III. CONDENSED MATTER THEORY

CONTENTS

LOW-ENERGY PHYSICS OF BCS HAMILTONIAN OF STRONGLY CORRELATED ELECTRONS

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The investigation of strongly correlated electron systems has been the central issue in solid state physics for more than four decades. The discovery of high-T_c superconductivity in copper-oxide based compounds (cuprates) revived interest in simple models displaying such strong correlations. Two much investigated models are the Hubbard model and its "descendant the t-J model. One of the main theoretical questions in that field is whether or not there is a superconducting phase in the t-J model [1]. Besides, the interplay between antiferromagnetism and superconductivity in the cuprates as well as their sensitivity to doping is still not very well understood.

An electron system is said to be strongly correlated if the leading energy scale in the problem is the on-site Coulomb repulsion energy. In this case, the low-energy sector of the underlying on-site Hilbert space should be modified to exclude a state occupied by two electrons. Such a modification results in an entirely new physics to account for the relevant low-energy excitations. Formally, strong correlations are encoded into the Gutzwiller-projected electron (Hubbard) operators, $X^{\sigma 0} = |\sigma\rangle\langle 0|$, where the electron spin projection $\sigma = \uparrow, \downarrow$, and vector $|0\rangle$ stands for a vacancy state. These operators act directly in the restricted Hilbert space as opposed to the conventional electron operators $c_\sigma^\dagger$ which describe the unconstrained system. In contrast with the conventional fermion operators, which generate the standard fermionic algebra, the Hubbard operators obey more complicated commutation/anticommutation relations and are closed into a superalgebra $su(2|1)$ [2].

The conventional Bardeen-Cooper-Schrieffer (BCS) Hamiltonian induced by phonon-electron interaction reads

$$H_{BCS} = -t \sum_{ij\sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + H.c. \right) + \Delta \sum_{ij} \left(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger + H.c. \right), \qquad (1)$$

where t and Δ are coupling constants and the summation is extended over nn lattice sites. It can easily be diagonalized in the momentum space, which results in the ground state represented by a phase-coherent condensate of Cooper pairs. On the other hand, in superconducting state induced by electron-electron interaction the formation of Cooper pairs must reflect strong electron correlations. As a result, the BCS effective Hamiltonian should be directly modified by the inclusion of the non-double occupancy (NDO) constraint to account for such an effect. The Gutzwiller-projected (or strongly correlated) BCS Hamiltonian then reads

$$H_{BCS}^G = -t \sum_{ij\sigma} \left(X_i^{\sigma 0} X_j^{0\sigma} + H.c. \right) + \Delta \sum_{ij} \left(X_i^{\uparrow 0} X_j^{\downarrow 0} - X_i^{\downarrow 0} X_j^{\uparrow 0} + H.c. \right). \qquad (2)$$

A few years back, Park discussed a close connection between the t-J model and the Gutzwiller-projected BCS Hamiltonian [3]. It was shown both numerically and analytically that the ground states of the t-J model at half filling (i.e. of the aniferromagnetic (AF) Heisenberg model) and of the strongly correlated BCS Hamiltonian are equivalent to each other. Moreover, at sufficiently small doping, there is numerical evidence of a strong overlap between those

two ground state wavefunctions, which provides further support for the existence of super-conductivity in the t-J model. Clearly, it is interesting to establish by analytical means such an equivalence at *nonzero* hole concentration. As is known, slightly away from half filling the long-range AF order is still observed in the cuprate superconductors. If the projected BCS Hamiltonian is indeed believed to contain close to half filling the low-energy physics of the t-J Hamiltonian, its ground state must also exhibit the AF order in the immediate vicinity of half filling.

However, an analytical treatment of strongly correlated BCS Hamiltonian (2) poses a sever technical problem. This Hamiltonian cannot be diagonalized either in a general case, or in the limiting cases of $t = 0$ or $\Delta = 0$. Due to the local NDO constraint the present problem is essentially at strong coupling. To derive a reliable approach, one should resolve the NDO constraint prior to any approximations.

This can explicitly be carried out within the $su(2|1)$ path-integral representation of the partition function. We employ this technique to derive the low-energy long-wavelength effective action for the lightly doped $2D$ projected BCS Hamiltonian (2) on a bipartite lattice. The action obtained is shown to be identical to that of the $2D$ quantum antiferromagnetic Heisenberg model explicitly represented by the classical $3D$ nonlinear σ-model [4]. In other words, close to half filling the ground state of the Gutzwiller-projected BCS Hamiltonian is antiferromagnetically ordered and non-superconducting. Since the conventional BCS Hamiltonian does not exhibit any magnetic ordering and always displays superconductivity, this result explicitly demonstrates that antiferromagnetism appears as a natural consequence of the strong Coulomb repulsion at low doped regimes. This result shows also that the ground state of the strong-pairing Gutzwiller-projected BCS Hamiltonian (2) can be considered as a reference state to a lightly doped Mott insulator. Technically, this is an important observation since it explicitly shows that the ordered magnetic state can evolve directly out of the strongly correlated spin-liuid phase.

On the other hand, at moderate doping the ground state of the Gutzwiller-projected BCS Hamiltonian becomes qualitatively similar to Anderson's resonating valence bond state which is known to fit nicely the properties of the t-J model in this regime. This indicates that the projected BCS Hamiltonian (2) captures the essential low-energy physics of the t-J model in the whole underdoped region [4].

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MOBILITY IN EPITAXIAL GaN: LIMITATION OF ELECTRON TRANSPORT DUE TO DISLOCATION WALLS

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It is well known that the extended defects of different types (mainly dislocations and dislocation substructures) frequently occur in thin semiconducting films and layers. In this context, the problem of their effect on carriers transport is of considerable present interest, both for theoretical and practical reasons [1].

Recently, these investigations have been stimulated additionally by the reason of new promising applications of GaN epitaxial films in optoelectronics [2, 3]. However, the performance of the devices based on GaN is limited by threading dislocations (exclusive of recently synthesized materials [4, 5]) with large densities 10^8-10^{11} cm^{-2}, which are the result from the large lattice mismatch between epilayer and substrate [6, 7, 8]. To improve the device characteristics, the effect of dislocations on the mobility should be studied.

To study the peculiarities in electron mobility at room temperature in application to GaN epitaxial films, we suggest a model based on the well-known Read approach [9, 10]. We explain the sharp mobility drop at some critical carrier density which, in turn, depends on the dislocation substructure [11, 12]. The total transverse mobility μ^* versus carrier density n is calculated when additional scattering due to electrostatic potential of a row of dislocations or a dislocation wall exists along with other mechanisms. The reason to consider dislocation walls is the fact found in most experiments that threading dislocations concentrate at subgrain boundaries lining up in row [11, 13]. In this picture, at some conditions (See discussion below) the mobility can be thermally activated because of the charged dislocation barriers present. The equation for the potential barriers is obtained here based on the model proposed in [14].

