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Theoretical studies of condensed matter

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This talk briefly reviews the basic directions the Theoretical Department of the Institute for High Pressure Physics, RAS, (IHPP) has been pursuing in condensed matter research during the 50-year existence of the institute.

In the 1960s, the IHPP Theoretical Department became one of the first research centers in our country to employ first principle computational methods — i.e., ones that involve no fitting parameters and thus are experiment-independent — to study the physical properties of and phase transformations in solids, in particular under high pressure conditions. This research is usually carried out in close cooperation with experimenters using experiment/theory comparisons to clarify the underlying physics of the phenomena being observed. Along with known materials, new high-pressure phases first obtained at the IHPP are being investigated. Starting in the 1960s and 1970s, appropriate computational techniques using electron density functional theory, such as the Augmented Plane Wave and Korringa–Kohn–Rostoker methods and their modifications and extensions, have been further developed and revised by IHPP theorists.

The early work by R G Arkhipov, E S Alekseev, and A P Kochkin [1] used the approximate Wigner–Seitz spherical cell method, with a unit cell replaced by an equal-sized sphere, to study the relation between the electronic structure and phase transformations in simple metals under high pressure at $T = 0$. A major finding of this study, a phase transition with a volume change in K, Rb, and Cs, was explained in terms of an electron s–d transition, i.e., as resulting from a pressure-induced change in the mutual arrangement the of s and d bands. The discovery, made due to advances in experimental techniques, and subsequent studies of new low-symmetry high-pressure phases in simple metals brought fresh relevance to this line of research. At present, IHPP researchers use modern theoretical methods (in particular, based on the first-principle pseudopotentials) not only to exactly determine structural sequences in simple metals under pressure at $T = 0$, but also to study $P - T$ phase diagrams at finite temperatures $T \neq 0$, on the basis of the phonon spectra calculations by the density-functional linear-response method [2].

The IHPP's M V Magnitskaya and colleagues from outside Russia [3] have calculated the electron and phonon spectra and the electron-phonon coupling (EPC) for a recently discovered high-pressure metallic phase of sulphur S-IV, which exhibits the incommensurate modulation of atomic positions in the direction [010] (charge density wave, CDW). The first-principle calculation produced a correct crystal structure for the modulated phase of S-IV. The transition to the CDW state can be interpreted as a distortion of the higher-density S-V phase (which has the β-Po type crystal structure). The results of calculations show that in the β-Po structure one of the transverse phonon modes on the vector $\mathbf{q}_{\mathrm{CDW}}$ becomes softer with decreasing pressure. Upon further decrease in pressure to $P \approx 135$ GPa, the frequency of this mode becomes zero, $\omega(\mathbf{q}_{\mathrm{CDW}}) = 0$, corresponding to the S-V phase being unstable relative to the transition to the S-IV phase in which this unstable phonon is 'frozen' into a CDW. The location of the minimum of the phonon mode is in excellent agreement with the experimental modulation vector $\mathbf{q}_{\mathrm{CDW}}$. To analyze the role of the electron–soft mode coupling, the contributions from various phonon modes to the matrix elements of the EPC were calculated. It has been established that the soft-mode contribution is maximum on the vector $\mathbf{q}_{\mathrm{CDW}}$, suggesting that the experimental jump at $p \approx 150$ GPa from 14 to 17 K in the superconducting transition temperature T_{c} can be due to the fact that at $p > p_{\mathrm{CDW}}$ the electron density of states at the Fermi level increases and the electron–soft mode coupling contributes significantly to T_{c}. This jump, as well as the subsequent increase in T_{c} in the interval to $P \approx 200$ GPa, is explained by the competition between the soft mode frequency $\omega(\mathbf{q}_{\mathrm{CDW}})$ and the electron–phonon coupling constant [3].

