

Biaxial Nematics of Hard Cuboids in an External Field

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I. METHODOLOGY

We performed Monte Carlo (MC) simulations in the canonical ensemble at constant number of particles, volume and temperature. The packing fraction was set in order to obtain, at equilibrium, isotropic or uniaxial nematic phases as found in the phase diagram of hard board-like particles (HBPs) [1]. Reduced particle length and width are respectively $L^* = L/T = 12$ and $W^* = W/T \in [1, 12]$, with T the particle thickness. The number of particles in the simulation box was set to $N = 2000$. All the results presented in this work have been obtained in a cubic simulation box. The initial configuration consisted of particles aligned along a common direction, with their center of mass randomly distributed. To equilibrate these systems, we first run simulations of approximately $2 \cdot 10^6$ MC cycles, where 1 MC cycle consists of N attempts of displacing (1/3), rotating (1/3) or displacing and rotating (1/3) a randomly selected HBP. At this stage, no external field was applied. After equilibration, the external field was switched on and a second simulation of $\approx 2 \cdot 10^6$ MC cycles was run. Finally, in the new equilibrium state, a third simulation of 10^6 MC cycles was run to evaluate the structural properties of the new phases. Maximum displacements and rotations were set to keep the acceptance rate at approximately 0.4.

It is well known that cubic simulation box could induce an asymmetry in the pressure tensor. Additionally, such a box shape could delay the formation of structured phases (*e.g.* smectic or columnar liquid crystals) due to the difficulty to accommodate the periodicity of the positional order of the fluid within the boundary conditions of the box. In order to check if the box shape would introduce any inconsistency into our results, we have used different box shapes for both isotropic and nematic phases. More specifically, we have used as initial configurations those obtained from *NPT* simulations of our recent work [1], where the three dimensions were different from each other. In this case, the number of HBPs is in the range [1100, 3648], depending on W^* . We have also run *NVT* simulations where the initial shape of the box was cubic, but, along the simulation, the box dimensions were left free to change independently, while keeping the volume constant. In this last case, the attempt of changing volume was the same as that of a standard *NPT* simulation. All these test simulations have been performed for HBPs of different sizes, field strengths and uniaxial and biaxial phases. The results revealed a sound consistency across all the systems, with some minor differences noticed in the magnitude of the order parameters (no more than 3%). No changes in the morphology of the phases was detected.

II. PARALLEL PAIR DISTRIBUTION FUNCTIONS

The pair distribution functions shown in Fig. 1 indicate the lack of positional order in the biaxial nematic phase, N_B , for a suspension of HBPs with $W^* = 3.46$, $\eta = 0.340$ and $\epsilon_f^* = 3.0$. A similar behaviour has been observed in all the remaining uniaxial and biaxial nematic phases investigated in this work.

III. UNIAXIAL AND BIAXIAL ORDER PARAMETERS

In the tables below, the uniaxial nematic order parameters $S_{2,L}$, $S_{2,T}$ and $S_{2,W}$, the biaxial nematic order parameter B_2 corresponding to the largest uniaxial nematic order parameter, and observed phase at different field strength ($\epsilon_f/k_B T$), for a fluid of HBPs with $L^* = 12$. The values in brackets denote statistical uncertainty - one standard deviation - in the last digit. The particle width and system packing fraction are indicated in the table captions. Tables I to XI refer to initial isotropic phases, whilst Tables XII to XXII to initial uniaxial nematic phases.