Let the wall of negatively charged dislocations be oriented along the y axis with the distance between them equal to D, and the lines of each dislocation are directed along the z axis. The negative charge in the dislocation line is compensated by a cylindrical positive space-charge region, with radius R around any dislocation. Thus, we have the periodically ordered cylinders with radius R. The Poisson equation in this case in the Schottky approximation can be written as

$$\frac{\partial^2 \phi(x,y)}{\partial x^2} + \frac{\partial^2 \phi(x,y)}{\partial y^2} = -\frac{e}{\epsilon\epsilon_0}\left[(N_d^+ - N_a^-)\theta(L(y) - |x|) - \frac{f\delta(x)}{c}\sum_{n=-\infty}^{\infty}\delta(y - nD)\right], \quad (1)$$

$$\theta(\xi) = \left\{\begin{array}{ll} 1, & \xi > 0 \\ 0, & \xi \le 0, \end{array}\right.$$

where N_d^+, N_a^- are the volume doping and unintentional acceptor densities, respectively. $D = b/2\sin\frac{\alpha}{2}$, b is the absolute value of the Burgers vector, f is the fraction of sites of dislocation that are occupied, ϵ is the dielectric constant, $L(y) = \sqrt{R^2 - y^2}$ is a periodic function along the y axis which is the screening length where the potential $\phi(x,y)$ is not equal to zero (by definition, $\phi(x,y) = 0$ when $|x| \ge L(y)$). Notice that $\phi(x,y)$ is an even function on y with the period D, and can be represented as a Fourier series

$$\phi(x,y) = \phi_0(x) + \sum_{n=1}^{\infty}\phi_n(x)\cos(\frac{2\pi ny}{D}), \quad (2)$$

where the explicit form of the expansion coefficients in Eq.(2) can be found in [15].
The barrier-limited mobility, generally, takes the form [16]

$$\mu_{GB} = \left(\frac{eL}{\sqrt{8kT\pi m^*}}\right) \exp\big(-V(0, y = R)/kT\big), \qquad (3)$$

where e is the absolute value of the electron charge, m^* its effective mass, k is the Boltzmann constant, T is the temperature, L is the average grain size, and $V(0, y = R) = -e\phi(0, y = R)$ is the value of the two-dimensional potential barrier caused by charged dislocations at $x = 0$. Notice that the potential $V(0, y = R)$ has quite a simple form when $2R \approx D$ [14]

$$V(0, y = D/2) = -e\phi(0, y = D/2) = \frac{4e^2(N_d^+ - N_a^-)R^3}{3\epsilon_0\epsilon D} - \frac{e^2 f}{2c\pi\epsilon_0\epsilon}\ln 2. \qquad (4)$$
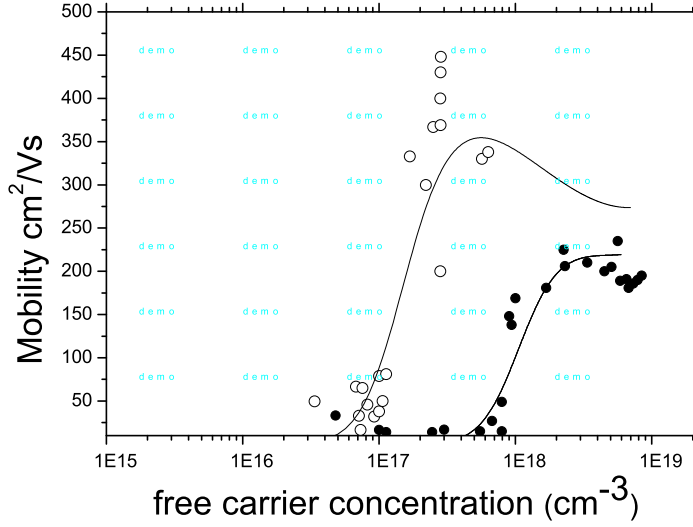

Figure 1: Room temperature mobility vs free carrier concentration for two samples with $N_{dis} = 5 \times 10^9 \text{cm}^{-2}$ (open circles), $N_{dis} = 2 \times 10^{10} \text{cm}^{-2}$ (closed circles) from Ref. [12]. Solids lines are theoretical curves. A set of the model parameters used in calculations: (open circles) $f = 0.05$, $D = 1000\text{Å}$, compensation ratio equal to 0.3, $L = 30000\text{Å}$; (closed circles) $f = 0.05$, $D = 900\text{Å}$, compensation ratio equal to 0.4, $L = 30000\text{Å}$. Other parameters are taken from Ref. [18]

Thus, the total effective mobility takes the form [16, 17]

$$\frac{1}{\mu^*} = \frac{1}{\mu_1} + \frac{1}{\mu_{GB}}, \qquad (5)$$

where μ_1 is the mobility caused by different mechanisms of scattering in GaN films except charged dislocation walls. We have used the explicit form for μ_1 and the main parameters for GaN from [18]. Using the proposed here model, we are able to reproduce quantitatively the drop of the mobility μ^* at some critical meanings of carrier density, as one can see from Figure 1. The sharp transition to the low mobility regime is caused by the domination of μ_{GB} as n falls.

The nature of this domination is the rise of the potential barrier as the dopant density decreases, since $V(0, y = R)$ is a function of the ratio $2R/D$, while $R \sim 1/\sqrt{N_d^+ - N_a^-}$. As

the result, μ_{GB} decreases as $n = N_d^+ - N_a^- - n_t$ decreases ($\mu_1 \gg \mu_{GB}$), and from Eq.(9) we have $\mu^* \simeq \mu_{GB}$. Since the doping level increases, the bulk single-crystal mobility starts to dominate. Also, at fixed $2R$, $V(0, y = R)$ will be greater for smaller D (increase of the local dislocation density in the dislocation wall). This explains the correlation between the position of the minimum of n and the dislocation density. However, the model does not allow to reproduce the rise of the mobility below the minimum ($2R/D > 1$). Most likely, this increase can be explained in the framework of the percolation theory [16, 19].

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DROPLET SHAPE WITHIN THE SPHERICAL MODEL OF LATTICE GAS

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Substances in the liquid state tend to form droplets. On the phenomenological level, the description of their shapes reduces to minimization of surface tension (the Wulff functional). However, in order to solve this problem from first principles (starting from a microscopic description of a macroscopic system), one has to overcome several fundamentally difficult obstacles. The first one is connected with the fact that in translation invariant systems the spatial location of the droplet is not fixed, and hence the natural state of the system under investigation is mixed (not pure). Average values of microscopic variables in a state like this inherit translation invariance of the Hamiltonian and, therefore, do not reveal the droplet shape. On the other hand, experimental observations are described by pure states.
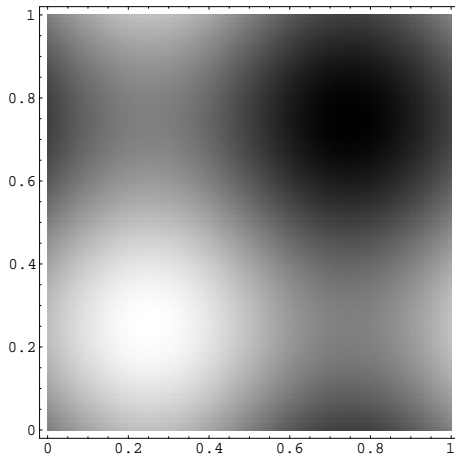

Figure 1: The shape of the maximally symmetric droplet.

One can try to single out pure states with the help of quasi-averages, but in doing so we encounter the second obstacle one has to overcome. Quasi-averaging proved to be quite an efficient tool for calculating observable values of intensive quantities, like density or magnetization. However, when it comes to surface properties, the situation becomes more complicated. An arbitrarily weak external field (of magnitude ε) deforms droplets unrecognisably and, therefore, is not helpful for finding such delicate characteristics as a droplet shape. Fortunately, there exists a more potent version of quasi-averaging, where the magnitude of external field tends to zero in the thermodynamic limit (as $\varepsilon n^{-\delta}$), see [1]. It turns out that if the field is switched off sufficiently fast, the obtained density profiles do not depend on the field magnitude ε and the switching-off exponent δ, and hence these profiles describe the true droplet shapes.

In paper [3], the shape of droplets of condensed matter is investigated within the spherical model of a lattice gas, see [2, 4], defined on a square lattice Z^d. The Hamiltonian of the model is given by

$$H_n = -J \sum_{j,k \in V_n} T_{jk} x_j x_k - \sum_{j \in V_n} h_j x_j,$$

where $J > 0$, and T_{jk} are the elements of the nearest-neighbour interaction matrix. In order to obtain a model with a physically sensible low-temperature phase, one can impose the so-called spherical constraint, $\sum_{j \in V_n} x_j^2 = n^d$. Finally, in order to prevent one of the thermodynamically stable phases filling the entire available volume V_n, we have to impose the density constraint $\sum_{j \in V_n} x_j = \rho n^d$.

It is shown in [3] that the droplet boundary within the spherical model is always diffuse, as opposed to sharp, and the corresponding density profiles (droplet shapes) can be described by exact formulae. The 2D slice of the maximally symmetric droplet is shown in Fig. 1.

