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Can superconductors be transparent?

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Superconducting circuits are among the most prominent platforms for quantum computing, communications, and sensing. Transparent superconductors are of particular interest, since they allow direct interfacing between stationary superconducting and flying photonic qubits. The latter are necessary for the transmission of quantum information because their quantum states are more resistant to decoherence. We here present a methodological approach for the development of superconductors with acceptable transparency and usefully high critical temperature, followed by discussion of representative characteristics of a number of already known oxides. In particular, we examine how the complex interplay of free carrier absorption and interband transitions can lead to the coexistence of comparatively high carrier density at the Fermi level and the needed transparency for visible light. The proposed design principles for discovering potential transparent superconductors are based on (i) the doping of wide band gap semiconductors or (ii) the tailoring of so-called degenerate gapped metals via controllable nonstoichiometry. To date, noticeable successes have been achieved using the first approach and, as a good example of its implementation, we overview detailed results obtained for electrochemically doped indium-tin-oxide compounds, which is a reference material for testing our ideas.

In this context, it is important to notice that transparent superconductors are often transition metal oxides where strong Coulomb interaction of partially occupied narrow electron bands renormalizes the properties of the charge carriers, resulting in a large increase in their effective electron mass. In such systems, strong electron-phonon coupling may occur, giving rise to polarons, a quasiparticle formed by an electron or a hole dressed by a cloud of virtual phonons. This response returns us to the idea of bipolaronic superconductivity, where the role of Cooper pairs (which can be named "bielectrons") is taken over by bipolarons, which are pairs of spatially delocalized electrons strongly coupled to the ionic lattice with a small correlation length.

Although the experimental and theoretical studies are still in the very early stages of research, their results appear to be very encouraging. A few materials have been developed primarily through structural engineering of oxide semiconductors. Their number should be increased to achieve two ambitious goals: greater transparency and higher critical temperature, with the prospect of creating a technology aimed to integrate multiple components into a transparent superconducting platform. The main area that can be occupied by transparent superconducting electronics is novel superconducting optoelectronic hardware that is addressing important needs of civilian and defense industries. Three main examples are quantum networking, quantum communications, and neuromorphic needs.

The joint activities in the field of electrochromic metal oxides for transparent superconducting electronics are supported by the NATO Science for Peace and Security Programme, proposal G6082. This work was partly supported by the German-Ukrainian collaborative project "Controllable quantum-information transfer in superconducting networks" (DFG project SE 664/21-1, AOBJ: 654837).

Binary ferromagnet-normal metal superlattices for quantum sensing

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As emphasized in a recent review [1], we are at the dawn of an era of layered quantum materials, which have proven their great potential as scalable components of quantum devices, including nanoscale sensors, and have made it possible to create new quantum phases of matter. In the contribution, we present our results on synthetic binary superlattices formed by nanometer-thick layers of normal and ferromagnetic metals, quantum transport through which unexpectedly demonstrates the formation of edge states, which are resistant to disorder and other mobile charge interactions. The idea of the experiments was inspired by a paradigmatic explanation of the plateaus in transversal transport characteristics in a 2D conductor at very low temperatures and strong magnetic fields (the integer quantum Hall effect) that is based on the existence of narrow near-boundary quantum channels of non-interacting electrons created at the Fermi level in strongly disordered electron systems [2]. The edge states are chiral in the sense that they can carry current only in one fixed direction. At the same time, the edge modes are topologically protected and their number cannot vary under continuous transformation of the system. This approach assumes the presence of a disordered and isotropic two-dimensional electron gas. Our aim was to create a strongly anisotropic 3D system with edge channels concentrated mainly at the hinges of the structure, i.e., a synthetic material with one or two 1D conducting modes.

The anisotropy is arising due to its layered structure where the diffusion coefficient for the charge motion across metallic layers ($D_\perp$) is much smaller than that along them ($D_\parallel$). In this case, the dephasing effect is characterized by the average $\langle \exp(-i\phi)\rangle$ of the phase factor ϕ calculated along all diffusive paths. If the related point belongs to the central region of the sample, a huge number of contributions with random signs largely cancel each other yielding $\langle \exp(-i\phi)\rangle$ to be proportional to $\exp(-d^2/l_B^2)$ with $l_B^2 = \Phi_0/\sqrt{D_\parallel/D_\perp}B$; here, Φ_0 is the magnetic flux quantum, and B is the magnetic flux density within the superlattice. In contrast to the central part of the superlattice, the presence of a nearby boundary imposes a sharp geometrical constraint on the allowed paths and near-surface trajectories are surviving. This is even more appropriate for 1D hinge states localized at the intersection of two surfaces. The presence of two hinge states at opposite edges of the superlattice can induce beats between the two contributions.

However, the disorder factor is insufficient to guarantee the chirality of the edge states in the absence of the magnetic field or in the presence of very weak field. For this, a source of the internally broken time-reversal symmetry is needed. It can be realized in a magnetically frustrated system where scattering off from spin clusters can generate an enhanced skew (asymmetric) scattering potential, one of the major mechanisms causing anomalous Hall effect in the absence of the magnetic field, and even without the spin-orbit interaction [3]. Hence, combination of the two factors - hinge states surviving in the strongly disordered and anisotropic material and the skew

scattering by small ferromagnetic nanoparticles - can generate the chiral edge currents.

One of the best ways to probe spatial current distributions is Josephson interferometry in a stacked (layered) configuration where the hybrid structure under study links two superconducting (S) electrodes. The figure of merit in such experiments is the maximum supercurrent (I_c) versus in-plane magnetic field (H). In our experiments, we applied this technique to study the transport of Cooper pairs through a periodic multilayer formed by ten normal metal (Al) - ferromagnetic metal (Ni or Ni-Fe alloy) bilayers. For the first time, we observed SQUID-like ($I_c(H)$) oscillations instead of conventional Fraunhofer patterns expected for trivial S-weak link-S junctions. Multilayers were deposited in situ by DC magnetron sputtering of the respective materials onto oxidized Si substrates at room temperature. The multilayered Josephson junctions (JJs) were patterned using optical lithography, reactive ion etching, Ar ion milling, and anodization followed by deposition of additional SiO_2 insulation. Our first experimental results on the multilayered samples can be found in the publications [4,5].