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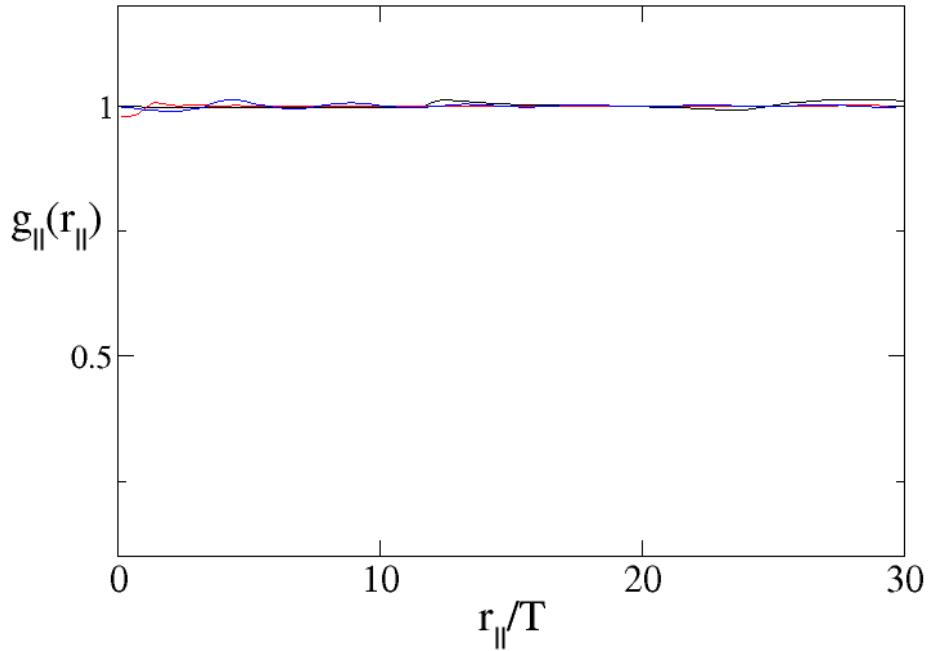


Figure 1: Parallel distribution function $g_{||}(r_{||})$ along the nematic directors \hat{m} (black line), \hat{p} (red line) and \hat{n} (blue line) calculated by computer simulation in a fluid of HBPs with $L^* = 12$ and $W^* = 3.46$, packing fraction $\eta = 0.340$, and field strength $\epsilon_f^* = 3.0$

Table I: $W^* = 1$; $\eta = 0.202$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.051(2)	0.033(1)	0.025(1)	–	I
0.10	0.086(2)	0.036(1)	0.057(1)	–	I
0.30	0.132(1)	0.038(1)	0.136(1)	–	I
0.50	0.194(1)	0.058(2)	0.205(1)	–	I
0.75	0.407(2)	0.178(1)	0.308(2)	0.183(1)	N_U^+
1.00	0.528(1)	0.272(4)	0.394(1)	0.259(2)	N_B^+
1.25	0.592(2)	0.347(1)	0.461(1)	0.316(1)	N_B^+
1.50	0.624(1)	0.402(1)	0.523(1)	0.407(1)	N_B
2.00	0.681(1)	0.503(1)	0.627(1)	0.509(2)	N_B
3.00	0.719(1)	0.614(2)	0.758(1)	0.631(2)	N_B

[1] A. Cuetos, M. Dennison, A. Masters and A. Patti, *Soft Matter*, 2017, **13**, 4720.

Table II: $W^* = 2.5$; $\eta = 0.277$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.154(3)	0.079(7)	0.039(9)	–	I
0.10	0.158(4)	0.068(8)	0.064(8)	–	I
0.30	0.466(3)	0.209(1)	0.181(1)	0.101(1)	N_U^+
0.50	0.613(4)	0.371(7)	0.308(9)	0.247(9)	N_B^+
0.75	0.685(2)	0.452(7)	0.395(3)	0.335(7)	N_B^+
1.00	0.733(8)	0.542(6)	0.487(8)	0.378(9)	N_B
1.50	0.792(7)	0.665(9)	0.624(7)	0.517(8)	N_B
2.00	0.821(5)	0.735(7)	0.705(6)	0.645(4)	N_B
3.00	0.858(5)	0.815(6)	0.806(4)	0.734(8)	N_B

Table III: $W^* = 3$; $\eta = 0.289$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.051(2)	0.050(2)	0.023(8)	–	I
0.10	0.146(3)	0.096(1)	0.066(1)	–	I
0.30	0.471(2)	0.313(1)	0.215(1)	0.194	N_U^+
0.50	0.600(2)	0.464(2)	0.348(3)	0.334(2)	N_B^+
0.75	0.679(2)	0.572(2)	0.458(8)	0.460(3)	N_B
1.00	0.723(4)	0.642(6)	0.538(8)	0.463(7)	N_B
1.50	0.788(7)	0.734(8)	0.661(7)	0.574(7)	N_B
2.00	0.824(6)	0.789(7)	0.734(5)	0.664(8)	N_B
3.00	0.861(5)	0.857(7)	0.821(7)	0.718(6)	N_B

