Helical coordinate system and electrostatic fields of double-helix charge distributions

P. J. Lin-Chung and A. K. Rajagopal
Naval Research Laboratory, Washington, D.C. 20375
(Received 23 February 1995; revised manuscript received 5 April 1995)

We present a helical coordinate system and illustrate its use in solving electrostatic problems due to charge distribution on a double helix. It is shown that for systems with helical symmetry the resulting expression provides the structural information in the solution in a transparent way, with a structure factor separated out displaying the proper symmetry. The expressions for vector operators and other invariants for this coordinate system are also presented. We believe that this method provides an elegant description of physical systems possessing inherent helical structures.

PACS number(s): 87.15.−v, 36.20.−r, 41.20.Cv, 42.15.Gs

Recently we employed a helical coordinate system in the investigation of electronic properties in graphitic tubules that possess helical symmetry [1]. Since many differential equations of mathematical physics have to be solved under boundary conditions that demand the introduction of the proper kind of curvilinear coordinates, we believe that our coordinate system is useful in solving other problems in systems with helical symmetry. The purpose of this paper is to demonstrate that in addition to solving problems of electronic structure of systems confined to the cylindrical surface, as in graphitic tubules [1], this coordinate system may also be used conveniently to obtain the electrostatic fields produced by ions that are located on a spiral, as in helical molecule. Because the helical coordinate system defined by us is a nonorthogonal curvilinear system, the expressions for vector operators of interest in this system are nontrivial. We present expressions for vector operators and other invariants of interest in the Appendix using the methods of tensor calculus [2].

Recently the electric potential emanating from a DNA macromolecule has been calculated using a cylindrical coordinate system [3]. In that work the DNA molecule was modeled as a helical charge distribution that was divided into line charges, and the total contribution of all the line charges to the potential were then summed up. The higher order terms that reflect the helical structure are then examined to determine the effective decay length for the helical information in the local electric field. Since the cylindrical coordinate system, that was used in that calculation does not represent the correct symmetry of the system under consideration, much of the structural information is not explicitly present in their final results. In the helical coordinate system the potential due to charges distributed on a double helix may be calculated directly, and the final expression contains the structural information in a transparent fashion in terms of the components in helical representation.

An alternative helical coordinate system was previously proposed by Waldron [4]. His system is similar to the one proposed by us in that the pitch of the helix is fixed but the pitch angle is allowed to vary as a function of the radius. The three basis vectors of his coordinate system are always nonorthogonal. We choose a curvilinear coordinate system that is orthogonal on the cylinder surface with radius a, but nonorthogonal elsewhere.

The helical system (ρ,t,s) we choose in three-dimensional space reduces to the two-dimensional one previously considered by us on a cylindrical surface when $\rho=a$ [1], where a is the radius of the cylinder on which the helical elements are situated. The detailed coordinate transformation from the cylindrical system $[\rho,\theta,z]$ to the present system can be found in the Appendix. In the present system we define the following relations for any radius:

$$
\begin{aligned}
s &= z\sin\beta + a\theta\cos\beta ,\\
t &= a\theta\sin\beta - z\cos\beta .
\end{aligned}
\tag{1}
$$

On the $\rho=a$ surface, $t=$constant describes a helix with pitch angle β and pitch $p=2\pi a\tan\beta$. For $p\neq a$, the s direction follows a helix with the same pitch but with pitch angle β', where $\tan\beta'=(a/\rho)\tan\beta$. The angle β'' between the t and $-z$ directions, as shown in Fig. 1 and proved in the Appendix, obeys $\tan\beta''=(\rho/a)\tan\beta$. Thus the s direction is perpendicular to the t direction only for $\rho=a$. However, in the cylindrical representation a helix is specified by a pair of displacements (h,α) on the $\rho=a$ surface given by $z\rightarrow z+h$, representing the translation, and $\theta\rightarrow\theta+\alpha$, the accompanying rotation, where $\alpha=h/a\tan\beta$. Because the helical system exhibits a symmetry lower than the cylindrical symmetry, there are distinct features in the helical representation that are absent in the cylindrical representation. For example, the cylindrical symmetry implies a periodicity of 2π in the angle variable θ. However, for a system with helical symmetry, the above periodicity in θ does not generally hold. This is due to the fact that the periodicity in the z direction of a general helical structure need not correspond to one pitch, i.e., the combined displacement $z\rightarrow z+p$ and $\theta\rightarrow\theta+2\pi$ need not reach a periodic site.

