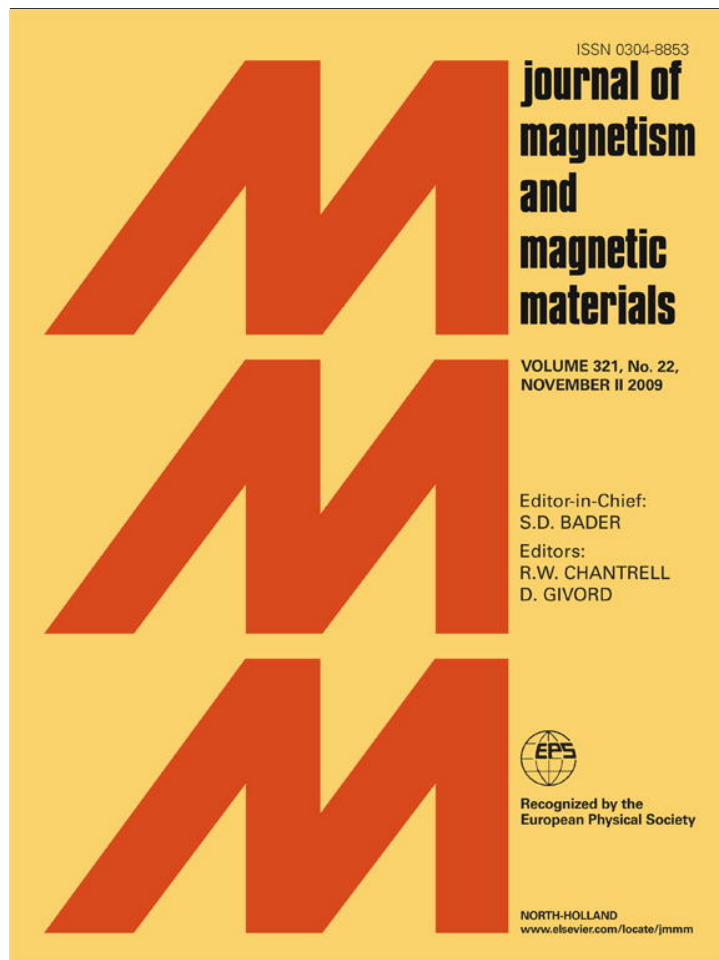


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Energy and force between two magnetic nanotubes

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ABSTRACT

The interaction energy and force between two parallel thin magnetic nanotubes is calculated using four different approaches. Although they agree for separation distances over 10 times the radius of any tube, some differences appear for shorter distances. Two exact methods giving identical results face handling difficulties in comparison with an approximate method based on a truncated expansion which produces fair enough results for distances to be found in the range of interest. Numerical calculations are done for cobalt particles of dimensions corresponding to nanotubes already manufactured and with properties reported in the literature. The force between two identical and parallel Co nanotubes ($L = 60 \mu\text{m}$, $D = 180 \text{nm}$), separated by a distance of 300 nm is of the order of few microdynes.

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1. Introduction

Low-dimensional ferromagnetic nanostructures attract attention both due to interesting fundamental properties and potential applications. Among several nanostructures are the magnetic nanotubes and nanowires. In particular magnetic nanotubes have advantage over the rest of non-magnetic nanotubes: they can be driven to the point of interest by means of externally applied magnetic fields. This is true whether the application of the magnetic nanotube is on a semiconductor chip or it is intended to reach an ill organ of a living body for drug delivery when filled with antibiotics or painkillers. The advantages of nanotubes over nanowires are easy to perceive: they have one more surface, their magnetization is easily reversed, nanotubes are lighter and can float in most liquids which usually do not penetrate completely the inner space due to its hydrophobic properties. The interest is stimulated by continuous improvements in the growth techniques using the self-assembly approach [1], like, for example, electro-deposition in combination with a porous template. Besides nanorods, whose magnetic properties have already been studied for many years, fabrication of more complicated structures, such as nanotubes either hollow or filled with a semiconductor material have been recently produced [2,3]. Simulations of such objects are focused on tubes with a small aspect ratio [4] or on

dynamic processes, like nucleation [5]. Reports on interacting nanotubes are scarce and no measurements or some estimation of the interacting forces is known to be reported so far. Recently, estimations on the interaction energy of two parallel and displaced nanocylinders have been calculated using magneto-static continuum theory in real space [6]. In this paper authors consider interactions between two nanowires and also between two thick nanotubes; in the present analysis we consider three pairs of nanotubes reflecting thin samples as characterized in recent experimental reports [3]. Moreover we extend the analysis to calculate the forces between the nanotubes. To accomplish this we use several approaches to cope with the calculation of the interacting energy between two parallel nanotubes. First, we use the magnetostatic continuum theory in the Fourier space to get an exact closed expression; second we use the approximation of tubes as wires for comparison purposes; third, we treat the hollow cylinder as a succession of wires around the circular cross section to do numeric simulations; fourth, we perform a series expansion of the last approach to truncate the series to the desired order of accuracy. This last expression is quite useful in comparison with the poor tube-as-wire approximation, converging well to the results obtained by the involved numeric and analytic work both reported here and in the recently quoted paper [6]. Moreover, we go beyond this point, extending the analysis to obtain the forces between these nanotubes by two different approaches: on one side the direct negative gradient of the interacting energy, while on the other side we obtain the magnetic field of one tube at the position of the other where interacts with the magnetization. Both approaches agree thus allowing a reliable estimation of the forces

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between two nanotubes with the idea this can be measured by experimentalists in the future. We understand this is the first report on estimated forces between magnetic nanotubes.

