1.3 Theory of Condensed Matter

Theoretical investigations in the Theory of Condensed Matter were performed in the framework of the following projects:

- Strongly correlated systems.
- Dynamical systems: chaos, intergability and self-organization.
- Disordered structures: glasses, topological defects, nanostractures and Josephson junction.
- Mesoscopic and coherent phenomena in quantum systems.

Major results of the investigations within these projects are presented below, while several topics are discussed in the attached brief reports.

Main results in the problem of strongly correlated systems were obtained in investigation of electronic spectrum and mechanisms of superconductivity in copper-oxide materials and in studies of magnetic properties of materials with complicated phase diagrams like transition metal oxides.

A microscopic theory of high-temperature superconductivity mediated by antiferromagnetic exchange and spin fluctuations was developed within the realistic p-d Hubbard model. It explains a strong variation of superconducting temperature with lattice constants in mercury superconductors recently discovered at the FLNP, JINR. New methods for calculation of thermoelectrical properties and the optical conductivity of real strongly correlated materials were developed. The dynamical mean-field theory was used to take into account strong electron interactions and thereby bring the self-energy into first-principal calculations. The results of computations for the optical conductivity for doped $LaTiO_3$ and thermopower for pyrites were found in good quantitative agreement with experiments. Relationships between structural and superconducting properties in the layered mercury cuprates were established within the proposed model of charge transfer between inequivalent layers. A system of highly correlated electrons strongly coupled with optical phonons was investigated in the framework of the Hubbard-Holstein model. A new mechanism of polaron pairing and superconductivity was proposed mediated by exchanging phonon clouds.

A phenomenological theory based on the group-theoretical analysis was developed to describe the orientational phase transition in $K_2Ba(NO_2)_4$ ferroelastic, the orbital phase transition in $Pr_{1-x}Ca_xMnO_3$ manganite, and a system of hydrogen bonds in the high–pressure phases of $CsHSO_4$ crystals which were studied by neutron scattering experiments at FLNP, JINR. Magnetic models of quasi one-dimensional spin systems were derived microscopically and applied to explain magnetic properties of a series of new transition metal oxides. A new mechanism of unconventional superexchange was proposed and studied to describe the ground state magnetic structure of a new complex manganese oxide. To describe an intriguing doping dependence of the exchange energies in the bilayer manganites $La_{2-2x}Sr_{1+2x}Mn_2O_7$ observed in neutron scattering experiments, a theory was developed which enabled one to explain the experimental data by taking into account the doping dependence of the orbital level splitting.

Main results in the problem of Dynamical systems: chaos, intergability and self-organization were obtained for two-dimensional equilibrium and one-dimensional nonequilibrium and quantum models of statistical mechanics. For the free-fermion models on

torus, exact asymptotic expansions of the free energy, the internal energy and the specific heat in the vicinity of the critical point were found. It is shown that there is a direct relation between the terms of the expansion and the Kronecker double series. The latter can be expressed in terms of the elliptic theta-functions in all orders of the asymptotic expansion.

The asymmetric stochastic process describing the avalanche dynamics on a ring was proposed. A general kinetic equation which incorporates the exclusion and avalanche processes was considered. The Bethe ansatz method was used for calculation of the generating function for the total distance covered by all particles. It gives the average velocity of particles which exhibits a phase transition from an intermittent to a continuous flow. We calculated also higher cumulants and the large deviation function for the particle flow. The latter has a universal form obtained earlier for the asymmetric exclusion process and conjectured to be common for all models of the Kardar-Parisi-Zhang universality class.

The universal formulation of spin exchange models related to Calogero-Moser models implies the existence of integrable hierarchies which have not been explored. We showed the general structures and features of the spin exchange model hierarchies by taking as examples the well-known Heisenberg spin chain with the nearest neighbour interactions. The energy spectra of the second member of the hierarchy belonging to the models based on the A_r root systems ($r = 3, 4, 5$) were explicitly and *exactly* evaluated. They show many interesting features and in particular, much higher degree of degeneracy than the original Heisenberg model, as expected from the integrability.

The investigations performed within the project: Mesoscopic and coherent phenomena in quantum systems were mostly concentrated on the following topics: atomic interactions in superfluid ^{4}He and in atomic traps, squeesed light teleportation, quasiparticle spectra in quantum wells, electron-phonon interaction in polar and covalent materials, mesoscopic fluctuations and transient coherence in nonequilibrium systems, toroid polarizations and nonlinear phenomena.

In studies of the superfluid ^{4}He the shift of the critical Bose-Einstein condensation temperature in an atomic trap by the gravitational field was estimated. This result concerns the recent NASA project of new precise physical experiments in the outer space. Low-density expansions were derived for the chemical potential, ground-state energy, pair distribution function, kinetic and interaction energies of the Bose gas in two-dimensions. It was shown that the ground-state energy was mostly kinetic in the low-density limit. The new form of the 2D Gross-Pitaevskii equation was proposed within our scheme. Resonant excitation of nonlinear coherent modes in trapped Bose-Einstein condensates was advanced. The dynamical theory of this phenomenon was developed.

The ultimate limits of continuous-variable single-mode quantum teleportation due to absorption was studied, with special emphasis on (quasi-)monochromatic optical fields propagating through fibers. It was shown that even if an infinitely squeezed two-mode squeezed vacuum were used, the amount of information that would be transferred quantum mechanically over a finite distance is limited and effectively approaches zero on a length scale that is much shorter than the (classical) absorption length.

In studies of the stability of a large bipolaron embedded in a polaron gas it was shown that an isolated nonstable bipolaron can be stabilized in the presence of a polaron gas exhibiting Fermi statistics. This study was performed for both for (3D) materials and thin (2D) films using the Hartree-Fock approximation. An approximate model to describe a multilayered heterostructure was generalized to the case of a asymmetrical quantum well.

The polaron energy and its effective mass were calculated for different quantum wells.

The method of stability indices was suggested describing the stability of stochastic systems. It is shown that quasi-isolated systems are stochastically unstable. The probabilistic approach to pattern selection was developed. This theory has to do with evolution equations of nonlinear nonequilibrium systems, when there appear a multiplicity of solutions corresponding to different spatiotemporal patterns. A probability measure characterizing these patterns was constructed and the principle of pattern selection was suggested. The theory was developed for describing turbulent photon filamenation in resonant media. The results of calculations were in very good agreement with experiments on lasers with high Fresnel numbers. Coherent phenomena in photonic bandgap materials, with localized light, were described. The effect of collective liberation of localized light was predicted.

Two approaches were developed to describe systems with a finite (countered) number of objects. In the first one a compound object is introduced directly via generation numbers of its components. Its behaviour is described with nonlinear equations of Lotka-Volterra-type with the skew-symmetric matrix of coefficients. All the solutions of the equations were obtained and the structure of their critical points was investigated. In the second approach probability equations (Smolukhovskyi type one), describing the processes coagulation as well as fragmentation, were proposed and solved.

