Research in Physics
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Theoretical Physics

- 10 Staff; 10 PDRAs; 22 PhDs;
- 219 articles; 2472 citations; £2.9M grant awards; £1.1M in-kind; 20 PhDs awarded

The main themes of research in Theoretical Physics are:
- Molecular & Materials Modelling;
- Complexity & Biological Physics;
- Quantum Condensed Matter.

The Theory Group has a breadth of expertise in materials modelling, esp. in molecular dynamics and electronic structure calculations. There is extensive collaboration with experimental groups on both hard condensed matter and bio-/soft matter. Recent strategy has also been to strengthen interdisciplinary links and make full use of high end computing facilities in the Centre for Scientific Computing (CSC). The study of complex matter has become an exciting focus for the future, with strong links to Maths, Chemistry, and Life Sciences coming through numerical modelling of crystal growth and phase stability of biological & functional materials (Quigley), applications of geometry and topology to liquid crystals (Alexander), and modelling of soft and biological condensed matter (Allen). The Complexity Centre (co-founded in 2007 by Ball) has developed into a dynamic environment for inter-disciplinary research into emergent behaviour and self-organisation (Ball) and for non-equilibrium biophysics systems (Turner). Theoretical Physics was a key driver in forming the new Biological Physics group and its interests in non-equilibrium systems overlap very well with the experimental work. The quantum condensed matter activity has been directed increasingly to understanding experimental developments in non-equilibrium phase transitions (Szymanska), magneto-responsive materials and spintronics (Staunton), electronic properties of disordered materials & transport in DNA (Römer), and quantum statistics in small devices (d’Ambrumenil). The strong and developing links with experimental activity (much of it in-house) in electron diffraction, PLD, magnetic resonance, neutron scattering and graphene offer excellent prospects for future development.
Three-dimensional colloidal crystals in liquid crystalline blue phases


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Applications for photonic crystals and metamaterials put stringent requirements on the characteristics of advanced optical materials, demanding tunability, high Q factors, applicability in visible range, and large-scale self-assembly. Exploiting the interplay between structural and optical properties, colloidal lattices embedded in liquid crystals (LCs) are promising candidates for such materials. Recently, stable two-dimensional colloidal configurations were demonstrated in nematic LCs. However, the question as to whether stable 3D colloidal structures can exist in an LC had remained unanswered. We show, by means of computer modeling, that colloidal particles can self-assemble into stable, 3D, periodic structures in blue phase LCs. The assembly is based on blue phases providing a 3D template of trapping sites for colloidal particles. The particle configuration is determined by the orientational order of the LC molecules: Specifically, face-centered cubic colloidal crystals form in type-I blue phases, whereas body-centered crystals form in type-II blue phases. For typical particle diameters (approximately 100 nm) the effective binding energy can reach up to a few 100 \(k_B T\), implying robustness against mechanical stress and temperature fluctuations. Moreover, the colloidal particles substantially increase the thermal stability range of the blue phases, for a factor of two and more. The LC-supported colloidal structure is one or two orders of magnitude stronger bound than, e.g., water-based colloidal crystals.

![Energetically favorable FCC colloidal crystal in Blue Phase I](image)
Power of the Poincaré Group: Elucidating the Hidden Symmetries in Focal Conic Domains


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Focal conic domains are typically the “smoking gun” by which smectic liquid crystalline phases are identified. The geometry of the equally spaced smectic layers is highly generic but, at the same time, difficult to work with. In this Letter we develop an approach to the study of focal sets in smectics which exploits a hidden Poincaré symmetry revealed only by viewing the smectic layers as projections from one-higher dimension. We use this perspective to shed light upon several classic focal conic textures, including the concentric cyclides of Dupin, polygonal textures, and tilt-grain boundaries.

Achronal boundaries for (a) a pair of spacelike and (b) timelike separated events, both in their rest frames (left-hand side) and in a general frame (right-hand side). The corresponding smectic textures (cross sections of realistic 3D structures) are shown below each surface, with focal lines that are the projections of cusps on the surface (indicated in red).
The Hopf fibration is an example of a texture: a topologically stable, smooth, global configuration of a field. Here we demonstrate the controlled sculpting of the Hopf fibration in nematic liquid crystals through the control of point defects. We demonstrate how these are related to torons by use of a topological visualization technique derived from the Pontryagin-Thom construction.

(a) Selected 3PEF-PM images from an image stack—the images are 16 μm wide and approximately 4 μm apart in the z direction. (b) The toron texture from Ref. [12]. The axis of symmetry of this structure is perpendicular to the substrate. (c) Top view, (d) side view: the “Pontryagin-Thom” surface constructed from this image stack. Despite the considerable noise, the robustness of this method allows us to recognize the nontrivial topology of the texture as the winding bands of color meeting at the two hedgehog defects on top and bottom.
Knots and knotted fields enrich physical phenomena ranging from DNA and molecular chemistry to the vortices of fluid flows and textures of ordered media. Liquid crystals provide an ideal setting for exploring such topological phenomena through control of their characteristic defects. The use of colloids in generating defects and knotted configurations in liquid crystals has been demonstrated for spherical and toroidal particles and shows promise for the development of novel photonic devices. Extending this existing work, we describe the full topological implications of colloids representing nonorientable surfaces and use it to construct torus knots and links of type \((p,2)\) around multiply twisted Möbius strips.