Using $I_c(H)$ characteristics for $S(NF)_{10}NI(NF)_{10}NS$ samples, we reconstructed the supercurrent-density spatial dependence. In chiral channels, an electron propagating along the interface with a superconductor could be reflected as a hole moving in the same chiral direction, then reflected as an electron and so on. Such combination of Andreev reflections with the chiral motion yields chiral Andreev edge states transferring superconducting correlations between S electrodes. We have found that the transport channels are strongly asymmetric with respect to the weak-link center and possibly one-dimensional. The strong asymmetry reveals itself also in the prominent upward shift of the periodic $I_c(H)$ curves while the amazing survival of edge transport in spite of the numerous scatterings at the boundaries of the neighboring layers remains unclear and may suggest a topological nature of the near-surface modes. Indeed, asymmetric hoppings in superlattice and non-Hermiticity can lead to new features in the energy band of non-Hermitian systems underpinning nontrivial topological features. Such phases of matter are of great interest for the future quantum technologies since they host edge modes which are robust information carriers.

Let us emphasize that compared with recent progress in non-electronic systems, in particular, optical ones, implementation of the non-Hermitian topological effects in condensed matter physics remains elusive. Currently, the issue of topological protection of the charge transport through a huge number of N/F interfaces remains open. Nevertheless, the discovery of stable hinge states in heterostructures based on traditional, well-studied and mature materials gives hope for their potential usage as a tunable platform for the controlled study of non-trivial edge physics and the practical implementations in quantum electronic circuits.

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Towards the problem of propagation of correlations in open systems

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One of the challenge problems of the theory of open quantum systems consists in the rigorous derivation of the master kinetic equation, that is, a kinetic equation of the Fokker-Planck quantum equation type, from the dynamics of many particles, including classical and quantum-classical open systems. The solution to this problem, in particular, is related to the question of the mechanism of stochastic behavior in dynamic systems of many particles.

In modern works, the main approach to the study of the collective behavior of open systems consists in the construction of scaling approximations, for example, the diffusion limit, the solution of evolution equations that describe the evolution of the state a system of many particles, which consists of a tracer particle in the environment of many particles, that is, a system of an infinite number of particles, in particular, a perturbative solution of the BBGKY (Bogolyubov - Born - Green - Kirkwood - Yvon) hierarchy of open systems.

Recently, in particular, when studying applied issues related to the propagation of correlations between the system and environment, the problems of the dynamics of the initially correlated open quantum systems began to be investigated systems.

In the talk, based on the non-perturbative solution of the hierarchy of von Neumann equations for the correlation operators of an open system, a new approach to the rigorous derivation of the Fokker –Planck kinetic equation of many particle system, which consists of a tracer particle and its environment in the presence of correlations of the initial states. In particular, this approach makes it possible to describe the process of propagation of initial correlations in open systems.

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Dynamics of quantum correlations and kinetic equations

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The talk provides an overview of some advances in the mathematical understanding of the nature of the kinetic equations of quantum systems of many particles. The fundamental equations of modern mathematical physics are studied, in particular, the hierarchies of evolution equations of quantum systems and their asymptotic behavior described by kinetic nonlinear equations.

Firstly, we discuss an approach to describing the correlations in a system of many quantum particles based on the hierarchy of evolution equations for the sequence of correlation operators, which are cumulants of the density operators (the von Neumann hierarchy). It is proved that the constructed dynamics of correlations underlies the description of the dynamics of both finitely and infinitely many quantum particles, governed by the BBGKY hierarchies for reduced (marginal) density operators or reduced correlation operators.

The structure of expansions by which are represented non-perturbative solutions of the Cauchy problem to these hierarchies of evolution equations of quantum systems is formulated. It is established that the concept of cumulants of the groups of operators of the von Neumann equations underlies non-perturbative expansions of solutions to hierarchies of fundamental equations that describe the evolution of observables and of the state of many quantum particles, as well as it forms the basis of the kinetic description of its collective behavior.

In the talk, we also consider a new approach to the problem of a rigorous description of kinetic evolution by means of reduced (marginal) observables governed by the dual BBGKY hierarchy. One of the advantages of the developed approach to the derivation of kinetic equations from underlying dynamics of many particles consists of an opportunity to construct kinetic equations with initial correlations, in particular, correlations characterizing the condensed states of a system, and to describe the processes of the propagation of initial correlations in suitable scaling limits.

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Quantum algorithms for detection of the energy levels of spin systems and graph properties with quantum programming

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We propose quantum algorithms for the detection of the energy levels of spin systems on a quantum computer. We show that the time dependence of the mean value of a physical quantity is related to the energies of a quantum system in the case when the operator of the physical quantity anticommutes with the Hamiltonian of the system [1]. Therefore, studying the evolution of the mean value of the operator with quantum programming gives the possibility to determine the energy levels. On the basis of the proposed algorithm energy levels of spin systems, namely spin in a magnetic field, spin chain, Ising model on the squared lattice are detected on IBM's quantum computers [1,2].

In the case when for a given Hamiltonian the anticommuting operator does not exist, we propose a quantum algorithm based on studies of the evolution of only one probe spin. Energy levels of the spin chain in a magnetic field, triangle spin cluster, and Ising model on a squared lattice in magnetic field are detected on IBM's quantum device with the algorithm [3].

It is worth noting that the proposed quantum protocols are efficient for the estimation of the energy levels of many-spin systems. The methods open a possibility to achieve quantum supremacy with the development of multi-qubit quantum computers.

On the basis of the proposed algorithms, we observe spin-1 tunneling on IBM's quantum computer [4]. We realize spin-1 with two spins-1/2. We detect the splitting of the energy levels as a result of tunneling on IBM's quantum device ibmq-bogota with studying of the evolution of probe spin.

Also, a quantum algorithm for the detection of the graph properties, namely the number of edges, triangles, and squares in a graph is developed [5]. We obtain that the geometric properties of evolutionary graph states of spin systems with Ising Hamiltonian are related to the properties. Namely, we found that such geometric characteristics as the velocity of quantum evolution, the curvature, and the torsion of the states are related to the total number of edges, triangles, and squares. Graph states corresponding to a chain, a triangle, and a square are studied. We apply the algorithm to detect the number of edges, triangles and squares in the corresponding graphs on IBM's quantum computer ibmq-manila [5]. The developed quantum algorithm gives a possibility to achieve quantum supremacy in finding number of edges, triangles, and squares in graphs with complicated structures with the development of quantum devices.