Main results in the problem of disordered structures were obtained in investigation of electronic structure of graphitic nanoparticles, in studies of the low-temperature thermal characteristics of topologically disordered materials, and in studies of some novel effects in Josephson junctions.

Within a gauge field-theory model, the local and total density of states (DOS) near the pentagonal defects (disclinations) were calculated for three geometries: sphere, cone, and hyperboloid. It was found that the low-energy total DOS has a cusp which drops to zero at the Fermi energy for disclinations with the Frank index $\nu < 1/2$. The appearance of an enhanced charge density near the Fermi level for nanocones with 60° opening angle (180° disclination at the apex) was predicted.

The problem of phonon scattering by long-range strain fields caused by wedge disclination dipoles and circular wedge disclination loops was studied. A combination of two scattering processes, the phonon scattering due to biaxial disclination dipoles and the Rayleigh-type scattering were shown to be of importance for amorphous dielectrics. The results are in good agreement with experimentally observed thermal conductivity in a-SiO_2, a-GeO_2, a-Se, and polystyrene. The frequency-dependent loss and specific heat due to twist disclinations were investigated by treating the disclination as an oscillating heterogeneous string. It was found that (1) the contribution to the specific heat depends linearly on the temperature, and (2) the decrement has a resonance-type character and is proportional to the fourth power of the disclination length.

Several novel phenomena in a twisted superconductor (containing a small annular SIS-type contact) under the influence of thermal gradient and applied magnetic field were predicted, including a torsional analog of Josephson piezomagnetism and magnetomechanical effect. A giant enhancement (reaching 500%) of electronic contribution to the thermal conductivity of a granular superconductor in applied electric field was predicted within a model of inductive Josephson junction arrays.

N.M. Plakida

ANTIFERROMAGNETIC EXCHANGE AND SPIN-FLUCTUATION SUPERCONDUCTING PAIRING IN CUPRATES

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A unique property of cuprates is that they belong to a charge-transfer insulators with a small splitting energy between $3d$ copper and $2p$ oxygen levels and a large Coulomb correlations in $3d$ copper states [1]. This results in a huge antiferromagnetic (AFM) superexchange interaction of the order of $J \simeq 1500$ K which brings the long-range AFM order in the undoped regime and causes strong AFM dynamical spin fluctuations in the superconducting state. It suggests that the AFM interaction can be responsible for the d-wave superconducting pairing in cuprates with high T_c, as was shown in studies of the one-band t-J model (see, e.g. [2]-[6]).

To prove the AFM pairing mechanism we consider the original p-d model for CuO_2 layer [1, 7]. In this report, we briefly present the results of these investigation, while details of the calculations can be found in the original papers [8, 9].

We consider an effective two-band Hubbard model with the lower Hubbard subband occupied by one-hole Cu d-like states and the upper Hubbard subband occupied by two-hole p-d singlet states [7]:

$$H = E_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22} + \sum_{i \neq j,\sigma} \{ t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma t_{ij}^{12} (X_i^{2\bar{\sigma}} X_j^{0\sigma} + \text{H.c.}) \}, \quad (1)$$

where $X_i^{nm} = |in\rangle\langle im|$ are the Hubbard [7] operators for the four states $n, m = |0\rangle, |\sigma\rangle, |2\rangle = |\uparrow\downarrow\rangle$, $\sigma = \pm 1/2 = (\uparrow, \downarrow)$, $\bar{\sigma} = -\sigma$. Here $E_1 = \epsilon_d - \mu$ and $E_2 = 2E_1 + \Delta$ where μ is the chemical potential and $\Delta = \epsilon_p - \epsilon_d$ is the p-d charge transfer energy. The effective hopping integrals $t_{ij}^{\alpha\beta} \simeq 0.1t \ll \Delta \simeq 2t$ where t is the p-d hybridization parameter (see [7]). The Hubbard model (1) corresponds to the strong correlation limit since the bandwidth $W \simeq 8|t_{ij}^{\alpha\beta}| \simeq t < \Delta$.

To discuss the superconducting pairing within the model Hamiltonian (1), we introduce the four-component Nambu operators $\hat{X}_{i\sigma}$ and $\hat{X}_{i\sigma}^\dagger = (X_i^{2\sigma}\ X_i^{\bar{\sigma}0}\ X_i^{\bar{\sigma}2}\ X_i^{0\sigma})$ and define the 4×4 matrix Green function (GF) $\tilde{G}_{ij\sigma}(t - t') = \langle\langle \hat{X}_{i\sigma}(t) \mid \hat{X}_{j\sigma}^\dagger(t') \rangle\rangle$. By applying the projection technique to the equation of motion method for the GF we derive the Dyson equation in the $(\mathbf{q}, \omega)$-representation [8, 9]:

$$\left(\tilde{G}_\sigma(\mathbf{q},\omega)\right)^{-1} = \left(\tilde{G}_\sigma^0(\mathbf{q},\omega)\right)^{-1} - \tilde{\Sigma}_\sigma(\mathbf{q},\omega), \quad \tilde{G}_\sigma^0(\mathbf{q},\omega) = \left(\omega\tilde{\tau}_0 - \tilde{E}_\sigma(\mathbf{q})\right)^{-1}\tilde{\chi}, \quad (2)$$

where $\tilde{\tau}_0$ is the 4×4 unity matrix and $\tilde{\chi} = \langle\{\hat{X}_{i\sigma}, \hat{X}_{i\sigma}^\dagger\}\rangle$. The zero-order GF within the generalized mean field approximation (MFA) is defined by the frequency matrix which in the site representation reads $\tilde{E}_{ij\sigma} = \tilde{\mathcal{A}}_{ij\sigma}\tilde{\chi}^{-1}$, $\tilde{\mathcal{A}}_{ij\sigma} = \langle\{[\hat{X}_{i\sigma}, H], \hat{X}_{j\sigma}^\dagger\}\rangle$. The self-energy operator in the Dyson equation (2) in the projection technique method is defined by the many-particle *irreducible* operators: $\hat{Z}_\sigma^{(ir)} = [\hat{X}_{i\sigma}, H] - \sum_l \tilde{E}_{il\sigma}\hat{X}_{l\sigma}$ in the form $\tilde{\Sigma}_\sigma(\mathbf{q},\omega) = \tilde{\chi}^{-1}\langle\langle\!\langle \hat{Z}_\sigma^{(ir)} \mid \hat{Z}_\sigma^{(ir)\dagger} \rangle\!\rangle\!\rangle_{\mathbf{q},\omega}^{(prop)}\ \tilde{\chi}^{-1}$ where $\langle\{\hat{Z}_\sigma^{(ir)}, \hat{X}_{j\sigma}^\dagger\}\rangle = 0$.