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MICROSCOPIC THEORY OF SPIN-EXCITATION SPECTRUM IN SUPERCONDUCTING CUPRATES

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1. General theory

To describe spin excitations in strongly correlated electronic systems, such as superconducting cuprates [4], the t–J model is commonly used. It can be written as

$$
H \;=\; -\sum_{i\neq j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \mu \sum_{i\sigma} X_i^{\sigma\sigma} + \frac{1}{4}\sum_{i\neq j,\sigma} J_{ij}\left(X_i^{\sigma\bar\sigma} X_j^{\bar\sigma\sigma} - X_i^{\sigma\sigma} X_j^{\bar\sigma\bar\sigma}\right), \tag{1}
$$

where t_{ij} is the hopping integral and J_{ij} is the exchange interaction. The Hubbard operators $X_i^{\alpha\beta} = |i,\alpha\rangle\langle i,\beta|$ describe transitions between three possible states at a site i on a square lattice: an empty (hole) state $|i,0\rangle$ and a singly occupied state $|i,\sigma\rangle$ with spin $\sigma = \pm(1/2)$, ($\bar\sigma = -\sigma$). The number and spin operators are given by: $N_i = \sum_\sigma X_i^{\sigma\sigma}, S_i^\sigma = X_i^{\sigma\bar\sigma}, S_i^z = \sum_\sigma \sigma X_i^{\sigma\sigma}$. The chemical potential μ is determined from the equation for the average electron density $n = \langle N_i\rangle = 1 - \delta$, where $\delta = \langle X_i^{00}\rangle$ is the hole concentration.

Applying the Mori-type projection technique, an exact representation of DSS in terms of the transverse spin-density operators $S_{\mathbf{q}}^\pm = S_{\mathbf{q}}^x \pm i S_{\mathbf{q}}^y$ was derived [1],

$$
\chi(\mathbf{q},\omega) = -\langle\langle S_{\mathbf{q}}^+ | S_{-\mathbf{q}}^-\rangle\rangle_\omega = \frac{m(\mathbf{q})}{\omega_{\mathbf{q}}^2 + \omega\,\Sigma(\mathbf{q},\omega) - \omega^2}, \tag{2}
$$

where $m(\mathbf{q}) = \langle [i\dot S_{\mathbf{q}}^+, S_{-\mathbf{q}}^-]\rangle = \langle [\,[S_{\mathbf{q}}^+, H],\, S_{-\mathbf{q}}^-]\rangle$, and $\omega_{\mathbf{q}}$ is the spin-excitation spectrum in a generalized mean-field approximation (MFA). The self-energy is given by the many-particle Kubo-Mori relaxation function

$$
\Sigma(\mathbf{q},\omega) = [1/m(\mathbf{q})]\,(\!(-\ddot S_{\mathbf{q}}^+\,|\,-\ddot S_{-\mathbf{q}}^-)\!)_\omega^{(\mathrm{proper})}, \tag{3}
$$

where $-\ddot S_{\mathbf{q}}^\pm = [\,[S_{\mathbf{q}}^\pm, H],\, H]$. The Kubo-Mori relaxation function is defined as

$$
(\!(A|B)\!)_\omega = -i\int_0^\infty dt\, e^{i\omega t}(A(t), B), \quad (A(t), B) = \int_0^\beta d\lambda\langle A(t - i\lambda)B\rangle, \tag{4}
$$

where $\beta = 1/k_{\mathrm{B}}T$. The "proper" part of the relaxation function (3) does not contain parts connected by a single-particle relaxation function which corresponds to the projected time evolution in the original Mori projection technique. The spin-excitation spectrum is given by the imaginary part of DSS $\chi''(\mathbf{q},\omega)$ in (2). The static susceptibility in (2) is defined by the equation $\chi_{\mathbf{q}} = \chi(\mathbf{q},0) = m(\mathbf{q})/\omega_{\mathbf{q}}^2$. The spin-excitation spectrum $\omega_{\mathbf{q}}$ was calculated from the equality $m(\mathbf{q}) = (-\ddot S_{\mathbf{q}}^+, S_{-\mathbf{q}}^-) = \omega_{\mathbf{q}}^2\,(S_{\mathbf{q}}^+, S_{-\mathbf{q}}^-)$, where the correlation function $(-\ddot S_{\mathbf{q}}^+, S_{-\mathbf{q}}^-)$ was evaluated in the mode-coupling approximation (MCA).

The self-energy (3) is defined in terms of the operators $-\ddot S_i^\pm = [[S_i^\pm, (H_t + H_J)], (H_t + H_J)] \equiv \sum_\alpha F_i^\alpha$ ($\alpha = tt, tJ, Jt, JJ$), where H_t and H_J are the hopping and the exchange parts of

the Hamiltonian (1). There are 16 contributions of type $((F_{\mathbf{q}}^{\alpha} | F_{-\mathbf{q}}^{\gamma}))_{\omega}$. As calculations show, at a finite hole doping $\delta > 0.05$ the largest contribution to the self-energy (3) is given by the term $\Sigma_t(\mathbf{q}, \omega) = ((F_{\mathbf{q}}^{tt} | F_{-\mathbf{q}}^{tt}))_{\omega}$ coming from the spin-electron scattering [2],

$$
F_i^{tt} = \sum_{j,n} t_{ij} \left\{ t_{jn} \left[H_{ijn}^- + H_{nji}^+ \right] - t_{in} \left[H_{jin}^- + H_{nij}^+ \right] \right\}, \tag{5}
$$

where $H_{ijn}^{\sigma} = X_i^{\sigma 0} S_j^+ X_n^{0\sigma} + X_i^{+0}(1 - N_j/2)X_n^{0-}$. We calculate the self-energy in the MCA assuming independent propagation of electronic ($X_i^{\sigma 0}$) and bosonic (S_j^+, N_j) excitations at different lattice sites in (5). This results in the decoupling of the time-dependent many-particle correlation function into a product of the corresponding single-particle functions:

$$
\langle X_{\mathbf{q}3}^{\sigma 0} S_{-\mathbf{q}2}^- X_{\mathbf{q}1}^{0\sigma} | X_{\mathbf{q}1}^{\sigma 0}(t) S_{\mathbf{q}2}^+(t) X_{\mathbf{q}3}^{0\sigma}(t) \rangle = \langle X_{\mathbf{q}1}^{0\sigma} X_{\mathbf{q}1}^{\sigma 0}(t) \rangle \langle S_{-\mathbf{q}2}^- S_{\mathbf{q}2}^+(t) \rangle \langle X_{\mathbf{q}3}^{\sigma 0} X_{\mathbf{q}3}^{0\sigma}(t) \rangle. \tag{6}
$$

Using the MCA and the MFA for the corresponding single-particle correlation function in (6) the imaginary part of the self-energy can be written as [3]

$$
\Sigma_t''(\mathbf{q}, \omega) = \frac{\pi(2t)^4}{\omega m(\mathbf{q})} \frac{Q^2}{N^2} \sum_{\mathbf{q}_1, \mathbf{q}_2} \sum_{\omega_1 = \pm E_{\mathbf{q}_1}} \sum_{\omega_2 = \pm \widetilde{\omega}_{\mathbf{q}_2}} \sum_{\omega_3 = \pm E_{\mathbf{q}_3}} \frac{m(\mathbf{q}_2)}{8\omega_1\omega_2\omega_3} \tag{7}
$$
$$
[N(\omega_2)n(-\omega_1)n(\omega_3) + N(-\omega_2)n(\omega_1)n(-\omega_3)]\delta(\omega + \omega_1 - \omega_2 - \omega_3)
$$
$$
[(\Lambda_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}^2 + \Lambda_{\mathbf{q}_3,\mathbf{q}_2,\mathbf{q}_1}^2)(\omega_1 + \varepsilon_{\mathbf{q}_1})(\omega_3 + \varepsilon_{\mathbf{q}_3}) - 2\Lambda_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}\Lambda_{\mathbf{q}_3,\mathbf{q}_2,\mathbf{q}_1}\Delta_{\mathbf{q}_1}\Delta_{\mathbf{q}_3}],
$$

