

Representing structural information of helical charge distributions in cylindrical coordinates

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(Received 13 September 1996; revised manuscript received 25 October 1996)

Structural information in the local electric field produced by helical charge distributions, such as dissolved DNA, is revealed in a straightforward manner employing cylindrical coordinates. Comparison of structure factors derived in terms of cylindrical and helical coordinates is made. A simple coordinate transformation serves to relate the Green function in cylindrical and helical coordinates. We also compare the electric field on the central axis of a single helix as calculated in both systems. [S1063-651X(97)14303-3]

PACS number(s): 87.15.-v, 36.20.-r, 41.20.Cv

A few years ago we developed an exact analytical solution for a model of the local electric potential and field arising from the double helix of phosphate groups of a single *B*-DNA molecule immersed in an aqueous solvent [1]. We subsequently extended our calculation to treat the full (sugar phosphate plus base pairs) discrete charge distribution of homopolymer *B*-DNA in a solvent modelled by concentric dielectric cylinders [2]. In both cases we found a characteristic length scale of $\approx 5 \text{ \AA}$ associated with the radial persistence length of either the helical imprint or individual base-pair identity. These detailed calculations are based on a theoretical model of *B*-DNA in solution together with Green function techniques to account for the contribution of each individual (partial) charge to the full net potential. As we discussed in detail in [1,2], although the helical configuration of point charges does not possess cylindrical symmetry, the individual charges making up the backbone as well as the base pairs can be assigned to a set of concentric cylindrical surfaces, and thus cylindrical coordinates provide the most natural system in which to *separate* Laplace's and Poisson's equations. The full power of the Green function technique can be brought to bear on the problem, which is made non-trivial by the presence of a nonuniform dielectric. Moreover, in cylindrical coordinates one may easily identify and separate out the featureless zero-mode contribution to the potential. The zero mode, which goes as $\sim \ln(\rho)$, corresponds to the cylindrically symmetric potential from a straight line of charge and is what one sees far from the DNA surface. The higher-mode terms in the potential therefore encode and reveal the specific helical conformation of the molecule. The structural information contained in these higher modes is complete, transparent and calculable [1,2].

Though the above points have been adequately discussed in [1,2], we wish to emphasize them in light of a recent claim that structural information of (double) helix charge distributions is better represented employing helical rather than cylindrical coordinates [3]. There it was argued that structure factors derived in a certain helical coordinate system reveal structural information in a more "transparent" fashion. The

purpose of the present Brief Report is to demonstrate that similar structural information may be represented just as easily in cylindrical coordinates.

STRUCTURE FACTORS

We turn to the derivation of structure factors in cylindrical coordinates. In the interests of clarity and brevity, we shall restrict our attention to the case of a *single* helix immersed in a *single* dielectric background medium. In our two previous papers we calculated explicitly both the electrostatic potential and electric field components due to *many* helices (to account for the phosphate backbones and base pairs) immersed in a medium modeled by a triply piecewise constant dielectric function. However, since the single helix in a uniform background is the only case treated by the methods in [3], we will stick to this simple example to facilitate comparison.

Before tackling the full helix, we begin by considering the electrostatic potential for a *single* point charge q embedded in a uniform dielectric medium ϵ , and located at the point (a, ϕ', z') . From [4], or expression (B26) in the Appendix of [1], we have

$$\Phi(\rho, \phi, z) = \frac{4q}{\pi\epsilon} \sum_{m=0}^{\infty}{}' \int_0^{\infty} dk I_m(k\rho_{<}) K_m(k\rho_{>}) \times \cos[k(z-z')] \cos(m[\phi-\phi']), \quad (1)$$

where I_m and K_m are the modified Bessel functions of integer order m , and the prime on the sum indicates that the zero mode is to be divided by two. From this we can build up the electrostatic potential corresponding to a finite or an infinite distribution of (identical) point charges distributed along a helix of constant radius a and pitch P . We regard a single helix of evenly spaced point charges as a two-dimensional regular lattice wrapped around the cylinder $\rho=a$. Instead of summing the charges along the helix, we decompose this equivalent lattice into a finite collection of one-dimensional vertical line charges that run parallel to the z axis, and then sum over this "bundle" of one-dimensional chains. Denote the number of such chains by the integer N_o and the number of charges along any such chain (this can be finite or infinite) by $2N+1$. The total number of charges living on the helix is