Table IV: $W^* = 3.46$; $\eta = 0.307$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.225(3)	0.215(4)	0.050(11)	–	I
0.10	0.417(2)	0.430(3)	0.189(2)	0.258(2)	N_B^-
0.30	0.561(2)	0.569(1)	0.345(3)	0.401(2)	N_B
0.50	0.622(8)	0.648(2)	0.447(1)	0.490(8)	N_B
0.75	0.682(1)	0.723(1)	0.540(1)	0.567(1)	N_B
1.00	0.730(7)	0.762(1)	0.607(8)	0.633(8)	N_B
1.50	0.796(8)	0.812(7)	0.711(8)	0.728(8)	N_B
2.00	0.827(5)	0.848(6)	0.765(6)	0.778(5)	N_B
3.00	0.871(4)	0.881(5)	0.841(4)	0.844(5)	N_B

Table V: $W^* = 4.0$; $\eta = 0.261$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.028(2)	0.037(2)	0.020(1)	–	I
0.10	0.039(1)	0.064(2)	0.046(1)	–	I
0.30	0.095(3)	0.182(4)	0.128(2)	–	I
0.50	0.191(4)	0.307(6)	0.217(3)	–	I
0.75	0.404(2)	0.549(3)	0.356(3)	0.290(1)	N _B [−]
1.00	0.504(2)	0.636(1)	0.454(2)	0.372(2)	N _B
1.25	0.571(2)	0.686(2)	0.525(2)	0.444(1)	N _B
1.50	0.628(1)	0.725(1)	0.587(3)	0.526(1)	N _B
2.00	0.716(4)	0.778(6)	0.686(8)	0-628(6)	N _B
3.00	0.794(7)	0.827(7)	0.790(5)	0.739(9)	N _B

Table VI: $W^* = 4.5$; $\eta = 0.250$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.036(2)	0.051(1)	0.025(1)	–	I
0.10	0.049(2)	0.090(3)	0.048(1)	–	I
0.30	0.064(2)	0.154(4)	0.122(1)	–	I
0.50	0.158(3)	0.298(4)	0.213(1)	–	I
0.75	0.151(3)	0.291(1)	0.213(2)	–	I
1.00	0.439(2)	0.615(2)	0.423(1)	0.323(2)	N _B [−]
1.25	0.511(2)	0.670(2)	0.500(1)	0.409(1)	N _B
1.50	0.570(2)	0.708(1)	0.633(1)	0.503(1)	N _B
2.00	0.663(1)	0.761(1)	0.660(1)	0.622(2)	N _B
3.00	0.759(1)	0.812(1)	0.773(1)	0.715(1)	N _B

Table VII: $W^* = 5.0$; $\eta = 0.248$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.056(2)	0.072(3)	0.031(1)	–	I
0.10	0.050(2)	0.100(5)	0.055(1)	–	I
0.30	0.063(2)	0.172(4)	0.138(1)	–	I
0.50	0.218(3)	0.445(4)	0.241(1)	0.152(0)	N _U [−]
0.75	0.336(2)	0.581(3)	0.343(2)	0.254(2)	N _U [−]
1.00	0.432(1)	0.657(2)	0.429(1)	0.328(2)	N _B [−]
1.25	0.509(2)	0.708(1)	0.501(1)	0.421(2)	N _B
1.50	0.564(1)	0.734(1)	0.560(1)	0.460(1)	N _B
2.00	0.653(1)	0.774(1)	0.660(1)	0.541(2)	N _B
3.00	0.758(1)	0.820(1)	0.779(1)	0.737(2)	N _B