In the MFA the electronic spectrum and superconducting pairing are described by the zero-order GF in Eq. (2). By applying the commutation relations for the Hubbard

operators the frequency matrix $\tilde{E}_{ij\sigma}$ can be easily derived. The normal component defines quasiparticle spectra of the model in the normal state which were studied in detail in [7]. The anomalous component defines the gap functions for the singlet and one-hole subbands, respectively, $(i \neq j)$: $\Delta^{22}_{ij\sigma} = -2\sigma t^{12}_{ij}\langle X^{02}_i N_j\rangle$, $\Delta^{11}_{ij\sigma} = -2\sigma t^{12}_{ij}\langle (2-N_j)X^{02}_i\rangle$, where the number operator $N_i = \sum_\sigma X^{\sigma\sigma}_i + 2X^{22}_i$. Using the definitions of the Fermi annihilation operators: $c_{i\sigma} = X^{0\sigma}_i + 2\sigma X^{\bar{\sigma}2}_i$ we can write the anomalous average as $\langle X^{02}_i N_j\rangle == \langle X^{0\downarrow}_i X^{\downarrow 2}_i N_j\rangle = \langle c_{i\downarrow} c_{i\uparrow} N_j\rangle$. Therefore, the anomalous correlation functions describe the pairing at one lattice site but in different subbands.

In our approach we perform a direct calculation of the correlation function $\langle X^{02}_i N_j\rangle$ without *any decoupling* by considering the corresponding commutator GF $L_{ij}(t-t') = \langle\langle X^{02}_i(t) \mid N_j(t')\rangle\rangle$. After writing the equation of motion for GF $L_{ij}(\omega)$ and applying the spectral theorem we obtain the following representation for the desired correlation function at sites $i \neq j$ for the singlet subband in the case of hole doping [9]: $\langle X^{02}_i N_j\rangle = -(1/\Delta)\sum_{m\neq i,\sigma} 2\sigma t^{12}_{im}\langle X^{\sigma 2}_i X^{\bar{\sigma}2}_m N_j\rangle \simeq -(4t^{12}_{ij}/\Delta)2\sigma\,\langle X^{\sigma 2}_i X^{\bar{\sigma}2}_j\rangle$, where the approximate value is obtained in the two-site approximation, $m = j$, usually applied to the t-J model. This finally allows us to write the expression of the gap function in MFA in the case of hole doping as follows: $\Delta^{22}_{ij\sigma} = -2\sigma\, t^{12}_{ij}\langle X^{02}_i N_j\rangle = J_{ij}\langle X^{\sigma 2}_i X^{\bar{\sigma}2}_j\rangle$. This result recovers the exchange interaction contribution to the pairing, with an exchange energy parameter $J_{ij} = 4\,(t^{12}_{ij})^2/\Delta$. We may therefore conclude that the anomalous contributions to the zero-order GF, Eq. (2), originate in conventional anomalous pairs of quasi-particles and their pairing in MFA is mediated by the exchange interaction which was studied in the t-J model (see, e.g., [2, 4]).

The self-energy matrix was calculated in the self-consistent Born approximation (SCBA) (or the noncrossing approximation). In SCBA, the propagation of the Fermi-like and Bose-like excitations in the many-particle GF in $\langle\langle \hat{Z}^{(ir)}_\sigma \mid \hat{Z}^{(ir)\dagger}_\sigma\rangle\rangle^{(prop)}_{\mathbf{q},\omega}$ are assumed to be independent, which results in the decoupling of the corresponding operators in the time-dependent correlation function $\langle B_{1'}(t)X_1(t)B_{2'}(t')X_2(t')\rangle \simeq \langle X_1(t)X_2(t')\rangle\langle B_{1'}(t)B_{2'}(t')\rangle$ for lattice sites $(1 \neq 1', 2 \neq 2')$. Using the spectral representation for these correlation functions we get a closed system of equations for the GF (2) and the self-energy of the Eliashberg type with the pairing interaction mediated by spin-fluctuations [9]. The latter is defined by the spin susceptibility $\chi''_s(\mathbf{q},\omega) = -(1/\pi)\mathrm{Im}\langle\langle \mathbf{S}_q \mid \mathbf{S}_{-q}\rangle\rangle_{\omega+i\delta}$ which comes from the correlation function $\langle B_{1'}(t)B_{2'}(t')\rangle$.

By considering the weak coupling approximation for calculation of the self-energy and taking into account the contribution from the exchange interaction in MFA, we arrive at the following equation for the singlet gap:

$$\Delta^{22}(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}[J(\mathbf{k}-\mathbf{q}) - \lambda(\mathbf{k},\mathbf{q}-\mathbf{k})]\frac{\Delta^{22}(\mathbf{k})}{2E_2(\mathbf{k})}\tanh\frac{E_2(\mathbf{k})}{2T}\,, \tag{3}$$

where $\lambda(\mathbf{k},\mathbf{q}-\mathbf{k}) = |t(\mathbf{k})|^2\chi_s(\mathbf{q}-\mathbf{k},\omega=0) > 0$ and $t(\mathbf{k}) \simeq t\,(1/2)(\cos k_x + \cos k_y)$. The gap equation (3) for model spin-fluctuation susceptibility $\chi_s(\mathbf{q})$ was numerically solved in [9], which gives the doping dependence of the superconducting transition temperature $T_c(\delta)$ and the gap function $\Delta^{22}(\mathbf{k})$ having d-wave pairing symmetry. The obtained results qualitatively agree with experiments in cuprates.

Further analytical studies was showed that for the exchange interaction, mediated by the interband hopping with large energy transfer $\Delta \gg W$, the retardation effects are negligible. It results in coupling of all electrons in the conduction band W and T_c

proportional to the electronic energy [5]

$$T_c \simeq \sqrt{\mu(W-\mu)}\exp(-1/\lambda), \quad \lambda \simeq J\,N(\delta), \tag{4}$$

where $N(\delta)$ is the density of electronic states for doping δ. The maximum T_c is achieved for the chemical potential $\mu = E_F \simeq W/2$ and even for a weak coupling, $\lambda \simeq 0.3$; it can be quite large of the order of 200 K.

The AFM pairing mechanism is further proved by considering the T_c dependence on the lattice constant [5]. While in conventional electron-phonon superconductors T_c decreases with pressure, in cuprates T_c increases. From Eq. (4) we get an estimation: $d\ln T_c/d\ln a = (d\ln T_c/d\ln J)\,(d\ln J/d\ln a) \simeq -50$ (for $\lambda \simeq 0.3$ and $d\ln J/d\ln a \simeq -14$) which is quite close to the experiments. Concerning the oxygen isotope effect in cuprates on substitution of ^{18}O oxygen for ^{16}O we can estimate it also from Eq. (4). By using the experimentally observed isotope shift for the Néel temperature in La_2CuO_4, $\alpha_N = -d\ln T_N/d\ln M \simeq 0.05$ with $T_N \propto J$ we get $\alpha_c = -(d\ln T_c/d\ln M) = -(d\ln T_c/d\ln J)\;(d\ln T_N/d\ln M) \simeq (\alpha_N/\lambda) \simeq 0.16$ for $\lambda \simeq 0.3$ which is close to experiments.