We illustrate the nature of the helical coordinate surfaces $s=$constant and $t=$constant in Fig. 2 for $\rho<4a$. The coordinate surfaces $\rho=$constant represent concentric cylindrical surfaces. Examples of surfaces with $t=0$ and $t=0.1074$ are shown in Figs. 2(a) and 2(b), with defining

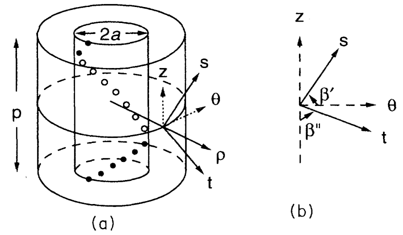

FIG. 1. Charges distributed on a single helix (solid dots and open circles indicate the charges situated on the front and the back of the cylinder, respectively), and the coordinate systems corresponding to the helical and cylindrical choices of representation.

parameters, pitch $p=4a$, radius $a=0.25$ ($\beta=32.48°$) of Eq. (1). The radial lines represent the directions along $\hat{\rho}$ and the spiral lines represent curves with ρ=constant. The tangent to the spiral at the point of intersection of the spiral with the radical line that has a positive component in the $+z$ direction gives the orientation of $\hat{s}$ at that point. Similarly the examples of surfaces with $s=0$ and $s=0.1687$ are given in Figs. 2(c) and 2(d), with the same parameters as in Figs. 2(a) and 2(b). The radial lines here also represent the directions along $\hat{\rho}$ and the spirals

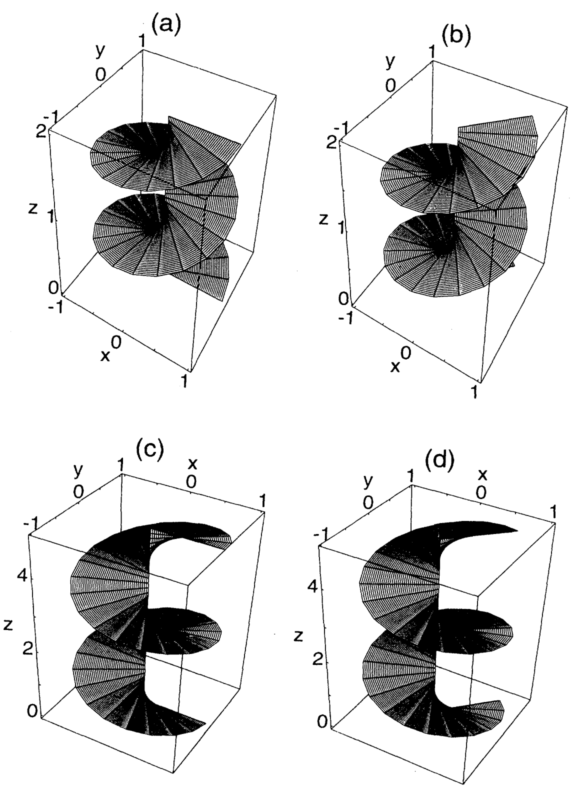

FIG. 2. Coordinate lines of the helical coordinate system for $\rho<4a$. We have chosen the parameters, pitch $p=4a$, radius $a=0.25$, which correspond to $\beta=32.48°$. (a) and (b) represent surfaces with $t=0$ and $t=0.1074$. (c) and (d) represent surfaces with $s=0$ and $s=0.1687$. See text for a detailed explanation of these surfaces.

represent cures with ρ=constant. But in these cases, the tangent at the point of intersection of the spiral with the radial line that has a positive component with the $-z$ direction gives the orientation of $\hat{t}$ at this point. Because of this feature, the senses of the spirals in Figs. 2(c) and 2(d) are the opposite of those in Figs. 2(a) and 2(b). We must point out that the unit vectors $\hat{s}$ and $\hat{t}$ are mutually perpendicular only for $\rho=a$; for $\rho\neq a$, they have an angle between them, as shown in Fig. 1. We also note that the scales of z in the upper and lower panels of Fig. 2 are different because the pitches of the s spiral and the t spiral are not equal.