Knots and linked disclinations in chiral nematics stabilized by the presence of twisted surfaces with homeotropic boundary conditions on the flat faces, and planar on the thin edges. They are torus knots and links of the form \((p, 2)\). Shown are (A) \(p=2\) Hopf link, (B) \(p=3\) trefoil knot, (C) \(p=4\) Solomon’s knot, and (D) \(p=5\) cinquefoil knot. The defects in the center are hedgehogs, existing in pairs above and below the strip.
Elastic constants of hard thick platelets by Monte Carlo simulation and virial expansion


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In this paper we present an investigation into the calculation of the Frank elastic constants of hard plate-like particles via molecular simulation and virial expansion beyond second order. We adopt the cut-sphere model, in which each particle consists of a hard sphere from which the top and bottom have been removed by cuts parallel to, and equidistant from, the equatorial plane. Monte Carlo simulations were carried out and director fluctuations measured as a function of wavevector k, giving the elastic constants through a fit in the low-k limit. Additionally, the virial expansion coefficients of the elastic constants up to sixth order were calculated, and the validity of the theory determined by comparison with the simulation results. The simulation results are also compared with experimental measurements on colloidal suspensions of plate-like particles.

Instantaneous configurations of a system of hard cut-spheres, H/D = 1/15, for ρD^3 = 7. (left) and ρD^3 = 8 (right), colour coded according to their angle relative to the vertical axis. The molecules are plotted conventionally (upper image) and as thin rods of length H (lower).
Improving the Wang-Landau algorithm for polymers and proteins.


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The 1/t Wang–Landau algorithm is tested on simple models of polymers and proteins. It is found that this method resolves the problem of the saturation of the error present in the original algorithm for lattice polymers. However, for lattice proteins, which have a rough energy landscape with an unknown energy minimum, it is found that the density of states does not converge in all runs. A new variant of the Wang–Landau algorithm that appears to solve this problem is described and tested. In the new variant, the optimum modification factor is calculated in the same straightforward way throughout the simulation. There is only one free parameter for which a value of unity appears to give near optimal convergence for all run lengths for lattice homopolymers when pull moves are used. For lattice proteins, a much smaller value of the parameter is needed to ensure rapid convergence of the density of states for energies discovered late in the simulation, which unfortunately results in poor convergence early on in the run.

![Graph](image.png)

Error $\Delta_{\text{rms}}$ against MC moves $M$ for an 18-monomer homopolymer using the Wang–Landau 1/t method with $\varphi = 0.8$ (black, full line), and the new version of Wang–Landau with various values of the parameter $p$: 16 (red, long dashes), 1 (orange, short dashes), 1/16 (green, dot-dashed), and 1/256 (cyan, dot-double-dashed).
Forces between cylindrical nanoparticles in a liquid crystal


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Using classical density functional theory, the forces between two cylindrical nanoparticles in a liquid crystal solvent are calculated. Both the nematic and isotropic phases of the solvent are considered. In the nematic phase, the interaction is highly anisotropic. At short range, changes in the defect structure around the cylinders leads to a complex interaction between them. In the isotropic phase, an attractive interaction arises due to overlap between halos of ordered fluid adsorbed on the surfaces of the cylinders.
Selective adsorption of lattice peptides on patterned surfaces

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To study the adsorption of individual peptides in implicit solvent, we propose a version of the Wang-Landau Monte Carlo algorithm that uses a single surface, with no need for a confining wall or grafting. Our “wall-free” method is both more efficient than the traditional ones and free of additional assumptions or approximations. We illustrate it by simulating an HP-model lattice peptide on planar surfaces with a variety of patterns of adsorption sites, discovering a temperature-induced switch of surface selection which is due to a balance of energetic and entropic effects.

Snapshots of the AC and AE configurations on the patterned surfaces of interest. The peptide is colored blue (polar, P) and yellow (hydrophobic, H); the monomer beads and the bonds between them are given the same radius to aid visualization. Surface sites that are attractive to polar beads are colored dark gray, nonattractive sites light gray. The AC phase on the uniform surface is essentially identical to that on P2×2; the AE phase is similar, but more disordered.
Pore-blockade times for field-driven polymer translocation


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We study pore-blockade times for a translocating polymer of length \(N\), driven by a field \(E\) across the pore in three dimensions. The polymer performs Rouse dynamics, i.e., we consider polymer dynamics in the absence of hydrodynamical interactions. We find that the typical time for which the pore remains blocked during a translocation event scales as \(\sim N^{(1+2ν)/(1+ν)} / E\), where \(ν\sim0.588\) is the Flory exponent for the polymer. We show, in line with our previous work, that this scaling behavior stems from polymer dynamics in the immediate vicinity of the pore—in particular, the memory effects in the polymer chain tension imbalance across the pore. This result, like numerical results from several other groups, violates the lower bound \(\sim N^{1+ν} / E\) suggested earlier in the literature. We discuss why this lower bound is incorrect and show, on the basis of the conservation of energy, that the correct lower bound for the pore-blockade time for field-driven translocation is given by \(ηN^{2ν} / E\), where \(η\) is the viscosity of the medium surrounding the polymer.

Snapshot of a translocating polymer in a two-dimensional projection of our three-dimensional system. Across the pore of size unity a voltage difference 2 \(V\) is applied. The monomer located within the pore is labeled \(s\).

Snapshot of a translocating polymer in a two-dimensional projection of our three-dimensional system. Across the pore of size unity a voltage difference 2 \(V\) is applied. The monomer located within the pore is labeled \(s\).
Polymer translocation out of planar confinements