In the 1970s, due to improvements in computational techniques, institute theorists started broad-scope studies of transition and rare-earth metals, intermetallic compounds, and alloys, covering in detail pressure-induced magnetic phase transitions, as well as alloying and phase stability, galvanomagnetic effects, optical and photoemission spectra, etc. Of particular note are the studies of the magnetic properties in double and triple Laves phase materials, including new compounds, first synthesized at the IHPP [4], of the magnetic 3d metals Fe, Co, and Ni with calcium. Considerable interest was generated by studies by N I Kulikov and colleagues of the effect of pressure on the properties of magnetically ordered metals and alloys, including complex — incommensurate and noncollinear — antiferromagnetic (AFM) structures, for example, chromium and yttrium and their respective alloys, the systems Pt_3Fe, FeRh, etc. [5]. In this context, the excitonic dielectric model combined with band calculations proved a very fruitful approach, offering a single framework for explaining how congruent Fermi surface regions give rise to various AFM orderings. For chromium, in which AFM ordering can be thought of as an incommensurate spin density wave the AFM-destroying effect of the EPC was investigated [6]. A series of publications by N I Kulikov and coworkers on the development of the coherent potential method and its application to disordered systems examined in detail the relation between structural disordering and the magnetic properties for various binary alloys of transition metals and for the disordered alloys of 3d metals with Si, Al, etc. [7].

Finally, one more area of research that emerged in the 1970s was the study of the compounds — carbides, nitrides, hydrides, etc. — which transition and rare earth metals form

with light elements. E S Alekseev and coworkers, who carried out the first principle calculations, and IHPP experimenters, who synthesized these compounds and explored them under high pressure, studied these compounds in close cooperation as promising construction materials (for example, the refractory and hard WC, ReC) and as possible high-temperature superconductors (NbN, TaN, etc.). The theoretical aspects considered were structural transitions, chemical bonding, superconductivity, electrical resistance, and other properties [8]. In a series of papers on hydrides, N I Kulikov and coworkers investigated phase transitions in the metal–hydrogen systems and provided simple approximation estimates for the EPC constant and the superconducting transition temperature T_c [9].

As is known, recently new, intermediate-T_c superconductors have been discovered, including Y_2C_3 ($T_c = 18$ K), MgB_2 ($T_c = 40$ K), and complex borocarbides ($T_c = 15$–23 K)—a discovery which rekindled interest in the compounds of metals with light elements (H, B, C, N, O) that exhibit phonon-mediated superconductivity. Calculations by M V Magnitskaya and A E Karakozov in cooperation with a research group from the P N Lebedev Physics Institute yielded the phonon spectra, EPC, and superconducting properties for a number of cubic carbides and nitrides of transition metals with a general chemical formula of AB over a wide range of pressures [10]. For NbC, the experimentally best studied carbide, the calculated optical and kinetic characteristics involving and related to the EPC are in excellent agreement with experiment, implying that the results of these first-principle calculations are sufficiently accurate to be used in the analysis of what affects the value of T_c in this class of compounds. Other than NbC, the effect of high pressure on phonon-related and superconducting properties was studied in much detail for the cubic nitrides ZrN and HfN, for which high-pressure experimental data are available. The theoretical phonon densities of states for ZrN and HfN are in reasonable qualitative agreement with the Raman spectra measured at various pressures in the range of up to 32 GPa. The spectral density of the EPC and the baric derivative of the critical temperature dT_c/dp for ZrN are in good agreement with measurements obtained at $p \approx 0$ and low pressures, respectively. At high pressures, T_c goes down (measurements at higher pressures were not carried out). Calculations performed suggest that upon further increase in pressure, T_c undergoes a linear decrease, and for $p > 10$ GPa the dependence $T_c(p)$ becomes nonlinear in a way that slows down the decrease in T_c. It is shown that the pressure-induced decrease in T_c results from a decrease in the EPC constant λ, which is due primarily to an increase in phonon frequencies rather than to electron-spectrum-related factors.

An analysis was made of the reasons why cubic carbides have a relatively low T_c compared, for example, with MgB_2. In most of the compounds studied, electrons in light atoms are coupled rather weakly to high-energy optical phonons because in a light atom B the partial electron density of states at the Fermi level, $N_B(E_F)$, is low. A typical example here is NbC. However, compounds with high $N_B(E_F)$—for example, the hypothetical cubic yttrium carbide YC not as yet synthesized stoichiometrically—have also been found to have a low T_c. It is established that in YC carbon's electrons and optical phonons are also weakly coupled, but the reason for this is not the low $N_B(E_F)$, as in NbC—it is the fact that the electron states at E_F are not hybridized and are almost pure p states of carbon. This leads to small matrix elements of EPC and thus to a low T_c. It seems it is only in carbides and nitrides with more complex crystal structures that the hybridization of C or N p states with s or d states can coexist with a high $N_B(E_F)$ (and hence with a high T_c) [10].