To conclude, the present investigation proves the existence of a singlet $d_{x^2-y^2}$-wave superconducting pairing for holes or electrons in the two-band Hubbard model mediated by the antiferromagnetic exchange interaction and spin-fluctuation scattering induced by the kinematic interaction characteristic of the Hubbard model. These mechanisms of superconducting pairing, generic for cuprates, are absent in the fermionic models.

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OPTICAL PROPERTIES OF STRONGLY CORRELATED SYSTEMS. DYNAMICAL MEAN FIELD THEORY

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Optical spectral functions such as conductivity or reflectivity are very important characteristics of solids which give us a direct probe of their electronic structure. In the past, very powerful numerical techniques based on density functional theory (DFT) and local density approximation (LDA) were developed, which allowed access to the one-electron spectrum in real materials via association of LDA energy bands with the real excitation energies. This approach works well for weakly correlated systems, where, for example, optical properties can be directly computed [1] via the knowledge of the band structure and the dipole matrix elements of the material.

Unfortunately, the treatment of materials with strong electronic correlations is not possible within this framework. Strong on-site Coulomb repulsion modifies the one-electron spectrum via appearance of satellites, Hubbard bands, strongly renormalized Kondo-like states, etc., which are no longer obtainable using static mean-field theories such as the Hartree-Fock theory or DFT. The wave functions in strongly correlated systems are not representable by single-Slater determinants and dynamical self-energy effects become important, thus requiring a new theoretical treatment based on the dynamical mean field theory [2] (DMFT). Recent advances in merging the DMFT with realistic LDA based electronic structure calculations has already led to solving such long standing problems as, e.g., temperature dependent magnetism of Fe and Ni, volume collapse in Ce, Mott transition in V_2O_3 and huge volume expansion of Pu.

We developed an approach to calculate the optical properties of strongly correlated systems based on combined LDA and DMFT framework. Realistic DMFT computations of optical properties would allow the test of DMFT predictions using more bulky sensitive probes. The DMFT based approach to the electronic structure problem considers both the charge density and the local Green function (GF) as parameters of a spectral density functional [3]. To find its extremum, a set of Dyson equations is solved self–consistently. The set also includes the local self-energy. The self-energy is found by solving the Anderson impurity model with a matrix of Coulomb interaction and a Weiss field function using the available many-body technique [2] such as Quantum Monte Carlo (QMC) method which is used in present calculations. Solutions of the Dyson equation are used in calculation of the optical conductivity which is expressed via the equilibrium state current-current correlation function.

The method was implemented for calculating optical conductivity of the paramagnetic doped insulator $La_{1-x}Sr_xTiO_3$. Local density approximation cannot reproduce the insulating behavior of this system when $x = 0$, indicating the importance of correlations. Upon doping the system becomes a correlated metal. The optical conductivity $\sigma_{xx}(\omega)$ obtained on the low frequency interval is shown in Fig. 1 at several doping levels $x = 0.1, 0.2$, and 0.3. The $x = 0$ case, which corresponds to undoped $LaTiO_3$ compound, is an insulator with a small gap equal to 0.2-0.5 eV. The gap between the lower Hubbard band and La $5d$ bands is the charge transfer gap. Optical transitions from the lower Hubbard band to La $5d$ give the main contribution to the optical conductivity in pure $LaTiO_3$, which is nicely reproduced in our calculations.

Upon doping, carriers are introduced into the conduction band, and the system shows metallic behavior.The optical conductivity at very low frequencies and for $x > 0$ exhibits a Drude peak whose strength increases with doping. As it is seen from Fig. 1, the optical conductivity has nonzero intensity all the way down to 1.1 eV. The contribution to this intensity is due to transitions from i) the coherent part of the spectrum near the Fermi level to the upper Hubbard and Lanthanum bands, ii) the transitions from the lower Hubbard band to the upper Hubbard band and Lanthanum bands and iii) transitions from the lower Hubbard band to the coherent part of the spectra.

This trend correctly reproduces the optical absorption experiments [4] performed for $La_{1-x}Sr_xTiO_3$. To compare our theoretical data with these measurements, Fig. 1 shows by symbols the measured optical conductivity at the doping level $x = 0.1$. Overall good agreement can be found from this comparison for both the frequency behavior of the theoretical and experimental curves and their relative intensities. We must emphasize that the corresponding calculations based on the local density approximation would completely fail to reproduce the doping behavior.The correct trend upon doping captured by the present calculation as well as proper frequency behavior can be considered as significant improvements brought by the realistic DMFT studies.

More insight into our calculations can be gained by comparing the effective number of carriers participating in the optical transitions.The main contribution in LDA case to the N_{eff} comes from the Drude part of the conductivity (90%) and only 10% is due to interband transitions. Hence, the main effect brought by DMFT suppresses those 90 % of the Drude contribution to get insulating behavior instead. Experimental doping dependence of the effective number of carriers was extracted from Ref. [5]. In the inset of Fig. 1 we plot the number of electrons as a function of hole concentration from both the theory and experimental measurements. Again, at zero doping the system is an insulator which gives very small N_{eff} for $x = 0$. The fact that our calculations predict the effective number behavior correctly indicates that the dynamical mean field method properly describes the system as a function of doping larger than 0.1.

Further we discuss our optical conductivity spectrum at higher frequency interval up to 16 eV. Figure 1 (right panel) shows the optical conductivity function $\sigma_{xx}(\omega)$ at doping $x = 0.1$ where we compare our results to the local density approximation result and with the measured data [4].

Even at low doping one can notice the difference between the LDA and DMFT results in the low-energy part of the conductivity (where the most differences are expected). A sharp increase in the optical conductivity at $\omega \sim 4$ eV is seen. This is attributed to the transitions from the oxygen p-band into unoccupied d states of Ti. The main peak of optical transitions is located between 5 and 10 eV, and major contribution to the peak comes from Oxygen to Lanthanum bands. It is predicted by both our (solid line) and LDA (dashed line) calculations. It is well compared with the measured spectrum (symbols). Since our self-energy corrections modify only the states near the Fermi level, we do not expect our spectrum to be essentially different from that given by the LDA in this frequency range which can also be concluded from Fig. 1. Overall, the agreement at high frequencies is quite good, which demonstrates reliability of the present theoretical study.

