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Prošnja za odobritev teme doktorske disertacije

Spoštovani,

podpisani Jure Aplinc prosim za odobritev teme doktorske disertacije z naslovom

"Field structures in active and passive liquid crystals"

(Strukture polja v aktivnih in pasivnih tekočih kristalih).

Prosim vas za odobritev pisanja disertacije v angleškem jeziku.

S spoštovanjem,

Jure Aplinc

Priloge:

- življenjepis
- osebna bibliografija
- utemeljitev teme disertacije v slovenskem in angleškem jeziku z literaturo

Življenjepis

Jure Aplinc

31. marec 2016

Jure Aplinc se je rodil 7. novembra 1989 v Slovenj Gradcu, osnovno šolo pa je začel obiskovati v Šoštanju leta 1996. V osnovni šoli se je udeležil mnogih tekmovanj in prejel nekaj srebrnih in eno zlato priznanje.

Po koncu osnovne šole se je vpisal na Gimnazijo Lava v Celju. V gimnaziji se je posvečal predvsem fiziki in matematiki. Jure se je vsako leto udeleževal tekmovanja iz fizike in leta 2007 dosegel drugo nagrado iz zlato priznanje, leto za tem pa tretjo nagrado in zlato priznanje. V četrtem letniku je po priporočilu učitelja fizike reševal zahtevnejše fizikalne probleme "Physics Challenge for Teachers and Students", ki so bili mesečno objavljeni v Ameriški reviji The Physics Teacher. V omenjeni reviji je bil zaradi tega tudi večkrat naveden kot uspešen tekmovalec.

Po zaključeni maturi leta 2008 se je vpisal na študij fizike na Fakulteti za matematiko in fiziko v Ljubljani. Leta 2011 je z najvišjim povprečjem v generaciji zaključil prvo bolonjsko stopnjo, s tem si je pridobil naziv diplomirani fizik (UN). V istem letu je študij nadaljeval na smeri matematična fizika, ki se izvaja na drugi bolonjski stopnji študija fizike. Študij je končal leta 2014 in si tako pridobil naziv Magister fizike. V času študija je bil eno leto tutor pri predmetu Matematika 3 in 4, več let pa tudi pri predmetu Matematična fizika 1. Leta 2012 se je udeležil poletne šole o fiziki delcev, ki je potekala pod okriljem DESY v Hamburgu.

Aplinc je trenutno zaposlen na projektu pri prof. Mihi Ravniku na Fakulteti za matematiko in fiziko. Ukvarja se s študijem struktur polja v pasivnih ter aktivnih tekočekristalnih sistemih in razvija metamaterialne koloide, ki lahko zaradi vplivov okoliškega tekočega kristala spontano tvorijo kristalno rešetko. Udeležil se je treh poletnih šol na temo mehke snovi in mrežne Boltzmannove metode. Imel je eno prispevano predavanje na konferenci Flowing matter 2016 v Portu in predstavitev s plakatom na dveh drugih. V objavo ima poslan en znanstveni članek z naslovom "Porous nematic microfluidics for generation of umbilic defects and umbilic defect lattices", trije drugi pa so v pripravi. Marca 2015 je bil tudi habilitiran na mesto asistenta na Fakulteti za matematiko in fiziko, kjer letos vodi vaje pri predmetu Računalniška orodja v fiziki.

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Strukture polja v aktivnih in pasivnih tekočih kristalih

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31. marec 2016

Tekoči kristali so kompleksne tekočine, ki lahko zaradi vplivov ograditve, zunanjih polj, toka ali vključenih koloidnih delcev tvorijo mnogotere strukture v polju. Tekoči kristal običajno sestavljajo podolgovate molekule organskega izvora, ki se pri določeni temperaturi ali koncentraciji spontano uredijo vzdolž preferirane smeri, ki ji pravimo direktor [1]. Prej omenjeni zunanji vplivi pokvarijo uniformno ureditev, zaradi tega se med posameznimi delci pojavijo elastične sile. Tovrstno polje sil je zavoljo anizotropne oblike molekul močno prostorsko odvisno, kar povzroči pojavitev kompleksnih struktur v polju in druge pojave.

Zaradi velike simetrije molekul tekočega kristala je ureditveni parameter simetrični brezsledni tenzor drugega reda Q_{ij}. Njegova glavna os is enakovredna direktorju, največja lastna vrednost pa opisuje stopnjo urejenosti. Tenzor ureditvenega parametra opisuje krajevno povprečje orientacije molekul v izbranem delu tekočega kristala.