Although similar to magnetic nanowires in their aspect and fabrication methods magnetic nanotubes show different properties. Thus, for example, it can be shown that Fe nanotubes exhibit larger anisotropic magnetic response than that of nanowires [7]. Furthermore, Fe nanotubes are physically robust to temperature changes when compared to nanowires because of a smaller thermal expansion coefficient. Therefore, the Fe nanotubes are a promising ferromagnetic material to make durable data storage devices operating in rough environment [7]. An interesting application for magnetic nanotubes is the possibility of fabricating them in multisegmented form [8] and then use this product for barcode designs as it has already been demonstrated for ferromagnetic nanowires [9].

The magnetic nanotubes we bear in mind while doing present calculations are those reported by Nielsch et al. [3] due to their different aspect ratios thus providing different geometrical arrangements to test the expressions produced below. These Co nanotubes are produced in alumina and silicon templates giving external radii as those summarized in Table 1. Previous to electrodeposition the hollow pores in the template are filled in with polymers which determines a very thin magnetic metallic deposition on the walls of the pore. In such thin nanotubes only two possible phases are possible: in-plane vortex alignment and magnetization parallel to the tube axis [10]. However, the later dominates for long tubes, which is the case for the study under consideration.

We assume here long tubes as those reported in the literature [11] where only a ferromagnetic phase with magnetization along the cylinder axis is to be found; in most cases we specialize to thin tubes. The main aims of the present paper are to calculate the interaction energy and the interaction force between two parallel nanotubes with geometries close to those already attained by the experimental groups. In doing so we will use different methods. They range from exact analytic expressions (under certain conditions) to the crude approximation of considering the nanotubes as wires; however, we also consider exact numerical calculations and series expansions. Results show consistency and they allow a reliable estimate of the interaction energy and interaction forces between two nanotubes. Thus, for instance, the force between two nanotubes could get to be about $100\ \mu\text{dyn}$ under appropriate conditions. The measurement of such forces could be a test for this classical approximation towards the nanoscopic magnetic materials (wall thickness is quite small). Eventually in this way some manifestations of quantum magnetism could become noticeable.

In the next section and in the appendix we do the theoretical treatment for the four methods in the following way. The analytic approach follows the method introduced by Beleggia [12] to describe the magnetization due to objects of different shapes. We have found more convenient to perform the analysis in the configuration space, and later use the Fourier transform of magnetization, field, potentials and energy, to bring them back to real space. We follow the general approach by Beleggia for interacting objects [13], where our analysis specializes for the geometries appropriate for nanotubes. This process is mediated by the use of the program Mathematica. In the appendix we give the steps leading to the evaluation of an integral that appears in the expression for the energy. It will turn out that even when the approximation of thin tubes is used the final analytic expression achieved is rather cumbersome. In the baseline of this analysis it is always the case when the two tubes can be considered as wires or magnetic lines, coinciding with the axes of the tubes; we will find that this approximation gives only a rough approximation

that worsens as tubes get wider. Then we launch a search for alternative ways of calculating the interacting energy, looking for simpler ways and closed approximate expressions. We will report here a numerical approach in real space which gives results that are equivalent to those obtained by the involved analytic expression. Additionally, we perform a series expansion for the interaction energy, which gives good enough results for the most interesting geometries where these nanotubes are to be found.

In Section 3 we present and discuss results getting to the point of obtaining magnitudes for the forces to encourage experimentalist to actually measure them. Although weak, they exist in the several microdynes range and manifest themselves in putting together bunches of nanotubes when they are freed from their template. In Section 4 we draw conclusions.

2. Theory

Let us begin by defining the parameters associated to the geometry as described in Fig. 1. The two tubes are of the same dimensions and exactly parallel: inner radius is R_1 , external radius R_2 , length $2L$ and separation distance between the axes is d .

2.1. Tubes as wires

One extreme approximation is to consider the tubes as just extremely narrow magnetic wires (reduced to magnetic lines), with all the magnetic charge M concentrated along the geometrical axes of the tubes. In such a case the interaction energy is simply given by [14]

$$E^w = \frac{M^2}{2L^2d} \left(1 - \left[1 + \left(\frac{2L}{d} \right)^2 \right]^{-1/2} \right). \quad (1)$$

With the condition $L > d$.