The fundamental periodicity requirement on the wave function describing the helical system is

$$\psi(\rho,t=2\pi a\sin\beta,s+2\pi a\cos\beta)=\psi(\rho,t=0,s) \quad \text{for all } s\ . \tag{2}$$

Thus this helical system has the advantage of incorporating an already present helix and is more suitable for certain problems where helical structures exist. A detailed description of the helical coordinate system may be found in [5,6]

As an example we consider the electrostatic potential $\phi(\rho,t,s)$ due to charges distributed on a double helix

$$\nabla^2\phi=\frac{-4\pi a}{\varepsilon\rho}\delta(\rho-a)\times\sum_{\nu=1}^{2}\sum_{n=-N}^{N}q_{\nu n}\delta(t-t_\nu)\delta(s-s_n-d_\nu)\ , \tag{3}$$

where the sum over ν corresponds to the two helices, and the sum over n represents the charges $q_{\nu n}$ on the νth helix. The relative positions of the two helices are given by $t_1=0$, $t_2=\pi a\sin\beta-2\zeta\cos\beta$, and the charge distributions on the helices are determined by $d_1=0$, $d_2=\pi a\cos\beta+2\zeta\sin\beta$, and s_n. 2ζ is the offset distance between two corresponding charges on the two helices [3]. For charges with equal magnitude and separated by equal distance $\bar{s}$ along a helix, we have $q_{\nu n}=a$ and $s_n=n\bar{s}$, where n takes integer values from $-N$ to N in steps of unity. $N=\infty$ represents an infinitely long helix. The left-hand side of Eq. (3) in the helical coordinate system is given in Eq. (A21).

The solution to Eq. (3) is given by

$$\phi(\rho,t,s)=\sum_{\nu=1}^{2}\sum_{n=-N}^{N}G(\rho,t,s;a,t_\nu,s_n+d_\nu)\ , \tag{4}$$

where the Green function $G(\rho,t,s;\rho',t',s')$ satisfies the equation

$$\nabla^2G(\rho,t,s;\rho',t',s')=\frac{-4\pi a}{\varepsilon\rho}\delta(\rho-\rho')\delta(t-t')\delta(s-s')\ . \tag{5}$$

This Green function is obtained by employing the method of separation of variables given in Morse and Feshbach [7] as follows. We first find the solution of $\nabla^2\phi(\rho,t,s)=0$ with the expressions in Eq. (A21). Let

$$\phi(\rho,t,s)=R(\rho)T(t)S(s)\ ,$$
$$T(t)=e^{-iM't}\ ,\ S(s)=e^{-iMs}\ , \tag{6}$$

then we obtain

$$\frac{R''}{R}+\frac{R'}{\rho R}-\frac{\lambda^2}{\rho^2}+k^2=0\ , \tag{7}$$

where

$$\lambda\equiv a(M'\sin\beta+M\cos\beta)\ ,$$
$$k\equiv -M'\cos\beta+M\sin\beta=\frac{-\lambda\cos\beta+aM}{a\sin\beta}\ . \tag{8}$$

In Eq. (7) primes denote differentiation with respect to ρ. The solution to Eq. (7) is, in general, of the form

$$R(\rho)=AI_\lambda(|k|\rho)+BK_\lambda(|k|\rho)\ . \tag{9}$$

In the case where the medium is in $0<\rho<\infty$ with a uniform dielectric constant ε (both inside and outside the cylinder on which the helix lies), the boundary conditions that exist when ρ approaches a from inside and from outside the cylinder determine the Green functions:

$$G(\rho,t,s;\rho',t',s')=\frac{q}{\pi a}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dM\,dM'\,A(M,M')\times e^{-iM(s-s')-iM'(t-t')}\times I_\lambda(|k|\rho_<)K_\lambda(|k|\rho_>)\ . \tag{10}$$

In the above, $I_\lambda(|k|\rho),K_\lambda(|k|\rho)$ are the modified Bessel functions, and the $\rho_<,\rho_>$ represent the smaller or the greater of the pair ρ,ρ'. As described in [1], and according to Eq. (2), λ is an integer and represents the discrete angular momentum in the cylindrical system when the M and M' represent the linear momenta along the s and t directions. We therefore can also replace the integral over M' by a sum over λ in Eq. (10). Equation (4) then becomes

$$\phi(\rho,t,s)=\frac{q}{\pi}\sum_{\nu=1}^{2}\sum_{n=-N}^{N}\sum_{\lambda=-\infty}^{\infty}\int_{-\infty}^{\infty}dM\ A(M,\lambda)\exp[-iM(s-n\bar{s}-d_\nu)]\times\exp\left[-i\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right](t-t_\nu)\right]I_\lambda(|k|\rho_<)K_\lambda(|k|\rho_>)$$
$$=\frac{q}{\pi}\sum_{\lambda=-\infty}^{\infty}\int_{-\infty}^{\infty}dM\ A(M,\lambda)H(M,\lambda)\exp\left[-i\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]t-(iMs)\right]I_\lambda(|k|\rho_<)K_\lambda(|k|\rho_>)\ . \tag{11}$$