where the vertex function is defined by $\Lambda_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = 4(\gamma_{\mathbf{q}_3+\mathbf{q}_2} - \gamma_{\mathbf{q}_1})\gamma_{q_3} + \gamma_{\mathbf{q}_2} - \gamma_{\mathbf{q}_1+\mathbf{q}_3}$, $\gamma_{\mathbf{q}} = 1/2(\cos q_x + \cos q_y)$ with $\mathbf{q}_3 = \mathbf{q} - \mathbf{q}_1 - \mathbf{q}_2$. In the electron spectrum $\varepsilon_{\mathbf{q}}$ we take into account only the nearest-neighbor hopping t and consider the energy dispersion in the Hubbard-I approximation: $\varepsilon_{\mathbf{q}} = -4t Q \gamma_{\mathbf{q}} - \mu$ where $Q = 1 - n/2$ is the Hubbard weighting factor. We consider here the superconducting state, where the spectrum of quasiparticles is given by the conventional formula $E_{\mathbf{q}} = \sqrt{\varepsilon_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2}$, where $\Delta_{\mathbf{q}}$ is the superconducting gap function. The Fermi and Bose functions are denoted by $n(\omega) = (e^{\beta\omega} + 1)^{-1}$ and $N(\omega) = (e^{\beta\omega} - 1)^{-1}$. It should be emphasized that the self-energy (7) is determined by the decay of spin excitation with the energy ω and wave vector $\mathbf{q}$ into three excitations: a particle-hole pair and spin excitation. This process is controlled by the energy and momentum conservation laws, $\omega = (\omega_3 - \omega_1) + \omega_2$ and $\mathbf{q} = \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3$, respectively. In the previous studies of the t-J model the self-energy was considered in a particle-hole bubble approximation, where the contribution of additional spin excitation was neglected or approximated by the static or mean-field-type expressions (see, e.g., [5]). This approximation resulted in the random-phase-type approximation for DSS. It is possible to derive the particle-hole bubble approximation from Eq. (7) by ignoring the spin-energy contribution ω_2 in comparison with the electron-hole pair energy $(\omega_3 - \omega_1)$ and excluding the spin-excitation wave-vector $\mathbf{q}_2$ from the wave-vector conservation law: $\mathbf{q} = \mathbf{q}_1 + \mathbf{q}_3$. In this approximation, a different behavior of the spin-excitation spectrum is observed in comparison with the results obtained for the full self-energy (7) [3].

2. Results and discussion

2.1. Static magnetic properties [2]. The spectrum of spin excitation and the static susceptibility were calculated by solving self-consistently the system of equations for the spectrum $\omega_{\mathbf{q}}$ and the static correlation function $C_{\mathbf{q}} = \langle S_{\mathbf{q}}^+ S_{-\mathbf{q}}^- \rangle = (m(\mathbf{q})/2\omega_{\mathbf{q}}) \coth(\beta \omega_{\mathbf{q}}/2)$
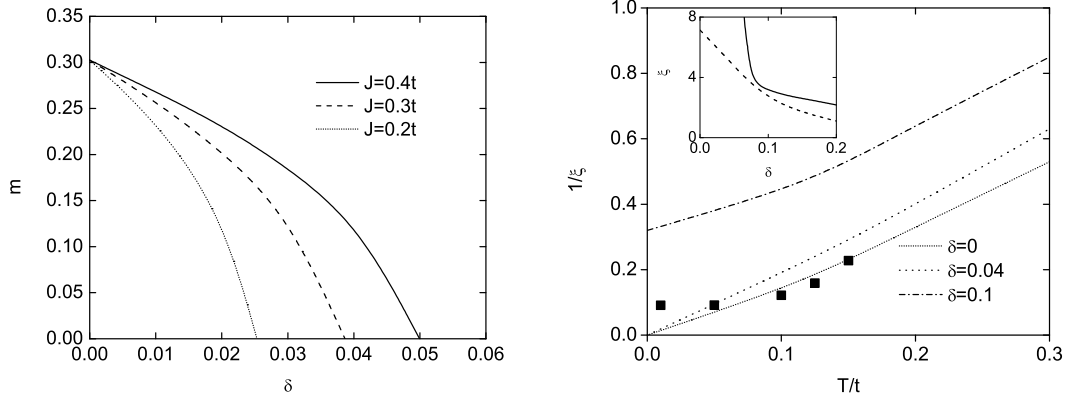
Figure 1: Left panel: Staggered magnetization $m(\delta)$ for different values of J/t. Right panel: Inverse AF correlation length $1/\xi(T)$ for different doping and neutron-scattering data (symbols). The inset exhibits $\xi(\delta)$ at $T = 0$ (solid line) and $T = 0.1t$ (dashed line).

which defines the spectrum. At zero temperature, $T = 0$, a long-range antiferromagnetic (AF) order (LRO) can emerge which manifests itself in the divergency of static susceptibility $\chi_{\mathbf{q}} = m(\mathbf{q})/\omega_{\mathbf{q}}^2$ at the AF wave vector $\mathbf{Q} = \pi(1,1)$ for a two-dimensional lattice, $\omega_{\mathbf{Q}} \to \infty$. The staggered magnetization $m^2 = 3C/2$, defined by the constant term in the pair spin-correlation function, $C_{\mathbf{R}} = (1/N)\sum_{\mathbf{q} \neq \mathbf{Q}} C_{\mathbf{q}}\exp(i\mathbf{q}\mathbf{R}) + C\exp(i\mathbf{Q}\mathbf{R})$, at zero temperature is plotted in Fig. 1 (left panel). We obtain strong suppression of LRO with increasing doping δ due to the spin-hole interaction. Above the critical doping $\delta > \delta_c$ LRO disappears. It is remarkable that δ_c is nearly proportional to J/t.

Figure 1 (right panel) shows the inverse correlation length $\xi^{-1}(T, \delta)$ at $J/t = 0.4$. At zero doping, $\xi^{-1}(T)$ exhibits the known exponential decrease as $T \to 0$. For $\delta > \delta_c$ we obtain finite values of ξ as $T \to 0$ corresponding to the vanishing LRO. The reasonable agreement with the neutron-scattering experiments on $La_{1.96}Sr_{0.04}CuO_4$ shown by symbols is obtained [6]. Concerning the doping dependence of $\xi(\delta, T)$ depicted in the inset of Fig. 1 (right panel), it can be described approximately by the proportionality $\xi(\delta, T) \propto 1/\sqrt{\delta}$ (dashed line, holding, at $T = 0$, for $\delta \geq 0.1$) which agrees with the experimental findings [6].