2.2. Summation of infinitesimal nanowires

On each tube of small thickness w an infinitesimal wire can be defined with lateral dimensions w and $Rd\phi$ and length $2L$. The interaction between such an infinitesimal nanowire of total magnetic charge dM_1 in tube 1 ($\phi = \alpha$) and another infinitesimal

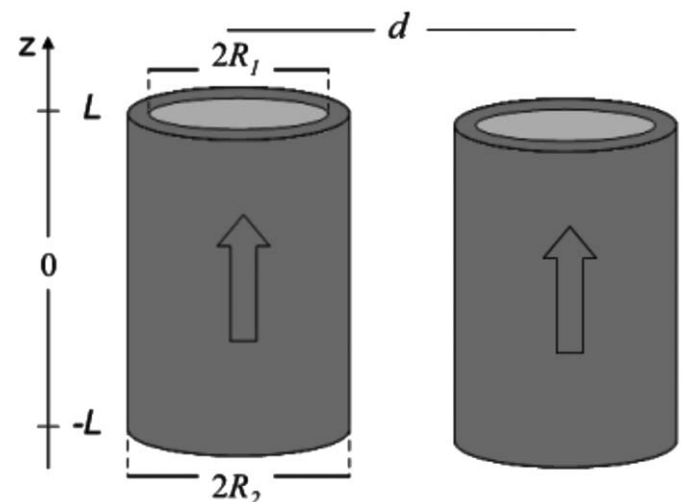


Fig. 1. Geometrical parameters defining the interaction between two identical and parallel nanotubes of length $2L$, inner radius is R_1 , and external radius R_2 . The $z = 0$ position coincides with the middle of the tubes length. The separation distance d will be our independent variable in the forthcoming analysis.

nanowire of total charge dM_2 in tube 2 ($\phi = \beta$) is illustrated in Fig. 2. The corresponding magnetostatic energy is

$$\delta E^w = \frac{dM_1 dM_2}{2L^2 \eta} \left[1 - \left[1 + \left(\frac{2L}{\eta} \right)^2 \right]^{-1/2} \right], \quad (2)$$

where η is the distance between these two infinitesimal nanowires.

The interaction energy between the two nanotubes is obtained as the sum among all possible infinitesimal nanowires sitting at different tubes, namely

$$E^S = \frac{M^2}{8\pi^2 L^2 R} \int_0^{2\pi} \int_0^{2\pi} d\alpha d\beta \times \left[\frac{d}{R} + (\cos\alpha - \cos\beta)^2 + (\sin\alpha - \sin\beta)^2 \right]^{-1/2} \times \left\{ 1 - \left\{ 1 + \frac{2L}{R} \left[\frac{d}{R} + (\cos\alpha - \cos\beta)^2 + (\sin\alpha - \sin\beta)^2 \right]^{-1/2} \right\}^{-1/2} \right\}. \quad (3)$$

So far we do not have a closed expression for the result of the integration so we will numerically integrate it to obtain this form E^S for the interaction energy obtained by computer simulation.

2.3. Series expansion

It is possible to expand the integrand in previous expression for the case $R < d$, which is always satisfied. Then we integrate term by term up to the desired order of accuracy. Thus we find

$$E^{X2} = \frac{M^2}{4L^2 d} \left[2 + \frac{R^2}{d^2} - \frac{d}{L} \right] \quad (4)$$

up to $(R/d)^2$, and

$$E^{X4} = \frac{M^2}{4L^2 d} \left[2 + \frac{R^2}{d^2} + \frac{27R^4}{16d^4} - \frac{d}{L} \right] \quad (5)$$

up to $(R/d)^4$, where the condition $d < L$ still holds.

2.4. General analytic approach

By using the continuum theory in the Fourier space, we can obtain an analytical expression for the magnetostatic interaction between two ferromagnetic nanotubes. Calculations in the Fourier space require the transformation of magnetization, local magnetic field and potentials. We followed the methodology introduced by Beleggia et al. [12]. In our case of two tubes with axial

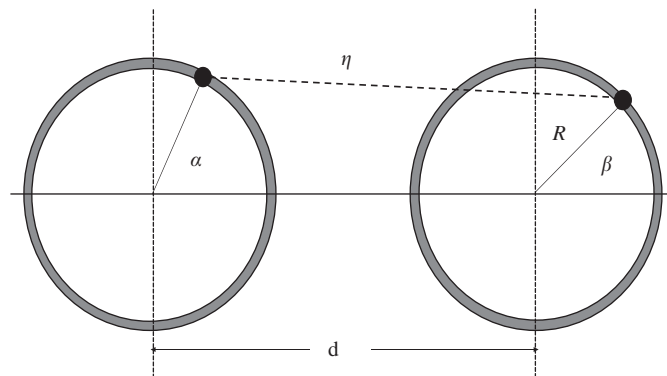


Fig. 2. Cross-section for the interaction between two nanotubes as due to the sum of interactions of pairs of infinitesimal nanowires: one on each tube.

magnetization we use the approximation of thin walls. This approximation is valid for most of the known systems anyhow. We consider tubes with thickness $w = (R_2 - R_1)$ much less than the external radius R_2 of the tube. In such case we have found a close expression E^A for the interaction energy (the details of calculation are given in Appendix A):

$$E^A = \frac{M^2}{2L^3} \left\{ \frac{L}{d^2} F_1^2 \left[\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2} \left(1 - \sqrt{1 - \left(\frac{2R}{d} \right)^2} \right) \right] - \sum_{m=0}^{\infty} \sum_{s=0}^{\infty} \eta(s, m) \left(\frac{d}{L} \right)^{2s} \left(\frac{R}{L} \right)^{2m} \right\} \quad (6)$$

with $R = (R_2 + R_1)/2$. M represents the total magnetization of each particle. The function $\eta(s, m)$ in this equation corresponds to

$$\eta(s, m) = \frac{(-1)^{s+m}}{(s!)^2 2^{4s+4m+1}} \frac{\Gamma[2m+2s+1]}{(m!)^2} {}_2F_1[-m, -m; 1; 1]. \quad (7)$$

We also make use of the hypergeometric function ${}_2F_1[a, b; c; z]$ and gamma function $\Gamma[x]$. Where we have used the program Mathematica to do some of the algebra. In addition the restriction $d < 2L$, applies, which is realistic for all known cases.