Summarizing, we have shown how the optical conductivity of realistic strongly correlated system can be computed using the recently developed DMFT-based electronic structure method. As application of the method, we have studied the optical conductiv-

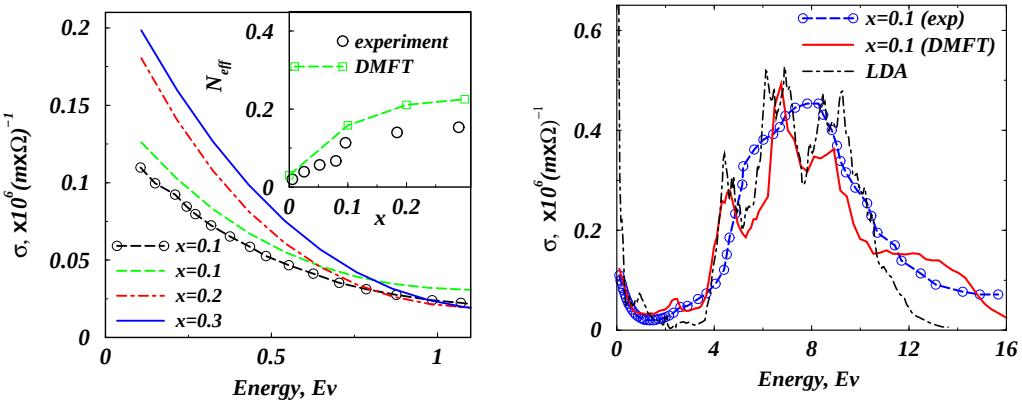

Figure 1: Low-frequency behavior of the optical conductivity for $La_{1-x}Sr_xTiO_3$ (left panel) at $x = 0.1, 0.2, 0.3$ calculated using the LDA+DMFT method. Experimental result is shown by symbols for the $x = 0.1$ case. In the inset we plot the effective number of carriers as a function of doping. Squares show theoretical result of the LDA+DMFT calculations. Circles are experimental data. Calculated optical conductivity spectrum for $La_{1-x}Sr_xTiO_3$, $x = 0.1$, in a large frequency interval (right panel) using theDMFT method (full line) as compared with the experimental data (symbols) and the results of the corresponding LDA calculations (dashed line).

ity of $La_{1-x}Sr_xTiO_3$ and found the correct dependence of this function as a function of both frequency and doping. Our results, reproducing well experimental data, significantly advance the studies based on static mean field approximations such as the LDA.

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DOUBLE KRONECKER SERIES AND EXACT ASYMPTOTIC EXPANSION FOR THE ISING MODEL ON TORUS

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Singularities of thermodynamic functions at the critical point arise only in the thermodynamic limit when the size L of a system tends to infinity. In this limit the correlation length $\xi_{\rm bulk}$ determines the degree of exponential decrease in correlation functions. In addition to these two fundamental scales L and $\xi_{\rm bulk}$ there also exists a microscopic interaction scale. Thus, thermodynamic quantities may depend on the scale-free ratios $\xi_{\rm bulk}/L$ and a/L. The finite-size scaling hypothesis [1] implies that near the critical point (where $a \ll \xi_{\rm bulk} \sim L$) the behaviour of any thermodynamic quantity can be described by a universal function of only one variable $t = \xi_{\rm bulk}/L$. Corrections to the finite-size scaling function can be treated as asymptotic series in powers of another variable a/L.

Two-dimensional exactly solvable models, in particular, the Ising model [2], have always been a certain testing ground used to verify general approaches to studying critical phenomena such as the finite-size scaling hypothesis and possible nonuniversal corrections to the scaling function. Asymptotic expansion of free energy of the Ising model on torus of the area S and with the relation of the sides τ near the critical point can be represented as a series

$$F_{T=Tc}(\tau, S) = f_\infty\ S + f_0(\tau) + \sum_{k=1}^{\infty} f_k(\tau)\ S^{-k}.$$

For the Ising model the coefficients of this expansion can be expressed through the elliptic theta functions

$$\begin{aligned} f_\infty &= -\frac{\ln 2}{2} - \frac{2\gamma}{\pi} \\ f_0(\tau) &= -\ln \frac{\theta_2 + \theta_3 + \theta_4}{2\eta} \\ f_1(\tau) &= -\frac{\pi^3 \rho^2}{180}\ \frac{\frac{7}{8}(\theta_2^9 + \theta_3^9 + \theta_4^9) + \theta_2\theta_3\theta_4\,[\theta_2^3\theta_4^3 - \theta_3^3\theta_2^3 - \theta_3^3\theta_4^3]}{\theta_2 + \theta_3 + \theta_4} \\ &\vdots \end{aligned}$$

Here the free energy per site f_∞ was calculated in [3] and the first term of the asymptotic expansion $f_0(\tau)$ was found in [4]. We derive recurrence formulae which though cumbersome allow one to write out explicit expressions for any term of the asymptotic expansion $f_k(\tau),\ k \geq 1$ in terms of the elliptic theta functions [5].

Our approach is based on the use of the double Kronecker series [6]

$$\mathrm{K}_p^{\alpha,\beta}(\tau) \sim \sum_{\substack{m,n \in Z \\ (m,n) \neq (0,0)}} \frac{e^{-2\pi i(n\alpha + m\beta)}}{(n + \tau\, m)^p}.$$

These series turned out to be directly associated with higher correction terms of the asymptotic expansion of the free energy for the model of free fermions on torus with twisted boundary conditions when the fermion wave function acquires a phase shift α

when going round one of the torus periods and β round the other. In this case one can show that

$$\ln Z_{\alpha,\beta}(\tau) = \left(-\tfrac{\ln 2}{4} - \tfrac{\gamma}{\pi}\right) S + \ln \left| \tfrac{\theta_{\alpha,\beta}(\tau)}{\eta(\tau)} \right| + \sum_{k=1}^{\infty} \hat{D}_{2k+2}\, \mathrm{K}^{\alpha,\beta}_{2k+2}(\tau)\; S^{-k},$$

where $\hat{D}_{2k+2}$ are the differential operators with respect to the variable τ [5].

Using this result one can calculate the asymptotic expansions for all free models of statistical mechanics (the Ising model, the dimer model, and the Gauss model). Indeed, the partition functions of these models are expressed in terms of that of free fermions on torus with the twisted boundary conditions as follows:

$$\begin{aligned}
Z_{\mathrm{Ising}}(\tau) &= 2^{MN/2-1} \left\{ Z_{\frac{1}{2},\frac{1}{2}}(\tau) + Z_{0,\frac{1}{2}}(\tau) + Z_{\frac{1}{2},0}(\tau) + Z_{0,0}(\tau) \right\} \\
Z_{\mathrm{Dimer}}(\tau) &= \frac{1}{2} \left\{ Z^2_{\frac{1}{2},\frac{1}{2}}(\tau) + Z^2_{0,\frac{1}{2}}(\tau) + Z^2_{\frac{1}{2},0}(\tau) - Z^2_{0,0}(\tau) \right\} \\
Z_{\mathrm{Gauss}}(\tau) &= 2^{MN/2} \left[\, Z_{0,0}(\tau) \,\right]^{-1}
\end{aligned}$$

Exact asymptotic expansions for other thermodynamic functions: internal energy and heat capacity, were found in an analogous way.