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Polymer translocation in three dimensions out of planar confinements is studied in this paper. Three membranes are located at \( z = -h \), \( z = 0 \) and \( z = h_1 \). These membranes are impenetrable, except for the middle one at \( z = 0 \), which has a narrow pore. A polymer with length \( N \) is initially sandwiched between the membranes placed at \( z = -h \) and \( z = 0 \) and translocates through this pore. We consider strong confinement (small \( h \)), where the polymer is essentially reduced to a two-dimensional polymer, with a radius of gyration scaling as \( R_g^{(2D)} \sim N^{\nu_{2D}} \); here, \( \nu_{2D} = 0.75 \) is the Flory exponent in two dimensions. The polymer performs Rouse dynamics. On the basis of theoretical analysis and high-precision simulation data, we show that in the unbiased case \( h = h_1 \), the dwell time \( \tau_d \) scales as \( N^{2+\nu_{2D}} \), in perfect agreement with our previously published theoretical framework. For \( h_1 = \infty \), the situation is equivalent to field-driven translocation in two dimensions. We show that in this case \( \tau_d \) scales as \( N^{2\nu_{2D}} \), in agreement with several existing numerical results in the literature. This result violates the earlier reported lower bound \( N^{1+\nu} \) for \( \tau_d \) for field-driven translocation. We argue, on the basis of energy conservation, that the actual lower bound for \( \tau_d \) is \( N^{2\nu} \) and not \( N^{1+\nu} \). Polymer translocation in such theoretically motivated geometries thus resolves some of the most fundamental issues that have been the subject of much heated debate in recent times.

The mean time \( \langle t \rangle \) required to unthread a distance \( [s - s(0)] \) for \( h = 3 \), \( h_1 = \infty \), \( s(0) = 3N/4 \) and \( [s - s(0)] = 5 \), 10, \ldots, \( N \). The \( \langle t \rangle \) values are obtained as the average over 2,048 realisations for each \( N \). The \( N \)-values used are (from left to right): 200, 280, 360, 400, 480, 520, 600, 680, 800. The \( \langle t \rangle \) values for \( N = 200 \) is the actual value of time, for the others, \( \langle t \rangle \)-values for each \( N \) are separated by a factor 2 along the \( x \)-axis. The solid line represents a power law with exponent \( 1/(2 + 2D) \), corresponding to \( \tau_d \sim N^{2 + 2D} \).
Shape of a Ponytail and the Statistical Physics of Hair Fiber Bundles


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A general continuum theory for the distribution of hairs in a bundle is developed, treating individual fibers as elastic filaments with random intrinsic curvatures. Applying this formalism to the iconic problem of the ponytail, the combined effects of bending elasticity, gravity, and orientational disorder are recast as a differential equation for the envelope of the bundle, in which the compressibility enters through an “equation of state.” From this, we identify the balance of forces in various regions of the ponytail, extract a remarkably simple equation of state from laboratory measurements of human ponytails, and relate the pressure to the measured random curvatures of individual hairs.

A ponytail. (a) Rotationally averaged image of a switch of N≈9500 fibers, approximately 25 cm long. Coordinate system for envelope shape $R(s)$ in terms of arc length $s(z)$. (b) Meanderings of hairs near ponytail edge.

Researchers have for the first time disentangled the factors that determine how hairs hang together, as reported in *Physical Review Letters*. The analytical model, which was based on a statistical characterization of ponytail shapes, treats the forces on individual hair fibers as continuous quantities inside a hair bundle. The resulting hair “equation of state” could apply to other fibers in biology and industry. Many scientists (and even more hairdressers) have wondered about the meanderings of hair. Leonardo da Vinci thought hair flowed like water, and this sort of fluid analogy has guided computer animators trying to recreate hair and fur on the movie screen. However, no model has yet addressed one of the most basic hair problems: what shape is a ponytail?

The authors obtained human hair switches (a type of commercially available hairpiece) and measured the random curvature (or curliness) of a sample of individual hairs. They then assembled different ponytails and recorded the average shape. This data helped in the formulation of an equation of state that balanced four competing effects: gravity, tension, an elastic restoring force, and a “swelling pressure” coming from the curliness. The model correctly predicted the shape of ponytails as the lengths of the switches were progressively shortened. The surprisingly simple equation of state could be used to study other hair “styles,” as well as dynamic problems like a swinging ponytail.
Collective Oscillations in Irreversible Coagulation Driven by Monomer Inputs and Large-Cluster Outputs


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We describe collective oscillatory behavior in the kinetics of irreversible coagulation with a constant input of monomers and removal of large clusters. For a broad class of collision rates, this system reaches a nonequilibrium stationary state at large times and the cluster size distribution tends to a universal form characterized by a constant flux of mass through the space of cluster sizes. Universality, in this context, means that the stationary state becomes independent of the cutoff as the cutoff grows. This universality is lost, however, if the aggregation rate between large and small clusters increases sufficiently steeply as a function of cluster sizes. We identify a transition to a regime in which the stationary state vanishes as the cutoff grows. This nonuniversal stationary state becomes unstable as the cutoff is increased. It undergoes a Hopf bifurcation after which the stationary state is replaced by persistent and periodic collective oscillations. These oscillations, which bear some similarities to relaxation oscillations in excitable media, carry pulses of mass through the space of cluster sizes such that the average mass flux through any cluster size remains constant. Universality is partially restored in the sense that the scaling of the period and amplitude of oscillation is inherited from the dynamical scaling exponents of the universal regime.

Main panel: Total mass $M_1(t)$ versus time for different values of $\Lambda$ with $\nu=\mu=3/4$. Inset: Collapse obtained by rescaling the data
Provided the measuring time is short enough, the full counting statistics (FCS) of the charge pumped across a barrier as a result of a series of voltage pulses are shown to be equivalent to the geometry of two planes. This formulation leads to the FCS without the need for the usual nonequilibrium (Keldysh) transport theory or the direct computation of the determinant of an infinite-dimensional matrix. In the particular case of the application of N Lorentzian pulses, we show the computation of the FCS reduces to the diagonalization of an N×N matrix. We also use the formulation to compute the core-hole response in the x-ray edge problem and the FCS for a square wave pulse-train for the case of low transmission.