3. Results and discussion

In order to analyze and compare these four approaches we will apply previous expressions to geometries of the already mentioned existing cobalt nanotubes. We begin with the widest tube as Case 1 (labelled c in the original paper). All dimensions are summarized in Table 1. Upon calculating the total magnetization of each tube we assume $1.5 \mu_B$ (Bohr magneton as unit) per Co atom.

The independent variable is d the distance between the axes of the two nanotubes which we vary from $2R$ (the closest possible approach) to $10R$, which covers the region of interest for practical purposes.

3.1. Energy

We compare now previous expressions for the interaction energy applying them to each of the three geometrical cases depicted in Table 1. The appropriate symbols to characterize each method are presented for Case 1 and are maintained as we proceed to report the other two cases.

Case 1: The energy curves for tube labelled Case 1 in Table 1 are given in Fig. 3. It is necessary to point out that expressions for E^A and E^S give entirely equivalent results so only one of these curves appears in Fig. 3. It can be noticed that the higher order expansion E^{X4} lays slightly below the exact results for short distances, while the wire approximation E^W is notoriously off for the most interesting part of the interval. A vertical dashed line marks the distance between nearest neighbors in the silicon template where these tubes were fabricated, serving as a useful reference distance. The inset enlarges the interval for the most probable distances, where there is also room to include the low order expansion E^{X2} which shows that first order expansion (although better than the

Table 1 Geometrical parameters for the three different Co nanotubes reported in Ref. [15].

Case	In Ref. [15]	$2L$ (nm)	R_2 (nm)	w (nm)
1	c	12 000	260	9.5
2	b	60 000	180	6.2
3	a	60 000	90	3.3

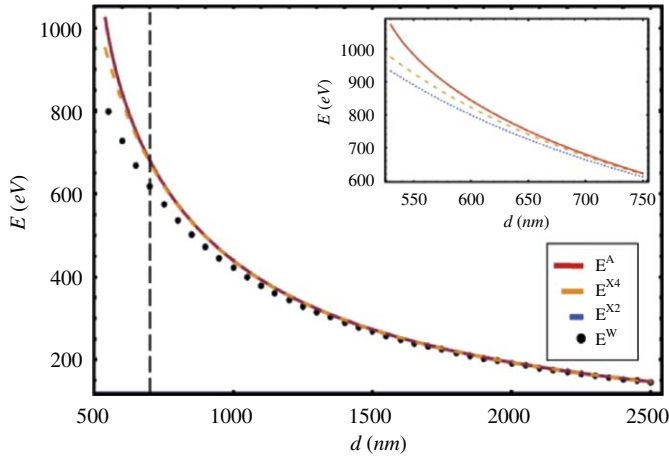


Fig. 3. Results for Case 1 (or nanotube c) of Table 1. The continuous curve corresponds both to E^A and E^S since they yield indistinguishable results. Discontinuous lines represent E^{X4} and E^{X2} (the latter in the inset only) which are the higher and lower order expansions respectively. Dotted line is used to represent E^W , the single wire approximation for the interaction between two nanotubes. The vertical dashed line in the main figure marks the distance for the average nearest neighbor distance between the axes of the nanotubes captured in the silicon template.

single wires approach) can still be notoriously improved to estimate interactions among magnetic nanotubes.

Case 2: The corresponding energy curves for tube are given in Fig. 4. Notice that values of energy are lower than those in previous case due to the smaller radius and thinner walls that by far compensates longer tubes. Once again E^A and E^S coincide and the expansion E^{X4} gives good general results for this system for the interval of interest, while the wire expression is still off exact values for most of the interval. Eventually this last approximation is becoming slightly better for long distances now due to the smaller radius of the tubes.

Case 3: The corresponding energy curves are given in Fig. 5. Notice that the interaction energy is lower than in two previous cases as these are the thinnest tubes and also the radius is the smallest among the three systems. As in previous cases E^A and E^S coincide. The expansion E^{X4} gives good general results for this system for the interval of interest and E^W is now closer to the exact results for this narrower tubes thus confirming previous hypothesis. Namely, as the radii of the nanotubes get smaller the expression for extremely narrow nanowires converges to the exact solution specially for long distances between nanotubes.

The expression for the energy found in Escrig et al. [6] agrees with ours in the long distance range, however, such expression fails to describe the interaction energy between two tubes in the short distance range.

3.2. Force

We maintain the indices and symbols used in previous subsection to identify each one of the approaches developed in Section 2.

One possible observable for the interaction between nanotubes is the interacting force between two such nanotubes, which can be obtained as the gradient of the corresponding interacting energy. Namely

$$F = -\nabla E, \quad (8)$$

where E represent the energy in any model as seen in the preceding section.