The structure factor $H(M,\lambda)$ in Eq. (11) is determined by the charge distribution on the double helix

$$H(M,\lambda)=\sum_{\nu=1}^{2}\sum_{n=-N}^{N}\exp\left[iM(n\bar{s}+d_\nu)+i\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]t_\nu\right]=H_1(M,\lambda)H_2(M)\ , \tag{12a}$$

where

$$H_1(M,\lambda)=\left[1+\exp\left\{-i\lambda\pi\left[1+\frac{4\xi}{P}\right]+iM\left[\frac{2\xi}{\sin\beta}\right]\right\}\right]\ , \tag{12b}$$

$$H_2(M)=\sum_{n=-N}^{N}\exp(-iM\bar{s}n)=\left[\sin\frac{(2N+1)M\bar{s}}{2}\right]\left[\sin\frac{M\bar{s}}{2}\right]^{-1}\ , \tag{12c}$$

$$H_2(M)=\frac{2\pi}{\bar{s}}\sum_{j=-\infty}^{\infty}\delta\left[M-\frac{2\pi j}{\bar{s}}\right]\quad\text{if } N=\infty\ . \tag{12d}$$

Note that in Eq. (12a) the two summations are separated into two factors, $H_1(M,\lambda),H_2(M)$. The first factor contains the summation over the number of helices and $H_1(M,\lambda)=1$ for a single helix. The second factor $H_2(M)$ represents the structure factor for a single helix and is independent of λ. It has simple forms given in Eqs. (12c) and (12d) for finite and infinite helices, respectively.

From the discontinuity in the derivative of the potential with respect to ρ as we approach $\rho=a$ from inside and outside, we have

$$\left[\frac{\partial\phi(\rho<a)}{\partial\rho}-\frac{\partial\phi(\rho>a)}{\partial\rho}\right]_{\rho=a}=\frac{4\pi q}{\varepsilon}\sum_{\nu=1}^{2}\sum_{n=-N}^{N}\delta(t-t_\nu)\delta(s-s_n-d_\nu)\ , \tag{13}$$

and thus we obtain the coefficients in Eq. (11),

$$A(M,\lambda)=\frac{1}{ka\varepsilon}\left[\frac{1}{I'_\lambda(|k|a)K_\lambda(|k|a)-K'_\lambda(|k|a)I_\lambda(|k|a)}\right]=\frac{1}{\varepsilon}\ , \tag{14}$$

where the prime stands for the derivative of the modified

Bessel functions. Note that the denominator within the parenthesis is the Wronskian $-\Delta(I_\lambda(x),K_\lambda(x))=1/x$. These relations may be found in [7].

The solution obtained in Eq. (11) differs from that given in [3] in that it is in terms of the helical coordinates, and the summation over the charge distribution on the double helix is separated into a characteristic structure factor, $H(M,\lambda)$. For simplicity we considered here a uniform dielectric constant. $\rho_<,\rho_>$ now represent the inside and outside of the cylinder corresponding to the smaller and the greater of ρ and a, respectively. Note that the variable k is a function of λ, and M and it represents the component of linear momentum along the z direction. The different dielectric materials involved in the real DNA system can easily be incorporated through appropriate boundary conditions. We shall not pursue this point here.