2.2. Spin dynamics in the normal state [2].

The spectrum of spin excitations $\omega_{\mathbf{q}}$ and the damping $\Gamma_{\mathbf{q}} = -(1/2)\Sigma''(\mathbf{q}, \omega_{\mathbf{q}})$ were calculated by using the equation for the imaginary part of the self-energy in the normal state $\Sigma_t''(\mathbf{q}, \omega)$ (7) with $\Delta_{\mathbf{q}} = 0$ and a similar expression for the self-energy $\Sigma_J''(\mathbf{q}, \omega)$ caused by the exchange interaction, $F^J = [[S_i^{\pm}, H_J], H_J]$. In the Heisenberg limit at $\delta = 0$ the spectrum of spin excitations and the damping $\Gamma_{J,\mathbf{q}}$ is shown in Fig. 2 (left panel). In the spin-wave region, at $q\xi \gg 1$, we get well-defined quasiparticles with $\Gamma_{\mathbf{q}} \ll \omega_{\mathbf{q}}$, as usually observed for the Heisenberg model. However, for nonzero doping the spin-hole scattering contribution $\Sigma_t''(\mathbf{q}, \omega)$ (7) increases rapidly with doping and temperature and already at moderate hole concentration far exceeds the spin-spin scattering contribution $\Sigma_J''(\mathbf{q}, \omega)$, as demonstrated in Fig. 2 (right panel). We conclude that depending on $\mathbf{q}$, doping and temperature, the spin excitations may have a different character and dynamics. At low enough doping and low temperatures, i.e., at small enough $\Gamma_{t,\mathbf{q}}$, well-defined high-energy spin-wave-like excitations propagating in the AF short-range order background are observed, while a crossover to diffusive-type spin excitations occurred for higher doping and temperatures in accordance with neutron-scattering experiments.
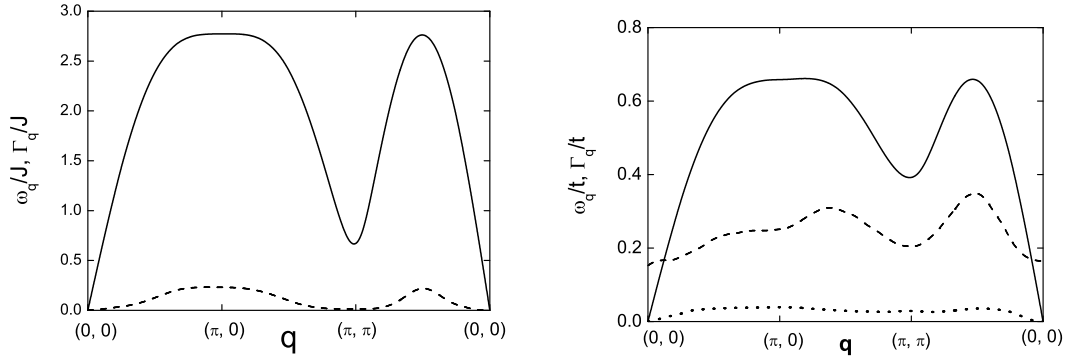
Figure 2: Left panel: Spectrum $\omega_{\mathbf{q}}$ (solid line) and damping $\Gamma_{\mathbf{q}}$ (dashed line) in the Heisenberg limit, $\delta = 0$, at $T = 0.35J$. Right panel: Spectrum $\omega_{\mathbf{q}}$ (solid line), and damping $\Gamma_{J,\mathbf{q}}$ (dotted line) and $\Gamma_{t,\mathbf{q}}$ (dashed line) at $T = 0.15t$ and $\delta = 0.1$.
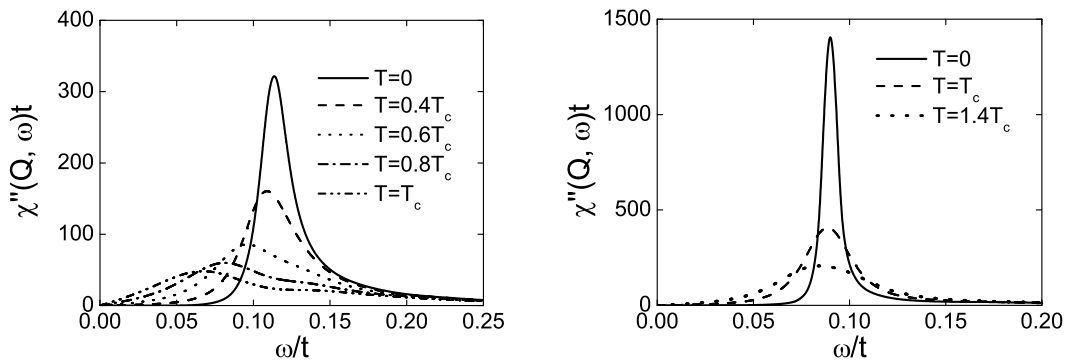

Figure 3: Temperature dependence of the spectral function $\chi''(\mathbf{Q}, \omega)$ at $\delta = 0.2$ (left panel) and at $\delta = 0.09$ (right panel).

2.3. Spin dynamics in the superconducting state [3]. In the superconducting state the spin-excitation spectrum of high-T_{c} cuprates is dominated by a sharp magnetic peak at the planar AF wave vector $\mathbf{Q}$ which is called *the resonance mode* (RM). It was discovered in the inelastic neutron scattering (INS) experiments which revealed a suppression of the spectral weight of low-energy spin excitations at low temperatures and its transfer to higher energies resulting in RM. Experimentally, the RM energy E_{r} decreases with underdoping following the superconducting transition temperature, $E_{\mathrm{r}} \simeq 5.3k_{\mathrm{B}}T_{\mathrm{c}}$, but only weakly depends on temperature. In many publications the RM phenomenon was explained by the opening of the energy gap $2\Delta_{\mathbf{q}}$ in the particle-hole excitations below T_{c}, which results in appearance of a bound state (spin-exciton) at the spin energy $E_{\mathrm{r}} < 2\Delta_{\mathbf{q}}$. However, in this scenario a strong temperature dependence of RM should be observed driven by $2\Delta(T)$ which has not been found in INS experiments.

To explain the appearance of RM above T_{c} and its weak temperature dependence, we have developed a microscopic theory of RM in [3] by generalizing our approach in [2] to the superconducting state. The temperature and doping dependence of the spectral function $\chi''(\mathbf{Q}, \omega)$ were calculated using the self-energy (7) for the d-wave gap function $\Delta_{\mathbf{q}} = (\Delta/2)(\cos q_x - \cos q_y)$. The DSS reveals RM at low temperatures due to a strong suppression of the damping of spin excitations. This is explained by the involvement of spin excitations in the decay process, as discussed above, besides the particle-hole continuum

usually considered in the bubble-type approximation (see, e.g., [5]). The spin gap in the spin-excitation spectrum at $\mathbf{Q}$ (see Fig. 2) plays a dominant role in limiting the decay of RM in comparison with the superconducting gap which results in the observation of RM even above T_c in the underdoped region. So as compared with the spin-exciton scenario based on the buble-type approximation, we propose an alternative explanation of RM which is driven by the spin gap at $\mathbf{Q}$ instead of the superconducting gap 2Δ.

The temperature dependence of the spectral function in the overdoped case $\delta = 0.2$ is shown in Fig. 3 (left panel). It has high intensity at low temperatures, but strongly decreases with temperature and becomes very broad at $T \sim T_\mathrm{c}$, as found in experiments. In Fig. 3 (right panel), the temperature dependence of the spectral function for the underdoped case $\delta = 0.09$ is plotted, whereas the resonance energy decreases with underdoping and the intensity of the RM greatly increases in accordance with experiments. The RM energy weakly depends on temperature and is still quite visible even at $T = 1.4T_\mathrm{c}$. Good agreement of our results for the temperature and doping dependence of the spin-excitation spectrum and RM with INS experiments provides a strong support for the proposed theory (for details see [3]).

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MULTI-PARTICLE SPACE-TIME TRANSITIONS IN THE TOTALLY ASYMMETRIC SIMPLE EXCLUSION PROCESS

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Recently, the totally asymmetric simple exclusion process (TASEP) was a subject of numerous investigations [1, 2]. In particular, several exact results about time dependent transition probabilities were obtained for the TASEP on the infinite lattice. Among them, there are determinant formulas for the Green functions, i.e. transition probabilities between particle configurations at different time moments, which were obtained first in [3] for continuous time TASEP and then generalized to discrete time dynamics [4, 5] and to the ring geometry [6, 7]. The next advance is calculation of correlation functions which are the transition probabilities for several tagged particles, while the positions of the others are integrated out. The first result was a distribution of the position of N-th particle at arbitrary time for the TASEP with parallel update and step initial conditions, [8]. It was generalized later to the backward sequential update, [4], and extended to flat initial conditions in [9]. The way to the multi-particle distributions was discovered in [10]. Then, extensive studies were undertaken of the distributions of positions of tagged particles at given time, [11, 12], and of particles on the space-like paths, [13]. The aim of present contribution is to extend the range of available multi-particle distributions. Specifically, we consider the TASEP with backward sequential update and step initial conditions, and obtain the joint distribution of times taken by selected particles to travel given distance.