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therefore equal to $N_o(2N+1)$. We now make this conceptual decomposition quantitative: the position in cylindrical coordinates of the n th charge on the s th vertical line with fixed angular coordinate ϕ_s is as follows: $(a, \phi_s, z_{n,s})$, where

$$\phi_s = \left(\frac{2\pi}{N_o}\right)s = \left(\frac{2\pi\Delta z}{P}\right)s, \quad z_{n,s} = nP + s\Delta z \quad (2)$$

for $0 \leq s \leq N_o - 1$ and $-N \leq n \leq N$, where Δz is the vertical rise per residue, and $N_o = P/\Delta z$ is the number of equally spaced residues per pitch length of the helix (see Fig. 1 of Ref. [1]). The single helix potential is obtained simply by replacing

$$z' \rightarrow z_{n,s} \quad \text{and} \quad \phi' \rightarrow \phi_s$$

in Eq. (1), and summing over the point charges,

$$\Phi_{\text{Helix}}(\rho, \phi, z) = \sum_{n=-N}^N \sum_{s=0}^{N_o-1} \Phi(\rho, \phi, z | a, \phi_s, z_{n,s}). \quad (3)$$

This leads to the following expression for the electrostatic potential from a single charged helix in a uniform background:

$$\begin{aligned} \Phi_{\text{Helix}}(\rho, \phi, z) &= \frac{2q}{\pi\epsilon} \sum_{m=0}^{\infty} \int_0^{\infty} dk G_1(k) \\ &\times \sum_{\pm} \{C^{\pm}(m, k) \cos(kz \pm m\phi) + S^{\pm}(m, k) \\ &\times \sin(kz \pm m\phi)\} J_m(k\rho_{<}) K_m(k\rho_{>}). \quad (4) \end{aligned}$$

The momentum-dependent structure factors appearing here are defined as follows:

$$\begin{aligned} G_1(k) &= \frac{\sin\left[(2N+1)\frac{kP}{2}\right]}{\sin\left(\frac{kP}{2}\right)} \quad (\text{for } N \text{ finite}) \\ &= \frac{2\pi}{P} \sum_{j=-\infty}^{\infty} \delta\left(k - \frac{2\pi j}{P}\right) \quad (\text{for } N \rightarrow \infty) \quad (5) \end{aligned}$$

and

$$\begin{aligned} C^{\pm}(m, k) &= G_2^{\pm}(m, k) \cos\left[(N_o - 1)\left(k \pm \frac{2\pi m}{P}\right)\Delta z/2\right], \\ S^{\pm}(m, k) &= G_2^{\pm}(m, k) \sin\left[(N_o - 1)\left(k \pm \frac{2\pi m}{P}\right)\Delta z/2\right]. \quad (6) \end{aligned}$$

The remaining structure factor appearing in Eq. (6) is defined by

$$G_2^{\pm}(m, k) = \frac{\sin\left[\frac{1}{2}(kP \pm 2\pi m)\right]}{\sin\left[\frac{1}{2N_o}(kP \pm 2\pi m)\right]}. \quad (7)$$

The final form in which we have written Eq. (4) results from working out the double sum in Eq. (3) and using one or more elementary series and/or trigonometric identities, as well as the Poisson summation formula, as for example, in Eq. (A3) of [1].

By inspection of Eq. (4), it is clear that structural information (as defined by the appearance of these so-called structure factors) of helical charge distributions is revealed in the cylindrical coordinate system. The structure factors depend explicitly on the pitch P and the rise per charge Δz which jointly parametrize the geometry of the helix.

