Backscattering between helical edge states via dynamic nuclear polarization

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We show that the nonequilibrium spin polarization of one-dimensional helical edge states at the boundary of a two-dimensional topological insulator can dynamically induce a polarization of nuclei via the hyperfine interaction. When combined with a spatially inhomogeneous Rashba coupling, the steady-state polarization of the nuclei produces backscattering between the topologically protected edge states leading to a reduction in the conductance which persists to zero temperature. We study these effects in both short and long edges, uncovering deviations from Ohmic transport at finite temperature and a current noise spectrum which may hold the fingerprints for experimental verification of the backscattering mechanism.

Experimental realization of the topological Haldane model

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The Haldane model on the honeycomb lattice is a paradigmatic example of a Hamiltonian featuring topologically distinct phases of matter. It describes a mechanism through which a quantum Hall effect can appear as an intrinsic property of a band-structure, rather than being caused by an external magnetic field. Although an implementation in a material was considered unlikely, it has provided the conceptual basis for theoretical and experimental research exploring topological insulators and superconductors. Here we report on the experimental realisation of the Haldane model and the characterisation of its topological band-structure, using ultracold fermionic atoms in a periodically modulated optical honeycomb lattice. The model is based on breaking time-reversal symmetry as well as inversion symmetry. The former is achieved through the introduction of complex next-nearest-neighbour tunnelling terms, which we induce through circular modulation of the lattice position. For the latter, we create an energy offset between neighbouring sites. Breaking either of these symmetries opens a gap in the band-structure, which is probed using momentum-resolved interband transitions. We explore the resulting Berry-curvatures of the lowest band by applying a constant force to the atoms and find orthogonal drifts analogous to a Hall current. The competition between both broken symmetries gives rise to a transition between topologically distinct regimes. By identifying the vanishing gap at a single Dirac point, we map out this transition line experimentally and compare it to calculations using Floquet theory without free parameters. We verify that our approach, which allows for dynamically tuning topological properties, is suitable even for interacting fermionic systems. Furthermore, we propose a direct extension to realise spin-dependent topological Hamiltonians.

Boundary Fidelity and Entanglement in the symmetry protected topological phase of the SSH model

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We present a detailed study of the fidelity, the entanglement entropy, and the entanglement spectrum, for a dimerized chain of spinless fermions---a simplified Su-Schrieffer-Heeger (SSH) model---with open boundary conditions which is a well-known example for a model supporting a symmetry protected topological (SPT) phase. In the non-interacting case the Hamiltonian matrix is tridiagonal and the eigenvalues and -vectors can be given explicitly as a function of a single parameter which is known analytically for odd chain lengths and can be determined numerically in the even length case. From a scaling analysis of these data for essentially semi-infinite chains we obtain the fidelity susceptibility and show that it contains a boundary contribution which is different in the topologically ordered than in the topologically trivial phase. For the entanglement spectrum and entropy we confirm predictions from massive field theory for a block in the middle of an infinite chain but also

consider blocks containing the edge of the chain. For the latter case we show that in the SPT phase additional entanglement---as compared to the trivial phase---is present which is localized at the boundary. Finally, we extend our study to the dimerized chain with a nearest-neighbour interaction using exact diagonalization, Arnoldi, and density-matrix renormalization group methods and show that a phase transition into a topologically trivial charge-density wave phase occurs.

Monte Carlo simultaions for Ising spins with spin greater than ½ applied to the square and triangular lattices with antiferromagnetic interactons and comparing results using Kawasaki and Glauber dynamics

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This paper has a pedagogical introduction. We describe the correct method for performing Monte Carlo simulations of Ising model systems with spin greater than one half. Correct and incorrect procedures are clearly outlined and the consequences of using the incorrect procedure are shown. The difference between Kawasaki and Glauber dynamics is then outlined and both methods are applied to the antiferromagnetic square and triangular lattices for S =1.

Periodic Subsystem Density-Functional Theory

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By partitioning the electron density into subsystem contributions, the Frozen Density Embedding (FDE) formulation of subsystem DFT has recently emerged as a powerful tool for reducing the computational scaling of Kohn--Sham DFT. To date, however, FDE has been employed to molecular systems only. Periodic systems, such as metals, semiconductors, and other crystalline solids have been outside the applicability of FDE, mostly because of the lack of a periodic FDE implementation. To fill this gap, in this work we aim at extening FDE to treat subsystems of molecular and periodic character. This goal is achieved by a dual approach. On one side, the development of a theoretical framework for periodic subsystem DFT. On the other, the realization of the method into a parallel computer code. We find that periodic FDE is capable of reproducing total electron densities and (to a lesser extent) also interaction energies of molecular systems weakly interacting with metallic surfaces. In the pilot calculations considered, we find that FDE fails in those cases where there is appreciable density overlap between the subsystems. Conversely, we find FDE to be in semiquantitative agreement (but still within chemical accuracy) with Kohn--Sham DFT when the inter-subsystem density overlap is low. We also conclude that to make FDE a suitable method for describing molecular adsorption at surfaces, kinetic energy density functionals that go beyond the GGA level must be employed.

On gradient field theories: gradient magnetostatics and gradient elasticity

Markus Lazar

In this work the fundamentals of gradient field theories are presented and reviewed. In particular, the theories of gradient magnetostatics and gradient elasticity are investigated and compared. For gradient magnetostatics, non-singular expressions for the magnetic vector gauge potential, the Biot-Savart law, the Lorentz force and the mutual interaction energy of two electric current loops are derived and discussed. For gradient elasticity, non-singular forms of all dislocation key-formulas (Burgers equation, Mura equation, Peach-Koehler stress equation, Peach-Koehler force equation, and mutual interaction energy of two dislocation loops) are presented. In addition, similarities between an electric current loop and a dislocation loop are pointed out. The obtained fields for both gradient theories are non-singular due to a straightforward and self-consistent regularization.