Orientational order determination in liquid crystals by x-ray diffraction

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The orientational distribution function f relative to the director of elongated molecules of liquid crystals and related materials can be determined, in principle, from the intensity distribution I along equatorial arcs in the x-ray-diffraction pattern. The integral equation relating these two quantities is solved here, yielding an analytic, closed-form expression for f in terms of the measured I. Analytic expressions for several important related quantities, like the second- and fourth-order order parameters, the average tilt angle, etc. are also derived. The accuracy obtainable in calculating these quantities from measured data is discussed, and examples demonstrating the use of the method are given. These examples show the robustness and accuracy of the solution and its related quantities even for highly noisy and/or sparse experimental input data I.

I. INTRODUCTION

Liquid-crystalline phases are characterized by the existence of long- or quasi-long-range orientational order for their elongated, rodlike molecules [1]. This is, in fact, the main feature distinguishing them from isotropic liquids and providing for their unique properties so important for basic and applied science as well as for commercial applications. The orientational order is quantified by the orientational distribution function (ODF), $f(\beta)$, of the long molecular axis relative to the director, and the orientational order parameters (OP), $\bar{P}_n$, defined as

$$\bar{P}_n = \int_0^{\pi/2} P_n(\cos\beta) f(\beta) d(\cos\beta) , \qquad (1)$$

where $P_n(x)$ is the nth Legendre polynomial. Although the order parameters $\bar{P}_2$ and $\bar{P}_4$ can be determined by various resonance and Raman techniques, the more important $f(\beta)$ cannot be measured directly. An x-ray method was developed, however, by Leadbetter, Norris, and Wrighton [2,3] that allows the determination of $f(\beta)$ for a large class of thermotropic liquid crystals from the intensity distribution I along equatorial arcs in the diffraction pattern. The two quantities are related by an integral equation, which must be inverted for the experimentally derived I to obtain f. As no analytic inverse is available for this equation, various numerical and series-expansion methods were employed in the numerous applications of the method published so far [2–7]. Although these methods were found to be satisfactory for the level of accuracy of most measurements to date, an analytic solution for the integral equation is desirable both on theoretical grounds and for obtaining higher computational accuracy and stability, not only for $f(\beta)$, but also for derived quantities strongly depending on f, such as $\bar{P}_n$. Furthermore, an analytic solution could benefit several other fields, such as grafted rods [8], viri in solutions [9,10] and Langmuir-Blodgett films [11], where

closely related methods can be, or have been, applied for ODF determination.

A closed-form, analytic solution for this integral equation was developed and is presented here. The mathematical formulation is given in the next section along with expressions for a number of physically important related quantities. The third section presents numerical results obtained for two examples and discusses some practical aspects of the calculations.