Table VIII: $W^* = 5.5$; $\eta = 0.242$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.048(2)	0.098(1)	0.034(1)	–	I
0.10	0.058(2)	0.118(1)	0.060(1)	–	I
0.30	0.089(3)	0.245(7)	0.152(2)	–	I
0.50	0.222(3)	0.481(4)	0.248(1)	0.146(2)	N _U [−]
0.75	0.328(2)	0.594(3)	0.340(1)	0.246(1)	N _U [−]
1.00	0.406(2)	0.651(2)	0.418(1)	0.325(2)	N _B [−]
1.25	0.476(1)	0.704(2)	0.484(1)	0.390(1)	N _B
1.50	0.545(1)	0.735(1)	0.553(1)	0.468(2)	N _B
2.00	0.637(1)	0.776(1)	0.652(1)	0.572(2)	N _B
3.00	0.740(1)	0.817(1)	0.769(1)	0.725(2)	N _B

Table IX: $W^* = 6.0$; $\eta = 0.224$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.036(3)	0.047(1)	0.024(2)	–	I
0.10	0.081(3)	0.198(1)	0.087(2)	–	I
0.30	0.189(2)	0.529(3)	0.196(2)	0.075(2)	N _U [−]
0.50	0.275(2)	0.609(3)	0.277(1)	0.158(2)	N _U [−]
0.75	0.354(2)	0.672(2)	0.362(1)	0.221(1)	N _B [−]
1.00	0.423(2)	0.707(2)	0.433(1)	0.320(2)	N _B [−]
1.25	0.487(1)	0.740(1)	0.498(1)	0.382(1)	N _B
1.50	0.548(1)	0.768(1)	0.560(1)	0.428(1)	N _B
2.00	0.626(1)	0.788(1)	0.651(1)	0.577(1)	N _B
3.00	0.741(1)	0.831(1)	0.769(1)	0.664(1)	N _B

Table X: $W^* = 8.0$; $\eta = 0.220$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.043(2)	0.072(2)	0.039(1)	–	I
0.10	0.088(2)	0.226(1)	0.101(2)	–	I
0.30	0.160(4)	0.482(7)	0.198(2)	0.066(2)	N _U [−]
0.50	0.236(2)	0.584(3)	0.270(2)	0.130(0)	N _U [−]
0.75	0.302(3)	0.634(4)	0.343(2)	0.205(1)	N _B [−]
1.00	0.370(2)	0.689(2)	0.409(2)	0.286(2)	N _B [−]
1.25	0.436(2)	0.718(2)	0.480(1)	0.364(2)	N _B
1.50	0.490(2)	0.739(2)	0.536(1)	0.404(2)	N _B
2.00	0.578(1)	0.770(2)	0.632(1)	0.497(1)	N _B
3.00	0.691(1)	0.800(1)	0.(1)	0.758(1)	N _B

Table XI: $W^* = 12$; $\eta = 0.183$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.075(3)	0.225(2)	0.084(1)	–	I
0.10	0.069(4)	0.166(6)	0.093(3)	–	I
0.30	0.084(3)	0.296(9)	0.192(3)	–	I
0.50	0.162(5)	0.470(7)	0.255(6)	0.110(4)	N_U^-
0.75	0.237(5)	0.562(9)	0.332(2)	0.180(3)	N_U^-
1.00	0.298(6)	0.586(1)	0.401(6)	0.262(4)	N_B^-
1.25	0.342(2)	0.602(2)	0.469(1)	0.325(1)	N_B^-
1.50	0.398(6)	0.632(7)	0.531(3)	0.398(1)	N_B
2.00	0.479(5)	0.662(8)	0.626(3)	0.472(3)	N_B
3.00	0.592(7)	0.708(7)	0.752(2)	0.603(2)	N_B

Table XII: $W^* = 1$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.893(4)	0.251(1)	0.233(1)	0.019(7)	N_U^+
0.10	0.887(3)	0.282(2)	0.260(1)	0.062(2)	N_U^+
0.30	0.902(6)	0.376(2)	0.355(2)	0.185(2)	N_U^+
0.50	0.899(5)	0.463(2)	0.438(2)	0.299(2)	N_B^+
0.75	0.906(3)	0.576(1)	0.546(1)	0.445(1)	N_B
1.00	0.919(1)	0.660(4)	0.632(1)	0.556(2)	N_B
1.50	0.911(3)	0.660(1)	0.632(1)	0.556(1)	N_B
2.00	0.920(3)	0.834(7)	0.806(7)	0.873(2)	N_B
3.00	0.932(2)	0.890(5)	0.872(1)	0.864(2)	N_B