Consider N particles on the one-dimensional integer lattice. A configuration of the system $\boldsymbol{x}$ takes its values in the set of strictly increasing integers $x_1 > x_2 > \cdots > x_N$. The TASEP is a random process which is given as a sequence of configurations $\boldsymbol{x}^0, \boldsymbol{x}^1, \ldots, \boldsymbol{x}^t$. We refer to such a sequence as a trajectory of the system up to time t. Every trajectory is realized with probability

$$P(\boldsymbol{x}^0, \ldots, \boldsymbol{x}^t) = P_1(\boldsymbol{x}^t | \boldsymbol{x}^{t-1}) \ldots P_1(\boldsymbol{x}^2 | \boldsymbol{x}^1) P_1(\boldsymbol{x}^1 | \boldsymbol{x}^0) P_0(\boldsymbol{x}^0), \tag{1}$$

where $P_0(\boldsymbol{x})$ is the initial probability of configuration $\boldsymbol{x}$. The one-step transition probability $P_1(\boldsymbol{x}|\boldsymbol{y})$ from configuration $\boldsymbol{y}$ to $\boldsymbol{x}$ takes the form

$$P_1(\boldsymbol{x}|\boldsymbol{y}) = \prod_{i=1}^{N} \theta \left(x_i - y_i, x_{i-1} - y_i \right), \tag{2}$$

where $\theta\left(k, l\right) = (q + p\delta_{l,1})\delta_{k,0} + p\delta_{k,1}$, and we formally define $x_0 = \infty$. The parameter p, the hopping probability, varies in the range $0 < p < 1$ and we define $q = 1 - p$.

Consider the probability for the system to be in a configuration $\boldsymbol{x}$ after t time steps, $t \geq 0$,

$$G_t(\boldsymbol{x}|\boldsymbol{y}) = \sum_{\{\boldsymbol{x}^0, \boldsymbol{x}^1, \ldots, \boldsymbol{x}^{t-1}\}} P(\boldsymbol{x}^0, \ldots, \boldsymbol{x}^t), \tag{3}$$

given $P_0(\boldsymbol{x}^0) = \delta_{\boldsymbol{y}, \boldsymbol{x}^0}$.

Proposition 0.1 *The GF has the determinantal form*

$$G_t(\boldsymbol{x}|\boldsymbol{y}) = \det[F_{j-i}(x_i - y_j, t)]_{i,j=1,\ldots,N}, \tag{4}$$

where

$$F_n(x,t) = \begin{cases} \frac{1}{2\pi i} \oint_{\Gamma_0} \frac{dw}{w} \left(q + \frac{p}{w}\right)^t (1-w)^{-n} w^x, & t \geq 0 \\ 0, & t < 0 \end{cases},$$ (5)

and the integration contour Γ_0 encircles the origin, while the point w=1 stays outside.

In present work we consider the TASEP at space-time points associated with different moments of time. To this end, we introduce a generalized Green function (GGF), [14]

Proposition 0.2 *Given two admissible N-point configurations $(\boldsymbol{x}, \boldsymbol{t})$ and $(\boldsymbol{x_0}, \boldsymbol{t_0})$, such that $t_i > t_i^0$ for $i = 1, \ldots, N$, the GGF can be expressed in the determinantal form:*

$$G\left((\boldsymbol{x}, \boldsymbol{t})|(\boldsymbol{x_0}, \boldsymbol{t_0})\right) = \det[F_{j-i}(x_i - x_j^0, t_i - t_j^0)]_{i,j=1,\ldots,N},$$ (6)

where $F_n(x,t)$ is defined in (5).

Consider N particles starting at the same moment of time $t = 0$ at positions separated by unit intervals, $x_i^0 = 1 - i$. Our aim is to have the joint distribution

$$\mathbf{P} = Prob\left(\{t_{n_1} \leq a_1\} \bigcap \{t_{n_2} \leq a_2\} \bigcap \cdots \bigcap \{t_{n_m} \leq a_m\}\right)$$ (7)

of times $t_{n_1}, \ldots, t_{n_m}$, when $m \leq N$ particles labeled by indices $n_1 < n_2 < \cdots < n_m$ jump off positions $x_{n_1}, \ldots x_{n_m}$ taken from an array $x_i = x + N - i, i = 1, \ldots, N$ and $t_{n_1} \leq t_{n_2} \leq \cdots \leq t_{n_m}$.

Consider a set of the N-paths consisting of N paths starting at the positions $(x - i + N, 0)$ and conditioned to make a step from $(x - i + N, t_i)$ to $(x - i + N + 1, t_i + 1)$, for $i = 1, \ldots, N$ respectively. The probability of a particular set $t_1, \ldots, t_N$ is given by GGF $G((\boldsymbol{x}, \boldsymbol{t})|(\boldsymbol{x^0}, \boldsymbol{t^0})$ multiplied by the last step probability p^N. The probability of interest (7) is a marginal of this N particle probability. Its derivation is simplified drastically when we observe that the GGF itself is a marginal of an auxiliary determinantal point process [15].

Consider an auxiliary signed point process over the subsets of $\mathbb{Z}_{\geq x} \times \{1, \ldots, n\}$ of the form

$$\mathcal{T} = \bigcup_{1 \leq n \leq N} \{\tau_n^n, < \tau_{n-1}^n, < \ldots, < \tau_1^n\} \subset \mathbb{Z}_{\geq(x-1)} \times \{1, \ldots, n\}$$ (8)

given by the measure

$$\mathcal{F}(\mathcal{T}) = \frac{1}{Z_N} \prod_{n=0}^{N-1} \det[\phi_n(\tau_i^n, \tau_j^{n+1})]_{i,j=1}^{n+1} \det\left[\Psi_i^N(\tau_{N-i}^N)\right]_{i,j=0}^{N-1},$$ (9)

where we define the functions

$$\phi_n(z, y) = \begin{cases} p, & y \geq z \\ 0, & y < z \end{cases}$$ (10)

and

$$\Psi_k^N(t) = (-1)^k \widetilde{F}_{-k}(x + N - k - 1, t),$$ (11)

where

$$\widetilde{F}_n(x,t) = \frac{1}{2\pi i} \oint_{\Gamma_0} \frac{dw}{w} \left(q + \frac{p}{w}\right)^t (1-w)^{-n} w^x,$$ (12)

The integral representation holds for $t \in \mathbb{Z}$.

We also introduce fictitious variables $\tau_n^{n-1}, 1 \leq n \leq N$, which are effectively less than any τ_j^n, so that $\phi_n(\tau_{n+1}^n, \tau_j^{n+1}) \equiv p$ for $j = 1, .., n+1$. If we consider τ_j^n as coordinates of fictitious particles at the n-th time step, then τ_{n+1}^n corresponds to a particle entering into the system from a reservoir on the left [10].

Now, we are able to interpret the GGF in the following way.

Proposition 0.3 *Let*

$$
\begin{align}
(\boldsymbol{x^0}, \boldsymbol{t^0}) &= ((0,0), \ldots, (-N+1, 0)) \tag{13} \\
(\boldsymbol{x}, \boldsymbol{t}) &= ((x+N-1, t_1), \ldots, (x, t_N)) \tag{14}
\end{align}
$$

with $t_1 \leq t_2 \leq \cdots \leq t_N \in \mathbb{Z}_{\geq x}$ and $x \geq -N+1$. Then we have

$$
p^N G((\boldsymbol{x}, \boldsymbol{t})|(\boldsymbol{x^0}, \boldsymbol{t^0})) = \mathcal{M} \left(\bigcup_{k=1}^N \{\tau_1^k = t_k\} \right) \tag{15}
$$

The measure $\mathcal{M}(\mathcal{T})$ has the same functional form as in [10, 15, 11]. In particular, Lemma 3.4 of [11] can be directly applied here. There is a difference in the form of functions $\Psi_n^N(t)$ and in the space where the variables τ_j^i live, which is $\mathbb{Z}_{\geq x}$ rather than $\mathbb{Z}$. This difference does not affect the applicability of the Lemma, which is formulated in a rather abstract fashion, though has to be taken into account when obtaining the final expressions. According to Lemma 3.4 the multi-point correlation functions of $\mathcal{M}(\mathcal{T})$ are determinantal.

