Report on the theme 01-3-1137-2019/2023

"Theory of complex systems and advanced materials"

During the reporting period, all planned tasks included in the PTP JINR were solved. Based on the research results, 268 articles were published in peer-reviewed journals, 3 monographs and 6 chapters in monographs, 3 review articles, 56 articles in scientific collections, more than 35 reports were presented at various international and Russian conferences, a number of international meetings were organized and held. Among the most important results, we note the following:

The multi-valley band structure of single-layer transition metal dichalcogenides (TMDs), which generates both intravalley and intervalley excitons, has been studied. By identifying excitons by irreducible representations of their point symmetry group, the exciton-exciton interaction is found, which depends on the symmetry of the interacting excitons. This interaction is generally repulsive, except in the case of excitons from different valleys, which are attracted, forming an intervalley biexciton. A semi-analytical dependence of the biexciton binding energy on the exciton mass and the dielectric characteristics of the material and the environment is established. This theoretical model covers the properties of exciton interaction and makes it possible to comprehensively study the structure and energy characteristics of the intervalley biexciton in single-layer TMDs.

A mechanism is proposed that makes it possible to overcome the well-known dichotomy between long-lived spin polarization and fast spin flip at a given time. A sample is considered connected to an electrical circuit that creates a feedback field acting on the spins. Turning on and off the variable quadratic Zeeman effect, one can implement spin flips with the desired delay time. The proposed spin flip control technique can be used in quantum information processing and spintronics.

Small-angle scattering (SAS) of X-rays, neutrons, and light waves by ensembles of deterministic fractal structures has been theoretically investigated. Their positions in space and orientation are assumed to be random. The standard technique for processing SAS data allows extracting only three characteristic parameters of the system: the size of the fractal and the lower and upper limits of the fractal range. It is shown that the self-similarity of deterministic fractal structures makes it possible to obtain their additional characteristics in real space. Exactly solvable models describing SAS on such systems are proposed and considered. The developed models make it possible to understand how to extract additional information about the fractal structure and analytically describe the intensity of the SAS, as well as offer efficient computational algorithms. Differences of SAS data for deterministic and random fractal structures are studied. The limits of applicability of the proposed models and prospects for future studies of deterministic fractal structures are discussed.

Numerical calculations have been performed for a number of materials used in radiation research at facilities available at FLNR and FLNP. The parameters of positron annihilation are obtained, which make it possible to characterize the structural changes caused by irradiation. Boron carbide B_4C and W_2B are considered. Characteristics of the structural and related magnetic phase transition in metallic terbium, measured under conditions of strong external pressure by the group of D.P. Kozlenko (FLNP JINR) received a quantitative explanation using the density functional theory methods.

Within the framework of cluster perturbation theory, the spectral properties of the weakly doped t-J model for cuprates are calculated. It is shown that the appearance of quantum oscillations in the density of electronic states can be explained by the appearance of effectively closed electron orbits in momentum space, which arise due to the Bragg reflection of electrons on charge density waves. This scenario made it possible to completely explain the possibility of the appearance of quantum oscillations in systems of strongly correlated electrons in the pseudogap phase.

It is shown that time reversal symmetry breaking in a 2d system of strongly correlated electrons leads to the appearance of the topological Hall effect, an integer quantum Hall effect, in the absence of an external magnetic field.

A theoretical study of the behavior of thermal and electrical conductivity in a promising material, polycrystalline graphene, has been carried out. It is shown that the role of grain boundaries in the suppression of thermal and electrical transport can increase significantly in a wide temperature range with a decrease in their size. It has also been found that grain boundaries can significantly suppress thermal and electrical transport even at room temperature if there are faults in the grain boundary misorientation angles.

Within the framework of stochastic molecular dynamics simulation, a method for generating fluorinated graphene structures with a tunable type of fluorine distribution has been developed. The electronic transport properties of fluorinated graphene have been studied in a wide range of the degree of fluorination and the method of ordering. An appreciable correlation was found between the degree of irregularity in the distribution of graphene and transport properties. In particular, the proposed consideration made it possible to reproduce two properties that were previously observed experimentally: electron-hole asymmetry and a peak in conductivity in the region of 10% fluorine concentration.