Note that our $G_1(k)$ has the same mathematical form as the function $H_2(M)$ calculated in [3]. The reason for this coincidence is clear: both structure factors result from performing the charge sum (whether finite or not) over (half) the coordinate lines corresponding to each coordinate system. That is, we obtain G_1 from summing charges along the coordinate line $\theta = \text{const}$ (a line parallel to the z axis), whereas H_2 results by summing along the coordinate line $t = \text{const}$, that is, along a helix. The linear momentum in the \hat{z} direction is k , while that in the helical direction \hat{t} is M . One has in fact the formal correspondence between summing over vertical lines and summing over helices,

$$k \leftrightarrow M, \quad P \leftrightarrow \bar{s}. \quad (8)$$

In the helical coordinate system, $H_2(M)$ is the full structure factor for a single helix. In cylindrical coordinates, $G_1(k)$ gives the structure factor for a line charge, and is not the complete ‘‘answer,’’ as it were. That is why we need the additional factors $C^{\pm}(m, k)$ and $S^{\pm}(m, k)$, as can be checked, by summing over the N_o vertical chains. In the cylindrical system, the helical structure is encoded in terms of the factorized set of structure factors $G_1(k)C^{\pm}(m, k)$ and $G_1(k)S^{\pm}(m, k)$. The necessity of C^{\pm} and S^{\pm} could have been anticipated on general grounds if one thinks of Fourier analysis on a cylinder, namely, one expands an arbitrary function of ϕ and z in terms of the complete set of functions of chiral ‘‘up’’ and ‘‘down’’ moving ‘‘waves’’: $\{\sin(kz \pm m\phi), \cos(kz \pm m\phi)\}$. These coefficient functions (C^{\pm}, S^{\pm}) are simply the projections of helical structure along the two helical directions, but expressed in cylinder coordinates. This is why these basis functions appear in our Φ_{Helix} . We already made use of this fact during an intermediate stage of our published calculation [see, e.g., Eq. (B8) in [1]].

We may derive another form for the structure factor by performing the sum over charges in a distinct way. For example, if we now sum the point charges *along* the helix, then an equally transparent factor results—even using cylindrical coordinates. Only a single sum need now be carried out because the helix sum means we are to make the replacements

$$\phi' \rightarrow \phi_n = n\Delta\phi, \quad z' \rightarrow z_n = n\Delta z \quad (9)$$

in Eq. (1) and summing over the helix charges to replace Eq. (3) such that m is in the range $-M \leq n \leq M$ [not be confused with the momentum variable M appearing in Eq. (8)], to obtain the corresponding single helix potential. The origin charge corresponds to $n=0$ and has coordinates $(a, 0, 0)$. Note that for a finite helix, the net charge must turn out to be

the same no matter how we carry out the sum. This implies that $2M+1=N_o(2N+1)$. By going through identical steps as above, we find that the single helix potential is now represented as

$$\Phi_{\text{Helix}}(\rho, \phi, z) = \frac{2q}{\pi \epsilon_m} \sum_{m=0}^{\infty} \int_0^{\infty} dk \sum_{\pm} \{G_3^{\pm}(m, k) \times \cos(kz \pm m\phi)\} I_m(k\rho_{<}) K_m(k\rho_{>}). \quad (10)$$

Here the structure factors turn out to be

$$G_3^{\pm}(m, k) = \frac{\sin[\frac{1}{2}(2M+1)(k\Delta z \pm m\Delta\phi)]}{\sin[\frac{1}{2}(k\Delta z \pm m\Delta\phi)]} \quad (11)$$

for finite M (and hence, finite N), or

$$G_3^{\pm}(m, k) = 2\pi \sum_{j=-\infty}^{\infty} \delta(k\Delta z \pm m\Delta\phi - 2\pi j), \quad (12)$$

for M (or N) infinite. Again, the basic parameters $\Delta z, P$ describing the helix geometry are manifest in the cylinder-based structure factors. Moreover, the cylinder and helix-based structure factors G_3 and H_2 , are mathematically identical in form. The formal replacement is

$$M\bar{s} \rightarrow k\Delta z \pm m\Delta\phi, \quad (13)$$

and allows us to obtain one from the other.

The extension to double helices is straightforward. One merely adds in the potential for the dyadically related charges and then sums over the j th backbone charge q^j , making up the group:

$$\Phi_{\text{double-helix}}^j(\rho, \phi, z) = \Phi_{\text{helix}}^j(\rho, \phi + \alpha_j, z + \delta_j) + \Phi_{\text{helix}}^j(\rho, \phi - \alpha_j, z - \delta_j), \quad (14)$$

where α_j and δ_j are the offset angles and distances, respectively [1,2].

