ $c_{10} \approx 177$ 	$c_4 \approx -129$ $c_8 \approx 191$ 	$c_6 \approx -222$ 	$c_8 \approx 43.6$ 	$c_{10} \approx -68.5$ 

the importance of an adequate design strategy for the production of nanostructured materials.

Finally, any application of this calculation method to real materials should take into account the inevitable existence of disorder. Since the results outlined above only depend on symmetry considerations, they should not be essentially affected by local disorder, as long as this disorder is isotropic and does not change the global symmetry of the system. This hypothesis has been checked by numerical calculations per-

formed on both quasicrystalline and disordered Bravais lattices. In the latter, the original lattice sites were given random displacements of up to 20% of the lattice constant. In this case, although the symmetry of the anisotropy energy is maintained, neither is the magnitude of the anisotropic nor the isotropic energy term. This is of course due to the shape of the interaction, which diverges as the interparticle distance approaches zero. If the distribution of interparticle distances is known, the lattice sums could be weighted accordingly,

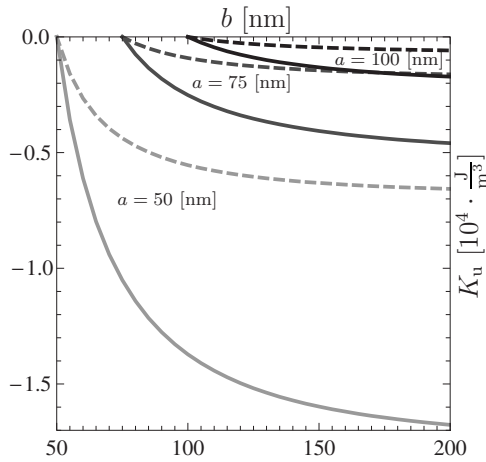


FIG. 5. Uniaxial anisotropy constant K_u of an array of in-plane magnetized permalloy disks (diameter 40 nm, height 5 nm) on a rectangular lattice with unit-cell side lengths a and b in the x and y directions, respectively. The anisotropy is given as a function of b for different a 's, and is zero in the limit of a square lattice ($a=b$). The dashed curves are first-order approximations; the solid ones contain third-order corrections. In detail: $a=50$ nm, - - - only dipole,—with octopolar corrections, $a=75$ nm, - - - only dipole,—with octopolar corrections, $a=100$ nm, (- - -) only dipole, (—) with octopolar corrections.

therefore allowing even the prediction of energies in disordered arrays.

Concerning quasicrystals it is important to mention that in principle the *disorder* can be measured. As only moments of large order l are important, in high symmetry lattices the energy converges very fast with distance and only next-nearest, or even nearest neighbors, have to be considered. In quasicrystals like the Penrose lattice, which can be generated by cut-and-project methods,³⁸ it is possible to count how many different surroundings a lattice site might have as well as the relative frequency with which one particular surrounding appears compared to others.³⁹ A more detailed study of quasicrystals could then give a more precise picture of the anisotropy in this type of lattices.

The results presented in this work are restricted to a very special case of anisotropy, i.e., coherent in-plane rotation in 2D lattices. The question may arise, if the results can be generalized to noncollinear states in three-dimensional (3D) lattices. This is in general possible and several results on multipole sums in three dimensions with fixed, collinear moments are known.^{40–42} As shown in Ref. 11, lattice sum and two particle interaction can still be separated. Nevertheless, simplifications based on symmetry will be more complicated and a more detailed treatment in terms of group theory might be required to decide whether there are vanishing terms in the anisotropy. On the contrary, the simple explanation furnished by Eq. (9) can be understood without knowledge of group theory.

Concerning noncollinear states in 2D the present results can be used in a modified version, if the system is periodic and can be decomposed into rectangular sublattices. The calculations then have to consider that the moments in different sublattices are different; in case of in-plane rotations they

have different phase factors. Nevertheless, the concept in such a system would be different, as, e.g., an increasing external field would transform the state—maybe continuously—into a collinear state instead of rotating each sublattice continuously in the same direction. Theoretically, it is possible to construct systems that would behave in the latter way, although it is questionable whether they can be realized in practice.

IX. SUMMARY

The energy of collinear multipole moments on a two-dimensional grid has been calculated analytically and numerically as a function of the moment's rotation angle. The analytical calculation shows that moments of order l are isotropic on lattices with rotational symmetry $C_{n>2l}$. On lattices with n -fold symmetry only zn -fold ($z \in \mathbb{N}$) anisotropy can appear. The calculation method described allows to separate the lattice geometry from the multipole moment properties.¹¹ For non-Bravais lattices like the honeycomb and the kagome, it has been shown that the energy of a single moment can differ from the average value, as the local symmetry differs from the global one.