Proposition 0.4 *The correlation kernel of the measure $\mathcal{M}$, (9), is*

$$
K(n_1, \tau_1; n_2, \tau_2) = \tag{16}
$$
$$
p \oint_{\Gamma_1} \frac{dv}{2\pi i v} \oint_{\Gamma_{0,v}} \frac{dw}{2\pi i w} \frac{(1 - p(\frac{w-1}{w}))^{\tau_1} (\frac{w-1}{w})^{n_1} (w/v)^{x+N}}{(1 - p(\frac{v-1}{v}))^{\tau_2+1} (\frac{v-1}{v})^{n_2} (w-v)}
$$
$$
- \mathbf{1}(n_2 - n_1) \oint_{\Gamma_{1,0}} \frac{pdz}{2\pi i z^2} \left(\frac{z-1}{z} \right)^{n_1-n_2} \left(1 - p\frac{z-1}{z} \right)^{\tau_1-\tau_2-1}.
$$

The previous results furnish us with all the means required to write the quantity of interest (7) as a Fredholm determinant, which is the content of the following theorem:

Theorem 0.5

$$
\mathbf{P} = \det \left(\mathbf{1} - \chi_{\mathbf{a}} \mathbf{K} \chi_{\mathbf{a}} \right)_{l^2(\{n_1, \ldots, n_m\} \times \mathbb{Z}_{\geq x})}, \tag{17}
$$

where $\chi_a(n_i)(t) = \mathbf{1}(t > a_i)$.

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DYNAMICS OF QUANTUM-DOT SUPERRADIANCE

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The theory of quantum-dot radiation is developed being based on microscopic equations. The possibility of realizing the superradiant regime is analyzed. The temporal evolution during all radiation stages is studied in detail. Special attention is payed to the process when coherence arises from an initially incoherent state. The description of this process is impossible by means of the standard semiclassical equations, because of which a more accurate method has been used in the paper, employing the stochastic mean-field approximation that has been developed earlier and applied for describing the dynamics of spin assemblies, Bose systems in random fields, and atomic squeezing [1-3].

It is necessary to emphasize that the radiation dynamics of quantum dots has several specific features distinguishing this dynamics from atomic radiation. This is connected, first of all, with rather different values of physical dot parameters, as compared to atomic parameters. Because of this, despite many analogies, the theory of dot radiation requires a separate investigation. The principal theoretical points that have been suggested in the present paper for the adequate description of dot radiation are as follows [4]:

(i) Because of essential current fluctuations in semiconductor, the standard semiclassical approximation, often used for atoms in free space, is not applicable for quantum dots. For the latter more elaborate techniques are required, such as the stochastic mean-field approximation.

(iii) For the correct description and principal understanding of the mechanism, triggering the beginning of the radiation process, it is important to stress the existence of triggering dipolar waves.

(iv) The single-mode picture is not applicable for quantum dots. It is necessary to consider a bunch of transverse modes forming spatial filaments. To reduce the consideration to a treatable problem, it is necessary to involve some tricks, like the transverse-mode expansion.

(v) The overall dynamics of dot radiation consists of several stages, which have been thoroughly studied and described, both analytically and numerically, for the parameters typical of quantum dots.

In the dynamics of dot radiation, it is possible to distinguish the following qualitatively different stages. The first is the *fluctuating stage* lasting during the time interval $0 < t < t_{int}$, when the radiation process is triggered by dipolar waves. At this stage, there is no yet sufficiently strong interaction between dots. The interaction time is of an order of $t_{int} \sim 10^{-15}s - 10^{-14}s$.

The second is the *quantum stage* in the temporal interval $t_{int} < t < t_{coh}$, when the dot interactions through photon exchange start playing a noticeable role, but coherence has not yet been developed. The coherence time, required for the appearance of the well-developed coherence is of an order of $t_{coh} \sim 10^{-14}s - 10^{-13}s$.

Then the *coherent stage* comes into play in the interval $t_{coh} < t < T_2$ when the dots emit a coherent superradiant pulse. For the quantum dot materials, the dephasing time is of an order of $T_2 \sim 10^{-13}s - 10^{-12}s$. The maximum of the pulse occurs at the delay time $t_0 \simeq 5t_{coh}$ and the pulse duration is $\tau_p \simeq 2t_{coh}$. The pulse duration is inversely proportional to the dot density, that is, inversely proportional to the number of dots involved in the process of radiation, which is a typical feature of superradiance.
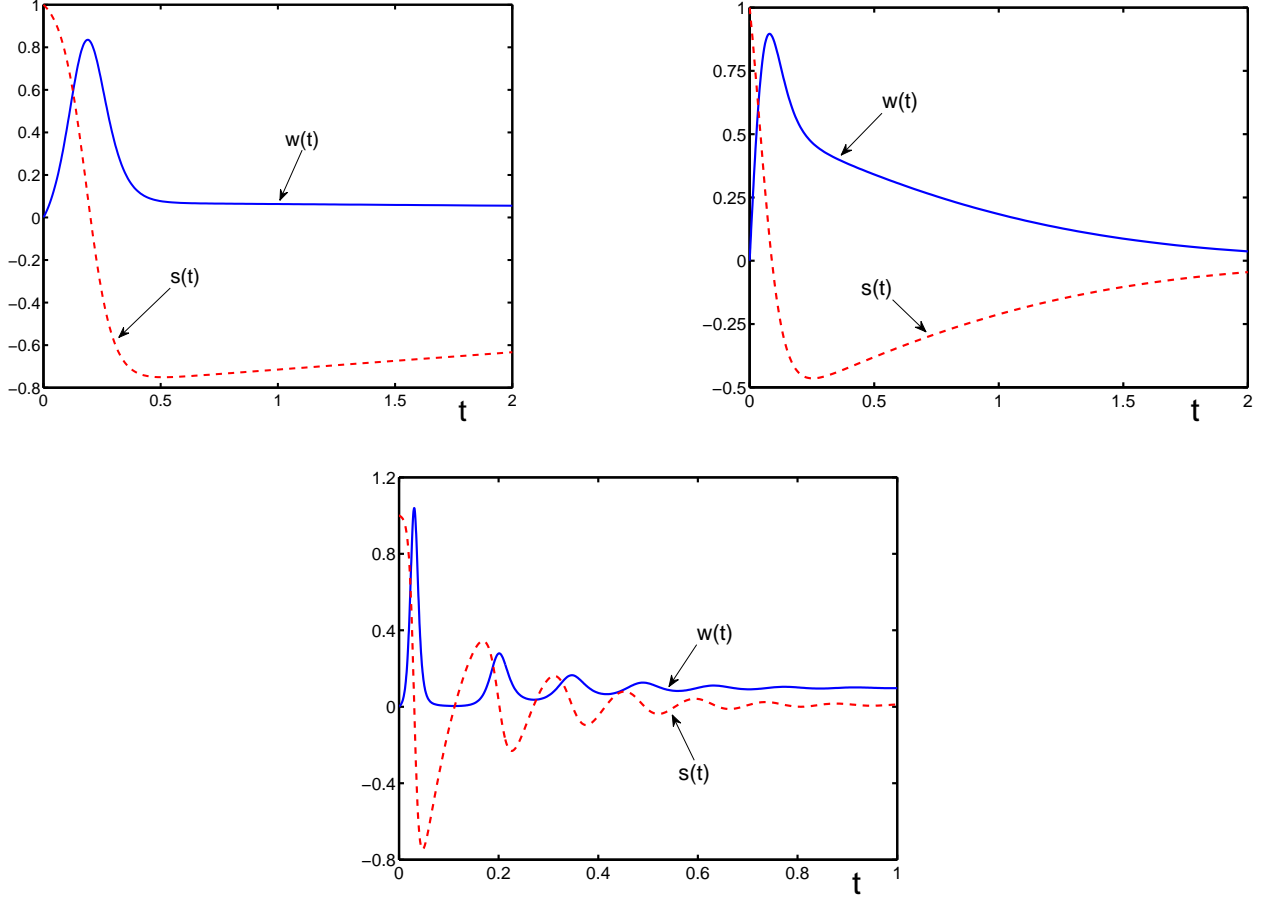
Figure 1: The upper left figure represents the behavior of the coherence intensity $w(t)$ (solid line) and population difference $s(t)$ (dashed line) as functions of dimensionless time (measured in units of T_2) for the attenuation parameters $\gamma_1 = 0.003, \gamma_3 = 1$ (measured in units of γ_2), for the coupling parameter $g = 10$, with the initial conditions $w_0 = 0, s_0 = 1$. The upper right figure presents the behaviour of the coherence intensity $w(t)$ (solid line) and population difference s as functions of dimensionless time (measured in units of T_2) for the attenuation parameters $\gamma_1 = 0.003, \gamma_3 = 10$ (measured in units of γ_2), for the coupling parameter $g = 10$, with the initial conditions $w_0 = 0, s_0 = 1$. A larger dynamic attenuation γ_3 makes the pulse more asymmetric. The lower figure presents the coherence intensity $w(t)$ (solid line) and population difference $s(t)$ (dashed line) as functions of dimensionless time (measured in units of T_2) in the case of external pumping, for the parameters $\gamma_1 = 10, \gamma_3 = 1$ (measured in units of γ_2), for the coupling parameter $g = 100$, with the initial conditions $w_0 = 0, s_0 = 1$. The coherence intensity, as well as population difference, exhibit five pulses with the decaying amplitude.