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A NEW LINE OF INVESTIGATION OF NONLINEAR EVOLUTION EQUATIONS SOLVABLE BY THE INVERSE SCATTERING METHOD

V.K. Mel'nikov

A new approach to the problem of finding nonlinear evolution equations solvable by the inverse sacttering method is proposed by the author. All existing approaches are based on the Lax representation [1] and its modifications [2, 3, 4], or on the study of a group of symmetries of the nonlinear equations under consideration [5], whereas in the proposed approach the evolution equations for the scattering data underlie it. This means that, first, a nonlinear evolution equation (or a system of these equations) and a linear differential operator to be used for investigation of the given equation (or the system) are taken. Then, we consider the evolution of the scattering data for this operator under the assumption that its coefficients vary with time in accordance with the nonlinear equation (or a system of these equations) taken. It turned out that under different assumptions on the structure of the evolution equations for the scattering data we can answer the question if there is a nonlinear evolution system generating this evolution of the scattering data and if yes, then how to find it (or describe it effectively).

At the present time, this issue obtained an effective and rather a simple solution for the Schrödinger and Dirac operators [6, 7]. It is shown that if the evolution equations for the scattering data are assumed to be differential (ordinary or with partial derivatives), the nonlinear evolution equations generating this evolution have the operator representation of which the Lax representation is a particular case [1]. Moreover, the structure of this operator relation is completely determined by the group of symmetries of the operator used. This group of symmetries determines transformations relating the solutions to these equations in the non-Lax case with those to the equations having the Lax representation. The procedure of solving this task is mostly new and its application in further investigations in this field seems promising.

The obtained results were reported at the seminars at the Bogoliubov Laboratory, JINR and the Currant Institute, New York, as well as at the International Conferences in Dubna, Prague, and Cambridge (Great Britain).

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ANALYTICALLY SOLVED KINETIC MODELS

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Many problem of physics, chemistry, biology and social science could be considered as a kinetic one which is nonlinear as a rule. Often that problem could be formulated in terms of population numbers or probability versus population numbers. We construct analytically solved problems in both the cases. These two variants are not necessarily alternative. A choice among them is defined, to a considerable extent, by a possibility to reveal, within the problem, a certain conserved dynamic quantity which assumes a nontrivial differential form. Being integrated that equation returns the above value as a function conserved on solutions [1, 2, 3].

A nontrivial r.h.s. of a nonlinear differential equation which is written in the normal form can get some additional symmetry as regards the original conservation law, some extra conservation laws. These extra symmetries could be comprehended as own dynamic properties which determine a complex system or transitions between its states, e.g., a balance rule which is related with position of representative point in co-space of coefficients (constants of interaction, etc.). Besides, a possibility arises to control an increase in of complexity of a system and a number of integrals. We constructed an example of this kind of system in terms of the population number approach.

A complex compound object of 3 species, whose population numbers converse dynamically as a result of interactions between them under a condition of conservation of their total sum, is described as nonlinear ODE's in the normal form with r.h.s. quadratic over population number of species and skew symmetric matrix of coefficients. We named it the 3D Lotka–Volterra System

$$\dot{x} = x(az - by)\,,\ \dot{y} = y(bx - cz)\,,\ \dot{z} = z(cy - ax) \tag{1}$$

Skew symmetry of the coefficient matrix of this system is a way to express some "coherent" balanced behaviour. The maximum of coherence corresponds to equality to unity modula of those ratios value. To this equation we investigated projective properties of functional space and the space of parameters as regards the families of integral curves in the functional space.

The same form of equations arises from different considerations (see [4, 5]). Finding out a bipartite finite oriented graph and the proper formal chemical reaction with periodic solutions owing to the linear balance condition leads to a reaction scheme involving three irreversible auto-catalytic reactions. In accordance with an accepted viewpoint, that irreversible scheme does not correspond directly to any real chemical phenomena, however, the conclusion was made that direct auto-catalytic steps provide a necessary condition for irregular oscillatory behavior in three–component closed and bimolecular schemes [3, 5].

Despite a common point of view on different LV tasks, we consider the problem at positive and negative values of variables, which gives a possibility to consider the case of equality to zero of a total sum of population numbers $\sum_{i=1}^{3} x_i = 0$. Moreover, a structure of all critical points and vector fields is examined. The method is more adequate at large population numbers.

A description of the problem in terms of probability function depending continuously on time is a more pertinent one, while population numbers are small and have been considered as integer ones. Probability functions depend upon these values as parameters. Say, processes of aggregation, fragmentation, or traffic at a little number of particles, and at not a little dimension of a system considered (i.e. low density) are the very cases.

Let a total probability be conserved to find a discussed system in some state. Then a conjecture about constancy of transition rates of processes allows to write down models, which are differential – difference linear as regards the above probability functions ones. It permits one to solve models exactly in terms of $W(s,t)$ – probability to find the system in a state with a given population number s at instant t. Aggregation and fragmentation are a couple of mutually inverse processes. So, it is important to describe this pair as a single whole by a unified equation analytically solved even in a probabilistic sense. This is done by us.

The clustering processes resemble to a certain degree the critical gas nucleation processes [6]. It is begotten in the mathematical description being general for kinetics of such processes. Clusters grow by coalescence of smaller clusters. Their kinetics of growth is like that of coagulation with conserved number of objects. The basic equation reads as

$$\begin{array}{c} \frac{dW(s,t)}{dt} \\ = \gamma_1[sW(s+1,t) - (s-1)W(s,t)] \\ -\gamma_2[(G-s)W(s,t) - (G-s+1)W(s-1,t)], \end{array} \tag{2}$$

with the initial conditions

$$W(G,0) = 1; \quad W(s,0) = 0, \quad if\ s \neq G, \tag{3}$$

where γ_1 and γ_2 are constant rates.

The r.h.s. of Eq. (2) consists of gain terms due to coagulation of clusters from an $(s+1)$-cluster state and dissociation of those clusters belonging to an $(s-1)$-cluster state and loss terms due to simultaneous coalescence and dissociation of clusters belonging to an s-cluster state. Solutions are given as

$$W(s,t) = \frac{\partial^s}{\partial z^s} \frac{\gamma\,(\frac{z\,\gamma_2 + \gamma_1\,e^{(-t\,\gamma)}\,z - \gamma_1\,e^{(-t\,\gamma)} + \gamma_1}{\gamma})^G}{(z\,\gamma_2 + \gamma_1\,e^{(-t\,\gamma)}\,z - \gamma_1\,e^{(-t\,\gamma)} + \gamma_1)} | z = 0,\ \gamma = \gamma_1 + \gamma_2. \tag{4}$$

Our results extend the possibilities of applications of the well-known Smoluchovsky and Lotka-Volterra approaches under stipulated conditions,

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DILUTE BOSE GAS IN TWO DIMENSIONS: DENSITY EXPANSIONS AND THE GROSS-PITAEVSKII EQUATION

A. Yu. Cherny and A. A. Shanenko

The leading term of the energy expansion in na^2 (here $n = N/S$ is the density in two dimensions) for a gas of hard discs was first obtained by Schick [1] who made use of the first-order Beliaev approximation [2] developed for the 3D Bose gas. To obtain the next-to-leading terms, the second-order Beliaev approximation is needed, which is a rather difficult problem in the 2D case due to the logarithmic singularity of the 2D Green function at small momenta. At the same time, our method [3, 4] successfully reproduces in the 3D case the famous next-to-leading term for the chemical potential, which ensures that our results are valid also in two dimensions.