The method can be applied in three different ways to experimental data. First, as the most general case, it is possible to check whether a system of unknown moments and symmetry shows anisotropy. If there is a nonzero anisotropy of order l , conclusions about the lowest mean symmetry and the lowest multipole moments can be drawn. In a second scenario the multipole moments can be calculated from the measured anisotropy, provided that lattices with known symmetry and no disorder are studied. If on the other hand the moments are known, a third application is to estimate the distribution function of disorder.

As a by-product of the calculation, it is also shown that the interaction between particles can be manipulated by an appropriate choice of the lattice symmetry, given the different range of the multipoles as a function of their order. It is suggested that, in order to minimize the effect of interparticle coupling, lattices with higher order symmetry should be used, while rectangular or square grids are to be avoided.

ACKNOWLEDGMENTS

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APPENDIX A: LATTICE SUMS

The sums that have to be evaluated for the interaction energy are of the form²⁷

$$S(\vec{r}, u, v, w) = \sum_{(i,j) \neq 0} \frac{(ai)^v (bj)^w}{[(ai)^2 + (bj)^2]^u}, \quad (\text{A1})$$

with $\vec{r}=(a, b)$. Here S , u , v , and w are used instead of T , α , β , and γ in contrast to Ref. 27, to avoid confusion with the

interaction tensor T and the Euler angles. Furthermore, the last two parameters are omitted, as they are always zero (as mentioned in the text, this is not the case for the hexagonal nor for the more complex honeycomb and kagome lattices). The isotropic term is a special case of this sum and has the form

$$S(\vec{r}, u, 0, 0) = S(\vec{r}, u). \quad (\text{A2})$$

For $a=b$ as well as $a=2b$ analytical solutions exist,^{43,44} i.e.,

$$S\left[\begin{pmatrix} 2 \\ 1 \end{pmatrix}, u\right] = (2 - 2^{1-u} - 2^{2-2u})\zeta(u) \frac{\zeta(u, \frac{1}{4}) - \zeta(u, \frac{3}{4})}{4^u},$$

$$S\left[\begin{pmatrix} 1 \\ 1 \end{pmatrix}, u\right] = 4^{1-u}\zeta(u) \left[\zeta\left(u, \frac{1}{4}\right) - \zeta\left(u, \frac{3}{4}\right) \right], \quad (\text{A3})$$

with the zeta function $\zeta(z)$ and the Hurwitz zeta function $\zeta(z, a)$. Furthermore, analytical solutions for the hexagonal lattice are known,³⁰

$$\sum'_{x,y} \frac{1}{(x^2 + xy + y^2)^u} = 2 \times 3^{1-u}\zeta(u) \left[\zeta\left(u, \frac{1}{3}\right) - \zeta\left(u, \frac{2}{3}\right) \right]. \quad (\text{A4})$$

For performing the summations, the formulas in Ref. 27 are simplified. As the modified Bessel functions $K_\nu(x)$ diverge for $x \rightarrow 0$, the sum for $l=0$ only exists in the sense of $\lim x \rightarrow 0$. Separating this summand and using the symmetry property that the sum required here does not change under $k \rightarrow -k$ and $l \rightarrow -l$, it can be written as

$$S(\vec{r}, u) = \sum_{k=1}^{\infty} \frac{8\sqrt{\pi} a^{(1/2)-u}}{\Gamma(u) b} \left[\frac{\Gamma(u - \frac{1}{2})}{4|k|^{2u-1} a^{u-(1/2)}} \right. \\ \left. + \sum_{l=1}^{\infty} \left| \frac{\pi l}{bk} \right|^{u-(1/2)} K_{u-(1/2)} \left(2a \left| \frac{\pi l k}{b} \right| \right) \right] + \frac{2}{b^{2u}} \zeta(2u). \quad (\text{A5})$$

The next sum that has to be calculated is $S(\vec{r}, \frac{5}{2}, 2, 0)$, which is equivalent to $S(\vec{r}, \frac{5}{2}, 0, 2)$ by changing $\vec{r}=(a, b)$ to $\vec{r}=(b, a)$. The simplified sum reads

$$S\left(\vec{r}, \frac{5}{2}, 2, 0\right) = \frac{8}{3b^3} \sum_{k=1}^{\infty} \left[\frac{b^2}{k^2 a^2} + \sum_{l=1}^{\infty} (2\pi l)^2 K_2 \left(a \left| \frac{2\pi l k}{b} \right| \right) \right]. \quad (\text{A6})$$

For the quadrupole, the following sum is required:

$$S\left(\vec{r}, \frac{7}{2}, 2, 0\right) = \frac{32}{15a^3 b^3} \sum_{k=1}^{\infty} \frac{1}{k^4} \\ \times \left[b^3 + 2 \sum_{l=1}^{\infty} (\pi l k a)^3 K_3 \left(\left| \frac{2\pi l k a}{b} \right| \right) \right]. \quad (\text{A7})$$