We also study the geometric measure of entanglement of quantum graph states [6,7]. Graph states prepared with the action of the operator of the evolution of the Ising model and those prepared with the action of the controlled phase shift operator are studied. We find analytically the geometric measure of entanglement of a spin with other spins for graph states corresponding to the arbitrary graph structure. It is obtained that the geometric measure of entanglement of a spin

is related to the degree of vertex which represents it in the graph. The geometric measure of entanglement of the graph states is calculated on IBM's quantum computers [6,7].

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Quantal and semiclassical study of the elastic scattering and charge transfer in cold H+H^+ collisions

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The study of the elementary processes occurring at proton impact on atomic hydrogen is important for many applications such as astrophysical and fusion plasma. In the present study, we compute the cross sections of the elastic scattering (EL)

$$\mathrm{H}(1s)+\mathrm{H}^+ \rightarrow \mathrm{H}(1s)+\mathrm{H}^+ \tag{1}$$

and the resonant charge transfer (CT)

$$\mathrm{H}(1s)+\mathrm{H}^+ \rightarrow \mathrm{H}^+ +\mathrm{H}(1s), \tag{2}$$

at proton collision with atomic hydrogen for the energy range of $10^{-10} \leq E_{\mathrm{c.m.}} \leq 10$ eV. Here $E_{\mathrm{c.m.}}$ is the collision energy in the center-of-mass frame. Reactions (1) and (2) have been the subject of active study for many decades [1-4].

For the energy range considered here, only the two lowest electronic states of $H_2{}^+$, the $1s\sigma_g$ *gerade* (g) and $2p\sigma_u$ *ungerade* (u), are involved. Thus, the cross sections for reactions (1) and (2) may be obtained from solutions of uncoupled single-channel Schrödinger equations of the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}R^2}+k^2-2\mu V_{g,u}^{(l)}(R)\right)\psi_{g,u}^{(l)}(R)=0, \tag{3}$$

where $k^2=2\mu E_{\mathrm{c.m.}}$, μ is the system reduced mass, l is the orbital angular momentum of the collision system, $V_{g,u}^{(l)}(R)$ is the adiabatic potential for either the $1s\sigma_g$ or $2p\sigma_u$ state, and $\psi_{g,u}^{(l)}(R)$ is the radial wave function for the corresponding reaction channel. The adiabatic potential $V_{g,u}^{(l)}(R)$ reads

$$V_{g,u}^{(l)}(R)=E_{g,u}^{\mathrm{BO}}(R)+\frac{l(l+1)}{2\mu R^2}, \tag{4}$$

where $E_{g,u}^{\mathrm{BO}}(R)$ is the Born-Oppenheimer energy of the corresponding reaction channel. We compute the $E_{g,u}^{\mathrm{BO}}(R)$ energy as the solution to the two-Coulomb-center problem eZ_1Z_2 by the method of the continued fractions.

The integral cross sections are determined from the scattering phase shifts. Due to the quantum indistinguishability of identical particles (as in the present case), the two different sets of elastic scattering cross sections, ELi (for indistinguishable) and ELd (for distinguishable) particles approach are produced. Both the fully quantal and the semiclassical (JWKB) approaches were utilized in the present calculations. Our computed cross sections (in a.u., $a_0^2=2.8003\times10^{-17}\mathrm{cm}^2$) are compared with the results of other authors and presented in Tab. 1 and Fig. 1.

Table 1: The integral cross section (in a_0^2) for charge transfer. The present fully quantal and JWKB calculations.

$E_{c.m.}$ (eV)	Present, quantal	Present, JWKB
0.1254	205.247	195.32
0.3	184.318	187.99
0.5100	166.518	165.99
1.0	162.251	162.16

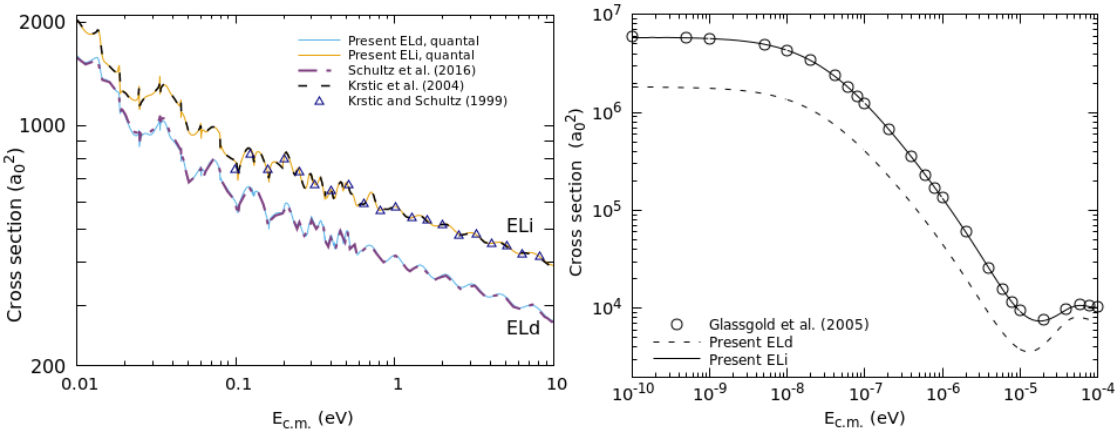

Figure 1: (left panel) Elastic distinguishable (ELd) and elastic indistinguishable (ELi) integral cross sections for center-of-mass collision energies within the range of 0.01–10 eV. Solid lines, the present quantal calculations; $- -$, the quantal calculations of Schultz *et al.* [1]; $- \cdot -$, the quantal calculations of [2]; $\bigtriangleup$, the JWKB calculations of [3]; (right panel) Integral elastic cross sections for the energy range of 10^{-10}–10^{-4} eV. Lines, the present calculations of $\sigma_{\rm EL}^{\rm (d)}$ and $\sigma_{\rm EL}^{\rm (i)}$; $\bigcirc$, the $\sigma_{\rm EL}^{\rm (i)}$ calculations of [4].