RELATION BETWEEN THE HELICAL AND CYLINDRICAL GREEN FUNCTIONS

From [4], the cylindrical Green function, that is, the potential for a unit ($q=1$) point charge in vacuum ($\epsilon=1$), is given by

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{2}{\pi} \sum_{m=-\infty}^{\infty} \int_0^{\infty} dk e^{-im(\phi-\phi')} \times \cos[k(z-z')] I_m(k\rho_{<}) K_m(k\rho_{>}). \quad (15)$$

A similar representation for the left hand side of Eq. (15) was given in [3], which involves the same set of basis functions (essentially products of exponentials and modified Bessel functions). Thus a coordinate transformation should suffice to relate these two Green functions. Since we are talking about the *same* function, and provided both coordinate representations are correctly worked out, then it must be the case that

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} \Big|_{\text{cylindrical}} = \frac{1}{|\mathbf{x}-\mathbf{x}'|} \Big|_{\text{helical}} \quad (16)$$

to be understood as an equality between one and the same function expressed in two different coordinate systems. Extending the range in the variable k in the above Green function (15) by replacing $k \rightarrow |k|$ in the arguments of the Bessel functions, use

$$\int_0^{\infty} dk \cos[k(z-z')] = \frac{1}{2} \int_{-\infty}^{\infty} dk e^{-ik(z-z')} \quad (17)$$

to rewrite the above Green function (15) (see also [4]). Now make (or define) the coordinate transformation $(\phi, z) \rightarrow (t, s)$:

$$z = s \sin\beta - t \cos\beta, \quad \phi = \frac{s}{a} \cos\beta + \frac{t}{a} \sin\beta, \quad (18)$$

which is just the transformation from cylindrical to helical coordinates defined in [3]. Here β is the pitch angle of the helix, and is related to the helix pitch by $P = 2\pi a \tan\beta$. This puts

$$e^{-im(\phi-\phi')} e^{-ik(z-z')} \equiv e^{-iM(s-s')} e^{-iM'(t-t')}, \quad (19)$$

provided we identify

$$M = \frac{m}{a} \cos\beta + k \sin\beta, \quad M' = \frac{m}{a} \sin\beta - k \cos\beta. \quad (20)$$

This identification can itself be inverted to yield

$$m = a(M' \sin\beta + M \cos\beta), \quad k = -M' \cos\beta + M \sin\beta. \quad (21)$$

In Eq. (21), m is an integer, while k represents the linear momentum along the z direction. These are written in terms of M' and M , which represent the components of linear momentum along the helical t and s -directions, respectively. Using Eqs. (17), (19), and (21), we can now rewrite the helical representation for $1/|\mathbf{x}-\mathbf{x}'|$ calculated in [3], and transform it back in terms of cylindrical variables. That expression was given as

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\pi} \int_{-\infty}^{\infty} dM dM' e^{-iM(s-s')} \times e^{-iM'(t-t')} I_{\lambda}(k\rho_{<}) K_{\lambda}(k\rho_{>}), \quad (22)$$

where $\lambda \equiv a(M' \sin\beta + M \cos\beta)$ and k is as above in Eq. (21). The first step is to insert the identity

$$\int_{-\infty}^{\infty} dm \delta(m - aM' \sin\beta - aM \cos\beta) = 1, \quad (23)$$

and perform the integration over M' . This gives a constant factor $(a \sin\beta)^{-1}$; this step is followed by replacing the integration over m by a discrete sum, $\int (dm/a) \rightarrow \sum_m$, in accord with the fact that m/a is the component of linear momentum in the ϕ direction of the cylinder. Next the identity

$$\int_{-\infty}^{\infty} dk \delta\left(k - \frac{aM - m \cos\beta}{a \sin\beta}\right) = 1 \quad (24)$$

allows one to carry out the integration over M . This produces a factor of $\sin\beta$ which cancels the $(\sin\beta)^{-1}$ from the previous step. Carrying out these steps together with the relations in Eqs. (19) and (20) demonstrates the equivalence (16) between the two representations calculated for the Green function.