From the solution in Eq. (11) and using Eq. (A20) we obtain the associated electric field due to the charges distributed on the helices. Define

$$\vec{E}=\hat{\rho}E_\rho+\hat{t}E_t+\hat{s}E_s \tag{15}$$

and note that this defines the components with respect to the unit basis vectors and not the covariant components.

$$E_\rho=\frac{q}{\pi\varepsilon}\sum_{\lambda=-\infty}^{\infty}\int_{-\infty}^{\infty}dM\,H(M,\lambda)W_\lambda(|k|\rho)\exp\left[-i\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]t-iMs\right], \tag{16}$$

where

$$W_\lambda(|k|\rho)=\begin{cases}|k|I'_\lambda(|k|\rho)K_\lambda(|k|a) & \text{for } \rho<a\\ |k|I_\lambda(|k|a)K'_\lambda(|k|\rho) & \text{for } \rho>a\,,\end{cases} \tag{17}$$

$$E_t=\frac{qi}{\pi\varepsilon}\left[\frac{a^2l_t}{\rho^2}\right]\sum_{\lambda=-\infty}^{\infty}\int_{-\infty}^{\infty}dM\,H(M,\lambda)\left[c^2M-l_s^2\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]\right]$$
$$\times\exp\left[-iMs-i\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]t\right]I_\lambda(|k|\rho_<)K_\lambda(|k|\rho_>)\,, \tag{18}$$

$$E_s=\frac{qi}{\pi\varepsilon}\left[\frac{a^2l_s}{\rho^2}\right]\sum_{\lambda=-\infty}^{\infty}\int_{-\infty}^{\infty}dM\,H(M,\lambda)\left[c^2\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]-l_t^2M\right]$$
$$\times\exp\left[-iMs-i\left[\frac{\lambda-aM\cos\beta}{a\sin\beta}\right]t\right]I_\lambda(|k|\rho_<)K_\lambda(|k|\rho_>)\,. \tag{19}$$

Equation (17) displays the discontinuity of the E_ρ component of the electric field across $\rho=a$ because of the presence of the charge distribution on that surface. The other two components are continuous across $\rho=a$.

The components of the electric fields in the cylindrical coordinates in terms of those of the helical system can be obtained using Eqs. (A18) and (A7):

$$E_\rho=E_\rho\,,\qquad E_\theta=\frac{E_t\sin\beta}{al_t}+\frac{E_s\cos\beta}{al_s}\,,\qquad E_z=\frac{-E_t\cos\beta}{al_t}+\frac{E_s\sin\beta}{al_s}\,, \tag{20}$$

with the notations defined in the Appendix.

The actual computations of the terms involving the Bessel functions in these formulas may be performed using the codes given by Press *et al.* [8]. An interesting special case of the components of the electric field at the central axis of the molecule can be evaluated analytically from Eqs. (16)–(19) and by using the known properties of the Bessel functions [7].

Thus the following expressions for the various components of the electric field along the central axis, defined by $\rho=0$ and arbitrary θ,z, are found to be

$$E_\rho(\rho=0,\theta,z)=\left[\frac{q}{\varepsilon}\right]\sum_{n,\nu}\frac{a\sin\beta\cos(\theta-u_{n\nu})}{[a^2+(z-\alpha_{n\nu}\sin\beta)^2]^{3/2}}\,, \tag{21a}$$

$$E_\theta(\rho=0,\theta,z)=\left[\frac{q}{\varepsilon}\right]\sum_{n,\nu}\frac{a\sin\beta\sin(\theta-u_{n\nu})}{[a^2+(z-\alpha_{n\nu}\sin\beta)^2]^{3/2}}\,, \tag{21b}$$

$$E_z(\rho=0,\theta,z)=\left[\frac{q}{\varepsilon}\right]\sum_{n,\nu}\frac{(\alpha_{n\nu}\sin\beta-z)\sin\beta}{[a^2+(\alpha_{n\nu}\sin\beta-z)^2]^{3/2}}\,, \tag{21c}$$

where $\alpha_{n\nu}\equiv n\bar{s}+d_\nu-t_\nu\cot\beta$ and $u_{n\nu}\equiv(n\bar{s}+d_\nu)\cos\beta+t_\nu\sin\beta$ are determined by the charge distribution on the double helix.

Since in these molecules the radius a is much smaller than the length of the molecule, we find from Eq. (21) that the z component E_z is the largest in magnitude. This appears to be in conformity with an observation reported recently on the fast motion of electrons through the DNA molecules [9]. Note that since our formulas involve the features of the structure of the DNA, their dependence on the lengths and nature of DNA strands are also obtained here explicitly.