Case 1. The force curves for tube labelled Case 1 in Table 1 are given in Fig. 6. Expressions for E^A and E^S give entirely equivalent

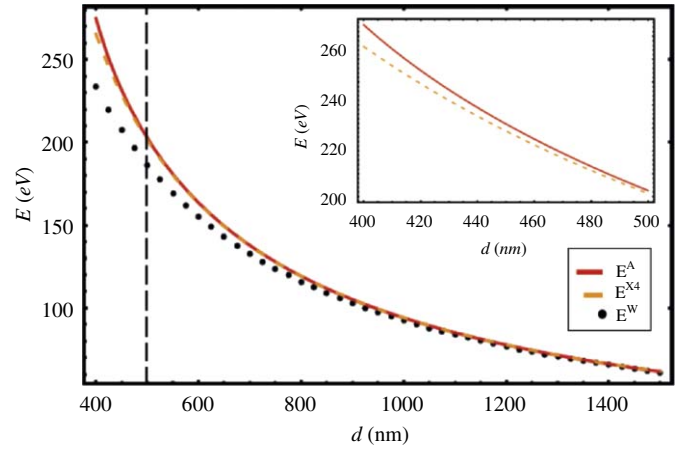


Fig. 4. Results for Case 2 (or nanotube b of Table 1). The solid curve corresponds both to E^A and E^S . Discontinuous line is for E^{X4} and dotted line represents E^W . The vertical dashed line is drawn at the average distance between neighboring nanotubes in the alumina template.

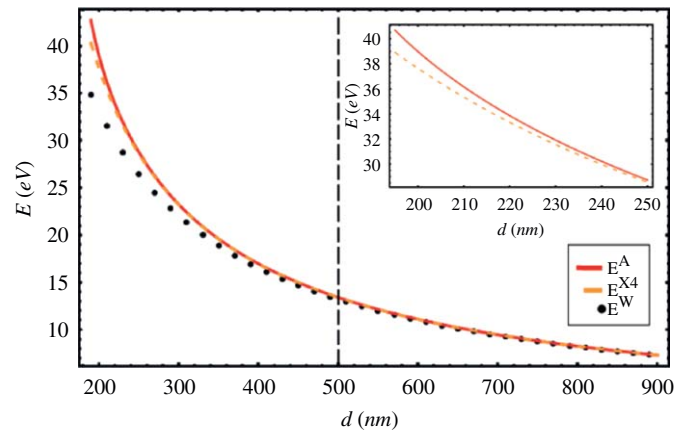


Fig. 5. Energies for Case 3 (or nanotube a of Table 1). The solid curve corresponds both to E^A and E^S , discontinuous line represents E^{X4} and dotted line is used to represent E^W . The dashed line is drawn at the average nearest neighbor distance between the axes of the nanotubes in the alumina template.

results so only one of these curves shows in Fig. 6. The higher order expansion E^{X4} lays slightly below the exact results for short distances, while the wire approximation E^W is clearly off for this interval. The dashed line marks the average distance between two of these nanotubes in the original array. The inset enlarges the interval for the most probable distances. In the inset we also include the low order expansion E^{X2} which shows that first order expansion (although better than the single wires approach) is not good enough to estimate forces among nanotubes.

Case 2: The force curves for tube labelled Case 2 in Table 1 are given in Fig. 7. Once again F^A and F^S coincide. The expansion F^{X4} gives good general results for this system for the interval of interest.

Case 3: The force curves for tube labelled Case 3 in Table 1 are given in Fig. 8. As in previous cases E^A and E^S coincide. The expansion E^{X4} gives good general results for this system for the interval of interest and even E^W is now closer to the exact results for this narrower tubes.

An alternative path to determine the magnetostatic force between two nanotubes is to consider the magnetic field generated by one tube acting on the second one. From standard magnetostatic theory, we can determine the force on a magnetized body exerted by an external field \mathbf{B}_e . For a uniformly magnetized body, with magnetization given by $\mathbf{M} = M_0\hat{z}$, and in

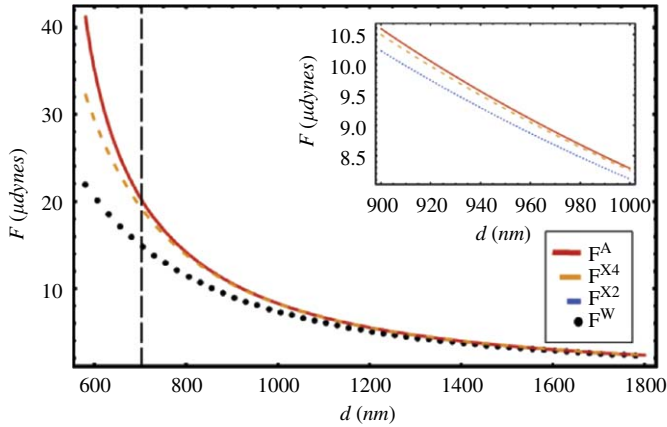


Fig. 6. Forces for Case 1 of Table 1. The solid curve corresponds both to F^A and F^S since they are indistinguishable for this interval. Discontinuous lines represent F^{X4} and F^{X2} (in the inset) which are the higher and lower order expansions respectively. Dotted line is used to represent F^W , the single wire approximation for the interaction between two nanotubes. The vertical dashed line is drawn at the average nearest neighbor distance between the axes of the nanotubes frozen in the silicon template.