The geometry of the FCS. In the space of single-particle states, orbitals occupied at zero temperature correspond to eigenstates of $h$ with eigenvalue 1 and define a mirror plane shown schematically as the $x$ axis. Unoccupied states at zero temperature (with eigenvalue -1) are in the complement of plane, one of these is the $y$ axis and the remainder are shown as the $z$ axis. In the insets the dashed line divides states into those above and below the unperturbed Fermi level but no other ordering by energy is implied. Application of a voltage pulse, biasing one electrode with respect to the other, transforms $h \rightarrow h' = U h U^\dagger$. Case (a): ($N_u=1$, $N_d=0$ see text) The corresponding plane has an added dimension and is shown as the shaded plane. Case (b): ($N_u=0$, $N_d=1$). The plane rotates by $\alpha/2$ about an axis perpendicular to $h$. The axis of rotation and the new occupied state are found from $[h, e^{-i\Phi(t)}]$ (see text). All other states are rotated as a function of time but remain eigenstates of both $h$ and $h'$. 
Optimal pumping of orbital entanglement with single-particle emitters


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We propose a method for the optimal time-controlled generation of entangled itinerant particles, using on-demand sources in a conductor in the quantum Hall regime. This entanglement pump is realized by applying periodic, tailored voltage pulses to pairs of quantum dots or quantum point contacts. We show that the pump can produce orbital Bell pairs of both electrons and holes at the optimal rate of half a pair per pumping cycle. The entanglement can be detected by a violation of a Bell inequality formulated in terms of low-frequency current cross correlations.

(a) Optimal orbital entanglement pump with two single-particle emitters, $C$ and $D$, connected to conductors in the quantum Hall regime. The emitted electrons and holes propagate along edge states to controllable electronic beam splitters at $A$ and $B$ and are detected at terminals 1–4. The sources $C$ and $D$ can be either (b) quantum dots or (c) quantum point contacts. Tailored voltage profiles $V_C(t)$ and $V_D(t)$ are applied to a gate in case (b) to move a localized level with energy $E(t)$ up (down) through the Fermi energy releasing an electron (hole), or in case (c) to cycle the transmission probability, $T(t)$, from zero through unity and back to generate a particle-hole excitation.
We present a model of dissipative transport in the fractional quantum Hall regime. Our model takes account of tunneling through saddle points in the effective potential for excitations created by impurities. We predict the temperature range over which activated behavior is observed and explain why this range nearly always corresponds to around a factor two in temperature in both integer quantum Hall and fractional quantum Hall systems. We identify the ratio of the gap observed in the activated behavior and the temperature of the inflection point in the Arrhenius plot as an important diagnostic for determining the importance of tunneling in real samples.

Band alignment and particle flow across a typical saddle point. Upper left: Breakup of a quantum Hall system. Incompressible fluid at filling fraction $\nu$ (white background) separates compressible regions in which QPs (dark diagonals on lighter shading) and QHs (light diagonals on darker shading) are nucleated [16]. Upper Right: Tunnelling of a QP through the saddle point from an equipotential line about the left region (chemical potential $\mu_l$) to one about the right. Main figure: Energy band alignment. For QP excitations with energies $E < E_s^p$, the transmission probability is significant if the point of closest approach to the saddle point, $x_0$, lies within a zone of width $\sim 2\ell_q$ about the saddle point. Potential variations in the incompressible region exceeding $\Delta_s$ are not possible. They would simply nucleate carriers and reduce the size of the incompressible region.
Thermopower in the Quantum Hall Regime


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We consider the effect of disorder on the thermopower in quantum Hall systems. For a sample in the Corbino geometry, where dissipative currents are not carried by edge states, we find that thermopower behaves at high temperatures like a system with a gap and has a maximum which increases as the temperature is reduced. At lower temperatures this maximum reduces as a function of temperature as a result of tunneling across saddle points in the background potential. Our model assumes that the mean saddle point height varies linearly with the deviation in filling factor from the quantized value. We test this hypothesis against observations for the dissipative electrical conductance as a function of temperature and field and find good agreement with experiment around the minimum.

Experimental data [13] and the theoretical fit for log $\sigma_{xx}$ at $\nu=12/5$ (right panel). The estimates of the saddle point gap $\Delta_s$, the width parameter $\alpha$, and $\delta B$, are used to predict the magnetic field dependence of the longitudinal resistance at different temperatures (left panel).
Stable prenucleation mineral clusters are liquid-like ionic polymers

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Calcium carbonate is an abundant substance that can be created in several mineral forms by the reaction of dissolved carbon dioxide in water with calcium ions. Through biomineralization, organisms can harness and control this process to form various functional materials that can act as anything from shells through to lenses. The early stages of calcium carbonate formation have recently attracted attention as stable prenucleation clusters have been observed, contrary to classical models. Here we show, using computer simulations combined with the analysis of experimental data, that these mineral clusters are made of an ionic polymer, composed of alternating calcium and carbonate ions, with a dynamic topology consisting of chains, branches and rings. The existence of a disordered, flexible and strongly hydrated precursor provides a basis for explaining the formation of other liquid-like amorphous states of calcium carbonate, in addition to the non-classical behaviour during growth of amorphous calcium carbonate.

(a,b) Illustration of the species observed at low and high pH, respectively, with snapshots of the simulation box for 0.5 M at the centre (animations of the time-evolution of the simulation are available as Supplementary Movies 1 & 2 for pH 10 and 9.5, respectively). Here atoms are represented as spheres where calcium, carbon of carbonate, carbon of bicarbonate, oxygen and hydrogen are coloured green, blue, yellow, red and white, respectively. Ca–C and C–C distances below the cutoffs of 3.9 and 5.0 Å, respectively, are highlighted by purple bonds. For the largest cluster (top of b), the oxygen atoms are omitted for clarity so that the connectivity is apparent.
Free energy and structure of calcium carbonate nanoparticles during early stages of crystallization


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We introduce a metadynamics based scheme for computing the free energy of nanoparticles as a function of their crystalline order. The method is applied to small nanoparticles of the biomimeral calcium carbonate to determine the preferred structure during early stages of crystal growth. For particles 2nm in diameter, we establish a large energetic preference for amorphous particle morphologies. Particles with partial crystalline order consistent with vaterite are also observed with substantially lower probability. The absence of the stable calcite phase and stability of the amorphous state support recent conjectures that calcite formation starts via the deposition of amorphous calcium carbonate.