II. THEORY

A. Formulation of the problem

A typical liquid crystal can be regarded as being made of elongated, rodlike molecules of an aspect ratio of approximately 4 or larger. In the liquid-crystalline phases, a magnetic field can be used to define a direction, called the director, along which the long axes of the molecules align. The alignment, however, is not perfect, and there is a finite probability $f(\beta)$ for a particular molecule to have its axis at an angle β to the director. $f(\beta)$ is the singlet orientational distribution function. A schematic x-ray-diffraction pattern of such a sample in its nematic phase is shown in Fig. 1. The meridional peak along the director q_z result from the order represented by the equal length of the individual molecules. The diffuseness of these peaks is due to the very-short-range order (a few molecules) in this direction. Upon transition to a smectic phase, where the sample develops quasi-long-range ordered layers in this direction, these peaks become very sharp. The equatorial arcs intersecting the q_x axis are due to diffraction perpendicular to the long molecular axis. With perfect alignment of the molecules along the director and equal intermolecular distances perpendicular to it, these arcs would condense into sharp peaks on the q_x axis, similar to those along q_z in the smectic case. Leadbetter and Norris [2] and Leadbetter and Wrighton [3] have shown that if the molecules cluster in small
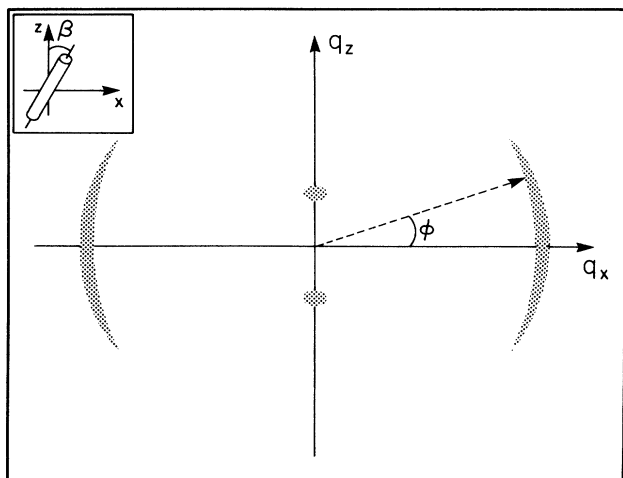
FIG. 1. A schematic x-ray-diffraction pattern of a liquid crystal. The director is along q_z. The inset shows the molecular orientation geometry, β being the molecular tilt angle away from the director.

domains of the order of approximately ten molecules or more, within which the orientations are well correlated but the domains have a distribution of orientations $f_d(\beta)$, the equatorial peaks smear into arcs, the intensity distribution along which is given by

$$I(\phi)=\int_\phi^{\pi/2} f_d(\beta)\sec^2\phi(\tan^2\beta-\tan^2\phi)(\sin\beta)d\beta \ . \quad (2)$$

Note that, in general, $f_d(\beta)$ is different from the singlet ODF $f(\beta)$. It has, however, been shown in a number of studies [2–7,12] that the ordering conditions under which the equation above is valid are well obeyed by thermotropic liquid crystals in general, and that $f_d(\beta)$ closely approximates the singlet ODF $f(\beta)$. We will therefore identify $f_d(\beta)$ with $f(\beta)$ in the following and drop the subscript d.

In order to obtain the ODF $f(\beta)$, the integral equation Eq. (2) has to be solved using the discrete, measured $I(\phi)$ values as input. Haase and co-workers [4] have shown recently that $I(\phi)$ should be taken as the intensity integrated radially across the arc for a given ϕ rather than the peak intensity at that ϕ. As the measured points include experimental errors and their number is necessarily finite and sometimes small, a numerical inversion of Eq. (2) is bound to increase the errors. For this reason, in most studies an analytic model is adopted for $f(\beta)$ and substituted in Eq. (2), which is then integrated analytically and the resultant expression is fitted to the measured $I(\phi)$ to obtain the best values for the parameters defining the model $f(\beta)$. This approach, while avoiding some of the difficulties of numerical inversion, has the disadvantage of biasing the solution by the particular choice of the model. For example, while some of the early studies adopted the Maier-Saupe model [13], more recent ones show that a truncated series of Legendre polynomials [12] or circular functions [4] yields a better agreement with the measured I data. To avoid these pitfalls, an exact analytic solution was derived and is presented below.

B. Analytic solution

To solve the integral equation (2) we make the substitution

$$y=\tan\phi, \quad r=\tan\beta \ . \quad (3)$$

After some algebraic manipulations, and denoting

$$J(y)=2I(y)/(1+y^2), \quad g(r)=f(r)/(1+r^2)^{3/2} \ , \quad (4)$$

we obtain

$$J(y)=2\int_y^\infty g(r)r(r^2-y^2)^{-1/2}dr \ . \quad (5)$$

This is immediately recognized as the Abel integral equation [14] for which three analytic solutions have been derived [14–16] was well as efficient numerical methods for their computation for experimentally derived data [17].