Since 1964, studies have been carried out on the use of classical statistical mechanics in the microscopic description of phase transitions, including the superconducting phase transition, orientational transitions in molecular crystals, the theory of melting in two and three dimensions, the Kosterlitz–Thouless transition, transitions in spin-glass systems, and liquid–glass and liquid–liquid transitions in real systems.

One example is an approach, developed by E E Tareyeva, in which superconductivity is treated in tight-binding approximation successfully adapted to describe the effect of pressure. The pressure dependence of the isotope effect in superconductors calculated in this way [11] later gained partial experimental support. The problem of symmetry-changing phase transitions gave rise to a research field using the mathematical theory of the branching solutions of nonlinear integral equations (Lyapunov–Schmidt theory). One of the major results in this area of work was the first microscopic explanation of the Landau symmetry change rules for the second-order phase transition [12].

The description of orientational disorder in molecular crystals was another successful application of this branching theory approach. One result was a detailed microscopic picture of the transition to the four-sublattice ferroquadrupole phase in solid molecular hydrogen [13]. Later applications to more complex problems—in particular, to the orientational transitions in fullerites—led to results in excellent agreement with experiment in terms of the transition temperature, the type of ordering, the order of transition, and the relative proportions of the preferred mutual orientations (the so-called P and H states) [14].

V N Ryzhov and E E Tareyeva [23, 28, 29] proposed using the equations for the conditional multiparticle distribution functions of classical statistical mechanics

$$F_{s+1}\left(\mathbf{r}_1|\mathbf{r}_1^0\ldots\mathbf{r}_s^0\right)=\frac{F_{s+1}(\mathbf{r}_1,\mathbf{r}_1^0,\ldots,\mathbf{r}_s^0)}{F_s(\mathbf{r}_1^0,\ldots,\mathbf{r}_s^0)}$$

to describe various space-symmetry-breaking situations, where $F_s(\mathbf{r}_1,\ldots,\mathbf{r}_s)$ is the usual s-particle distribution function. The conditional functions satisfy the equations

$$\frac{\rho F_{s+1}(\mathbf{r}_1|\mathbf{r}_1^0\ldots\mathbf{r}_s^0)}{z}=\exp\left\{-\beta\sum_{k=1}^{s}\Phi(\mathbf{r}_1-\mathbf{r}_k^0)\right.$$
$$+\sum_{k\geqslant 1}\frac{\rho^k}{k!}\int S_{k+1}(\mathbf{r}_1,\ldots,\mathbf{r}_{k+1})$$
$$\left.\times F_{s+1}(\mathbf{r}|\mathbf{r}_1^0\ldots\mathbf{r}_s^0)\ldots F_{s+1}\left(\mathbf{r}_{k+1}|\mathbf{r}_1^0\ldots\mathbf{r}_s^0\right)\mathrm{d}\mathbf{r}_2\ldots\mathrm{d}\mathbf{r}_{k+1}\right\},$$

where z is the activity, ρ is the density, $S_{k+1}(\mathbf{r}_1,\ldots,\mathbf{r}_{k+1})$ are irreducible Mayer diagrams, and $\beta = 1/k_B T$.

Using the fact that the symmetry-breaking analysis of a single-particle function yields the liquid–crystal transition, a fundamentally new approach to the theory of crystallization was proposed and developed [15–17], which later came to be known as the density functional method in crystallization theory. The essential point is that with this method, knowing the liquid direct correlation function alone, it is possible to

obtain the crystallization temperature and the volume change due to the transition and also to predict which type of lattice will result. It is mostly this method which is currently used in melting curve calculations and which has enabled, in particular, concrete calculations for a number of model systems, as well as melting curve calculations for molecular hydrogen [18] and, later, for fullerite [19].

In the 1990s, the melting theory of three-dimensional systems was extended to the case of two dimensions [20, 21]. The microscopic theory of two-dimensional melting depends to a large extent on the description of the orientational ordering of bonds in simple liquids (in terms of the violation of isotropy of the two-particle distribution function) and on the correct account of fluctuations. An important development here was the derivation of microscopic formulas for elastic and Frank moduli of two-dimensional systems and their application to constructing a theory of two-stage melting. Using this theory, it proved possible to determine potentials for which two-dimensional melting proceeds via two continuous transitions and those for which it occurs via a single first-order transition [22–27].