In summary, since we can separate the structure factor in the above expressions for the potential and the electric fields, it is easier to examine the structural information using the present coordinate system than using the cylindrical system [3]. This approach may also be employed in other contexts, such as helical wave guides [4], helical optical beams [10], and helical magnetic fields [11]. In general we note that the procedure developed here is a useful method in studying system with inherent helical symmetry.

This work was supported in part by the Office of Naval Research.

APPENDIX: COORDINATE TRANSFORMATION FROM CYLINDRICAL $[\rho,\theta,z]$ TO HELICAL (ρ,t,s) SYSTEMS AND EXPRESSIONS FOR THE DIFFERENTIAL INVARIANTS IN THE HELICAL SYSTEM

In a general nonorthogonal curvilinear coordinate system, a position vector $\vec{r}$ may be expressed in terms of its contravariant components x^i with a fixed set of basis vectors, $\vec{e}_i$, or its covariant components x_i with the adjoint set of basis vectors, $\vec{e}^{\,i}$. The expressions for the position vector are

$$\vec{r}=\sum x^i\vec{e}_i=\sum x_i\vec{e}^{\,i} . \tag{A1}$$

The differential line element in this system is

$$ds^2=d\vec{r}\cdot d\vec{r}=g_{ij}dx^i dx^j , \tag{A2}$$

where

$$g_{ij}\equiv\vec{e}_i\cdot\vec{e}_j , \tag{A3}$$

and g_{ij} are the covariant components of the second-order symmetric metric tensor of the system. The respective contravariant components of vectors and tensors in curvilinear systems are obtained from their covariant components by

$$g_{ij}\vec{e}^{\,j}=\vec{e}_i , \quad g^{ij}\equiv\vec{e}^{\,i}\cdot\vec{e}^{\,j} , \quad \sum_\alpha g^{i\alpha}g_{\alpha j}=\delta_{ij} , \tag{A4}$$

where δ_{ij} is the usual Kronecker delta symbol, 1 for $i=j$ and 0 for $i\neq j$.

The above basis vectors and metric tensors are fundamental in defining a curvilinear coordinate system, as they are employed in deriving the basic differential invariants and covariants of mathematical entities in such systems.

In the following we use $\vec{e}_i$, x^i, and g_{ij} ($\vec{f}_i$, $\bar{x}^i$, and $\bar{g}_{ij}$) to represent the corresponding quantities in the cylindrical (helical) coordinate system. A position vector $\vec{r}$ in the helical coordinate system defined here and in the cylindrical system is then given by

$$\vec{r}=\sum\bar{x}_i\vec{f}^{\,i}=\sum\bar{x}^i\vec{f}_i=\rho\vec{f}_\rho+t\vec{f}_t+s\vec{f}_s$$
$$=\sum x_i\vec{e}^{\,i}=\sum x^i\vec{e}_i=\rho\vec{e}_\rho+\theta\vec{e}_\theta+z\vec{e}_z . \tag{A5}$$

The components x^i are (ρ,θ,z) in the cylindrical system and the components $\bar{x}^i$ are (ρ,t,s) in the helical system. A detailed analysis of the cylindrical system may be found in Morse and Feshbach [7].

The coordinate transformation between these two systems is represented by

$$\vec{f}_i=a_i^j\vec{e}_j, \quad \bar{x}^i a_i^j=x^j \tag{A6}$$

where

$$a_i^j=\begin{bmatrix}1 & 0 & 0\\ 0 & \dfrac{\sin\beta}{a} & -\cos\beta\\ 0 & \dfrac{\cos\beta}{a} & \sin\beta\end{bmatrix} \tag{A7}$$

is the transformation matrix derived from Eq. (1) in the text. The transformation of the second-order metric tensor is

$$\bar{g}_{tu}=a_t^r a_u^s g_{rs} , \tag{A8}$$

where

$$\bar{g}_{ij}\equiv\vec{f}_i\cdot\vec{f}_j . \tag{A9}$$

Since in the cylindrical system we have $\vec{e}_\rho=\hat{\vec{\rho}}$, $\vec{e}_\theta=\rho\hat{\vec{\theta}}$, $\vec{e}_z=\hat{\vec{z}}$ for the basis vectors in terms of the unit vectors $\hat{\vec{\rho}},\hat{\vec{\theta}},\hat{\vec{z}}$ [7], we obtain from Eqs. (A3) and (A4),

$$g_{rs}=\begin{bmatrix}1 & 0 & 0\\ 0 & \rho^2 & 0\\ 0 & 0 & 1\end{bmatrix} , \quad g^{rs}=\begin{bmatrix}1 & 0 & 0\\ 0 & \rho^{-2} & 0\\ 0 & 0 & 1\end{bmatrix} . \tag{A10}$$