The analytic solution can be obtained now by using the Abel inversion formulas

$$g_1(r)=-\pi^{-1}\int_r^\infty [dJ(y)/dy](y^2-r^2)^{-1/2}dy \quad (6a)$$

and

$$g_2(R)=-(\pi r)^{-1}\frac{d}{dr}\left[\int_r^\infty J(y)y(y^2-r^2)^{-1/2}dy\right] \ . \quad (6b)$$

g_1 and g_2 are two different forms of the same solution and are related by a single integration by parts. However, error amplification for experimentally derived I is considerably reduced [16,17] when using g_2. Note also that $I(\phi)$ is measured in a diffraction experiment. As *absolute* diffracted intensities are notoriously difficult to measure accurately, $I(\phi)$ will almost always be unnormalized, i.e., it will include an arbitrary multiplicative constant that is commonly eliminated by normalizing $f(\beta)$. Using now Eqs. (6), back substituting from Eq. (4), and normalizing, we finally obtain

$$f_1(\beta)=-(N\cos^3\beta)^{-1}\int_\beta^{\pi/2}\{d[I(\phi)\cos^2\phi]/d\phi\}$$
$$\times(\tan^2\phi-\tan^2\beta)^{-1/2}d\phi \quad (7a)$$

and

$$f_2(\beta)=-(N\sin\beta)^{-1}\frac{d}{d\beta}$$
$$\times\left[\int_\beta^{\pi/2}I(\phi)\tan\phi(\tan^2\phi-\tan^2\beta)^{-1/2}d\phi\right] \ . \quad (7b)$$

The normalizing constant N is given by

$$N=\int_0^{\pi/2}f(\beta)(\sin\beta)d\beta=\int_0^{\pi/2}I(\phi)d\phi \ , \quad (8)$$

where a factor of $(2/\pi)$ common to Eqs. (7) and (8) was eliminated.

Equations (7) are the requested analytic solutions of the integral equation, Eq. (2).

C. An analytic example

To illustrate the solution obtained above, consider the case of the Maier-Saupe ODF:

$$f_{MS}(\beta) = A \exp(a \cos^2\beta) \ . \tag{9}$$

Using Eq. (2) the intensity distribution along the equatorial arcs is

$$I_{MS}(\phi) = (A\pi^{1/2}/2v)\exp(v^2)\mathrm{erf}(v) \ , \tag{10}$$

where A is a normalizing constant, $\mathrm{erf}(x)$ is the usual error function, and $v = a^{1/2}\cos\phi$. By substituting Eq. (10) into the analytic solution Eq. (7b) and using $\cos\phi = u$ and $\cos\beta = t$, we obtain

$$f(\beta) = (A/\pi^{1/2})(d/dt)$$
$$\times \left[t \int_0^{a^{1/2}t} \exp(v^2)\mathrm{erf}(v)v^{-1}(at^2 - v^2)^{-1/2}dv \right] \ . \tag{11}$$

Using a table of integrals [18] and a minimum amount of algebra one obtains

$$f(\beta) = (A\pi^{1/2}/2)d[\mathrm{erf}(z)]/dz \ , \tag{12}$$

where $z = -ia^{1/2}\cos\beta$. Straightforward calculation [19] recovers Eq. (9), as required.

D. Derived quantities

The layer spacing in the smectic phases can be obtained from the molecular length and the average cosine of the molecular tilt relative to the normal [20]. Higher-order even moments of $\cos\beta$ are also of interest in optical studies of liquid crystals [11,21]. These averages are weighted, as in the case of $\bar{P}_n$ in Eq. (1), by the ODF. We need to calculate, then,

$$\bar{F} = N^{-1}\int_0^{\pi/2} F(\cos\beta)f(\beta)d(\cos\beta) \ , \tag{13}$$

where F denotes the function averaged upon. Substituting now Eq. (7b) for f and integrating by parts one obtains

$$\bar{F} = N^{-1}\left[\int_0^{\pi/2} I(\phi)d\phi - \int_0^{\pi/2}\sin\beta[dF(\cos\beta)/d(\cos\beta)]\int_\beta^{\pi/2} I(\phi)\tan\phi(\tan^2\phi - \tan^2\beta)^{-1/2}d\phi \right] \ . \tag{14}$$