Tekoči kristali so tekočine in lahko tečejo, njihova dinamika pa je precej drugačna in mnogo bolj komplicirana kot dinamika izotropnih tekočin. Do teh razlik prihaja zato, ker je materialni tok tekočega kristala sklopljen z orientacijo molekul. Zaradi tega lahko tok vpliva na orientacijo direktorja in obratno, rotacija direktorja lahko požene tok. Ta pojav je znan tudi kot pojav povratnega toka. Tekoči kristali tečejo zgolj zaradi zunanjih sil kot so tlačni gradienti, težnost in električna polja, zato spadajo v razred pasivnih tekočin. Aktivne tekočine, ki opisujejo široko paleto bioloških sistemov (oziroma biološko navdahnjenih sistemov) od mikrotubulov [2, 3, 4], suspenzij bakterij, [5, 6, 7, 8], suspenzij alg [9], kovinskih palčk [10, 11] do sperme [12] pa ravno nasprotno tečejo kar same od sebe.

Defekti v tekočih kristalih lahko zaradi ograditve, vključenih koloidnih delcev, zunanjih polj in toka tvorijo kaotične ali celo urejene strukture. Ograjenost in površinsko sidranje lahko tvori in vpliva na defekte v tekočem kristalu. V primeru ko je struktura, ki ograjuje tekoči kristal pravilna je prehod iz kaotične strukture defektov v urejeno mogoče kontrolirati [13], tovrstni sistemi pa imajo spominski efekt. Tudi koloidni delci v tekočem kristalu ustvarjajo defekte na svoji površini. Defekti se glede na predznak privlačijo oziroma odbijajo, ako koloide pravilno oblikujemo se lahko povezujejo v kristale, ki se lahko sami izgrajujejo [14]. Tudi pasivni in aktivni tok povzroča reorientacijo direktorja preko mehanizma povratnega toka. Ta lahko v določenih pogojih povzroči nastanek struktur v direktorskem polju [15].

Kompleksni sistemi defektnih struktur so skupaj z ograditvijo in koloidi zanimivi kot 1D, 2D ali 3D fotonski kristali [16] s spremenljivimi in nastavljivimi fotonskimi pasovi. Fotonski pasovi v takšnih sestavljenih fotonskih materialih so posledica tako orientacijskega profila defektnih struktur kot tudi pravilne mreže ograditve ali koloidnih delcev. Samo-sestavljeni koloidni kristali [17, 18] so zanimivi tudi za fotonske aplikacije in lahko delujejo kot uklonske reže. Primerna oblika in izbira materiala koloidnih delcev lahko vodi do zelo zanimivih fotonskih lastnosti samo-sestavljenih koloidnih kristalov, kot je na primer negativni lomni količnik [19].

Dinamika tekočih kristalov se močno razlikuje od dinamike izotropnih tekočin, saj se hkrati obnaša kot viskozen in elastičen medij [1]. Viskozni odziv na zunanje sile je kompliciran zaradi orientacijskega urejanja, kar privede do efektivno anizotropne viskoznosti. Hitrostno polje je določeno z generalizirano Navier-Stokesovo enačbo, ki vključuje anizotropno viskoznost in elastičnost in aktivnost. Kombinacija Navier-Stokesove enačbe in enačb nematske elastičnosti nas privede do Ericksen-Leslijevih enačb [1], ki pa predpostavljajo konstantno stopnjo reda. Ta pogoj pogosto ni izpolnjen zato uporabimo Beris-Edwardsov model, ki namesto direktorja uporablja tenzor ureditvenega parametra. Model vključuje reduciran set materialnih parametrov - samo eno rotacijsko translacijsko viskoznost in eno elastično konstanto.

Sistemi, ki jih bomo študirali v tej doktorski disertaciji, zaradi kompliciranih robnih efektov običajno nimajo analitične rešitve. Zaradi tega bomo uporabili različne numerične tehnike za reševanje enačb. Za simuliranje polne hidrodinamike tekočih kristalov bomo uporabljali hibridno mrežno Boltzmannovo metodo. Metoda je sestavljena iz dveh delov (i) metode končnih diferenc za evolucijo ureditvenega parametra in (ii) mrežne Boltzmanove metode za reševanje generalizirane Navier-Stokesove enačbe za hitrostno polje.