From Eq. (A8) we then obtain the corresponding tensor in the helical system,

$$\bar{g}_{rs}=\begin{bmatrix}1 & 0 & 0\\ 0 & l_t^2 & c^2\\ 0 & c^2 & l_s^2\end{bmatrix} , \tag{A11}$$

where

$$l_t^2\equiv\cos^2\beta+\left[\frac{\rho\sin\beta}{a}\right]^2 ,$$
$$l_s^2\equiv\sin^2\beta+\left[\frac{\rho\cos\beta}{a}\right]^2 , \tag{A12}$$
$$c^2\equiv\sin\beta\cos\beta\left[\frac{\rho^2}{a^2}-1\right] .$$

We also have

$$\bar{g}\equiv\det|\bar{g}_{rs}|=\frac{\rho^2}{a^2} . \tag{A13}$$

The basis vectors $\vec{f}_i$ are expressed in terms of the unit vectors $\hat{\vec{\rho}},\hat{\vec{t}},\hat{\vec{s}}$ based on Eqs. (A9) and (A11)

$$\vec{f}_\rho=\hat{\rho}\ , \quad \vec{f}_t=l_t\hat{t}\ ,$$
$$\vec{f}_s=l_s\hat{s}\ , \quad \hat{s}\cdot\hat{t}=\frac{c^2}{l_s l_t}\ . \tag{A14}$$

Note that the $\hat{s},\hat{t}$ are not orthogonal for $\rho\neq a$ in the helical system, and the lengths of the basis vectors $\vec{f}_t,\vec{f}_s$ are l_t,l_s, respectively.

From Eqs. (A6) and (A14) we have

$$\vec{f}_s=\frac{\cos\beta}{a}\rho\hat{\theta}+(\sin\beta)\hat{z}=l_s\hat{s}\ ,$$
$$\vec{f}_t=\frac{\sin\beta}{a}\rho\hat{\theta}-(\cos\beta)\hat{z}=l_t\hat{t}\ . \tag{A15}$$

Thus the pitch angle β' of the helix along s direction and the angle β'' shown in Fig. 1 for $\rho\neq a$ are determined from

$$\sin\beta'=\frac{\sin\beta}{l_s}\ , \quad \cos\beta''=\frac{\cos\beta}{l_t}\ ,$$
$$\text{i.e., } \tan\beta'=\left[\frac{a}{\rho}\right]\tan\beta\ , \quad \tan\beta''=\left[\frac{\rho}{a}\right]\tan\beta\ . \tag{A16}$$

$\beta'=\beta''$ ($\hat{s}\perp\hat{t}$) only when $\rho=a$.

The adjoint set of the basis vectors is determined from similar relations given in Eq. (A4),

$$\vec{f}^\rho=\vec{f}_\rho=\hat{\rho}\ ,$$
$$\vec{f}^t=\frac{a^2}{\rho^2}(-c^2\vec{f}_s+l_s^2\vec{f}_t)=\frac{a^2 l_s}{\rho^2}(-c^2\hat{s}+l_s l_t\hat{t})\ , \tag{A17}$$
$$\vec{f}^s=\frac{a^2}{\rho^2}(l_t^2\vec{f}_s-c^2\vec{f}_t)=\frac{a^2 l_t}{\rho^2}(l_s l_t\hat{s}-c^2\hat{t})\ .$$

An arbitrary vector $\vec{A}$ in the helical system is decomposed into either its covariant components, contravariant components, or the components with respect to the basis vectors in the following form:

$$\vec{A}=\sum_i \overline{A}_i\vec{f}^i=\sum_i \overline{A}^i\vec{f}_i=A_\rho\hat{\rho}+A_t\hat{t}+A_s\hat{s}\ . \tag{A18}$$

The various components are related by the equations

$$\overline{A}_i=g_{ij}\overline{A}^j\ , \quad \overline{A}_\rho=A_\rho\ ,$$
$$\overline{A}_t=\frac{c^2}{l_s}A_s+l_tA_t\ , \quad \overline{A}_s=l_sA_s+\frac{c^2}{l_t}A_t\ . \tag{A19}$$