Interchanging the order of the two integrals in the second term, changing the variable $x = \cos\beta$ in the inner integral, and using Eq. (8) yields

$$\bar{F} = 1 - N^{-1}\int_0^{\pi/2}(\sin\phi)I(\phi)d\phi\int_{\cos\phi}^1 [dF(x)/dx]x(x^2 - \cos^2\phi)^{-1/2}dx \ . \tag{15}$$

This equation can now be used to calculate ODF-averaged quantities directly from the measured intensity $I(\phi)$ without having to calculate $f(\beta)$ first. This is particularly advantageous in cases when error amplification proves to be a serious problem in calculating f due to large experimental errors in, or sparsity of, the I data.

The average cosine of the tilt angle is obtained by taking $F(\cos\beta) = \cos\beta$ in Eq. (15). This yields

$$\overline{\cos\beta} = N^{-1}\int_0^{\pi/2} I(\phi)(\cos^2\phi)d\phi \ . \tag{16}$$

The higher-order moments of $\cos\beta$ are obtained by choosing $F(\cos\beta) = \cos^n\beta$. Noting that only even moments are of interest and using a table of integrals [22] we obtain

$$\overline{\cos^n\beta} = N^{-1}\int_0^{\pi/2} I(\phi)\left[1 - n(\sin^2\phi)\sum_{r=1}^{n/2} D_r(\cos\phi)^{n-2r} - n\sin\phi(\cos\phi)^n\ln[(1+\sin\phi)/\cos\phi] \right]d\phi \ , \tag{17}$$

where $D_r = r!(r-1)!/(2r)!$.

The order parameters $\bar{P}_n$ are obtained by taking $F(\cos\beta) = P_n(\cos\beta)$. The explicit expression for the Legendre polynomials [23] is inserted into Eq. (15). Since only even orders, $n = 2l$, are of interest, we obtain

$$\bar{P}_{2l} = 1 - (4^l N)^{-1}\sum_{k=0}^{l-1} C_{l,k}\int_0^{\pi/2} I(\phi)(\sin\phi)d\phi\int_{\cos\phi}^1 x^{2l-2k}(x^2 - \cos^2\phi)^{-1/2}dx \ , \tag{18}$$

where $C_{l,k}$ are constants. The inner integral can now be evaluated [22] and we finally obtain

$$\bar{P}_{2l} = 1 - N^{-1}\int_0^{\pi/2} I(\phi)\left[\sin^2\phi\sum_{k=0}^{l-1}\sum_{i=1}^{l-k} A_{l,k,i}(\cos\phi)^{2(l-k-i)} + (\sin\phi)\ln[(1+\sin\phi)/\cos\phi]\sum_{k=0}^{l-1} B_{l,k}(\cos\phi)^{2(l-k)} \right]d\phi \ , \tag{19}$$

where $A_{l,k,i}$ and $B_{l,k}$ are the following constants:

$$A_{l,k,i} = \frac{i!(i-1)!(4l-2k)!(-1)^k(2l-2k)}{(2i)![(l-k)!]^2k!(2l-k)!2^{2(2l-k-i)+1}} , \tag{20a}$$

$$B_{l,k} = \frac{(4l-2k)!(-1)^k(2l-2k)}{4^{2l-k}[(l-k)!]^2k!(2l-k)!} . \tag{20b}$$