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Azobenzene-Based Polymer as a Photoactive Material: Simulation, Preparation and Properties

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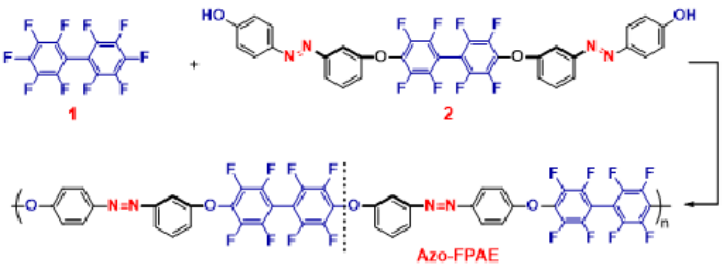
Light-responsive polymers show great promise in various applications, such as reconfigurable photonic elements and optical-to-mechanical energy conversion. Azobenzene chromophores are popular for their reversible conformational changes (trans-cis-trans photoisomerization) absorption of UV or visible light. An intriguing aspect of light-responsive polymers is their capacity to exhibit anisotropic behavior under polarized light irradiation. Thus, during azobenzene's trans-cis-trans isomerization within the polymer, the orientation of the units shifts, becoming perpendicular to the incident light polarization. This induces a conformational change in the macromolecules, resulting in photoinduced alignment of the azobenzene fragments. As a consequence, the polymer film exhibits birefringence upon illumination. This phenomenon is particularly relevant for the design of polarization holographic gratings and the efficient control of photoalignment. In this context, polymers with azobenzene side chains are widely used, while polymers with azobenzene moieties in the backbone face problems due to limited solubility, mechanical properties and film forming ability. Overcoming these challenges is essential to unlock the full potential of light-responsive polymers with azobenzene functionalization in the main chain.

In this study, we synthesized and characterized a polymer that combines azobenzene and octafluorobiphenylene (OFB) units alongside with meta-linked fragments in the backbone. The resulting polymer is azo-containing fluorinated poly(arylene ether) (Azo-FPAE). The incorporation of OFB units improves solubility (due to the lipophilicity of fluorine atoms), enhances chemical and thermal stability, and influences molecular packing due to the nonplanarity of OFB's aromatic rings. Furthermore, according to the literature, the incorporation of fluorinated units is known to improve the optical and electro-optical properties of the polymer, leading to a lower refractive index, reduced optical losses, and enhanced hyperpolarization. We also incorporated meta-phenoxy units based on our previous research, which demonstrated improved solubility, thermostability, and mechanical properties in such meta-connected polymers.

The Azo-FPAE was synthesized by the aromatic nucleophilic substitution reaction from decafluorobiphenyl 1 (DFB) and hydroxyl-substituted azo-based monomer 2 (4,4'-{(2,2',3,3', 5,5',6,6'-octafluorobiphenyl-4,4'-diyl)bis[oxy-3,1-phenylenediazene-2,1-diyl]}diphenol) in dimethylacetamide (DMAc) in the presence of excess potassium carbonate as a base.



We introduced an azo group into the structure of polymer through the OH-based component, namely V-type monomer 2 (conjugation system D-π-A-π-D), in which the electron acceptor component (A) is situated between the two donor (D) units. Remarkably, monomer 2 can be regarded as an a-b-a trimer, comprising a DFB residue (b) and a para/meta-substituted azo-diphenol residue (a). Consequently, the polymer structure can be simplified as the result of the interaction between DFB (**b** in **a**-**b**-**a** trimer) and 3-((4-hydroxyphenyl)diazenyl)phenol (**a** in **a**-**b**-**a** trimer). Nevertheless, in our perspective, monomer 2 was obtained more easily through a straightforward diazotization reaction of the corresponding fluorinated meta-linked aromatic diamine followed by azo coupling with phenol.

The Azo-FPAE polymer, obtained as an orange fibrous solid, exhibited complete solubility in chloroform and DMAc, while it was insoluble in alcohols. This solubility behavior allows for the casting of the copolymer from solution, yielding high-quality self-supporting films that are mechanically strong and easy to handle. The success of the synthesis of the Azo-coFPAE was confirmed with ^{1}H NMR, ^{19}F NMR, FTIR and Raman spectroscopy techniques. The electronic absorption spectrum of the prepared azobenzene-modified polymer in DMAc solution exhibit two characteristic absorption bands. The high intensity band at around 336 nm is related to π-$\pi*$ transition of the trans form of the azobenzene moiety. The weak band at $\sim$440 nm originates from typical n-$\pi*$ transition.

Thermal properties of the resulting Azo-FPAE were investigated by differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA). Owing to the high content of fluorinated units, the polymer had good thermal stability and exhibited a one-step pattern of decomposition. It demonstrated a temperature of 405°C at 5% weight loss ($T_{5\%}$), indicating its suitability for various applications. DSC measurements revealed the amorphous nature of the copolymer because no melting endotherm peak was found from the first and second heating DSC scans. Note, two glass transition temperatures (T_g) are revealed for Azo-FPAE: T_{g1} is about 151 ^{o}C and T_{g2} is about 184 ^{o}C. This indicates that the polymer structure consists of two different amorphous regions.

Generally, various interactions can occur within the polymer, including H- and J-aggregation of azobenzene fragments, π_{Ar}-π_{ArF} (fluorine) stacking interactions between non-fluorinated aromatic units and perfluoroaromatic fragments, and other weak interactions. The nonplanarity of the OFB fragment rings is caused by the covalent bonds between perfluorinated phenylene fragments, which leads to the contortion of polymer chains. All these factors influence the packing of polymer chains and the available free volume within the polymer, which are crucial for processes such as photoisomerization and photoorientation.

To address these questions and gain further insights into the chain conformations and interactions, we first develop a coarse-grained computational model aimed at preserving the relevant geometry of the Azo-FPAE monomer for use in molecular dynamics simulations. Specifically,

our model directly incorporates the shape of each subunit of the monomer as opposed to conventional spherical-bead approximations. This approach enables us to preserve the relevant stacking of the aromatic units using a minimal model that can capture hierarchical, mesoscale organization – particularly relevant for subsequent property characterization. As such, results from both theoretical and experimental studies combine to provide comprehensive understanding of the azo-based system.