Examples of amorphous (A) and ordered (B) particle configurations explored during a metadynamics simulation of a 75 CaCO₃ unit nanoparticle in water.
Growing a good egg: Metadynamics simulations show that the eggshell protein ovocleidin-17 induces the formation of calcite crystals from amorphous calcium carbonate nanoparticles. Multiple spontaneous crystallization and amorphization events were simulated; these simulations suggest a catalytic cycle that explains the role of ovocleidin-17 in the first stages of eggshell formation (the picture shows one intermediate of this cycle).

Two binding configurations of protein to the calcite (10.4) surface. The residues that bind to the surface are highlighted. The neutralising chloride ions are depicted in green. Binding energies are (left) $-53\pm42$ kJ/mol and (right) $-422\pm43$ kJ/mol. The residues bound to the surface are (left) SER 27, 31 and 85; ARG 28, 34, 35, 86, 89 and 112; and ALA 83 and (right) ARG 46, 86 and 89. Note that the binding energy is much lower for the configuration with fewer ARG in contact with the surface, demonstrating the importance of minimising the disruption of the structured surface water.
Metadynamics simulations of ice nucleation and growth


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The metadynamics method for accelerating rate events in molecular simulations is applied to the problem of ice freezing. We demonstrate homogeneous nucleation and growth of ice at 180 K in the isothermal-isobaric ensemble without the presence of external fields or surfaces. This result represents the first report of continuous and dynamic ice nucleation in a system of freely evolving density. Simulations are conducted using a variety of periodic simulation domains. In all cases the cubic polymorph ice Ic is grown. The influence of boundary effects on estimates of the nucleation-free energy barrier are discussed in relation to differences between this and earlier work.

Representative snapshots at the specified metadynamics step number during crystallization of 576 water molecules. Molecules are color coded by phase.
Quantum Hall Transition in Real Space: From Localized to Extended States


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Using scanning tunneling spectroscopy in an ultrahigh vacuum at low temperature (T=0.3 K) and high magnetic fields (B≤12 T), we directly probe electronic wave functions across an integer quantum Hall transition. In accordance with theoretical predictions, we observe the evolution from localized drift states in the insulating phases to branched extended drift states at the quantum critical point. The observed microscopic behavior close to the extended state indicates points of localized quantum tunneling, which are considered to be decisive for a quantitative description of the transition.

LDOS of lowest LL. (a)–(g) Measured dI/dV (x,y); B=12 T, Vs=−116.3 mV (a), -111.2 mV (b), -104.4 mV (c), -100.9 mV (d), -99.2 mV (e), -92.4 mV (f), -89.0 mV (g), Istab=0.1 nA, Vstab=150 mV, Vmod=1.0 mV; same dI/dV color scale in each image; white (green) arrows in (a), (b), (f), and (g) mark drift states encircling potential minima (maxima); red, yellow arrows in (c) and (e) mark tunneling connections existing at identical positions; crosses in (d) mark extended LDOS areas at saddle points. (h) Spatially averaged dI/dV curve with circles at the Vs used in (a)–(g). (i) Calculated LDOS at the center of LL0↓ at B=12 T; red arrows mark tunneling connections at the saddle points; white crosses mark extended areas. (j) dI/dV image close to the center of LL0↑ at B=6 T, Vs=−99 mV; image includes the area of (a)–(g) within the marked rectangle.
Point-Mutation Effects on Charge-Transport Properties of the Tumor-Suppressor Gene $p53$


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We report on a theoretical study of point mutations effects on charge transfer properties in the DNA sequence of the tumor-suppressor $p53$ gene. On the basis of effective tight-binding models which simulate hole propagation along the DNA, a statistical analysis of mutation-induced charge transfer modifications is performed. In contrast to noncancerous mutations, mutation hot spots tend to result in significantly weaker changes of transmission properties. This suggests that charge transport could play a significant role for DNA-repairing deficiency yielding carcinogenesis.

Schematic models for hole transport in DNA. The nucleobases are given as (gray) circles. Electronic pathways are shown as lines, and dashed lines and circles denote the sugar-phosphate backbone. Graph (a) shows effective models $1L$ and $FB$ (with dashed backbone) for transport along a single channel, whereas graph (b) depicts possible two-channel transport models $2L$ and $LM$ (with dashed backbone).
Multifractal Analysis with the Probability Density Function at the Three-Dimensional Anderson Transition


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The probability density function (PDF) for critical wave function amplitudes is studied in the three-dimensional Anderson model. We present a formal expression between the PDF and the multifractal spectrum $f(\alpha)$ in which the role of finite-size corrections is properly analyzed. We show the non-Gaussian nature and the existence of a symmetry relation in the PDF. From the PDF, we extract information about $f(\alpha)$ at criticality such as the presence of negative fractal dimensions and the possible existence of termination points. A PDF-based multifractal analysis is shown to be a valid alternative to the standard approach based on the scaling of inverse participation ratios.