Our approach is based on the analysis [3] of the eigenvalues and eigenfunctions of the two-body density matrix, which allows for obtaining all thermodynamic characteristics of the system. The maximum eigenvalue $N_0(N_0-1) \sim N_0^2$ corresponds to the state of two particles in the condensate; its eigenfunction $\varphi(r)/S$ (here $\varphi(r) = \langle\hat{\psi}(\mathbf{r})\hat{\psi}(0)\rangle/n_0$, n_0 is the condensate density) can be interpreted as a pair wave function *in medium* of the condensate-condensate type. The other macroscopic eigenvalues $2N_0n_q$ correspond to the two-body states with one particle in the condensate and another one beyond the condensate; its eigenfunctions $\varphi_{\mathbf{q}/2}(\mathbf{r})\exp[i\mathbf{q}\cdot(\mathbf{r}_1+\mathbf{r}_2)/2]/S$ are of the condensate-supracondensate type where $\hbar\mathbf{q}$ is the total momentum of the pair of bosons. For a dilute gas, only small momenta are of importance, and we can replace the condensate-supracondensate wave functions by their limiting value [3] $\sqrt{2}\varphi(r) = \lim_{p\to 0}\varphi_{\mathbf{p}}(\mathbf{r})$. Thus, contrary to the standard approaches, we use the low-momentum approximation that keeps the coordinate dependence in the eigenfunctions of the two-body matrix. It is a crucial point that leads to accurate treatment of the short-range particle correlations. In this way, one can write down the simple low-momentum ansatz for the pair distribution function and chemical potential

$$\begin{aligned} g(r) &= \varphi^2(r)[1+2(n-n_0)/n+\cdots], \\ \mu &= nU(0)[1+(n-n_0)/n+\cdots]. \end{aligned} \tag{1}$$

Here we introduce the "in-medium" scattering amplitude $U(k) = \int \mathrm{d}^2r\,\varphi(r)V(r)e^{-i\mathbf{k}\cdot\mathbf{r}}$, which obeys the equation of the Lippmann-Schwinger type [4]

$$U(k) = V(k) - \frac{1}{2}\int \frac{\mathrm{d}^2q}{(2\pi)^2}\frac{V(|\mathbf{k}-\mathbf{q}|)U(q)}{\sqrt{T_q^2+2nT_qU(q)}},$$

where $T_q = \hbar^2q^2/(2m)$ and $V(q)$ are the kinetic term and the Fourier transform of the pairwise interaction potential $V(r)$, respectively. It is not difficult to linearize the latter

equation in the dilute limit $n \to 0$ and thus obtain in a self-consistent manner the short-range behaviour of $\varphi(r)$ (at $r \lesssim 1/\sqrt{n}$) and the in-medium scattering amplitude $U(0)$

$$\varphi(r) \simeq 2u\varphi^{(0)}(r), \quad U(0) = \int \mathrm{d}^2 r\, \varphi(r) V(r) \simeq (4\pi\hbar^2/m)u. \tag{2}$$

Here $\varphi^{(0)}(r)$ is the solution of the two-body Schrödinger equation in the centre-of-mass system with asymptotics $\varphi^{(0)}(r) \to \ln(r/a)$ at $r \to \infty$ [by definition, a is the two-dimensional scattering length for arbitrary short-range potential $V(r)$], and the parameter u is given by the relation ($\gamma \simeq 0.5772$ is the Euler constant)

$$1/u + \ln u = -\ln(na^2\pi) - 2\gamma. \tag{3}$$

Equation (3) has no solution for u when $\delta > 1$ and has two positive ones when $na^2 < 0.0369\ldots$. The solution with a greater value of u should be ignored because of its unphysical behaviour [$u \sim 1/(na^2)$ at $n \to 0$]. Equations (1), (2), (3), and thermodynamic relation $\mu = \partial(\varepsilon n)/\partial n$ yield the following results:

$$g(r) = [\varphi^{(0)}(r)]^2 4u^2[1 + 2u + \cdots], \tag{4}$$

$$\varepsilon = \frac{2\pi\hbar^2 n}{m}[u + u^2/2 + + \cdots], \tag{5}$$

$$\varepsilon_{\mathrm{int}} = \frac{n}{2}\int \mathrm{d}^2 r V(r) g(r) = \frac{2\pi\hbar^2 n\alpha}{m}[u^2 + 2u^3 + \cdots], \tag{6}$$

$$\varepsilon_{\mathrm{kin}} = \left\langle \sum_i p_i^2 \right\rangle /(2mN) = \frac{2\pi\hbar^2 n}{m}[u + (1/2 - \alpha)u^2 + \cdots] \tag{7}$$

for the pair distribution function (4) at $r \lesssim 1/\sqrt{n}$, the total (5), interaction (6) and kinetic (7) energies at zero temperatures. In Eqs. (6) and (7) we put by definition $\alpha = \dfrac{m}{\pi\hbar^2}\displaystyle\int \mathrm{d}^2 r\, [\varphi^{(0)}(r)]^2 V(r)$. It is seen from Eq. (5), (6) and (7) that in the leading order, proportional to nu, the total energy is purely kinetic. Thus, whatever a particular shape of the potential $V(r)$, at sufficiently small densities the energy becomes mostly kinetic. The energy expansion (5) leads to the 2D Gross-Pitaevskii equation

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2\nabla^2\phi}{2m} + V_{\mathrm{ext}}(\mathbf{r})\phi + \frac{4\pi\hbar^2 u}{m}|\phi|^2\phi$$

with the unusual nonlinear term. Here $\phi = \phi(\mathbf{r}, t) = \langle\hat{\psi}(\mathbf{r}, t)\rangle$ is the order parameter with the normalization $N = \int \mathrm{d}^2 r\, |\phi|^2$, and u is given by Eq. (3) with $n = |\phi|^2$.

The above results are described in details in the paper [5].