Acknowledgments

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Quantum Anomalies have Classical Origin

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Quantum anomalies (ie, the violation of the conservative nature of the classical Noether currents by quantum radiative corrections, for a review see [1]) are one of the most intriguing and mysterious phenomena of quantum field theory. It is commonly believed that they have a purely quantum origin (they are an artifact of the renormalization procedure) and therefore, they in principle cannot be derived within the framework of the classical theory. The purpose of the current research is to demonstrate that the anomalies can arise naturally in the classical theory of spatially bounded field systems. Exploring as an example the classical electrodynamics of massless fermions in the space-time domain Ω of a finite size, we show that the famous Adler-Bell-Jackiw (ABJ) anomaly $\partial_\nu j^\nu_{5vac} = cF_{\mu\nu}{}^*F^{\mu\nu}$ is a simple consequence of the requirements of the spatial boundedness of the field system under consideration (ie non-spreading of the fields beyond the region Ω) and the gauge invariance. The main stages of our research are as follows.

We consider first the theory of the free massless Dirac field ψ in the region Ω ($\partial\Omega = \Sigma_1 \cup \Sigma_2 \cup B_{12}$, where Σ_1, Σ_2 are spacelike, and B_{12} is timelike). We require that during the evolution the field must remain localized in Ω, and the Dirac equation is fulfilled everywhere in $\overline{\Omega} = \Omega \cup B_{12}$ (that is, both in the bulk Ω, and *on its boundary* B_{12}). These requirements can be satisfied only if we introduce a *surface (i.e localized on* B_{12}*) fermion source* ζ. It is shown that the including of its in the Lagrangian makes the variational problem well-posed, and the variational principle allows us to obtain the Dirac equation $i\gamma^\mu\partial_\mu\psi = 0$ (the equation of motion in the bulk Ω), as well as *the junction conditions* $\psi|_{B_{12}} = \mu\zeta$ (the equation of motion on the boundary B_{12}). The last relation will be chirally invariant if ζ has the same transformation properties as ψ.

We consider then the electromagnetic field $F^{\mu\nu}$ interacting with an external electric current j^ν. The requirements of the localization of the field in Ω (both its electric $\vec{E}$ and magnetic $\vec{H}$ components) and fulfillment of the Maxwell equations in $\overline{\Omega}$ forces us to introduce *surface electric* i^ν *and magnetic* ${}'i^\nu$ *currents*. It is shown that they can be combined into a unique tensor $i^{\mu\nu}$ ($i^\nu = i^{\perp\nu}$, ${}'i^\nu = {}^*i^{\perp\nu}$), so the surface sources are of the dipole type (here $\perp$ means the component orthogonal to B_{12}, and $*$ is the Hodge star). The standard Maxwell action functional allows us to derive junction conditions for $F^{\perp\nu}$ components only. We overcome this difficulty by constructing a *complex* action functional whose imaginary part is the Chern-Simons form. It is shown that the inclusion of the surface currents $i^{\mu\nu}$ leads to a well-posed variational problem and allows us to obtain both, the Maxwell equation $\partial_\mu F^{\mu\nu} = -j^\nu$ and the juction conditions $F^{\mu\nu}|_{B_{12}} = i^{\mu\nu}$ *for all components* of the electromagnetic field. The resulting theory can be formulated in terms of the self-dual field $F^{\mu\nu}_- = F^{\mu\nu} - i^*F^{\mu\nu}$ (*the Riemann-Silberstein vector* $\vec{\varepsilon} = \vec{E} + i\vec{H}$) and the self-dual sources $i^{\mu\nu}_- = i^{\mu\nu} - i^*i^{\mu\nu}$. The analysis of the canonical structure of the theory shows that, unlike the case of an electromagnetic field in the infinite space, in our case the components of the vector $\vec{\varepsilon}$ are kinematically independent (ie they commute). Alternatively, but equivalently, the theory can be formulated in terms of antiself-dual quantities $F^{\mu\nu}_+$, $i^{\mu\nu}_+$. It should be noted that the Riemann-Silberstein vector $\vec{\varepsilon}$ plays an important role in modern studies of optical helicity (see, for example, [2] and references therein).

Finally, we consider the full dynamical theory of interacting the massless electron-positron

and the electromagnetic fields localized in Ω. The fermionic surface source ζ is a charged field, and therefore it must contribute to the surface currents $i^{\mu\nu}$. The interaction of ψ and ζ with the electromagnetic field (with the potential A_μ) is fixed by the requirement of the gauge invariance of the theory in $\overline{\Omega}$. The analysis of the dynamical conservation of the total electric current J^ν (which includes both bulk j^ν and surface i^ν currents) leads to the identification $i^{\mu\nu} = e\mu\overline{\zeta}S^{\mu\nu}\zeta = e\mu\overline{\zeta}_L S^{\mu\nu}\zeta_R + e\mu\overline{\zeta}_R S^{\mu\nu}\zeta_L = i_+^{\mu\nu} + i_-^{\mu\nu}$ and to the junction conditions $F_\pm^{\mu\nu}|_{B_{12}} = i_\pm^{\mu\nu}$ (here $S^{\mu\nu}$ is the spin matrix, and ζ_R and ζ_L are the right and left spinors, respectively). Unlike the bulk current vector $j^\nu = e\overline{\psi}\gamma^\nu\psi = e\overline{\psi}_R\gamma^\nu\psi_R + e\overline{\psi}_L\gamma^\nu\psi_L = j_R^\nu + j_L^\nu$, each of $i_\pm^{\mu\nu}$ contains fields of *opposite* chirality and therefore the are not invariant under chiral transformations (γ_5-rotations). When $\psi \to \exp(i\alpha\gamma_5)\psi$, then $i_\pm^{\mu\nu} \to \exp(\pm i2\alpha)i_\pm^{\mu\nu}$. Therefore, in order to ensure the fulfillment of the junction conditions (the field equations on B_{12}!), every γ_5-rotations of fermions must be accompanied by dual rotations ($*$-rotations) of the electromagnetic field $F_\pm^{\mu\nu} \to \exp(2\alpha*)F_\pm^{\mu\nu} = \exp(\pm i2\alpha)F_\pm^{\mu\nu}$. We show that for such extended (γ_5- plus $*$-) chiral rotations, the corresponding current J_5^ν is nothing but the *total helicity current* (the sum of the helicity currents of the electron-positron J_{5EP}^ν and the electromagnetic J_{5EM}^ν fields), and that its conservation *reproduces the chiral anomaly of ABJ*, $\partial_\nu J_5^\nu = \partial_\nu J_{5EP}^\nu - cF_{\mu\nu}{}^*F^{\mu\nu} = 0$.