Closely related to the studies of two-dimensional melting was the 1990s research on the statistical mechanics of a system of vertices in a thin superconducting film. A microscopic approach developed within this research has, among other things, provided the description of the Kosterlitz–Thouless transition and also allowed the analysis of vortex–vortex interactions in a finite thickness thin film [30–36], whose results compared well with experiments on a niobium film in which a system of vortices passes through a hexatic phase occupying a large region of the H–T phase diagram (where H is an external magnetic field).

Soon after the first classical publications on the theory of spin glasses, its extension to a number of more complex systems was proposed by E E Tareyeva and her colleagues. In this way, a description of quadrupole glass in a mixture of para- and ortho-hydrogen was developed, in which — and this is a fundamental point — the order parameter increases smoothly and without a phase transition with decreasing temperature, as is indeed the case experimentally [37]. Another important, but later, development was a theory describing the transition to the orientational glass state in molecular para-hydrogen under pressure, when the system can be thought of as a mixture of $J = 0$ and $J = 2$ molecules [38]. The calculated results are in quantitative agreement with experiment. Interesting results, also in quantitative agreement with experiment, were obtained for orientational glass in fullerite. An example is the first theoretical calculations of the relative proportions of the P and H states for a wide range of temperatures and pressures [39].

The cluster-model description of the liquid–glass transition is yet another interesting application of spin-glass-theoretical methods. This description was made possible by showing, using the distribution function method, that the orientational interaction of cluster changes sign as a function of cluster size [40, 41].

Based on the above research into complex spin glass systems, and considering the results of a number of model studies (in particular, a detailed study of the Potts model [42–45]), it has proved possible, first, to establish a number of regularities (universality) in the behavior of glasses depending on the presence (or absence) of reflection symmetry and, second, to develop a consistent theory of non-Ising spin glasses.

Whereas first-order phase transitions in crystals as a function of external parameters is quite a mature field both experimentally and theoretically, the study of pressure- and temperature-induced phase transitions in disordered condensed matter, including liquids and amorphous solids, is still in its infancy. In the work by V N Ryzhov and S M Stishov [46, 47], a system with a purely repulsive potential of 'collapsing' hard spheres, i.e., a hard sphere potential with an added repulsive step, was used to model the liquid–liquid transition. The thermodynamic functions were calculated by the thermodynamic second-order perturbation theory in the step-height-to-temperature ratio; the zeroth order approximation was taken to be a system of solid spheres, whose properties were calculated in the Perkus–Yevick approximation. Note that this theory is analogous to the van der Waals theory for the liquid–gas transition. Using this theory, the thermodynamic functions of the system were calculated, including the free energy and isotherms. A major result was the discovery on low-temperature high-density isotherms of van der Waals loops corresponding to the liquid–liquid transition. Using the Maxwell rule, the liquid–liquid transition line was calculated, as was the friction coefficient between different liquid phases along it. The transition line was shown to terminate at a critical point. The isotherms obtained for the potential of 'collapsing' hard spheres characteristically intersect in the region of low densities — implying that the temperature extension coefficient becomes negative in a certain temperature–density range. Note that this anomalous behavior is characteristic of a number of liquids, including water. The transition line lies below the melting curve and can be observed only in the metastable region, as appears to be the case for a supercooled water. However, by varying the potential parameters, it is in principle possible to move the transition line to the stability region of the system. Melting curve calculations for the potential of 'collapsing' hard spheres using the Hansen–Verlet criterion show that in the neighborhood of the liquid–liquid transition line the melting curve in the pressure–temperature plane goes successively through a maximum and a minimum before becoming a straight line characteristic of the hard sphere potential. Note that adding an attractive term to the potential of 'collapsing' hard spheres leads, in a certain range of parameters, to the appearance of a second critical point, that of the liquid–gas transition [48].