PDF at criticality for $\Delta \alpha=0.04$. The gray lines correspond to L from 30 (bottom) to 90 (top). Standard deviations are within the line width. For $L \leq 100$ and $L > 100$ we average over $5 \times 10^4$ and $100$ states, respectively. The vertical dashed line marks the mean value for $\alpha_0=4.027 \pm 0.016$ using $L$ from 50 to 200. Inset (a) shows $P(L)\alpha_0$ vs $L$. Standard deviations are contained within symbol size. The solid line is the fit $a \ln(L/l)^b$, with $a=0.297 \pm 0.002$, $b=0.490 \pm 0.005$. Inset (b) shows the collapse of all the PDF from $L=30$ to 240 onto the $f(\alpha)$. 
Exciton Storage in a Nanoscale Aharonov-Bohm Ring with Electric Field Tuning


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We study analytically the optical properties of a simple model for an electron-hole pair on a ring subjected to perpendicular magnetic flux and in-plane electric field. We show how to tune this excitonic system from optically active to optically dark as a function of these external fields. Our results offer a simple mechanism for exciton storage and readout.

![Diagram](https://example.com/diagram.png)

Excitonic probability density $|\Psi(\theta_e, \theta_h)|^2$ at $v_0=\frac{2}{\pi^2}$ and (a) $u_0=0$, $\Phi=0$, (b) $u_0=0$, $\Phi=0.4999$, (c) $u_0=0.5$, $\Phi=0$, and (d) $u_0=0.5$, $\Phi=0.4999$. The solid lines and dashed lines are contour lines separated in height by $1/10\pi^2$. 
The complex correlation of structure and magnetism in highly coercive monoatomic FePt surface alloys is studied using scanning tunneling microscopy, x-ray magnetic circular dichroism, and ab initio theory. Depending on the specific lateral atomic coordination of Fe either hard magnetic properties comparable to that of bulk FePt or complex noncollinear magnetism due to Dzyaloshinski-Moriya interactions are observed. Our calculations confirm the subtle dependence of the magnetic anisotropy and spin alignment on the local coordination and suggest that 3D stacking of Fe and Pt layers in bulk $L1_0$ magnets is not essential to achieve high-anisotropy values.

STM images of Fe$_{x}$Pt$_{1-x}$ SAs formed during deposition of Fe atoms onto Pt(997) at 525 K. (a) Fe$_{50}$Pt$_{50}$: Mixture of Fe and Pt atoms in the surface layer consistent with the expected stoichiometry. Fe 2×2 and 2×1 superstructures on a local scale are clearly visible (right side). (b) Fe$_{25}$Pt$_{75}$: Partial Fe$_{50}$Pt$_{50}$ SA with preferential 2×1 superstructure confined close to the step edges.
Theoretical Physics

**Theory of electronic transport in random alloys with short-range order: Korringa-Kohn-Rostoker nonlocal coherent potential approximation**


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We present an *ab initio* formalism for the calculation of transport properties in compositionally disordered systems within the framework of the Korringa-Kohn-Rostoker nonlocal coherent potential approximation. Our formalism is based on the single-particle Kubo-Greenwood linear response and provides a natural means of incorporating the effects of short-range order upon the transport properties. We demonstrate the efficacy of the formalism by examining the effects of short-range order and clustering upon the transport properties of disordered AgPd and CuZn alloys.

![Graph](image)

The resistivity of randomly disordered alloys Ag$_c$Pd$_{1-c}$ alloys as a function of concentration $c$. The full lines are the NLCPA results [pink (green) lines with squares (diamonds) show those without (with) vertex corrections]. The dashed curves show the CPA results [long dashes (dots)—without (with) vertex corrections]. The experimental results of Guenault are shown for comparison (full blue lines with filled circles).
Atomic-scale engineering of magnetic anisotropy of nanostructures through interfaces and interlines
Nature Communications 3, 1313 (2012) 10.1038/ncomms2316
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The central goals of nanoscale magnetic materials science are the self-assembly of the smallest structure exhibiting ferromagnetic hysteresis at room temperature, and the assembly of these structures into the highest density patterns. The focus has been on chemically ordered alloys combining magnetic 3\textit{d} elements with polarizable 5\textit{d} elements having high spin–orbit coupling and thus yielding the desired large magneto-crystalline anisotropy. The chemical synthesis of nanoparticles of these alloys yields disordered phases requiring annealing to transform them to the high-anisotropy L1\textsubscript{0} structure. Despite considerable efforts, so far only part of the nanoparticles can be transformed without coalescence. Here we present an alternative approach to homogeneous alloys, namely the creation of nanostructures with atomically sharp bimetallic interfaces and interlines. They exhibit unexpectedly high magnetization reversal energy with values and directions of the easy magnetization axes strongly depending on chemistry and texture. We find significant deviations from the expected behaviour for commonly used element combinations. \textit{Ab-initio} calculations reproduce these results and unravel their origin.

Blocking temperature $T_b$ of Co-core islands as a function of the shell coverage $\Theta_s$ and element, Fe (red), Co (blue) and Pt (green). Lines are guides to the eye and error bars reflect the uncertainty of the $\chi''(T)$ peak position. For simplicity, we drew the islands circular, the real ones are more irregular, as shown in \textit{Supplementary Fig. S1}. The arrows represent the direction and magnitude of the magnetic anisotropy emerging from the respective interlines. Growth of Co-cores: coverage $\Theta_c=0.12$ ML for Fe shells and 0.18 ML for Pt shells, 1 ML is defined as one atom per Pt(111) substrate atom, deposition flux $F_{\text{Co}}=0.18\pm0.01$ ML min$^{-1}$, deposition temperature $T_{\text{dep}}=150$ K, annealing temperature $T_{\text{ann}}=250$ K; growth of shells: $T_{\text{dep}}=250$ K, $F_{\text{Fe}}=0.12\pm0.01$ ML min$^{-1}$, $F_{\text{Pt}}=0.009\pm0.001$ ML min$^{-1}$. 
Tuning the metamagnetism of an antiferromagnetic metal


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We describe a “disordered local moment” first-principles electronic structure theory which demonstrates that tricritical metamagnetism can arise in an antiferromagnetic metal due to the dependence of local moment interactions on the magnetization state. Itinerant electrons can therefore play a defining role in metamagnetism in the absence of large magnetic anisotropy. Our model is used to accurately predict the temperature dependence of the metamagnetic critical fields in CoMnSi-based alloys, explaining the sensitivity of metamagnetism to Mn-Mn separations and compositional variations found previously. We thus provide a finite-temperature framework for modeling and predicting different metamagnets of interest in applications such as magnetic cooling.