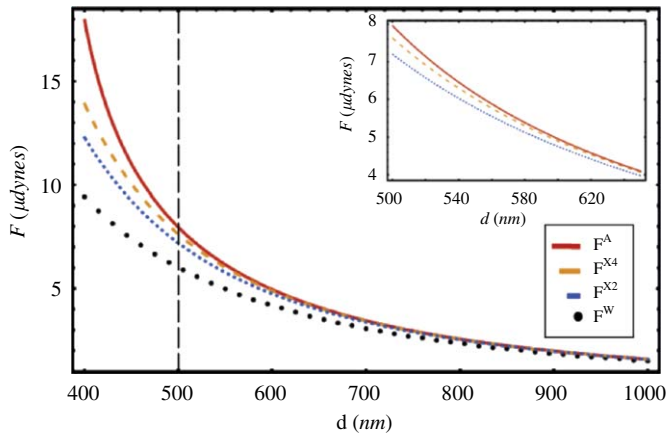


Fig. 7. Results for Case 2 of Table 1. The solid curve corresponds both to F^A and F^S . Discontinuous lines represent F^{X4} . Dotted line is used to represent F^W . The dashed line is drawn at the average nearest neighbor distance between the axes of the nanotubes frozen in the alumina template.

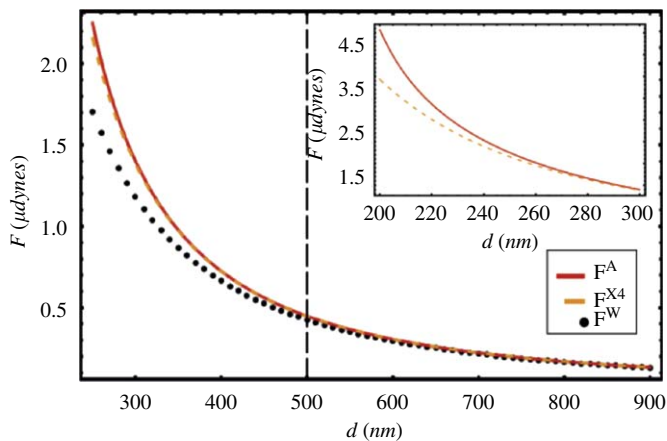


Fig. 8. Forces for Case 3 of Table 1. The solid curve corresponds both to F^A and F^S . Discontinuous lines represent F^{X4} . Dotted line is used to represent F^W . The dashed line is drawn at the average nearest neighbor distance between the axes of the nanotubes frozen in the alumina template.

the absence of macroscopic currents, the force acting on a nanotube is given by the following expression [16]:

$$\mathbf{F}(\mathbf{r}) = M_0 \int_S \mathbf{B}_e(\mathbf{r}) ds, \quad (9)$$

where the integration needs to be performed over the two end surfaces of the tube at $z = \pm L$ only, and $\mathbf{B}_e(\mathbf{r})$ represents the magnetic field generated by the second tube, which can be determined throughout the following relationship:

$$\mathbf{B}_e(\mathbf{r}) = \frac{\mu_0 M_0}{4\pi} \int_S \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2} ds', \quad (10)$$

where \mathbf{r}' is vector on the tube surface and \mathbf{r} represents the position where we like to calculate the field. The integral appearing in Eq. (10) has to be solved numerically. In Fig. 9 we show the variation of the magnetic field with respect to distance between the objects (main body). We have chosen Case 1 from Table 1 to illustrate this study. It shows how the magnetic field of one nanotube decreases with distance at the position $z = \pm L$ where surface integral given by the last equation must be evaluated; notice that B_{ez} is always zero and the rest of the field is radial. In Fig. 10 we show the variation of the field components with respect to z axis for a fixed intertube distance of 700 nm; it is clear that the main presence and variations of the magnetic field is at the ends of the tubes.

Now, once the field is known, we can determined the force acting over the second nanotube according to Eq. (9), where we numerically determined the field average on the top and bottom surfaces of the tube. Results are presented in Fig. 11, where the dots represent these numerical evaluations for different distances, designated by F^C , which is compared to the force obtained by the exact analytical method F^A (indistinguishable from F^S). The agreement is remarkable considering the entirely different approaches followed to obtain these results, thus providing confidence on the numerical evaluation of these forces. This is of importance since studies on the interactions between magnetic nanotubes are scarce and no reports of measurements of the interacting forces are known so far. Hopefully this estimation of the magnitude of these forces, in the range of some microdynes, can stimulate such experiments.

4. Conclusions

We have found both the interacting energy and the interacting force between two thin nanotubes by means of different analytic

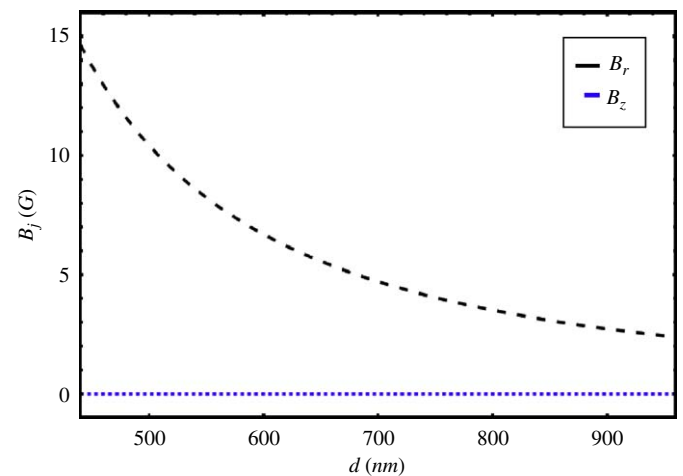


Fig. 9. Absolute value of magnetic field components generated by one nanotube, evaluated at $z = \pm L$, as a function of the distance of d to the axis of the tube. We have used parameters corresponding to the Case 1 (see Table 1).