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UNIVERSAL BEHAVIOR OF REMANENT MAGNETIZATION IN LOW-T_C AND HIGH-T_C JOSEPHSON JUNCTION ARRAYS

S.A. Sergeenkov

Despite the fact that Josephson Junction Arrays (JJAs) have been actively studied for decades, they continue to contribute to the variety of intriguing and peculiar phenomena [1]. To give just a few recent examples, it is sufficient to mention Josephson analogs of thermoelectric [2, 3], magnetoelectric [4] and deformation induced effects (including piezomagnetism [5, 6] and thermomagnetic effects in a twisted weak-link-bearing superconductor [7]). On the other hand [8], $3D$ disordered JJAs fabricated from either conventional (LTS) or high-T_c (HTS) superconductors may, upon excitation by a magnetic field, exhibit a temperature-dependent magnetic remanence, $M_R(T)$. In this report we briefly discuss the latest results [9] on a comparative study of three different samples with a rather spectacular remanent behavior and suggest a possible interpretation of the observed temperature dependence of the remanent magnetization (RM) of both LTS and HTS tridimensional disordered JJAs. Our analysis shows that all the experimental data can be rather well fitted using the explicit temperature expressions for the activation energy and the inductance-dominated contribution to the magnetization of the array within the so-called phase-slip model. All three samples, prepared from Nb, $YBa_2Cu_3O_{7-\delta}$ (YBCO) and $La_{1.85}Sr_{0.15}CuO_{4-\delta}$ (LSCO) exhibit the predicted remanence and other characteristic features of Josephson arrays. The remanence was obtained measuring the sample magnetization after application and removal of a train of sinusoidal pulses. Since the observed RM in our samples appears only below the so-called phase-locking temperature T_J (which marks the establishment of phase coherence between the adjacent grains in the array and always lies below a single grain superconducting temperature T_C), it is quite reasonable to assume that the origin of RM is related to thermal fluctuations of the phases of the superconducting order parameters across an array. In the present approach we consider the sample as a single plaquette with four Josephson junctions (JJs), each of which is treated via an effective single junction approximation. Within this approximation, the phase-slip scenario yields then $\Delta M_R(T) \equiv M(T) - M_R$ for the observed remanent magnetization where $M(T) = 2\pi M_0(T)\gamma(T)e^{-\gamma(T)}$. Here, $M_0(T)$ is an inductance-induced contribution to the magnetization of the array (see below), $\gamma(T) = U(T)/k_BT$ is the normalized barrier height for thermal phase slippage, and $M_R = M(T_J)$ is a residual temperature-independent contribution. Figure 1 shows the temperature dependence of the normalized remanent magnetization $m_r(T) = \Delta M_R(T)/\Delta M_R(T_p)$, where T_p is the peak temperature. The data are found to be well fitted with the following explicit expression for the array magnetization $M(t) = A(1-t^4)^{5/2}\exp[-\alpha(1-t^4)]$ where $t = T/T_C$. The best fits through all the data points (shown in Fig.1 by solid, dotted and dashed lines for YBCO-, Nb- and LSCO-based JJAs, respectively) using the known critical parameters (i) $YBCO$: $T_C = 90K$, $T_J = 82K$, $T_P = 0.88T_J$; (ii) $LSCO$: $T_C = 36.5K$, $T_J = 19.87K$, $T_P = 0.7T_J$; and (iii) Nb: $T_C = 9.1K$, $T_J = 8.2K$, $T_P = 0.92T_J$ yield $\alpha_{YBCO} = 7$, $\alpha_{LSCO} = 2$ and $\alpha_{Nb} = 9$ for the estimates of the model parameters. To understand the observed behavior of the remanent magnetization, we need to specify the temperature dependencies of the activation energy $U(T)$ and the inductance-dominated contribution $M_0(T)$ to the magnetization of the array. Assuming that $U(T) = \Phi_0 I_C(T)/2\pi$ and $M_0(T) = LI_C(T)/\mu_0 S$, where $I_C(T)$ is an average value of the critical current, L is an average inductance of the

Josephson network, S is an effective projected area of the contact, Φ_0 is the flux quantum, and μ_0 is the vacuum permeability, we arrive at the following relationships between the fitting and the model parameters: $A = LI_C(0)\alpha/(\mu_0\lambda_L(0)l)$ and $\alpha = \Phi_0 I_C(0)/2\pi k_B T_C$ with $\lambda_L(0)$ being the London penetration depth and l the thickness of a SIS-type contact.

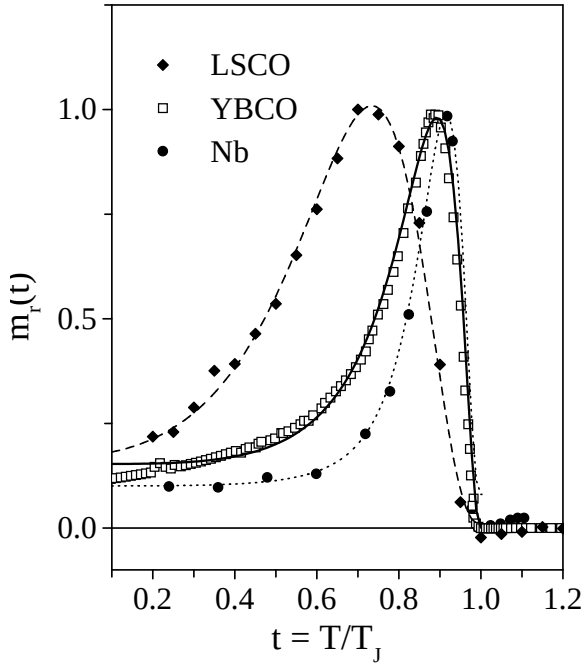

Figure 1: Temperature dependence of the normalized remanent magnetization $m_r(t)$, showing the experimental data for three different samples and the corresponding fittings.

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RESONANT BOSE CONDENSATE: ANALOG OF RESONANT ATOM

V.I. Yukalov and E.P. Yukalova

Dilute atomic gases, trapped and cooled down to temperatures when almost all atoms are in the Bose-condensed state, are described by the Gross-Pitaevskii equation (see review [1]). The mathematical structure of the latter is that of the nonlinear Schrödinger equation which, due to the presence of the trapping potential, possesses a discrete spectrum. The equilibrium Bose-Einstein condensate corresponds to the ground state associated with the lowest energy level of the spectrum. If not the ground but an excited state would be macroscopically populated, this would correspond to a *nonground-state* Bose condensate. The possibility of creating such a nonequilibrium condensate was advanced in Ref. [2, 3]. This can be done by applying an alternating field with a frequency tuned to the transition frequency between the ground state and a chosen excited state. The latter states are called the nonlinear coherent modes and they are described by the stationary solutions to the Gross-Pitaevskii equation. The properties of these modes have been considered theoretically in several publications [4]–[9] and a nonlinear dipole mode was observed experimentally. A known example of such a mode is a vortex that can be formed by means of a rotating laser spoon.

Nonlinear coherent modes are the collective states of trapped Bose atoms, corresponding to different energy levels. These modes can be created starting from the ground state condensate that can be excited by means of a resonant alternating field. A thorough theory for the resonant excitation of the coherent modes is presented. The necessary and sufficient conditions for the feasibility of this process are found. Temporal behaviour of fractional populations and of relative phases exhibits dynamic critical phenomena on a critical line of the parametric manifold. The origin of these critical phenomena is elucidated by analyzing the structure of the phase space. An atomic cloud, containing the coherent modes, possesses several interesting features, such as interference patterns, interference current, spin squeezing, and massive entanglement. The developed theory suggests a generalization of resonant effects in optics to nonlinear systems of Bose-condensed atoms.

We stress the analogy of the resonant Bose condensate with a resonant atom. And we show that, because of its coherent collective nature, the resonant Bose condensate possesses a number of properties distinguishing it from a single resonant atom. We describe several interesting novel effects that can be observed in a nonequilibrium Bose condensate.

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