The validity of the proposed classical mechanism of the generation of the chiral anomaly can be verified experimentally. The predictable effect will consist in the helicity flip of a circularly polarized electron beam moving along an optical circular waveguide in which an electromagnetic field of the suitable configuration is excited (an optical instanton). The theoretical calculation of such a field, as well as a multiplicity of various other processes having place in such a system, can be performed by the methods of the Penrose twistor theory [3].

Some features, in particular symmetry properties, of the electrodynamics with dipole-type currents are also discussed. Based on them, a possible theoretical explanation of the problem (of non-existence) of the electric dipole moment of the electron is proposed.

The current investigation is a part of a broader research program of the investigation of the classical and quantum kinematics and dynamics of spatially bounded field systems. Some directions of further investigations and their perspectives are outlined.

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Variational optimization of iPEPS with CTMRG on the original lattice

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Tensor networks provide an effective framework to study many-body problems in strongly-correlated systems, since they can capture the structure of entanglement of the ground state wave function [1]. For two-dimensional quantum systems infinite projected entangled pair states (iPEPS) have proven themselves as an efficient wave-function ansatz capable to represent both symmetry-broken phases and topological orders [2-4]. To represent the entanglement structure of the ground state the PEPS tensor network usually mimics the lattice on which the original model is defined. There are several ways to calculate observables with PEPS tensor network: the corner transfer matrix renormalization group (CTMRG) [5], the boundary matrix product states [6], the tensor renormalization group [7] with CTMRG scheme being the most widely employed. Unfortunately, the CTMRG is usually applied in a straightforward manner only on the square lattice geometry. This initiated the development of various methods to map the original lattice into the square lattice, with the mapping process usually not respecting the original lattice symmetries and possibly enlarging the necessary unit cell [8-11].

We report on a successful application of the generalization of the CTMRG approach to the honeycomb lattice geometry [12,13] with the calculation of relevant physical observables and optimization of the iPEPS wave function directly on the honeycomb lattice. The optimization is realized by means of variational optimization, where gradients are obtained from the automatic differentiation through the CTMRG algorithm. We benchmark our method on both the antiferromagnetic Heisenberg and Kitaev models and obtain the state-of-the-art accuracy of the corresponding results. In particular, the obtained iPEPS are able to capture both symmetry-broken gapless magnetic and the gapless Kitaev spin-liquid states.

We also generalize the theoretical approach to other lattice geometries. In particular, we develop the CTMRG algorithm on triangular and Kagome lattices and generalize the honeycomb CTMRG to the two-site unit cells. We also discuss how CTMRG can be extended to the more general lattice geometries, in particular, dice or ruby lattices. We also demonstrate a potential extension and capability of the approach to study quantum many-body problems on hyperbolic lattices.

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Free-space quantum channels: Numerical simulations

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Quantum channels in free space attract great attention from the perspective of their practical applications in many important communication scenarios. For example, they are applied to establish secure communication through hard-to-reach regions, communication with and between moving objects, global satellite-mediated communication, etc. Beyond the task of quantum key distribution, these channels could be used for quantum digital signature, connecting quantum devices with quantum teleportation or entanglement swapping protocols, etc. Atmospheric turbulence is a leading disturbance factor for such channels. Therefore, an accurate theoretical description of its impact on the quantum states of a light mode is important for both fundamental and applied research in quantum optics and quantum communication.

We consider a group of protocols that do not involve the spatial structure of light modes. In this case, the input state at the transmitter is related to the output state at the receiver via the input-output relation,

$$P_{\rm out}(\alpha) = \int_0^1 {\rm d}\eta \frac{1}{\eta} P_{\rm in}\left(\frac{\alpha}{\sqrt{\eta}}\right) \mathscr{P}(\eta), \tag{5}$$

see Ref. [1]. Here $P_{\rm in}(\alpha)$ and $P_{\rm out}(\alpha)$ are the Glauber-Sudarshan P-functions characterizing the quantum states of a light mode at the transmitter and receiver, respectively. The quantity $\eta \in [0,1]$ describes the channel transmittance, while the function $\mathscr{P}(\eta)$ is the probability distribution of transmittance (PDT). The latter represents the main characteristic of atmospheric quantum channels. The PDT depends on the beam parameters at the transmitter, the channel length, the turbulence parameters, and the receiver characteristics.

Several analytical models for the PDT have been proposed in literature. One of them is focused on the impact of beam wandering [2]. The elliptic-beam model [3] also incorporates beam-spot distortions, which are approximated by Gaussian elliptic beams with randomly oriented semi-axes. The truncated log-normal distribution, discussed in Ref. [4], is applicable in cases where the beam-spot distortion plays a critical role. Furthermore, under the assumption of statistical independence between beam wandering and beam-spot distortion, the PDT can be derived using the law of total probability, as outlined in Ref. [5].

The direct application of analytical models is faced with the problem of properly determining the domain of their applicability. Typically, it is considered to depend on the strength of the turbulence. In this contribution, for details see Ref. [6], we report on numerical simulations of atmospheric quantum channels and use the results for validation of analytical models. This enables, among other applications, to conclude on the range of their applicability.

The random component of the channel transmittance is caused by fluctuations in the index of refraction due to atmospheric turbulence. This, in turn, leads to random fluctuations in the shape of

the beam and its fraction passing through the receiver aperture. Considering a classical field with amplitude $u(\mathbf{r};z)$, the channel transmittance is defined as

$$\eta = \int_{\mathscr{A}} d^2\mathbf{r}|u(\mathbf{r};z)|^2, \tag{6}$$

where $\mathscr{A}$ is the amplitude opening. Thus, to sample the channel transmittance η, it is necessary to first sample the field amplitude $u(\mathbf{r};z)$ at the aperture plane. We have performed this task with the sparse-spectrum model [7] for the phase-screen method [8].

We have also introduced an empirical model of the PDT based on the beta distribution. This distribution can be parameterized by the moments $\langle\eta\rangle$ and $\langle\eta^2\rangle$, which can be calculated from the classical theory of optical radiation in the turbulent atmosphere. For a wide range of channel parameters, the beta distribution model provides better agreement with numerical simulations than other analytical models.

Having implemented this method, we studied the three channels with different turbulence impact: weak, moderate and strong. We compared all the mentioned models with simulated PDTs. Our results have shown that the applicability of the analytical models depends mainly on the radius of the receiver aperture and only slightly on the turbulence strength. Our numerical results are applied to study the transmission of non-classical properties of quantum light through free-space channels.