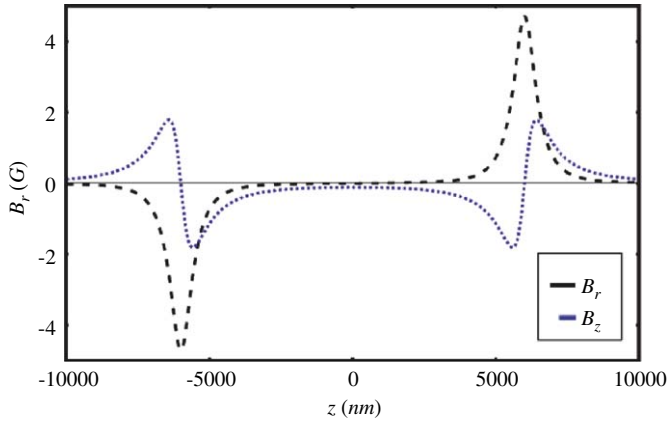


Fig. 10. Components of the field for fixed distance $d = 700$ nm as a function of the height z along the axis of the nanotube. We have used parameters corresponding to the Case 1 (see Table 1).

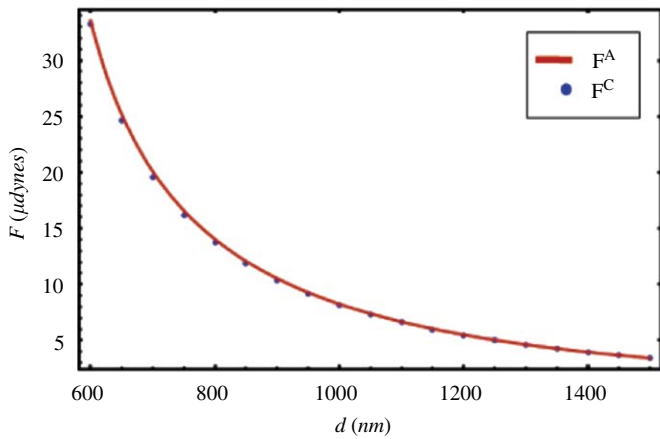


Fig. 11. Force for Case 1 of Table 1. The solid curve is obtained from either E^A or E^S using Eq. (18). Dots represents the force obtained by means of the magnetic field.

and numeric methods. Such treatments were applied to obtain numeric evaluations using parameters of real magnetic nanotubes available in the literature. One way to obtain the interacting force is to apply the negative gradient over the interacting energy. We do this by four different methods.

First, analytic expression E^A and F^A (energy and force respectively) were obtained by means of magnetostatic continuum theory in Fourier space; the program Mathematica was used to cope with some complex mathematical steps. Second, we divided the tube into longitudinal stripes along the axis, each one considered as a nanowire. The interaction between two such nanowires (one on each nanotube) is summed up to numerically get the E^S and F^S . It turns out that these results are indistinguishable from the previous ones. The disadvantages are that the analytic expression given by Eq. (6) is rather involved, while the numeric approach requires numeric integration which masks the functional dependence on the physical parameters. Third, we do a series expansion of the general expression obtained by previous treatment in terms of R/d (tube radius over distance). It turns out that the expression up to $(R/d)^4$ for E^{X4} and up to $(R/d)^5$ for F^{X4} give good enough results as compared with those obtained by previous exact results. The advantage of these truncated series expressions is their simplicity. Fourth, we can always think of a tube as a wire in first approximation, however, this approximation is very poor and by no means advisable to estimate energies or forces.

Independently of previous approach we also obtained the interacting force as the interaction of the magnetic field produced by one nanotube over the other one. The calculation once again is mathematically involved and requires numerical integration. However, these results by means of F^C agree very well with the exact forces F^A and F^S .

The evaluation of interaction energies by the four alternative methods leads to interaction energies of a few hundreds of eV, which eventually could reach 1 keV upon optimizing the geometry in the fabrication of the nanotubes. By the same token, interaction forces could reach $100 \mu\text{dyn}$. Such forces could be measured by opposing two of these nanotubes in a torsion balance or by any other experimental method. If experimental results confirm previous calculations, the extension of the theory of continuous magnetization to systems with walls of a few nm would be established. If this is not the case and the forces are quite different from those calculated above, the possibility of corrections coming from quantum magnetism is a real possibility.