From the general expressions Eqs. (19) and (20) one can obtain easily the two lowest and most important order parameters

$$\bar{P}_2 = 1 - N^{-1}\frac{3}{2}\int_0^{\pi/2} I(\phi)\{\sin^2\phi + (\sin\phi)(\cos^2\phi)\ln[(1+\sin\phi)/\cos\phi]\}d\phi \tag{21a}$$

and

$$\bar{P}_4 = 1 - N^{-1}\int_0^{\pi/2} I(\phi)\{\sin^2\phi(\tfrac{105}{16}\cos^2\phi + \tfrac{15}{24}) + (\sin\phi)\ln[(1+\sin\phi)/\cos\phi](\tfrac{105}{16}\cos^4\phi - \tfrac{15}{4}\cos^2\phi)\}d\phi . \tag{21b}$$

In these expressions the order parameters are obtained from an integral over the measured intensity $I(\phi)$. Although the integrands are quite different, such use of I resembles Vainshtein's [7,24] method, where $f(\beta)$ is simply *replaced* by $I(\phi)$ in calculating $\bar{P}_n$ in Eq. (1). It is important to note, however, that Vainshtein's method is an empirical approximation. It is found to work well mostly for Maier-Saupe type ODF's having relatively small widths. By contrast, Eqs. (20) and (21) above are exact and are thus applicable to any ODF, regardless of width or shape. The accuracy achievable in calculating the various quantities discussed above is limited only by the quality and density of the measured $I(\phi)$ data, assuming, of course, that sufficiently accurate numerical methods of integration, interpolation, etc. are employed. This point is discussed further in the next section.

III. RESULTS AND DISCUSSION

The expressions derived above were subjected to extensive numerical tests by simulating "experimental" $I(\phi)$ data from a given analytic ODF and inverting it to obtain the "experimental" ODF and quantities derived from it. The results were then compared with those calculated directly from the analytic ODF. A number of ODF's were investigated, ranging from the conventional Maier-Saupe type (denoted MS in the following) through a distribution peaking at $\beta_0 \neq 0$, i.e., tilted molecules (denoted t), to a less realistic, simple square-window ODF. The results obtained for the first two of these are presented in the following.

For the examples presented here, the "measured" $I_{MS}(\phi)$ data were generated from Eq. (10) using $a=8$, while the data of $I_t(\phi)$ were calculated by numerically integrating Eq. (2) for an ODF given by

$$f_t(\beta) = A\{\exp[a\cos^2(\beta-\beta_0)] + \exp[a\cos^2(\beta+\beta_0)]\} \tag{22}$$

using $a=8$ and $\beta_0=40°$. One hundred equidistant points were calculated in each case, and Gauss-distributed random errors of a specified magnitude were then added to I to simulate statistical measurement errors. Using this data as input, the integral equation, Eq. (2), was inverted by employing the analytic solution Eq. (7). The integra-

tion routine used in the inversion used a least-squares-fitted spline function to interpolate the integrand. The code used was a slightly modified version of the Abel inversion program of Beniaminy and Deutsch [17]. In addition to the inverted f, we also calculated in each run the second- and fourth-order OP and the normalized and weighted Legendre polynomials $\hat{P}_2(\beta)$ and $\hat{P}_4(\beta)$ defined by [4]

$$\hat{P}_n(\beta) = N^{-1}P_n(\cos\beta)f(\beta)\sin\beta . \tag{23}$$

The "measured" I data, including random errors of a Gaussian distribution with a half-width of 1%, and the f, $\hat{P}_2$, and $\hat{P}_4$ obtained thereof are plotted in Figs. 2 and 3 for the Maier-Saupe and tilted ODF's, respectively, along with the exact results for each quantity. Note the excellent agreement between the exact and calculated results for all calculated quantities in both examples. The slight deviations observable at $\beta \sim 90°$ reflect the poorer fit of the spline function used in the integration routine to interpolate I near the high-angle termination of the "experimental" data. Both a decrease in the total number of values spanning the angular range and an increase in the random errors in I tend to increase the deviations in the calculated quantities from their exact values, particularly near their endpoints. Note, however, that the deviations of the calculated quantities from their exact values were invariably found to be smaller than the input errors even when those were as large as $\pm 20\%$. This is due, in part, to the ability of the spline routine to follow trends in the data while smoothing local scatter, which is shown by statistical tests to be random [17].