The next higher order sum, namely $S(\vec{r}, \frac{9}{2}, 2, 2)$, converges already so fast that direct summation is sufficient, though for comparison purposes it was calculated, too:

$$S\left(\vec{r}, \frac{9}{2}, 2, 2\right) = \frac{64}{105 ab} \sum_{k=1}^{\infty} \frac{1}{k^4} \\ \times \left\{ \frac{1}{2a^3} + \sum_{l=1}^{\infty} \left[\left| \frac{\pi l k}{b} \right|^3 K_3 \left(a \left| \frac{2\pi l k}{b} \right| \right) \right. \right. \\ \left. \left. - 2a \left| \frac{\pi l k}{b} \right|^4 K_2 \left(a \left| \frac{2\pi l k}{b} \right| \right) \right] \right\}. \quad (\text{A8})$$

For all higher order sums direct summation is applied.

APPENDIX B: MULTIPOLE MOMENTS OF AN IN-PLANE MAGNETIZED DISK

Let us assume a disk of radius R_0 and height h so the volume is $V = \pi R_0^2 h$. If the magnetization lies in-plane with an azimuthal angle ψ the l th order moment reads

$$Q_{l1} = \mu_0 M_S V e^{i\psi} \sum_{n=0}^{l-1} p_n(l, 1) \sum_{g=0}^{(l-n-1)/2} \binom{(l-n-1)/2}{g} \\ \times \sqrt{\frac{(l-1)!}{(l+1)!}} \frac{R_0^{2g} \left(\frac{h}{2}\right)^{l-2g-1}}{l-2g}, \quad (\text{B1})$$

with

$$p_n(l, 1) = \frac{1 + (-1)^{l+1-n}}{2} \frac{(-1)^{(l+1-n)/2}}{2^l} \\ \times \frac{(l+1+n)!}{\left(\frac{l-1-n}{2}\right)! \left(\frac{l+1+n}{2}\right)! n!} \quad (\text{B2})$$

and the binomial coefficient $\binom{l}{l}$. Negative m 's are obtained via the relation $(-1)^m Q_{lm} = Q_{l-m}^*$. The results for the dipole and octopole used in Sec. VII are

$$Q_{11} = -\mu_0 M_S \frac{V}{\sqrt{2}},$$

$$Q_{31} = -\mu_0 M_S \frac{V}{4\sqrt{3}} (h^2 - 3R_0^2). \quad (\text{B3})$$

Further results for $\psi=0$ are listed in Ref. 45.

APPENDIX C: MULTIPOLE EXPANSION OF A SCALAR POTENTIAL

A given potential Φ that fulfills Laplace's equation can be expanded in the form⁴⁶

$$\Phi(r, \theta, \varphi) = \sum_{lm} (A_{lm} r^l + B_{lm} r^{-(l+1)}) Y_{lm}(\theta, \varphi). \quad (\text{C1})$$

If there are no sources in the volume of interest, one must have $B_{lm}=0$ and naturally the A_{lm} depend on the choice of origin of the expansion,

$$A_{lm}(r) = \int_0^\pi d\theta \int_0^{2\pi} d\varphi \sin \theta \Phi(r, \theta, \varphi) Y_{lm}^*(\theta, \varphi). \quad (C2)$$

Therefore, the potential is a sum of harmonic functions and each term fulfills Laplace's equation.

Multipole-potential interaction

To calculate the interaction of the potential Φ with the multipoles Q_{lm} that describe the charge distribution $\varrho(\vec{r})$ we consider the general expression

$$\begin{aligned} E &= \int_V d\vec{r} \varrho(\vec{r}) \Phi(\vec{r}) = \int_V d\vec{r} \varrho(\vec{r}) \sum_{lm} A_{lm} r^l Y_{lm}(\theta, \varphi) \\ &= \int_V d\vec{r} \varrho(\vec{r}) \sum_{lm} A_{lm} \sqrt{\frac{2l+1}{4\pi}} R_{lm}(\vec{r}) = \sum_{lm} \sqrt{\frac{2l+1}{4\pi}} A_{lm} \int_V d\vec{r} \varrho(\vec{r}) R_{lm}(\vec{r}) = \sum_{lm} \sqrt{\frac{2l+1}{4\pi}} A_{lm} Q_{lm}. \end{aligned} \quad (C3)$$

The interchange of integration and summation requires the uniform convergence of the sum and it is further assumed that the potential is expanded around the center of charge of $\varrho(\vec{r})$. Hence, different orders l' and l of the expansions of the potential and the charge distribution do not interact.

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