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Landau-Zener-Stuckelberg-Majorana transitions for controlling states of quantum systems

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Since the pioneering works by Landau, Zener, Stuckelberg, and Majorana (LZSM), it has been known that driving a quantum two-level system results in tunneling between its states. Even though the interference between these transitions is known to be important, it is only recently that it became both accessible, controllable, and useful for engineering quantum systems [1]. We study systematically various aspects of LZSM physics and review the relevant literature, significantly expanding the review article in Ref. [2]. In particular, we address such aspects as Majorana's approach, LZSM logic gates, and dynamics of multi-level systems [3].

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Separable or Entangled? – How to deduce these quantum ensemble properties from density matrix elements

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How can one deduce by using only the information about present quantum state of arbitrary open quantum system whether any act of entanglement took place between its counterparts in the system's "history"? – This fundamental question has been debated for more than twenty years in the framework of a modern quantum science (see, e.g., Ref. [1]). The search of the most universal and physically transparent forms of separability tests for arbitrary density matrices represents one of the most fundamental challenging problems in the quantum entanglement theory. Besides its fundamental importance the successful solution of this problem can open new perspectives in a wide range of important applications in the area of quantum computation and quantum algorithms optimizations. The first important step in such a solution was made in the end of twenty century independently by A. Peres (1996) [2] and Horodecki family [3]. This was known in the literature as "Peres-Horodecki (or PPT- positive partial transpose) separability criterion" [1-3]. However, the applicability of the most famous PPT-criterion of separability is restricted by two-qubits density matrices only [2,3] while its general physical background has not been clarified until the appearance of the paper [4] . Especially, the general solution of this common separability problem has been proposed by the author in Ref. [4]. Here the general physical background behind the Peres–Horodecki positive partial transpose (PPT-) separability criterion has been revealed [4] for the first time. Especially, a general physical sense of partial transpose operation is shown to be equivalent to what one can call as the *"local causality reversal"* (LCR-) procedure for all separable quantum systems, or to the demonstration of *a global time arrow direction uncertainty* in all entangled cases [4]. Using these two universal causal considerations two brand new fundamental universal probabilistic relations which encode new heuristic causal separability criterion have been proposed for density matrices of arbitrary (even infinite) dimensionality D^N, describing arbitrary ensembles of N quantum systems of D eigenstates each [4]. Resulting general formulas have been then analyzed for the widest specific type of one-parametric density matrices of arbitrary dimensionality, those modelling a number N of equivalent quantum subsystems of a dimensionality D in each subsystem's Hilbert subspace, being all equally connected (EC-) with each other to arbitrary degree by means of a single entanglement parameter p (see Ref. [4]). As the result, a number of remarkable features of the entanglement thresholds $p_{th}(D,N)$ for such EC-density matrices have been described for the first time in Ref. [4]. All novel results being obtained for the family of arbitrary EC-density matrices are shown to be applicable to a wide range of both interacting and non-interacting (at the moment of measurement) multi-partite quantum systems, such as arrays of qubits, spin chains, ensembles of quantum oscillators, strongly correlated quantum many-body systems, etc. (see Ref. [4] for details).

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Many-body correlations and ordered phases of cold alkaline-earth atoms in state-dependent optical lattices

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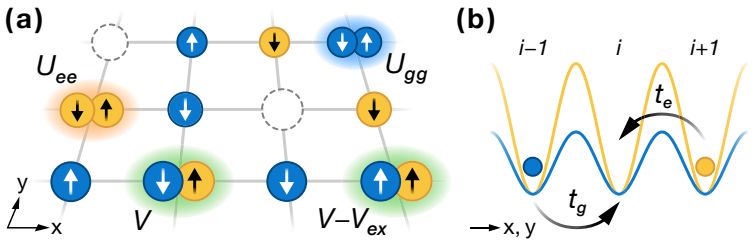
We explore the rich nature of correlations in the ground state and ordered phases of ultracold atoms trapped in state-dependent optical lattices. In particular, we consider interacting fermionic ytterbium or strontium atoms, realizing a two-orbital Hubbard model with two spin components. We analyze the model in one-dimensional setting with the experimentally relevant hierarchy of tunneling and interaction amplitudes by means of exact diagonalization and matrix product states approaches, and study the correlation functions in density, spin, and orbital sectors as functions of variable densities of atoms in the ground and metastable excited states [1]. We show that in certain ranges of densities these atomic systems demonstrate strong density-wave, ferro- and antiferromagnetic, as well as antiferroorbital correlations.

By employing a dynamical mean-field theoretical analysis, we extend the description of systems to quasi-two-dimensional state-dependent optical lattices and study low-temperature phases in multicomponent gases of fermionic alkaline-earth(-like) atoms [2]. Using the example of ^{173}Yb atoms, we show that a two-orbital mixture with two nuclear spin components is a promising candidate for studies of not only magnetic but also staggered orbital ordering peculiar to certain solid-state materials. We calculate and study the phase diagram of the full Hamiltonian with parameters similar to existing experiments and reveal an antiferro-orbital phase. This long-range-ordered phase is inherently stable, and we analyze the change of local and global observables across the corresponding transition lines, paving the way for experimental observations. Furthermore, we suggest a realistic extension of the system to include and probe a Jahn-Teller source field playing one of the key roles in real crystals.



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Semiclassical limit of quantum logic and information loss

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As Feynman mentioned in 1982, quantum systems cannot be imitated by classical computing machines [1]. The greatest interest to quantum computers appeared in 1994, after the discovery of Shor's factoring algorithm [2]. Since then a lot has been done in the field, and today both industry and academic institutes are investing a lot to quantum information processing and computation.

Despite that, the origin of quantum calculation efficiency still seems to be a challenge. Both superposition principle and linearity of unitary operators are widely believed to be responsible for the advantage of quantum algorithms. Unfortunately, these might conflict with the Gottesmann-Knill theorem. One may consider quantum entanglement, which has no classical analog, as another possible solution to the problem. Indeed, it violates Bell's inequalities and is crucial for the implementation of various quantum information transfer protocols. However, its role can also be argued [3,4].