Table XIII: $W^* = 2.5$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.883(6)	0.252(1)	0.231(1)	0.021(1)	N_U^+
0.10	0.889(3)	0.282(2)	0.260(1)	0.061(2)	N_U^+
0.30	0.893(5)	0.380(2)	0.354(1)	0.190(2)	N_U^+
0.50	0.906(4)	0.462(1)	0.440(1)	0.298(2)	N_B^+
0.75	0.904(4)	0.569(1)	0.539(1)	0.437(1)	N_B
1.00	0.908(4)	0.663(1)	0.631(1)	0.559(2)	N_B
2.00	0.924(2)	0.833(7)	0.809(6)	0.877(3)	N_B
3.00	0.928(2)	0.889(5)	0.870(4)	0.895(3)	N_B

Table XIV: $W^* = 3.0$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.839(1)	0.256(1)	0.215(1)	0.029(1)	N_U^+
0.10	0.843(5)	0.315(2)	0.268(2)	0.104(2)	N_U^+
0.30	0.867(4)	0.445(2)	0.401(2)	0.271(2)	N_B^+
0.50	0.851(5)	0.571(2)	0.507(2)	0.430(2)	N_B
1.00	0.855(7)	0.760(1)	0.681(1)	0.668(1)	N_B
2.00	0.905(3)	0.867(5)	0.823(5)	0.823(7)	N_B
3.00	0.923(3)	0.905(4)	0.879(4)	0.881(5)	N_B

Table XV: $W^* = 3.46$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.731(8)	0.279(3)	0.190(2)	0.053(3)	N_U ⁺
0.10	0.641(2)	0.577(2)	0.347(1)	0.398(2)	N_B
0.30	0.711(5)	0.687(1)	0.493(1)	0.525(2)	N_B
0.50	0.750(6)	0.742(1)	0.575(1)	0.619(2)	N_B
0.75	0.750(6)	0.742(1)	0.575(1)	0.619(2)	N_B
1.00	0.814(4)	0.827(8)	0.704(7)	0.688(5)	N_B
1.50	0.814(4)	0.827(8)	0.704(6)	0.688(5)	N_B
2.00	0.887(4)	0.889(5)	0.828(5)	0.800(1)	N_B
3.00	0.911(3)	0.916(3)	0.876(3)	0.862(7)	N_B

Table XVI: $W^* = 4.0$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.265(6)	0.864(8)	0.231(6)	0.040(6)	N_U ⁻
0.10	0.323(9)	0.863(8)	0.287(8)	0.114(1)	N_U ⁻
0.30	0.511(8)	0.864(7)	0.457(8)	0.354(2)	N_B
0.50	0.635(3)	0.858(1)	0.567(8)	0.508(4)	N_B
1.00	0.783(1)	0.876(7)	0.719(1)	0.708(2)	N_B
2.00	0.860(4)	0.909(4)	0.823(4)	0.813(3)	N_B
3.00	0.865(2)	0.924(5)	0.844(2)	0.831(2)	N_B

Table XVII: $W^* = 4.5$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.279(8)	0.895(7)	0.260(8)	0.048(8)	N_U ⁻
0.10	0.289(7)	0.898(6)	0.271(5)	0.066(9)	N_U ⁻
0.30	0.402(5)	0.902(5)	0.378(5)	0.218(6)	N_B ⁻
0.50	0.415(5)	0.909(4)	0.398(5)	0.238(7)	N_B ⁻
0.75	0.589(6)	0.908(6)	0.560(6)	0.462(8)	N_B
1.00	0.683(4)	0.909(4)	0.650(6)	0.547(7)	N_B
2.00	0.842(4)	0.919(4)	0.815(5)	0.719(6)	N_B
3.00	0.891(4)	0.931(3)	0.872(3)	0.853(4)	N_B