Prosto energijo minimiziramo numerično z Euler-Lagrangeovim formalizmom in relaksacijskim algoritmom [20]. Problem rešimo numerično s kodo, ki je bila razvita v ta namen, temelji pa na metodi končnih diferenc na kubični mreži. Obstaja mnogo metod s katerimi lahko minimiziramo funkcional proste energije, na primer metoda končnih elementov (FEM) in spust po konjugiranem gradientu (conjugate gradient descent) [21]. Predvsem metode končnih elementov imajo mnogo prednosti, na primer adaptivnost mreže, kar lahko pospeši simulacije in omogoči računanje z veliko natančnostjo na določenih področjih. Prav zaradi adaptivnosti mreže je tovrstne metode težko implementirati. Glavna prednost metode končnih diferenc je v tem, da jo lahko inkorporiramo v mrežno Boltzmannovo metodo in tako dobimo polno rešitev nematske dinamike.

Mrežna Boltznannova metoda je numerična shema, ki se je razvila iz avtomatov za mrežni plin (lattice gas automata). Za razliko od običajnih metod, ki rešujejo enačbe numerično, mrežna Boltzmannova metoda modelira tekočino z navideznimi delci. Ti delci zaporedoma doživljajo propagiranje po diskretni mreži in trke. Prav zaradi tega ker mrežna Boltzmannova metoda operira z delci ima mnogo prednosti pred drugimi običajnimi metodami, izpostavimo lahko dve: dokaj enostavno obravnavanje in opis kompliciranih robnih površin in zelo dobra paralelizacija algoritma. Algoritem je sestavljen iz diskretnih korakov, ki jih lahko interpretiramo kot propagacije in trki distribucijskih funkcij. Z izbiro primernega operatorja trka in uporabo Chapman-Enskogovega razvoja, dinamika delnih distribucijskih funkcij ustreza dinamiki posplošene Navier-Stokesove enačbe.

Naša skupina je razvila hibridno mrežno Boltzmannovo metodo, ki omogoča študij pasivnega in aktivnega tekočekristalnega toka. Ta je dobro paralelizirana za računanje na večih procesorskih jedrih. Ta metoda je torej namenjena simulacijam toka v aktivnih in pasivnih tekočih kristalih in je kombinacija mrežne Boltzmannove metode in relaksacije z metodo končnih diferenc. To nam odpira možnost da lahko simuliramo tako pasivne in aktivne tokove, kot tudi relaksacijo statičnega tekočega kristala brez toka.

Kompleksna nematska tekočina ima izjemno zanimivo zmožnost samo-sestavljanje urejenih struktur različnih simetrij in dimenzionalnosti, ki so odvisne predvsem od geometrije koloidnih delcev in sidranja. Predlagamo raziskavo samo-sestavljanje kompliciranih koloidnih delcev v obliki podkve, ki v fotoniki služijo kot resonatorji in so potencialno zanimivi kot metamateriali. Tudi kompleksne geometrijske in topološke strukture v zadnjem času vzbujajo vse več pozornosti, saj imajo ti materiali uporabne in zanimive lastnosti. Giroid je kompleksna tri-periodična cevasta struktura, ki se samo-sestavi v določenih surfaktantih ali maščobnih mezofazah. Predlagamo študij struktur v nematskem in holesteričnem tekočem kristalu v tej že sami po sebi kiralni strukturi, ki je gotovo zanimiva tudi kot fotonski kristal. Zaradi nedavnih eksperimentalnih rezultatov je zanimiv tudi študij 64-polnih nematskih koloidov, ki jih trenutno raziskuje eksperimentalna skupina Profesorja Ivana I. Smalyukha iz Univerze v Kolorado Boulderju.

Tekoči kristali so zanimivi tudi v mikrofluidiki, saj tok omogoča postopno prižiganje struktur [15, 22]. Raziskali bomo tok tekočih kristalov v mikrokanalih različnih geometrijskih presekov in z dodatkom cilindričnih vlaken v kanale uvedli poroznost. Zaradi teh vlaken dobimo široka in ozka mesta, ki pomembno spremenijo notranjost mikrokanalov. Glede na naše preliminarne rezultate pričakujemo, da tok deformira direktorsko polje preko mehanizma povratnega toka in tako ustvari zvezne deformacije direktorskega polja, ki jim pravimo umbilični defekti [23]. Umbilični defekti so celoštevilski defekti, pobegli v tretjo dimenzijo. Umbiliki s pozitivnim nabojem nastanejo na območjih z več maksimumi v toku, število teh pa je povezano z njihovim nabojem. Umbilični defekti z negativnim nabojem nastajajo na mestih, kjer ima tokovni profil sedla, število dolin je takisto povezano z nabojem umbilika. Tako uvedena urejena poroznost nas privede do nastanka različnih mrež umbiličnih defektov, ki lahko delujejo kot fotonski kristali, ki jih lahko nastavljamo s tokom. To delo se že izvaja v sodelovanju s prof. Stephenom Morrisom iz univerze v Oxfordu.