Over more than 30 years, A F Barabanov's team at the IHHP's theoretical department has been investigating the highly topical subject of strongly correlated systems, including in particular systems with heavy fermions, mixed valency systems, manganites, magnetic semiconductors, and compounds that exhibit high-temperature superconductivity (HTSC) when doped. Because such compounds contain rather strongly localized f or d electrons, they fail to be described by conventional band theory, which is a one-particle approach, and their microscopic theory is as yet far from complete. The fundamental questions which still remain open concern current carriers and the magnetic subsystem (namely, their spectra and their mutual influence as a function of temperature); the number of carriers, and the dimensionality of the system; the nature of the normal state and the possible existence of the superconducting state; and the anomalous behavior of kinetic coefficients.

In the field discussed, new results have been obtained and new approaches developed. In particular, a diagrammatic technique was developed for the regular Anderson model

[49 – 51]. Calculations to high order in the hybridization interaction exactly revealed the presence of large logarithms $\ln(D/T)$ and $\ln(D/\varepsilon_f)$ in this model, where D is the conduction band width and ε_f is the position of a localized level with respect to the chemical potential. The developed technique allowed these logarithms to be taken into account in the analysis of phase transitions in mixed valency systems (in particular, in cerium under pressure) [51, 52]. Two further developments were the construction of RVB-type no-sublattice states for low-dimensional systems [53 – 55] and the study of the motion of carriers on an RVB sublattice (RVB standing for resonant valence bond).

The discovery of HTSC triggered the study of the spectrum of carriers in a two-dimensional $S = 1/2$ doped antiferromagnet, which provided the basis for the small-radius spin-polaron approach and for investigating the kinematic mechanism of superconducting pairing by taking into account strong correlation effects [55 – 57]. To correctly describe the spin subsystem, a self-consistent, spherically symmetric theory of a two-dimensional (2D) antiferromagnet was developed [58 – 60]. In particular, the damping of spin excitations was taken into account [61], enabling the analytical derivation of the scaling behavior of spin susceptibility for weakly doped cuprates [62],

$$\frac{\chi_{2D}(\omega, T)}{\chi_{2D}(\omega, T \to 0)} = f\left(\frac{\omega}{T}\right),$$

$$\chi_{2D}(\omega, T) = \int \mathrm{d}\mathbf{q}\ \mathrm{Im}\ \chi(\mathbf{q}, \omega, T)$$

$$f\left(\frac{\omega}{T}\right) = \pi\Theta\left[\left(\frac{\omega}{T}\right)^2 - \beta^2\right] + \arctan\left\{\frac{\alpha\omega/T}{\left[\beta^2 - (\omega/T)^2\right]}\right\},$$

and verifying the linear temperature behavior of the gap, $\Delta = \beta T$, and of the damping, $\gamma = \alpha T$.

The experimental data for the non-spin-wave (nonSW) behavior of magnetic susceptibility of cuprates in the superconducting state are reproduced using a spherically symmetric self-consistent approach within the framework of the frustrated Heisenberg model and introducing a polarization operator resonant with the superconducting state (scs) [63]:

$$\chi''_{\mathrm{scs}}(\mathbf{q}, \omega) = \frac{\Gamma F_{\mathbf{q}}}{Z^2 + \Gamma^2},$$

$$\Gamma = \gamma\omega + M''_{\mathrm{scs}}(\mathbf{q}, \omega) = \gamma\omega + \frac{\lambda\omega\Phi_{\mathbf{q}}}{(\omega^2 - \varepsilon^2)^2 + \lambda^2\omega^2},$$

$$Z = \omega^2 - \omega_{\mathbf{q}}^2 - M'_{\mathrm{scs}}(\mathbf{q}, \omega);$$

$$M'_{\mathrm{scs}}(\mathbf{q}, \omega) = \frac{\Phi_{\mathbf{q}}(\omega^2 - \varepsilon^2)}{(\omega^2 - \varepsilon^2)^2 + \lambda^2\omega^2}.$$

With this approach it proved possible to explain

(a) the appearance of a lower spin excitation branch (incommensurate peaks), which splits off from the resonance **Q** peak (the calculated resonance energy of 40 meV is close to the observed value);