The robustness of the formulas given above and the numerical procedures employed is further reflected in the values obtained for the two order parameters $\bar{P}_2$ and $\bar{P}_4$. The OP calculated for "experimental" errors of varying magnitude are given in Table I for the MS example. The values were calculated using several different procedures.

(a) Numerical integration of Eq. (1) using the analytic f of Eq. (9) without restrictions on the number of integrand values used. An alternative procedure using the analytic I of Eqs. (10) and (21) yielded identical values. Note that in this case random errors are not included in the calculations.

(b) Numerical integration of Eq. (1) using a spline function to interpolate 100 values of f calculated from Eq. (9).

TABLE I. Order parameters for a Maier-Saupe-type orientational distribution function. The values were calculated using four different methods, as discussed in the text. The simulated experimental data used as input in c and d includes Gauss-distributed random errors of a percentage specified in the header. Each Δ is the deviation, in percent, of the preceding value from the exact one given in a.

| Method | $\bar{P}_2$ | | | | | | $\bar{P}_4$ | | | | | |
	0%	Δ	10%	Δ	20%	Δ	0%	Δ	10%	Δ	20%	Δ
a	0.7931						0.4801					
b	0.7933	0.03					0.4801	0.01				
c	0.7932	0.02	0.7924	0.09	0.7910	0.26	0.4801	0.01	0.4792	0.19	0.4780	0.43
d	0.7933	0.03	0.7930	0.02	0.8028	1.22	0.4801	0.01	0.4792	0.18	0.4794	0.13

Here, again, no random errors are included.

(c) Numerical integration of Eq. (21) using a spline to interpolated 100 I values, calculated from Eq. (10), with random errors added as discussed above.

(d) Numerical integration of Eq. (1) using spline interpolation of 100 f values. These were calculated, in turn, from Eq. (7b) using 100 I values including random errors.