Aktivni sistemi so posebej zanimivi saj medsebojni vpliv nematskega urejanja in aktivnosti privede do kolektivnega gibanja. V dovolj aktivnih sistemih to gibanje postane nestabilno in preide v turbulentno obnašanje, ki je zelo podobno kot turbulenca, ki jo poznamo v pasivnih tekočinah pri visokih Reynoldsovih številih. Topološki defekti, značilni za nematske materiale, močno interagirajo s tokom in so lahko, za razliko od tistih v pasivnih tekočih kristalih, dinamično ustvarjeni in anihilirani zaradi toka, ki nasprotuje elastičnim silam. Defektne strukture in dinamika same aktivne tekočine pod in v turbulentnem režimu so slabo poznane, posebej v tri-dimenzionalnih ograjenih sistemih. Zato predlagamo raziskavo dinamike in tvorbe struktur v preprostih sistemih z različnim genusom in sidranjem.

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Field structures in active and passive liquid crystals

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March 31, 2016

Liquid crystaline fluids can be designed into various field structures that are characterised by confinement, external fields, flow or included colloidal particles. Liquid crystals usually consists of elongated organic molecules, which at given temperature or molecular concentration spontaneously order along a preferred direction called the director [1]. Aforementioned effects distort its order, thus structural elastic forces between particles appear. Such force field is highly spatially dependent due to the inherent anisotropy of the liquid crystal molecules and give rise to complex director field structures and phenomena.

The symmetry of the liquid crystal molecules require the order parameter of the liquid crystal to be a symmetric traceless tensor Q_{ij}, whose major axis is equivalent to the director and largest eigenvalue prescribes the liquid crystal degree of order. Order parameter tensor describes spatial average of the molecular orientations in a chosen part of liquid crystal.

Liquid crystals are liquids and can flow, but their dynamics is quite different and more complex than the dynamics of isotropic liquids. The difference arise from the fact that the material flow of liquid crystal is coupled with the molecular orientation, thus the flow can affect the director orientation and vice versa, rotation of the director can induce the flow. This phenomena is known as backflow. However, liquid crystals flow only by the presence of an external forces like pressure gradients, gravity electric fields etc., so they are characterised as passive fluids. Complementary active matter that describes a broad class of biological and bioinspired systems renging from microtubule nematic [2, 3, 4], bacterial suspensions [5, 6, 7, 8], algal suspensions [9], self-propelled rods [10, 11] to even sperm cells [12], flows inherently. These nonequilibrium systems generally consists of anisotropic particles that are able to convert ambient or stored energy into motion.

Defects in liquid crystals can form chaotic or even regular structures, depending on the type of confinement, inserted colloidal particles, external fields and flow. Confinement and the surface anchoring can impose and affect defects in liquid crystal. If the confinement has a regular structure, the transition from chaotic to regular structures is controllable [13] and the created system has a memory effect. Colloidal particles inserted in the liquid crystal introduce the topological defects on their surface. This defects attract each other, so if the colloids have an appropriate design, this can cause self-assembly of colloidal crystals [14]. Even the passive or active flow itself can cause the reorientation of the director via backflow mechanism, at certain circumstances this gives birth to the structures in the director field [15].

Complex systems of periodic structures of defects in liquid crystal, together with the regular confinement or inserted colloidal particles, are particularly interesting as 1D, 2D or 3D photonic crystals [16] with variable and micro-controllable photonic band structures. In such composite photonic materials one contribution to the band structure is determined by the periodic birefringent orientational profile of the defect structures, whereas the second contribution emerges from the regular array of the confinement or colloidal particles. Self-assembled colloidal crystals [17, 18] are also interesting for photonic applications and can act as diffraction layers. Clever design of colloids could result in interesting photonic properties of the self-assembled colloidal crystal, such as negative refraction index [19].

The velocity field of liquid crystal is governed by the Navier-Stokes equation, which is generalised to account for the viscosity anisotropy, elastic stresses and activity. Combining the Navier-Stokes equation with the equations for liquid crystal elasticity results in the Ericksen-Leslie equations [1]. However, the Ericksen-Leslie equations assume that the liquid crystal degree of order is constant, which is usually not the case. To account also spatial changes of scalar order parameter we use the Beris-Edwards model that uses the tensorial order parameter instead. Model includes a reduced set of material parameters - only one rotational translational viscosity and one elastic constant.

The systems that will be investigated in this thesis generally do not have analytical solutions due to complex boundary conditions. Therefore, we have to employ different numerical techniques to solve the governing equations. Hybrid lattice Boltzmann method is used to simulate the full hydrodynamics of the nematic liquid crystal. It comprises of the (i) finite difference time evolution for the order parameter tensor and (ii) the lattice Boltzmann method for solving the generalised Navier-Stokes equation for the volocity field.