Table XVIII: $W^* = 5.0$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.257(9)	0.912(5)	0.246(9)	0.031(1)	N_U ⁻
0.10	0.292(1)	0.916(5)	0.280(1)	0.069(1)	N_U ⁻
0.30	0.391(6)	0.915(4)	0.378(5)	0.207(2)	N_B ⁻
0.50	0.432(4)	0.920(5)	0.418(5)	0.256(5)	N_B ⁻
0.75	0.532(1)	0.923(4)	0.517(1)	0.386(1)	N_B
1.00	0.708(7)	0.919(4)	0.683(8)	0.618(1)	N_B
2.00	0.834(3)	0.928(3)	0.813(3)	0.788(3)	N_B
3.00	0.854(1)	0.936(3)	0.841(1)	0.817(1)	N_B

Table XIX: $W^* = 5.5$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.251(4)	0.916(5)	0.243(7)	0.016(4)	N _U ⁻
0.10	0.278(1)	0.914(6)	0.268(1)	0.054(2)	N _U ⁻
0.30	0.351(2)	0.920(5)	0.342(2)	0.152(2)	N _U ⁻
0.50	0.428(2)	0.923(6)	0.417(1)	0.246(2)	N _B ⁻
0.75	0.523(2)	0.920(5)	0.511(1)	0.369(2)	N _B
1.00	0.596(1)	0.923(5)	0.584(1)	0.462(1)	N _B
2.00	0.798(9)	0.930(3)	0.782(8)	0.699(1)	N _B
3.00	0.872(5)	0.937(3)	0.863(5)	0.812(7)	N _B

Table XX: $W^* = 6.0$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.256(4)	0.929(4)	0.250(3)	0.017(3)	N _U ⁻
0.10	0.277(6)	0.931(6)	0.272(6)	0.051(6)	N _U ⁻
0.30	0.322(6)	0.932(4)	0.317(6)	0.112(8)	N _U ⁻
0.50	0.401(3)	0.932(4)	0.395(4)	0.218(5)	N _B ⁻
0.75	0.447(5)	0.934(4)	0.441(5)	0.280(5)	N _B ⁻
1.00	0.585(1)	0.934(4)	0.576(2)	0.432(4)	N _B
1.50	0.703(4)	0.937(3)	0.693(4)	0.616(4)	N _B
2.00	0.791(8)	0.939(3)	0.781(7)	0.735(1)	N _B
3.00	0.871(5)	0.943(3)	0.865(4)	0.842(5)	N _B

Table XXI: $W^* = 8.0$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.248(4)	0.939(4)	0.244(4)	0.011(3)	N _U ⁻
0.10	0.306(2)	0.945(3)	0.303(3)	0.089(3)	N _U ⁻
0.30	0.340(6)	0.945(3)	0.337(5)	0.134(7)	N _U ⁻
0.50	0.348(4)	0.947(2)	0.346(5)	0.144(6)	N _U ⁻
0.75	0.429(2)	0.948(2)	0.427(2)	0.250(3)	N _B ⁻
1.00	0.654(1)	0.948(3)	0.651(1)	0.547(1)	N _B
2.00	0.755(6)	0.951(3)	0.753(5)	0.687(7)	N _B
3.00	0.818(8)	0.953(3)	0.820(8)	0.769(1)	N _B

Table XXII: $W^* = 12.0$; $\eta = 0.340$.

$\epsilon_f/k_B T$	$S_{2,L}$	$S_{2,T}$	$S_{2,W}$	B_2	Phase
0.00	0.252(1)	0.947(3)	0.252(1)	0.013(8)	N _U ⁻
0.10	0.269(8)	0.950(3)	0.270(8)	0.035(9)	N _U ⁻
0.30	0.321(7)	0.950(2)	0.322(6)	0.098(7)	N _U ⁻
0.50	0.367(7)	0.952(2)	0.368(7)	0.156(8)	N _U ⁻
0.75	0.447(5)	0.952(2)	0.450(6)	0.246(6)	N _B ⁻
1.00	0.503(1)	0.948(5)	0.511(1)	0.357(2)	N _B
1.50	0.628(1)	0.952(4)	0.635(1)	0.523(2)	N _B
2.00	0.721(7)	0.952(3)	0.729(7)	0.648(9)	N _B
3.00	0.832(5)	0.954(3)	0.845(5)	0.797(6)	N _B