The accuracy of the first method is limited only by the convergence limits set for the numerical integration routine, 10^{-6} in our case. Thus, the values listed under a in Table I can be considered exact. Note that the restriction of using 100 f values, method b, introduces only negligible errors of approximately 0.01%. Methods c and d show remarkably good results even for input error values as high as 20%. In most cases listed, the error is roughly that of b, i.e., the numerical integration error only.
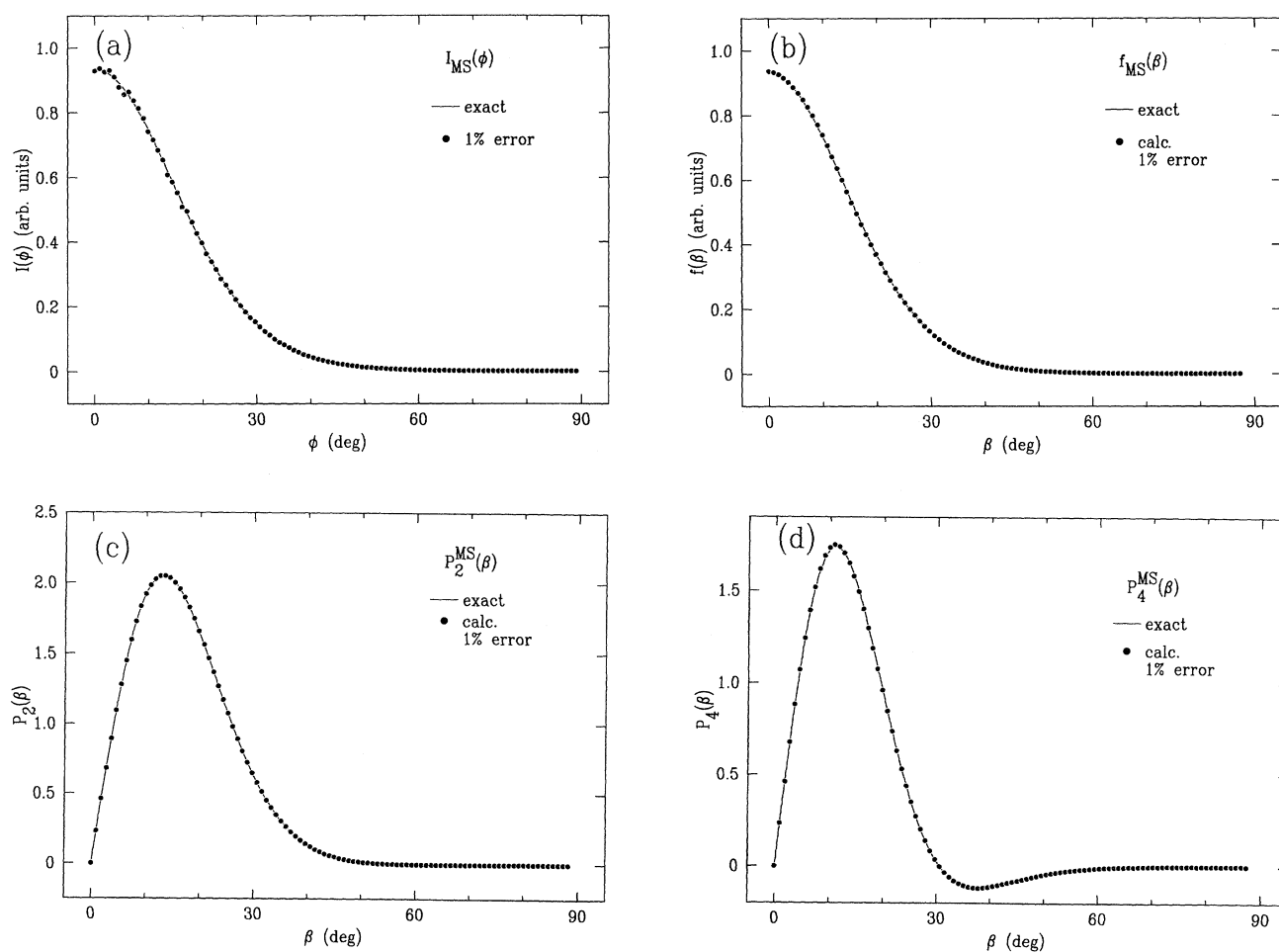