Minimisation of the free energy is numerically done with the Euler-Lagrange formalism. We use the relaxation algorithm [20], which treats the order parameter tensor as time dependent. Numerically the problem is tackled using a costum code based on the finite difference method on a cubic mesh. There are many other numerical techniques that can minimise the free energy functional, like finite-element methods (FEM) or conjugate gradient descent [21]. Especially FEM methods have numerous advantages, like the mesh adaptivity, which can speed up the simulations and calculate the desired regions with high precision, but it is difficult to implement. However the main advantage of the finite difference method is that it can be incorporated into a lattice Boltzmann method for a full nematodynamics solution.

The lattice Boltzmann method is a numerical scheme, derived from the lattice gas automata. Unlike the traditional methods, which solve the conservation equations of macroscopic properties numerically, lattice Boltzmann method models the fluid consisting of fictive particles. Such particles perform consequentive propagation and collision processes over a discrete lattice mesh. Due to its particle nature and local dynamics lattice Boltzmann method has several advantages over other conventional methods, especially in dealing with complex boundaries and parallelization of the algorithm. The numerical algorithm consists of discrete map, which can be interpreted as the propagation and collisions of partial distribution functions. By choosing a suitable collision operator and using the Chapman-Enskog expansion, the dynamics of the partial distribution functions obey generalised Navier-Stokes equation dynamics.

At the moment, our group already has implemented the hybrid Lattice Boltzmann method that allows the study of passive and active liquid crystal flow. This implementation has been custom-developed in our group and is parallelized to work on multiple CPUs. This method is dedicated to simulate flow of active or passive liquid crystals and is the combination of Lattice Boltzmann method and finite difference relaxation. This gives us the opportunity to simulate both complex active and passive flows and also static liquid crystal relaxation without fluid flow.

In this thesis, we propose to explore the director field structures in active and passive liquid crystals, which emerge due to various combinations of confinement, inserted colloidal particles, flow and inherent activity.

Complex liquid crystaline fluids have the remarkable capability for self-assembling regular structures of various symmetries and dimensionality, depending largely on the geometry of the colloidal particles and anchoring. We propose to research the self-assembly of more complex horseshoe-like particles, that could work as a split ring resonators in metamaterials. Complex geometrical and topological structures have recently raised a lot of attention because of their applications in material design. A gyroid is a complex three periodic structure of labyrinth passages that self-assemble in certain surfactant or lipid mesophases. We propose to study the structures of nematic and cholesteric liquid crystals in this complex and inherently chiral confinement, which could be interesting as a photonic crystal. Also, a recent research interest is to explore 64-polar nematic colloids which is a work with the experimental group of Prof. Ivan I. Smalyukh from University of Colorado Boulder.

In addition to simple isotropic fluids, there is considerable fundamental and applied interest in the microfluidics of complex liquid crystaline fluids, as the internal structures of the fluid allow for novel mechanisms of manipulation, driving and steerage [15, 22]. We will investigate the flow of liquid crystal in the microchannels of various geometrical cross sections and introduce the porosity, inserting long cylindrical fibres into the microchannel. Cylindrical fibres will change the landscape of the microchannel, introducing wide and narrow regions. According to our preliminary results we expect that the flow deforms the director field via the backflow mechanism, creating a continuous deformation of the director field, called umbilic defect [23]. Umbilic defects are integer defects, escaped in the third dimension. Umbilics of positive umbilic strength are found to emerge from multipeak flow profiles, with the number of flow peaks corresponding the umbilic strength. Alternatively, umbilic defects of negative strength are found to emerge at saddle points in the flow profile, with the number of the valleys of the saddle determining the the umbilic strength. Introduced regular porosity lead to formation of various lattices of umbilic defects, which could act as microfluidics tunable photonic crystals. This work is being done in collaboration with experimental group of Prof. Stephen Morris from the University of Oxford.

Active systems are particularly interesting, since the interplay between nematic ordering and activity results in a collective motion. For sufficiently active systems, the motion undergoes instability and transitions into turbulent behaviour, similar to turbulence seen in passive fluids at high Reynolds numbers. Topological defects, a signature feature of nematic materials, strongly interact with the flow and can be, unlike the defects in passive liquid crystal, dynamically created and annihilated by flows opposing the elastic forces. Defect structures and fluid dynamics below and in the turbulent regime are poorly known especially in the three dimensional confined systems. We propose to explore the behaviour and the structures in some simple systems of various genus and anchoring.

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