(b) a marked decrease in the spectral weight in the neighborhood of the point ($\widetilde{q}_{x,\,\mathrm{nonSW}} \approx 0.065$ r.l.u., $\omega_0 \approx \varepsilon \approx 60 - 80$ meV), a neighborhood which corresponds to the experimentally observed 'dark region' located near point ($\widetilde{q}_x = \widetilde{q}_y \approx 0.1$ r.l.u., $\omega_0 \approx 50$ meV) (the abbreviation r.l.u. stands for reduced lattice unit, meaning that the vectors **q** are defined relative to the reduced lattice); and

(c) traces of the so-called 'silent band' lying in a narrow (in $\widetilde{q}_x$) region near $\widetilde{q}_{x,\,\mathrm{nonSW}}$: if, based on the positions of the maxima of $\chi''_{\mathrm{scs}}(\mathbf{q}, \omega)$ with respect to ω (at fixed **q**), we introduce an 'effective' spectrum $\widetilde{\omega}^+_{\mathrm{scs}}(\mathbf{q})$ for the upper branch, then, as q increases, the spectrum $\widetilde{\omega}^+_{\mathrm{scs}}(\mathbf{q})$ passes through an inflection point, and the intensity of the maxima of $\chi''_{\mathrm{scs}}[\mathbf{q}, \widetilde{\omega}^+_{\mathrm{scs}}(\mathbf{q})]$ will have a minimum.

Further, in the framework of various strongly correlated models (Emery, regular s-d, Hubbard), a theory of charge excitations was developed for a doped antiferromagnet taking into account the scattering of a spin polaron by spin fluctuations [64, 65]. The obtained results are simplest to understand for the regular s – d model with a Hamiltonian of the form

$$\widehat{H} = \widehat{h} + \widehat{J} + \widehat{I}, \quad \widehat{h} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^+_{\mathbf{k}\gamma} a_{\mathbf{k}\gamma},$$

$$\widehat{I} = \frac{1}{2} I(1-p) \sum_{\mathbf{R},\,\mathbf{g}} S^{\alpha}_{\mathbf{R}+\mathbf{g}} S^{\alpha}_{\mathbf{R}} + \frac{1}{2} Ip \sum_{\mathbf{R},\,\mathbf{d}} S^{\alpha}_{\mathbf{R}+\mathbf{d}} S^{\alpha}_{\mathbf{R}},$$

$$\widehat{J} = \frac{J}{\sqrt{N}} \sum_{\mathbf{k},\,\mathbf{q}} a^+_{\mathbf{k}+\mathbf{q},\,\gamma_1} S^{\alpha}_{\mathbf{q}} \hat{\sigma}^{\alpha}_{\gamma_1\gamma_2} a_{\mathbf{k}\gamma_2},$$

where $\widehat{h}$ describes bare Fermi carriers and contains the spectrum $\varepsilon_{\mathbf{k}}$ of bare holes; $\widehat{I}$ refers to the frustrated antiferromagnetic (AFM) interaction between spins $S = 1/2$; vectors **g** and **d** are for the first and second neighbors; $I_1 = (1-p)I$ and $I_2 = pI$ are the corresponding AFM interaction constants; and p $(0 \leqslant p \leqslant 1)$ is the frustration parameter.

The term $\widehat{J}$ in this expression describes the interaction of carriers with the subsystem of localized spins $\mathbf{S}_{\mathbf{R}}$, $\widehat{\sigma}^{\alpha}$ are the Pauli matrices, and repeated indices — both Cartesian α and spin-related γ_1, γ_2 — are summed over. For characteristic values of $J \simeq 0.1$ eV, the Hamiltonian $\widehat{J}$ is that of a bare hole strongly interacting with the spin subsystem.

A 'good' minimum to take as a site set is the following set of basic operators:

$$\varphi^{(1)}_{\mathbf{r}\sigma} = a_{\mathbf{r}\sigma}, \quad \varphi^{(2)}_{\mathbf{r}\sigma} = \left(\frac{3}{4}\right)^{-1/2} S^{\alpha}_{\mathbf{r}} \hat{\sigma}^{\alpha}_{\sigma\sigma_1} a_{\mathbf{r}\sigma_1},$$

$$\left\langle [\varphi^{(i)}_{\mathbf{r}\sigma}; \varphi^{(j)+}_{\mathbf{r}\sigma}]_+ \right\rangle = \delta_{i,j},$$

$$\langle \widehat{A} \rangle = \mathrm{Tr}\{\hat{\rho}^0 \widehat{A}\}, \quad \hat{\rho}^0 = Z_0^{-1} \exp\left(-\frac{\widehat{H}_0}{T}\right).$$