In this study, we analyze the problem from the perspective of propositional logic [5]. Within the approach any calculation can be interpreted as some logical expression which can be either true or false, depending on whether a system possesses some property λ. In terms of the classical Boolean logic, this implies dealing with characteristic functions χ_λ determined on the system's phase space $\mathbb{P}$. For the quantum case, one should work with the relevant projector operators P_λ from the Hilbert space $\mathbb{H}$.

For any atomic expression $P_\lambda |\psi\rangle$, where $|\psi\rangle \in \mathbb{H}$ is the system's vector state, we consider how it transforms under the semiclassical limit $\lim_{\hbar\to 0}$. During the transition, all possible trajectories reduce to a single one, which describes the classical evolution in $\mathbb{P}$. The corresponding information loss can estimated with the help of the Shannon and the von Neumann entropies and can be represented as some function of the number of involved qubits (bits) n. Taking the limit may change the problem the algorithm was designed for, so our method differs from the Kolmogorov complexity [6].

The proposed technique is generalized to any quantum logical expression consisting of elementary quantum gates which make up a complete set. The largest information loss is observed for the expressions containing non-commuting operators. For elementary expression consisting of non-commuting projectors, the loss is upper bounded by the dimensionality of space defining the commutator.

The obtained results are illustrated by the analysis of two different algorithms: the quantum discrete Fourier transform and the Grover search algorithm. As known, their classical counterparts require $\mathcal{O}(n2^n)$ and $\mathcal{O}(2^n)$ amount of time correspondingly. Within the approach, the estimated information loss equals to $\mathcal{O}(n2^n)$ for the first algorithm and to $\mathcal{O}\left(n^2 2^{n/2}\right)$ for the second one.

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Quantum correlations and magnetic properties of ultracold Fermi gases with SU(4) spin symmetry in anisotropic cubic optical lattices

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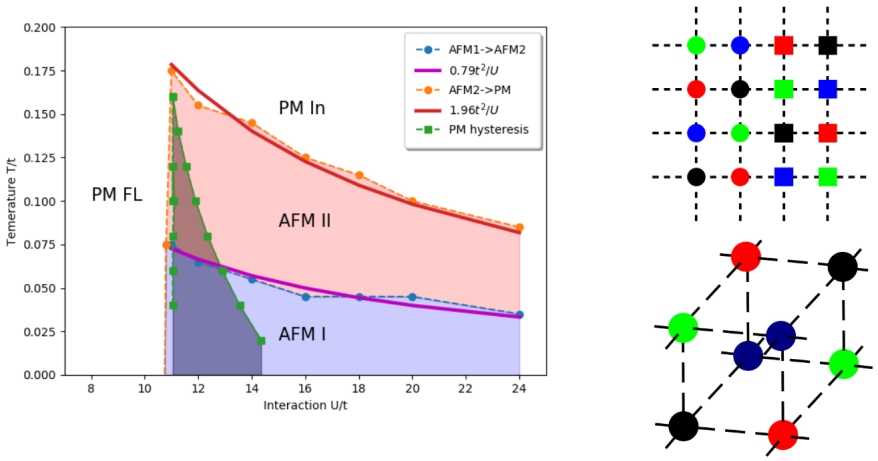
Optical lattice represents itself as a periodic potential in space produced by coherent laser beams, where ultracold atomic gas is trapped [1]. By means of the electric field formed by the lasers, the dipole moment of atoms is induced and interacts with the field. If the frequency of lasers is adjusted close to the resonance frequency of atoms, the trapping potential can be formed due to the ac Stark effect. Thus, one can consider such systems as analogs of real crystals with neutral atoms instead of electrons. This enables the usage of optical lattices for both experimental and theoretical purposes as a tool to simulate the real crystalline materials and verify results of different models, for instance the Ising or Hubbard models.

In our research, we are mainly interested in the description of systems with high spin symmetries, specifically SU(4)-symmetric fermionic mixtures. In practice, this particular high spin symmetry can be obtained if we choose atoms of ^{173}Yb or ^{87}Sr, and cool them down to the temperatures $1\ \mu$K, so they could be trapped in an optical lattice. Such a particular choice is based on the unique properties of alkaline earth-like atoms. Since fermionic isotopes of ^{173}Yb and ^{87}Sr have 6 and 10 nuclear spin projections [2], respectively, one can separate atoms with the needed amount of projections via Stern-Gerlach method. Remaining components are commonly referred to as the pseudospin flavors. The symmetry of the interaction between flavors appears due to the fact that the outer electron shell is filled, while the nuclear spin negligibly affects the interaction of the flavors.

In order to study quantum correlations and define magnetic properties of SU(4)-symmetric systems, we apply the Dynamical Mean Field Theory algorithm to the Hubbard model on 3D cubic lattice. The model itself was introduced by J. Hubbard to describe the behavior of electrons in the crystals, allowing the electrons to tunnel to neighboring sites on the lattice and interact with each other, under the condition they are located on the same site [3]. The same model can be applied to optical lattices and the atoms instead of electrons, which gives an opportunity to observe certain exotic phenomena.

Specifically, we interested in the dependence on the change of tunneling amplitude in a chosen direction, i.e., in a cubic lattice with three equal tunneling amplitudes alongside crystallographic lattice, we pick one amplitude and trace how its change affects the phase diagram. When the chosen amplitude equals zero, we arrive at the case of non-interacting 2D planes, which gives the same phase diagram as just for a 2D square lattice. Here, the system can be located in one of four different phases: a paramagnetic Fermi-liquid state in the region of small interaction amplitudes and three insulator states (one paramagnetic and two different antiferromagnetic) which have specific type of ordering (long-range correlation) [4].

In the opposite limit of the value of the chosen tunneling amplitude, one can find a system in an isotropic cubic lattice. In this case, the phase diagram still has four phases, though in slightly different regions of temperatures and interaction amplitudes. The main difference, which can't



Left: Phase diagram for the cubic lattice of non-interacting planes. *Right top*: antiferromagnetic plaquette-type ordering for square lattice at low temperatures. *Right bottom*: antiferromagnetic ordering for isotropic cubic lattice at low temperatures.

be directly seen from the diagram, is that the low-temperature antiferromagnetic states for the layered square and cubic lattice geometries are sizebly different and cannot be transformed into each other under a continuous transition. Hence, the discontinuity must occur at a certain value of tunneling amplitude, which we determine numerically. In addition to this anisotropy-induced phase transition, we also study the evolution of the boundaries of magnetic phases, as for the mentioned cases they differ from each other.

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