Phenomenological models to the ± 1 disclination core structure: comparison with computer simulation results

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June 19, 1999

1 Introduction

The phenomenological approach to the investigation of the line defects was first described by Schopohl and Sluckin [1]. To study the structure of the disclination core they worked with full order parameter tensor $Q_{\alpha\beta}$ in the frame of Landau-de Gennes theory. The *full* order parameter $Q_{\alpha\beta}$ was used because of two reasons: a) to avoid *divergent* terms in the elastic energy; b) to take into account possible *biaxiality* of the defect core.

Then, the general idea was implemented for the particular problem of the core structure of the ± 1 strength defect. Biscari and Virga [2] and Mottram and Hogan [3] solved the equations for the order tensor and obtained the profiles for the order parameter and biaxiality. Finally, Sigillo et al [4] studied the problem in contest of Maier-Saupe mean-field approach. We recapitulated their results to fit the simulation data.

2 Basic equations

The equations for the second order moment $\mathbf{M}$ of the orientational distribution function of the molecules, related to the tensorial order parameter as $\mathbf{S} = \frac{3}{2}\mathbf{M} - \frac{1}{2}\mathbf{I}$, can be rewritten as

$$\begin{aligned} \frac{d^2 M_{\rho\rho}}{d\rho^2} + \frac{1}{\rho}\frac{dM_{\rho\rho}}{d\rho} - \frac{2}{\rho^2}\left(M_{\rho\rho} - M_{\theta\theta}\right) - f_1\left(M_{\rho\rho}, M_{\theta\theta}\right) = 0 \\ \frac{d^2 M_{\theta\theta}}{d\rho^2} + \frac{1}{\rho}\frac{dM_{\theta\theta}}{d\rho} + \frac{2}{\rho^2}\left(M_{\rho\rho} - M_{\theta\theta}\right) + f_2\left(M_{\rho\rho}, M_{\theta\theta}\right) = 0 \end{aligned} \tag{1}$$

subject to the boundary conditions

$$M'_{\rho\rho}\Big|_{\rho=0}, \;\; M'_{\theta\theta}\Big|_{\rho=0} = 0, \tag{2}$$

$$M_{\rho\rho}|_{\rho=R} = \frac{1}{3}\left(2S_s + 1\right), \;\; M_{\theta\theta}|_{\rho=R} = \frac{1}{3}\left(1 - S_s\right).$$

Here the functions f_1, f_2 are theory-specific and have the form:

1. P. Biscari, E. G. Virga

$$f_1 = 2AS,$$
$$f_2 = AS - B\alpha$$

2. N. J. Mottram, S. J. Hogan

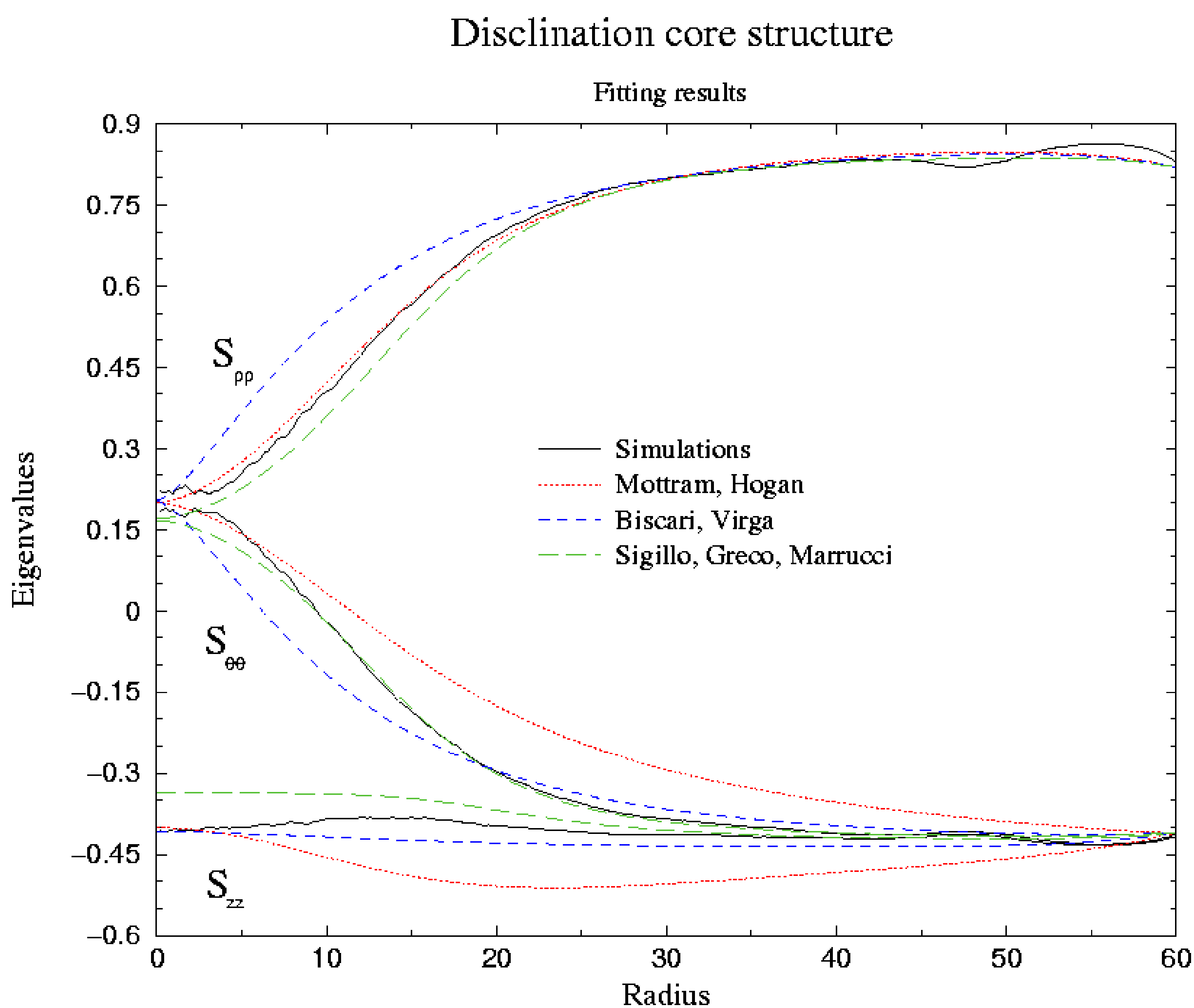
$$f_1 = 2AS\,(S - S_u)\,(S - S_b)\,S_b^{-1}\,(S_b - S_u)^{-1}\,,$$
$$f_2 = \tfrac{1}{2}f_1 - B\alpha$$

where $S = \frac{3}{2}M_{\rho\rho} - \frac{1}{2}$, $\alpha = M_{\theta\theta} + \frac{1}{2}M_{\rho\rho} - \frac{1}{2}$.

3. I. Sigillo, F. Greco, G. Marrucci

$$f_1 = \{B_2\,(M_{\rho\rho} - P_{\rho\rho}) - A_2\,(M_{\theta\theta} - P_{\theta\theta})\}\,D^{-1},$$
$$f_2 = \{B_1\,(M_{\rho\rho} - P_{\rho\rho}) - A_1\,(M_{\theta\theta} - P_{\theta\theta})\}\,D^{-1}$$

The boundary problem (1,2) was solved using *relaxation method* [5].



Disclination core structure
Fitting results
Eigenvalues
Radius
Simulations
Mottram, Hogan
Biscari, Virga
Sigillo, Greco, Marrucci
$S_{\rho\rho}$
$S_{\theta\theta}$
S_{zz}
0.9
0.75
0.6
0.45
0.3
0.15
0
−0.15
−0.3
−0.45
−0.6
0
10
20
30
40
50
60

The slope of the fitting curves in general reflects the structure of the core: the center of the core is strongly biaxial, setting in a few units of length, as shown by the splitting of the eigenvalues $S_{\theta\theta}$ and S_{zz}.

At the same time, the difference between the descriptions is also evident: Biscari and Virga's theory gives incorrect shape of $S(\rho)$ for small values of S. This is fairly predictable, since the quadratic expansion of the free energy density $f\tilde{}\ (S - S_b)^2$ was used, which is valid only for small deviations of the order parameter from the bulk value S_b. More sophisticated form of free energy used by Mottram and Hogan (up to the fourth order in S) corrects the slope of the curve for the order parameter $S = S_{\rho\rho}$. However, the biaxial part, $S_{\theta\theta} - S_{zz}$, still has only qualitative agreement with simulation results, which is probably because of quadratic approximation to the biaxial part of the free energy.

The most correct structure of the core predicts the Maier-Saupe theory. However, the potential intensity U is the only parameter we can adjust to fit the simulations results. Therefore, we have slightly lower than obtained in simulations value of the core biaxiality.

References

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Acknowledgments:

The funding of EPSRC grant and the International Soros Science Education Program grant (No. PSU082002) is gratefully acknowledged by D.Andrienko