ELECTRIC FIELD ON THE CENTRAL AXIS

Another point of direct comparison with the results of [3] is obtained by considering the calculation of the electric field on the central axis of the helix. It is not necessary to employ complicated Green functions in order to calculate the components of the electric field on the central axis in a *uniform* medium. The potential for a single point charge located at $\mathbf{x}' = (a, \phi', z')$ in a uniform dielectric medium is just

$$\begin{aligned} \Phi(\mathbf{x}) &= \frac{q}{\epsilon} \frac{1}{|\mathbf{x} - \mathbf{x}'|} \\ &= \frac{q}{\epsilon} \frac{1}{(\rho^2 + a^2 - 2a\rho \cos(\phi - \phi') + (z - z')^2)^{1/2}}. \end{aligned} \quad (25)$$

A textbook calculation yields the electric field on the central axis:

$$\begin{aligned} E_\rho(0, \phi, z) &= -\frac{q}{\epsilon} \sum_{n,s} \frac{a \cos\left(\phi - \frac{2\pi s \Delta z}{P}\right)}{(a^2 + (z - nP - s\Delta z)^2)^{3/2}}, \\ E_\phi(0, \phi, z) &= \frac{q}{\epsilon} \sum_{n,s} \frac{a \sin\left(\phi - \frac{2\pi s \Delta z}{P}\right)}{(a^2 + (z - nP - s\Delta z)^2)^{3/2}}, \\ E_z(0, \phi, z) &= \frac{q}{\epsilon} \sum_{n,s} \frac{(z - nP - s\Delta z)}{(a^2 + (z - nP - s\Delta z)^2)^{3/2}}. \end{aligned} \quad (26)$$

Since these formulas involve the features of the structure of the DNA (clearly through the two parameters Δz and P), their dependence on the lengths and nature of the DNA strands are also obtained here explicitly.

The much lengthier calculations for the electric field components on the (double)-helix central axis in [3] lead to the same results only after that calculation is corrected for a spurious factor of $\sin\beta$ [5]. Indeed, the step invoking the replacement of integration over M' in Eq. (22) by a sum

over $\lambda (= m)$ in [3] overlooked this factor of $(\sin\beta)^{-1}$ which results, as we see, from correct use of identity (23). Once this is done, the two sets of electric field components as calculated in terms of cylindrical and helical coordinates do agree.

Some concluding remarks are in order. First of all, and most importantly as demonstrated above, not only are cylindrical coordinates adequate for calculating potentials and fields due to helical charge distributions, they also lead to simple structure factors admitting a straightforward physical interpretation.

In regards to the helical coordinate system advocated in [3], it is a fact that Laplace's equation does not separate in helical coordinates. Indeed, it has been known for some time that there are exactly 11 coordinate systems in which the three-dimensional Laplacian is separable [6]; the helical system is not one of them. Nevertheless, the helical Laplacian in [3] was separated assuming an *a priori*, but not general, form for the t - and s -dependent factors of the product ansatz. For this reason, it is important to establish the validity of the Green function so constructed, and the coordinate transformation between cylindrical and helical systems leads, as shown above, to independent confirmation of the correctness of the helical Green function. At this stage, insofar as one restricts attention to charged helices in uniform dielectric media, which coordinate system one prefers to employ is simply a matter of taste. However, for the more realistic case of a nonuniform dielectric or solvent, the cylindrical coordinate system offers an advantage [1,2]. In this situation the question of the matching of solutions at the dielectric interfaces arises. Charges within a dielectric induce a surface charge at the interface between that dielectric and a region with a different dielectric constant. Since helical coordinates are nonorthogonal and curvilinear, we expect that matching solutions of Laplace's or Poisson's equations across the boundary will lead to a nontrivial albeit solvable problem in differential geometry. We in fact had already considered, but rejected, using helical coordinates, in 1993 for some of the above reasons. Finally, even though helical coordinates are not separable, we can always take the potential and electric field computed in cylindrical coordinates, and then simply transform them to helical coordinates to find their correct forms in these latter coordinates.

ACKNOWLEDGMENTS

We thank A. K. Rajagopal for a careful reading of the manuscript and for making useful comments which helped to clarify the connection between the helical and cylindrical Green functions.

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