With the above quantities defined for the helical coordinate system, the fundamental differential invariants and covariants, namely, the gradient and Laplacian of a scalar field, the divergence and curl of a vector field are readily derived. They are

$$\nabla\phi=\vec{f}^i\frac{\partial\phi}{\partial\overline{x}^i}$$
$$=\left[\hat{\rho}\frac{\partial}{\partial\rho}+\hat{s}\left[\frac{a^2 l_s}{\rho^2}\right]\left[l_t^2\frac{\partial}{\partial s}-c^2\frac{\partial}{\partial t}\right]+\hat{t}\left[\frac{a^2 l_t}{\rho^2}\right]\left[-c^2\frac{\partial}{\partial s}+l_s^2\frac{\partial}{\partial t}\right]\right]\phi\ , \tag{A20}$$

$$\nabla^2\phi=\frac{1}{\sqrt{g}}\frac{\partial}{\partial\overline{x}^i}\left[\sqrt{g}g^{ij}\frac{\partial}{\partial\overline{x}^j}\right]\phi$$
$$=\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right]+\frac{\partial^2}{\partial t^2}+\frac{\partial^2}{\partial s^2}+\left[\frac{a^2}{\rho^2}-1\right]\left[\sin\beta\frac{\partial}{\partial t}+\cos\beta\frac{\partial}{\partial s}\right]^2\right]\phi\ , \tag{A21}$$

$$\operatorname{div}\vec{A}=\frac{1}{\sqrt{g}}\frac{\partial}{\partial\overline{x}^i}(\sqrt{g}\,\overline{A}^i)$$
$$=\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A_\rho)+\frac{1}{l_t}\frac{\partial A_t}{\partial t}+\frac{1}{l_s}\frac{\partial A_s}{\partial s}\ , \tag{A22}$$

$$\operatorname{curl}\vec{A}=\frac{1}{\sqrt{g}}\left[\left[\frac{\partial\overline{A}_k}{\partial\overline{x}^j}-\frac{\partial\overline{A}_j}{\partial\overline{x}^k}\right]\vec{f}_i+(ijk\ \text{cyclic})\right]$$
$$=\frac{a}{\rho}\left[\left[\frac{\partial\overline{A}_s}{\partial t}-\frac{\partial\overline{A}_t}{\partial s}\right]\hat{\rho}+\left[\frac{\partial\overline{A}_\rho}{\partial s}-\frac{\partial\overline{A}_s}{\partial\rho}\right]l_t\hat{t}+\left[\frac{\partial\overline{A}_t}{\partial\rho}-\frac{\partial\overline{A}_\rho}{\partial t}\right]l_s\hat{s}\right]\ . \tag{A23}$$

(ijk cyclic) means terms obtained by cyclic permutation of i, j, k. In Eqs. (A22) and (A23) the various forms of the components of the same vector are defined by Eq. (A19). It is interesting to note that in Eq. (A23) the covariant components of $\vec{A}$ are used to get the contravariant components of curl $\vec{A}$.

[1] P. J. Lin-Chung and A. K. Rajagopal, J. Phys. C **6**, 3697 (1994).

[2] C. Lanczos, in *Handbook of Physics*, edited by E. U. Condon and H. Odishaw (McGraw-Hill, New York, 1958), Chap. 10.

[3] D. Hochberg, T. W. Kephart, and G. Edwards, Phys. Rev. E **49**, 851 (1994); also see G. Edwards, D. Hochberg, and T. W. Kephart, Phys. Rev. E **50**, R698 (1994).

[4] R. A. Waldron, Q. J. Mech. Appl. Math. **11**, 439 (1958).

[5] P. J. Lin-Chung and A. K. Rajagopal, in *Local Order in Condensed Matter Physics*, edited by P. Jena and S. D. Mahanti (NOVA Science, New York, in press).

[6] A. K. Rajagopal and P. J. Lin-Chung, in *Clusters and Nanostructure Materials*, edited by P. Jena and S. N. Behera (NOVA Science, New York, in press).

[7] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. I, Chap. 7.2.

[8] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, New York, 1986), Chap. 6.

[9] D. Clery, Science **267**, 1270 (1995), and references therein.

[10] P. L. Overfelt, Phys. Rev. A **46**, 3516 (1992).

[11] M. Calvo, Phys. Rev. B **18**, 5073 (1978).