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Appendix A. Interaction energy calculation in the Fourier space

The interaction energy between the two objects can be cast into the following form [12]:

$$E^{int} = \text{Re} \left[\frac{\mu_0 M_1 M_2}{8\pi^3} \int \frac{d^3 \mathbf{k}}{|\mathbf{k}|^2} |\hat{\mathbf{m}}_1 \cdot \mathbf{k} | \hat{\mathbf{m}}_2 \cdot \mathbf{k} (\mathbf{D}_1(\mathbf{k}) \mathbf{D}_2^*(\mathbf{k})) e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} \right], \quad (\text{A.1})$$

where Re denotes the real part of the expression to the right. At this point we have considered uniform magnetization within the particle, namely, $\mathbf{D}_j(\mathbf{k}) = D_j(k) \hat{\mathbf{m}}_j$.

In the presence of two identical tubes and after some manipulations, the previous expression can be transformed into the following form:

$$E^{int}(r) = \frac{\mu_0 M_0^2}{4\pi r^3} S_2(r, R, L), \quad (\text{A.2})$$

where function S_2 is given by

$$S_2(r, R_1, R_2, L) = \frac{2r^3}{L^2(R_2^2 - R_1^2)^2} \int_0^\infty \frac{dk}{k^2} (1 - e^{-2kL}) J_0(kr) \times [R_2 J_1(kR_2) - R_1 J_1(kR_1)]^2, \quad (\text{A.3})$$

in terms of $J_i(x)$ which are i th order Bessel's functions.

Therefore by changing variables $x = kL$ we can rewrite Eq. (A.3) as follows:

$$S_2(r, R, L) = \frac{2r^3}{L(R_2^2 - R_1^2)^2} \int_0^\infty \frac{dx}{x^2} (1 - e^{-2x}) J_0\left(\frac{r}{L}x\right) \times \left[R_2 J_1\left(\frac{R_2}{L}x\right) - R_1 J_1\left(\frac{R_1}{L}x\right) \right]^2. \quad (\text{A.4})$$

Now, we do the approximation for a nanotube with a very thin wall. $R_1 = R_2 = w$ with $w \rightarrow 0$. Then, by using a series expansion,

expression (A.3) reduces to

$$S_2(d, R, L) = \frac{d^3}{2L^3} \left\{ \int_0^\infty dx (1 - e^{-2x}) J_0\left(\frac{d}{L}x\right) J_0^2\left(\frac{R}{L}x\right) \right\}, \quad (\text{A.5})$$

where $d = r$ and $R = (R_1 + R_2)/2$. We can rewrite this as follows:

$$S_2(d, R, L) = \frac{d^3}{2L^3} \int_0^\infty J_0\left(\frac{d}{L}x\right) J_0^2\left(\frac{R}{L}x\right) dx - \frac{m_z^2 d^3}{2L^3} \int_0^\infty e^{-2x} J_0\left(\frac{d}{L}x\right) J_0^2\left(\frac{R}{L}x\right) dx. \quad (\text{A.6})$$

The integrals of Eq. (A.6) can be determined by using standard integration tables [17], where we find that

$$\begin{aligned} \text{Intg}^1 &= \int_0^\infty J_0\left(\frac{d}{L}x\right) J_0^2\left(\frac{R}{L}x\right) dx \\ &= \frac{L}{d^2} F_1^2 \left[\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2} \left(1 - \sqrt{1 - \left(\frac{2R}{d}\right)^2} \right) \right]. \end{aligned} \quad (\text{A.7})$$

To evaluate the second integral in (A.6) we do the approximation $d \ll L$ and we use the series expansion of the Bessel function $J_0(x)$

$$J_0(x) = \sum_{s=0}^\infty \alpha(s) x^{2s} \alpha(s) = \frac{(-1)^s}{2^{2s} (s!)^2} \quad (\text{A.8})$$

then,

$$\text{Intg}^2 = \sum_{s=0}^\infty \alpha(s) \left(\frac{d}{L}\right)^{2s} \int_0^\infty e^{-2x} x^{\lambda-1} J_0^2\left(\frac{R}{L}x\right) dx, \quad (\text{A.9})$$

where $2s = \lambda - 1$. Therefore the result for this integral is

$$\begin{aligned} \text{Intg}^2 &= \sum_{m=0}^\infty \sum_{s=0}^\infty \frac{(-1)^s}{(s!)^2 2^{4s+1}} \left(\frac{d}{L}\right)^{2s} \\ &\times \frac{\Gamma[2m+2s+1]}{(m!)^2} {}_2F_1[-m, -m; 1; 1] \left(-\frac{R^2}{16L^2}\right)^m. \end{aligned} \quad (\text{A.10})$$

Consequently, the function S_2 is given by the following expression:

$$\begin{aligned} S_2 &= \frac{1d^3}{2L^3} \left\{ \frac{L}{d} F_1^2 \left[\frac{1}{2}, \frac{1}{2}, 1; \frac{1}{2} \left(1 - \sqrt{1 - \left(\frac{2R}{d}\right)^2} \right) \right] \right. \\ &\quad \left. - \sum_{m=0}^\infty \sum_{s=0}^\infty \eta(s, m) \left(\frac{d}{L}\right)^{2s} \left(\frac{R}{L}\right)^{2m} \right\}, \end{aligned} \quad (\text{A.11})$$

where

$$\eta(s, m) = \frac{(-1)^{s+m}}{(s!)^2 2^{4s+4m+1}} \frac{(2(m+s))!}{(m!)^2} F[-m, -m; 1; 1]. \quad (\text{A.12})$$

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