The influence of the factor of the transverse dimension of tunnel nanocontacts on the magnitude of the magnetoresistance has been studied. A sharp change in the tunneling magnetoresistance in contacts with a mismatched cross section is found, which is explained by the features of the spatial distribution of the electron density, which is different for the states of the major and minor spin directions. The results obtained have important applications for the creation of nanodevices operating on the basis of the phenomenon of tunneling magnetic resistance.

The reversal of the magnetization of a ferromagnet by electric current pulses in Josephson junctions of a superconductor/ferromagnetic insulator/superconductor on the surface of a topological insulator has been studied. It is shown that such a system is promising for low-dissipation spintronics due to the presence of a rigid coupling between the momentum and spin of a quasiparticle in the surface states of a topological insulator. This property provides an ideally strong coupling between the orbital and spin degrees of freedom, making it possible to reverse the magnetic moment of a ferromagnet by electric current pulses with an amplitude below the critical Josephson current, which greatly reduces the energy dissipation in the system. A method for simultaneous electrical detection of a flip is proposed.

The possibility of indirect capture of the magnetic precession in the SFS junction by Josephson oscillations under the action of an external periodic signal is shown, which is expressed by the appearance of synchronization steps in the dependence of the magnetization on the current through the junction. The position of the step is determined by the radiation frequency and the shape of the resonance curve. In transitions with strong spin-orbit coupling, states with a negative differential resistance appear on the I–V characteristic, which leads to an additional synchronization step. It is found that the corresponding oscillations have the same frequency as the oscillations in the first stage, but have a different amplitude and a different dependence on the radiation frequency. This allows us to control not only the frequency, but also the amplitude of the magnetic precession in the capture area.

The exact densities of contractible and non-contractible loops are obtained in the O(1) model on a strip of a square lattice folded into an infinite cylinder with a finite even base perimeter L=2N. They are also equal to the densities of critical percolation clusters on a 45-degree rotated square lattice rolled into a cylinder, which do not enclose and enclose the cylinder, respectively. The results are presented as explicit rational functions of N that take rational values for any N. Their asymptotic expansions in the limit of large N have irrational coefficients that reproduce the results obtained earlier in leading orders. This result provides a unique example of the exact calculation of an observable in a bounded system that becomes critical in the limit of infinite size.

A model of a dimer on a rectangle with free boundary conditions is considered. Exact expressions are obtained for the coefficients in the asymptotic volume expansion of the free energy up to the 22nd order. It is shown that the ratio of coefficients for an open strip and a square tends to 1/2. In addition, it is predicted that the coefficients in the free energy expansion for arbitrary rectangles are related to the coefficients for a square. A simple exact expression for the free energy of an open band of arbitrary width is also obtained. Within the framework of conformal field theory, it is shown that the angular contribution to the free energy for the dimer model on rectangular lattices with free boundary conditions is zero.

The statistics of avalanche flows in the Raise and peel model is described. Functions of large deviations are constructed that describe the dynamics of these flows in the limit of large time. Their first cumulants, such as mean, dispersion, etc., are explicitly calculated. A phase transition is described that occurs in the model when the time-averaged flow deviates from its most probable value.

A family of states of the Schrödinger cat type is described in the form of superpositions of coherent states of a harmonic oscillator with coefficients determined by quadratic Gauss sums. These states arise as eigenfunctions of lowering operators resulting from the canonical transformations of the Heisenberg-Weyl algebra associated with the ordinary and fractional Fourier transforms. The first member of this family is given by the well-known Yurke-Stoler coherent state.

The renormalization group and epsilon expansion method is used to calculate the dynamic critical index z, which determines the rate of relaxation of the order parameter of a ferromagnet in the vicinity of the phase transition point (critical deceleration). The calculations are performed in the fifth order of the epsilon expansion. The value of this index obtained as a result of resummation is in good agreement with both the results of computer simulation and experiment.

Theme leader V.A. Osipov