FIG. 2. Simulated data for a Maier-Saupe–type orientational distribution function with (a) 1% Gauss-distributed random errors added, (b) the inverted ODF and (c) the calculated weighted Legendre polynomials $\hat{P}_2$ and (d) $\hat{P}_4$. For details see text. Note the excellent agreement between the exact results (———) and those calculated from the ODF obtained using the present method (●).
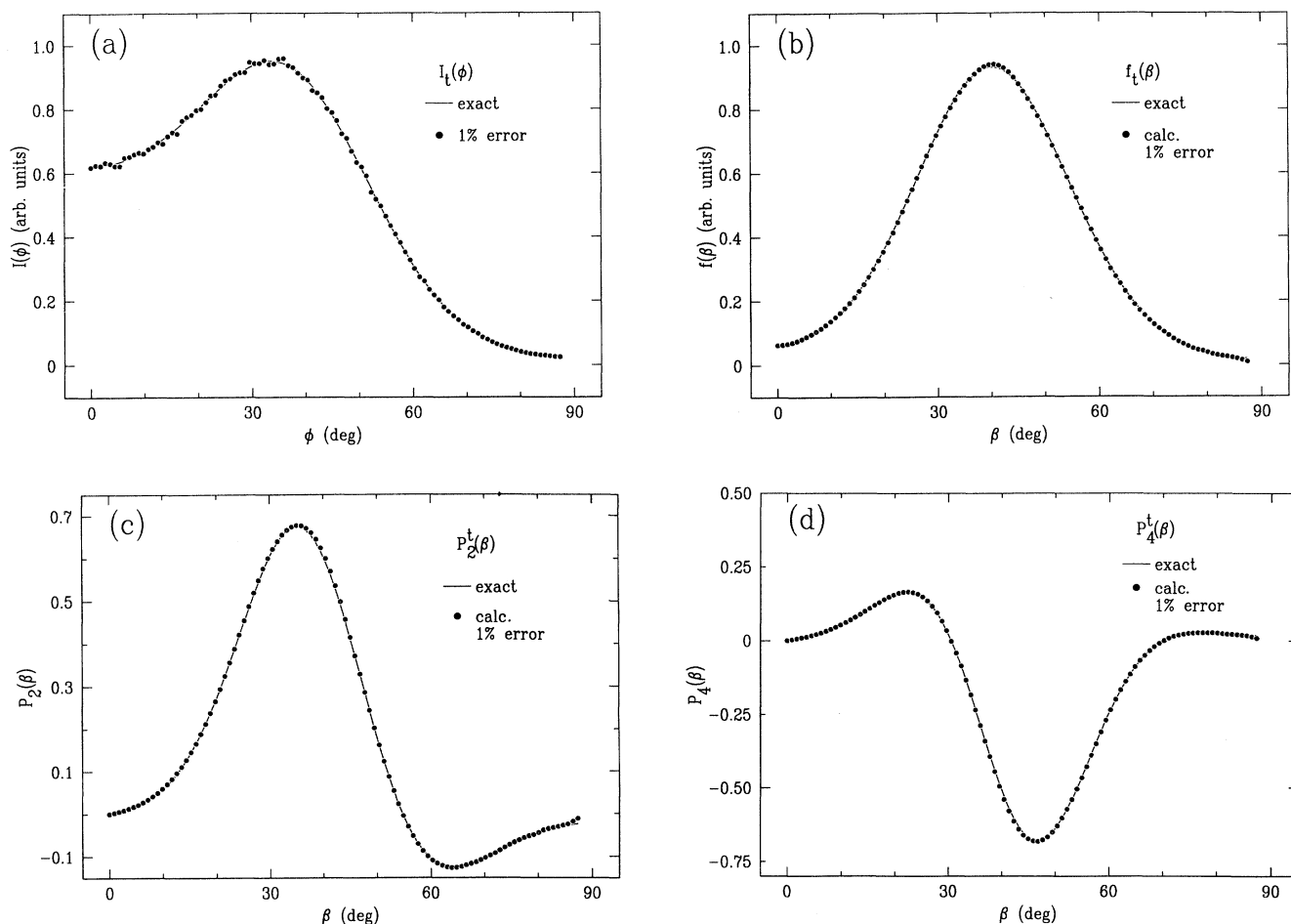
FIG. 3. Same as Fig. 2 but for a tilted orientational distribution function, given in Eq. (22).

While the accuracy of the calculated OP for methods c and d deteriorates when increasing the input random errors above 20% and up to 60%, the deviations of the calculated OP from their exact values remain smaller than the input errors by at least one order of magnitude. In all ODF studied, more accurate results were obtained by calculating the derived quantities, including the OP, directly from I by method c, as compared to calculating f first and using it to calculate the derived quantities as in method d. This holds particularly true for large random errors in I and/or for sparse I data, which are the most demanding cases.

From the extensive number of examples studied, some of which were presented above, we conclude that the present method allows an accurate determination of the ODF and the quantities derived from it even when the measured intensity data contain fairly large random errors and/or are sparse. This, along with the advantages of having a closed-form analytic solution and the ability to calculate a number of physically significant quantities directly from the measured intensity, important for data analysis as well as theory, are bound to render the analytic solution presented here a useful tool for the study of liquid crystals and related materials.

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