(a) Experimental $B_c(T)$ for CoMnSi, $\text{Co}_{0.95}\text{Ni}_{0.05}\text{MnSi}$, and $\text{CoMn}_{0.98}\text{Cr}_{0.02}\text{Si}$ (Ref. 30). (b) Theoretical $B_c(T)$ for the same three systems, modeled using the lattice parameters found from neutron diffraction (Ref. 30) in zero field. The $B_c(T)$ of the Ni- and Cr-doped systems modeled using the CoMnSi structural data is also shown (dashed lines) to highlight the relative importance of accurate structural data.
After the discovery of zero viscosity in liquid helium, other fundamental properties of the superfluidity phenomenon have been revealed. One of them, irrotational flow, gives rise to quantized vortices and persistent currents. Those are the landmarks of superfluidity in its modern understanding. Recently, a new variety of dissipationless fluid behaviour has been found in microcavities under the optical parametric regime. Here we report the observation of metastable persistent polariton superflows sustaining a quantized angular momentum, m, after applying a 2-ps laser pulse carrying a vortex state. We observe a transfer of angular momentum to the steady-state condensate, which sustains vorticity for as long as it can be tracked. Furthermore, we study the stability of quantized vortices with m=2. The experiments are analysed using a generalized two-component Gross–Pitaevskii equation. These results demonstrate the control of metastable persistent currents and show the peculiar superfluid character of non-equilibrium polariton condensates.

Calculated TOPO signal emission for an m=2 triggering probe at \( k_{pb}=0.1 \, \mu m^{-1} < k_{pb}^{cr} \) (first row) and at \( k_{pb}=0.7 \, \mu m^{-1} > k_{pb}^{cr} \) (second row) at the arrival of the probe (t=0) and 42 ps after. The supercurrents are plotted in the frame of the group velocity of the moving vortex. In the second row, the net current felt by the m=2 vortex causes it to split (Supplementary Video S5).
Spontaneous and Triggered Vortices in Polariton Optical-Parametric-Oscillator Superfluids


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We study nonequilibrium polariton superfluids in the optical-parametric-oscillator regime by using a Gross-Pitaevskii equation with pumping and decay. We identify a regime above the optical-parametric-oscillator threshold, where the system undergoes spontaneous symmetry breaking and is unstable towards vortex formation without any rotating drive. Stable vortex solutions differ from metastable ones; the latter can persist but can be triggered only externally. Both spontaneous and triggered vortices are characterized by a generalized healing length, specified by the optical-parametric-oscillator parameters only.

Generation of an $m=+1$ metastable vortex solution into the OPO signal ($f_p=1.24f_{p}^\text{th}$ and $\sigma_p=70 \ \mu m$). First row: OPO filtered signal spatial profile together with currents (left) and interference fringes (right) are plotted at $t=-24 \ \text{ps}$ before the arrival of either a strong enough vortex probe (2) or a strong enough noise pulse. The metastable vortex lasts for as long as our simulation (last row, $t=1.8 \ \text{ns}$) and requires a threshold in the intensity of the perturbation breaking the $y\to-y$ symmetry.
Onset and Dynamics of Vortex-Antivortex Pairs in Polariton Optical Parametric Oscillator Superfluids

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We study, both theoretically and experimentally, the occurrence of topological defects in polariton superfluids in the optical parametric oscillator (OPO) regime. We explain in terms of local supercurrents the deterministic behavior of both the onset and dynamics of vortex-antivortex pairs generated by perturbing the system with a pulsed probe. Using a generalized Gross-Pitaevskii equation, including photonic disorder, pumping and decay, we elucidate the reason why topological defects form in couples and can be detected by direct visualizations in multishot OPO experiments.

Simulated profile and supercurrents of the steady state OPO signal before the arrival of the probe (a) and associated interference fringes (b).

Location of antivortices [dots (c)] and vortices [stars (e)] at the arrival (t=0 ps) of a vortex [stars (c)] or an antivortex [dots (e)] probe, for 1000 realizations of the random relative phase between pump and probe, $\Phi_{\text{rdm}}$. The size of the dots in (c) [stars in (e)] is proportional to the number of times the antivortices (vortices) appear in that location.

Panel (d) [(f)] shows single shot interference fringes relative to the plot in (c) [(e)]. Contour-level lines in (c) and (e) represent the photonic disorder $V(r)$. The white circle represents the edge of the probe.
We create a large exciton-polariton condensate and employ a Michelson interferometer setup to characterize the short- and long-distance behavior of the first order spatial correlation function. Our experimental results show distinct features of both the two-dimensional and nonequilibrium characters of the condensate. We find that the gaussian short-distance decay is followed by a power-law decay at longer distances, as expected for a two-dimensional condensate. The exponent of the power law is measured in the range 0.9–1.2, larger than is possible in equilibrium. We compare the experimental results to a theoretical model to understand the features required to observe a power law and to clarify the influence of external noise on spatial coherence in non-equilibrium phase transitions. Our results indicate that Berezinskii–Kosterlitz–Thouless-like phase order survives in open-dissipative systems.