Here, $\varphi^{(1)}_{\mathbf{r}\sigma}$, $\varphi^{(2)}_{\mathbf{r}\sigma}$ provide a full set of local, single-hole spin-polaron operators, $\varphi^{(2)}_{\mathbf{r}\sigma}$ and $\varphi^{(1)}_{\mathbf{r}\sigma}$ being analogues of singlet and triplet one-site states, respectively. Even in the local operator basis, the bare band $\varepsilon_{\mathbf{k}}$ splits into two bands, the spectral weight of a bare hole in the lower band being strikingly different from unity. A further inclusion of spin polaron damping in the lower band permits the description of how a pseudogap develops close to the boundary of the magnetic Brillouin zone. The well-known kink structure of the spectral density and the closure of the pseudogap with increasing doping are also accounted for using this theory.

A kinetic equation derived by using the polaron approach and a many-moment solution method developed by accounting for the extremely anisotropic scattering of holes by spin fluctuations [66] have allowed the description of the anomalous kinetics (electrical resistance $\rho(T)$ and the Hall coefficient $R(T)$), providing a single framework for ade-

quately treating the dielectric regime, the low-doping regime, and the regime close to optimum doping. It has been shown [67] that the energies $E_{\mathbf{k}}^{(s)}$ and residues $Z_{\mathbf{k}}^{(s)}$ in the collision term

$$P_{ll_1}^{s,s_1} = J^2 \frac{1}{N^2} \sum_{\mathbf{k},\mathbf{q}} \left[F_l^s(\mathbf{k}) - F_l^s(\mathbf{k}+\mathbf{q})\right] \times \left[F_{l_1}^{s_1}(\mathbf{k}) - F_{l_1}^{s_1}(\mathbf{k}+\mathbf{q})\right] Z_{\mathbf{k}}^{(s)} Z_{\mathbf{k}+\mathbf{q}}^{(s_1)} \times n_{\mathrm{F}}(E_{\mathbf{k}}^{(s)}) \left[1 - n_{\mathrm{F}}\left(E_{\mathbf{k}+\mathbf{q}}^{(s_1)}\right) n_{\mathrm{B}}(E_{\mathbf{k}+\mathbf{q}}^{(s)} - E_{\mathbf{k}}^{(s_1)})\right] \times \chi''\left(\mathbf{q}, E_{\mathbf{k}+\mathbf{q}}^{(s_1)} - E_{\mathbf{k}}^{(s)}\right)$$

should be those of polaron bands. This provides an adequate description of the anomalous temperature dependence exhibited by the resistance and Hall effect in cuprates.

The observation over ten years ago of Bose–Einstein condensation in diluted metal vapor opened up new possibilities for the study of macroscopic quantum phenomena in degenerate systems. These systems, typically diluted and spatially inhomogeneous, usually consist of several tens of thousands of atoms gathered into a limited size cloud near a minimum of the external potential. The atoms involved are cooled by laser cooling followed by a partial evaporation from a trap. Because higher energy atoms evaporate at a higher rate, the evaporation causes the gas to cool, leading to temperatures of hundreds of nK and allowing the observation of Bose condensation.

The modern theoretical description of a dilute Bose gas in a trap has as its basis the famous 1947 work by N N Bogolyubov, in which it was shown that weak repulsion leads to a qualitative change in the excitation spectrum. The key point of Bogolyubov's approximation was the separation from the second-quantized boson annihilation operator ψ of its classical part, which describes the condensate. The Gross–Pitaevskii equation for a trapped Bose condensate is obtained by extending Bogolyubov's theory to the spatially nonuniform case. This equation looks like a nonlinear Schrödinger equation and is essentially classical even though it contains a quantum constant.

Many interesting new effects in the behavior of trapped Bose condensates show up in experiments on mixtures of supercooled gases. Some important aspects of such mixtures — namely, phase separation and vortical states in binary mixtures of condensates in the case of coincident and shifted trap centers; and the stability of the Bose system in a Bose–Fermi mixture with attraction between bosons and fermions — were studied by V N Ryzhov and E E Tareyeva and their coworkers [68–77]. The obtained results fit well the experimental data on condensate mixtures consisting of rubidium atoms in two spin states and on a mixture of boson atoms of rubidium and Fermi atoms of potassium.

For a Bose condensate with coincident traps and with two components corresponding to two spin states of the rubidium atom, the following results have been obtained [69, 70]. It has been shown that interaction between the condensates leads to phase separation and the formation of shells. Critical angular rotation velocities of the condensate have been obtained, the term critical meaning critical for the formation of stable vortical states. How this picture depends on particle concentration in the condensates has been examined. Further, for the same problem but with initially displaced trap centers [71, 72], (1) it was shown, in agreement with experiment, that the resulting center-of-mass displacement of the condensates is considerably larger due to the interaction between the condensates; and (2) vortex stability in the external and internal condensates was investigated as a function of trap potential minimum displacements along the rotation axis.

Although primarily of interest for creating degenerate (and possibly superconducting) Fermi systems, the behavior of the boson–fermion mixture is also of interest in itself. For example, because spin-polarized fermions do not interact in the s-wave approximation due to the Pauli principle, the evaporative cooling of a Fermi system can be effective due to indirect interaction (if any) with a fermion subsystem in a different spin state or, alternatively, due to interaction with the boson subsystem of the Fermi–Bose mixture.

V N Ryzhov and E E Tareyeva [73–77] derived an effective Hamiltonian for the Bose component in a fermion–boson system and analyzed the stability of this system for the case of attraction between bosons and fermions. Because the absence of the fermion–fermion interaction in the s-wave approximation makes the action quadratic in fermion operators, the exact integration over the Fermi fields can be performed formally, leading to an effective action which depends on the temperature and the number of fermions and which contains only boson fields. Using the quasiclassical Thomas–Fermi approximation, the effective action was obtained in an explicit form, which can be expanded in a series in the boson field. It is shown that interaction with fermions decreases the effective boson–boson interaction corresponding to the fourth-order expansion. If there is attraction between bosons and fermions, then the behavior of the system is determined by the negative sixth-order term in the boson field. In this case, by analogy with a system of attracting bosons, a variational principle with a Gaussian bosonic wave function can be used to estimate the energy of the system. The behavior of the system is determined by the competition between the positive kinetic energy of zero-point oscillations (which is due to the existence of the trap), the positive energy of the interboson repulsion, and the negative energy due to the sixth-order term in the boson field. As the number of fermions increases, the last term increases in magnitude, resulting in an increased density of bosons at the center of the trap. At a certain critical value of the number of bosons, the sum of the positive kinetic energy and the interboson repulsion energy is insufficient to stabilize the system, leading ultimately to the collapse of the boson component. The critical number of bosons depends on the number of fermions and the temperature. The results of the calculations were applied to a system consisting of fermionic ^{40}K atoms and bosonic ^{87}Rb atoms and gave good agreement with experiment. For the same system, the structure and stability of vortex states was investigated using the variational approach and the Thomas–Fermi approximation. It was shown that in the presence of a vortex more bosons are needed for the system to collapse. The dependence of the critical velocities for the formation of vortices on the number of bosons and fermions was examined. Using the numerical solution of the generalized Gross–Pitaevskii equation corresponding to the effective Hamiltonian, it was shown that the Thomas–Fermi approximation is highly accurate in describing the behavior and collapse of the system.

Further, based on the effective Hamiltonian for the boson subsystem in the mixture of harmonically trapped degenerate Bose and Fermi gases, the critical temperature displacement

of a Bose gas was calculated as a function of the number of bosons and fermions. It was shown that the presence of the Fermi component results in the displacement behaving differently from the case of a single interacting Bose gas in a trap: the dependence of the critical Bose condensation temperature T_C on the number of bosons N_B has a different curvature in the presence of the Fermi component [78].

To summarize, the fifty years of the Theoretical Department of the IHPP, RAS, were those of wide-ranging research in the most topical areas of condensed matter physics, whose results not only matched but indeed established the world level. On the other hand, the department staff is actively involved in teaching activities — one aspect of which is that a number of able young scientists have joined the staff after obtaining candidate or doctoral degrees. So, all in all, the department has every reason to be optimistic about its future.

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