Measured $g^{(1)}(\Delta x)$ vs. $\Delta x$ for various pumping spot radii $R_0$. All data is taken above threshold and is chosen such that $\lambda_{\text{eff}} \sim 4.1 \text{ \mu m}$. As the condensate size increases, $g^{(1)}(d\Delta x)$ converges to a power-law decay.
Weather and seasons together demand complex biological clocks


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The 24-hour rhythms of the circadian clock allow an organism to anticipate daily environmental cycles, giving it a competitive advantage. Although clock components show little protein sequence homology across phyla, multiple feedback loops and light inputs are universal features of clock networks. Why have circadian systems evolved such a complex structure? All biological clocks entrain a set of regulatory genes to the environmental cycle, in order to correctly time the expression of many downstream processes. Thus the question becomes: What aspects of the environment, and of the desired downstream regulation, are demanding the observed complexity? To answer this, we have evolved gene regulatory networks in silico, selecting for networks that correctly predict particular phases of the day under light/dark cycles. Gradually increasing the realism of the environmental cycles, we have tested the networks for the minimal characteristics of clocks observed in nature: oscillation under constant conditions, entrainment to light signals, and the presence of multiple feedback loops and light inputs. Realistic circadian gene networks are found to require a nontrivial combination of conditions, with seasonal differences in photoperiod as a necessary but not sufficient component.

The general form of the four-gene networks that we considered as candidates for generating circadian rhythms. Gene regulatory interactions may be positive, negative, or absent, and genes may be activated by light.
Lipid and protein lateral mobility is essential for biological function. Our theoretical understanding of this mobility can be traced to the seminal work of Saffman and Delbrück, who predicted a logarithmic dependence of the protein diffusion coefficient (i) on the inverse of the size of the protein and (ii) on the “membrane size” for membranes of finite size [Saffman P, Delbrück M (1975) Proc Natl Acad Sci USA 72:3111—3113]. Although the experimental proof of the first prediction is a matter of debate, the second has not previously been thought to be experimentally accessible. Here, we construct just such a geometrically confined membrane by forming lipid bilayer nanotubes of controlled radii connected to giant liposomes. We followed the diffusion of individual molecules in the tubular membrane using single particle tracking of quantum dots coupled to lipids or voltage-gated potassium channels KvAP, while changing the membrane tube radius from approximately 250 to 10 nm. We found that both lipid and protein diffusion was slower in tubular membranes with smaller radii. The protein diffusion coefficient decreased as much as 5-fold compared to diffusion on the effectively flat membrane of the giant liposomes. Both lipid and protein diffusion data are consistent with the predictions of a hydrodynamic theory that extends the work of Saffman and Delbrück to cylindrical geometries. This study therefore provides strong experimental support for the ubiquitous Saffman–Delbrück theory and elucidates the role of membrane geometry and size in regulating lateral diffusion.

Experimental approach to diffusion measurements on tubular membranes. (A) Schematic of the tracer molecule (KvAP in this case) embedded in the tubular membrane and labeled with QD. (B) Fluorescence of individual QD-labeled molecules diffusing on the lipid nanotube (center) and the parent vesicle (left). The nanotube is pulled using a micropipette (dotted lines on the left) holding the vesicle and an optically trapped bead (dotted circle on the right) attached at the distal tube end.
Microphase Separation in Nonequilibrium Biomembranes


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Compositional heterogeneities of cell membranes are thought to play an important role in many physiological processes. We study how variations in the membrane composition can be driven by nonthermal fluctuating forces and therefore show how these can occur relatively far from any critical point for the membrane. We show that the membrane steady state is not only controlled by the strength of the forces and how they couple to the membrane, but also by their dynamics: In a simple class of models this is captured by a single force correlation time. We conclude that the coupling of membrane composition to normal mechanical forces, such as might be exerted by polymerizing cytoskeleton filaments, could play an important role in controlling the steady state of a cell membrane that exhibits transient lateral modulations of its composition on length scales in the 10–100 nm regime.

The dynamics of a membrane containing multiple force centers (of density $\rho$) depends on the ratio of the membrane length $\lambda$ (see text) to the distance between force centers, $\lambda\sqrt{\rho}$, and the ratio of the composition diffusion length $\sqrt{D\tau}$ to the distance between force centers $\sqrt{D\tau}\rho$. Each illustration represents two neighboring force centers, with a typical separation $\rho^{-1/2}$, and shows (not to scale) the diffusion length in red (thin), the membrane length in blue (thick), and the region of substantial compositional variation in dark gray shading. The controlling length scale is shown as a continuous colored line and the other length scale is shown dotted. The shaded region indicates where domains are substantially noninteracting.
Theoretical Physics

**Force Transduction by the Microtubule-Bound Dam1 Ring**

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The coupling between the depolymerization of microtubules (MTs) and the motion of the Dam1 ring complex is now thought to play an important role in the generation of forces during mitosis. Our current understanding of this motion is based on a number of detailed computational models. Although these models realize possible mechanisms for force transduction, they can be extended by variation of any of a large number of poorly measured parameters and there is no clear strategy for determining how they might be distinguished experimentally. Here we seek to identify and analyze two distinct mechanisms present in the computational models. In the first, the splayed protofilaments at the end of the depolymerizing MT physically prevent the Dam1 ring from falling off the end, and in the other, an attractive binding secures the ring to the microtubule. Based on this analysis, we discuss how to distinguish between competing models that seek to explain how the Dam1 ring stays on the MT. We propose novel experimental approaches that could resolve these models for the first time, either by changing the diffusion constant of the Dam1 ring (e.g., by tethering a long polymer to it) or by using a time-varying load.

Two general classes of models of Dam1 ring-microtubule coupling. In both cases, the force is Brownian motion; that is, the ring diffuses to the right and the MT happens to unzip one segment or it is driven to the right by a powerstroke associated with unzipping. (Dotted line) Point reached by MT unzipping (x = 0). (A) The ring is sterically confined to the MT by PFs (protofilament model). (B) The ring is attractively bound to the MT surface with a free energy of binding ΔGDam1 (binding model). Below each model, the potential profile V in which the ring diffuses is shown as a function of the distance x of the ring from the MT end, and a dotted line indicates the connection between profile and model.