After the superradiant pulse is emitted, the system relaxes to an incoherent state during the *relaxation stage* in the interval $T_2 < t \ll T_1$. The population difference reverses. For the system of dots in a semiconducting material, the longitudinal relaxation time is $T_1 \sim 10^{-9}s$. However, this is not yet the final stage of evolution.

The *stationary stage* is reached for $t \gtrsim T_1$ if there is no external permanent pumping or the effective dot interactions are weak, so that $|g\zeta| \ll 1$. Then the system tends to a stationary

incoherent state representing a stable node.

If the system of dots is subject to a sufficiently strong external permanent pumping, the regime of *pulsing superradiance* occurs. Then a series of about 10 superradiant bursts can appear, flashing in the intervals of time $T_{eff} \sim 10^{-13}s$.

Figure 1 shows the evolution of coherence intensity and population dynamics as functions of dimensionless time t, measured in units of $T_2 \equiv 1/\gamma_2$, for several typical cases. We assume that at the initial time, the system is inverted, but coherence is absent and develops in a self-organized way. The upper figures correspond to the case of no external pumping when $\zeta = -1$. The difference between these figures is in the value of the dynamical attenuation rate. As we see, a larger γ_3 decreases the delay time and makes the superradiant pulse strongly asymmetric. The essential asymmetry of superradiant pulses is the feature typical of quantum-dot radiation. Another typical feature of the quantum-dot dynamics, also caused by the large rate γ_3, is a much faster, than for atoms in free space, tendency of the population difference to the stationary state. The lower figure demonstrates the radiation dynamics in the case of external pumping, when $\zeta = 1$, and there appear several superradiant pulses with decaying amplitude.

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LOW-TEMPERATURE ELECTRICAL RESISTIVITY IN THE GEOMETRICALLY FRUSTRATED NEARLY ANTIFERROMAGNETIC METALLIC SYSTEM LiV$_2$O$_4$

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The metallic vanadium oxide LiV$_2$O$_4$ has attracted much attention after a heavy fermion behavior in this $3d$-electron system was discovered about a decade ago. LiV$_2$O$_4$ has the cubic spinel structure with the magnetic vanadium ions (in the mixed valence state V$^{3.5+}$) occupying the pyrochlore lattice sites. At low temperatures, the spin system of LiV$_2$O$_4$ exhibits pronounced short-range antiferromagnetic (AFM) correlations, but no long-range magnetic ordering was detected at any measured temperatures. The geometrical frustration of the pyrochlore lattice is likely to be a crucial aspect of the problem. The frustration may suppress at any T a long-range ordering of strongly correlated itinerant electrons, but instead, the system is placed near a magnetic instability. The emergence of largely degenerate nearly critical (low-energy) AFM spin excitations in the ground state of LiV$_2$O$_4$ is expected to be responsible for low-T properties of this material, including its heavy fermion behaviour. Actually, the quasiparticle mass enhancement is expected when a metallic system is driven by strong electron correlations to the vicinity of a charge and/or spin phase transition at low T. This appealing picture has been suggested [1] and examined further [2, 3, 4, 5] by comparing the theoretical results with experimental data obtained by different techniques, like the inelastic neutron scattering and the nuclear magnetic resonance. In our theory, the temperature evolution of nearly critical spin fluctuations is treated in the framework of the self-consistent renormalization (SCR) approach. In the present report, I give a short review of our latest results obtained along this line and presented together with my colleagues in Ref.[6].

Specifically, we show that the low-T Fermi liquid behaviour of the resistivity and a deviation from this behavior for higher T may also be understood within that context. We calculate the temperature dependence of the electrical resistivity $\rho(T)$ assuming that two basic mechanisms of the quasiparticle scattering, resulting from impurities and spin-fluctuations, operate simultaneously. A peculiar behavior of $\rho(T)$ in LiV$_2$O$_4$ is related to the properties of low-energy spin fluctuations whose T-dependence is obtained from the SCR theory in a wide temperature range up to 40 K, where the SCR approach is valid.

In the linear response theory, in an applied electric field $\mathbf{E}$ the quasiparticle distribution function $f_{\mathbf{k}}$ is linearized around the equilibrium Fermi distribution $f_{\mathbf{k}}^0$, according to $f_{\mathbf{k}} = f_{\mathbf{k}}^0 - \Phi_{\mathbf{k}} df_{\mathbf{k}}^0/d\epsilon_{\mathbf{k}}$. The electronic transport can be found from the Boltzmann equation

$$-e(\mathbf{E}\mathbf{v_k})\frac{df_{\mathbf{k}}^0}{d\epsilon_{\mathbf{k}}} = \sum_{\mathbf{k}} W_{\mathbf{kk}'}\Phi_{\mathbf{k}'}. \tag{1}$$

The scattering operator $W_{\mathbf{kk}'}$ can be expressed through the total equilibrium transition probability $\mathcal{P}_{\mathbf{kk}'} = \mathcal{P}_{\mathbf{kk}'}^{imp} + \mathcal{P}_{\mathbf{kk}'}^{sf}$ as ($k_B = \hbar = 1$):

$$W_{\mathbf{kk}'} = \frac{1}{T}\left(\delta_{\mathbf{kk}'}\sum_{\mathbf{k}''}\mathcal{P}_{\mathbf{kk}''} - \mathcal{P}_{\mathbf{kk}'}\right), \tag{2}$$

provided the spin fluctuations are in thermal equilibrium, i.e., there is no drag effect.

For the elastic impurity scattering one has

$$\mathcal{P}^{imp}_{\mathbf{kk'}} = 2\pi n_i |T_{\mathbf{kk'}}|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k'}}) f^0_{\mathbf{k}}(1 - f^0_{\mathbf{k'}}). \tag{3}$$

To a sufficiently good approximation, the T-matrix in Eq.(3) is frequently assumed to be a constant $|T_{\mathbf{kk'}}|^2 \approx V^2_{imp}$ and $n_i V^2_{imp}$, where n_i is the impurity density, is regarded as a free parameter to be chosen so as to give a realistic value of the measured residual resistivity ρ_{imp}. We avoid this approximation and treat below the matrix elements of $\mathcal{P}^{imp}_{\mathbf{kk'}}$ generally.

For the spin-fluctuation (sf) scattering one has

$$\mathcal{P}^{sf}_{\mathbf{kk'}} = 3J^2_{sf} f^0_{\mathbf{k}}(1 - f^0_{\mathbf{k'}})[n(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k'}}) + 1]\mathrm{Im}\chi\left(\mathbf{k} - \mathbf{k'}, \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k'}}\right), \tag{4}$$

where $n(\epsilon)$ is the Bose distribution function, $\chi(\mathbf{q}, \epsilon)$ is the dynamical spin susceptibility describing the low-T paramagnetic state of LiV$_2$O$_4$ and J_{sf} is an effective coupling constant which is the second free parameter. It is worth emphasizing that in the present study the other parameters of the phenomenological SCR theory determining the behavior of $\chi(\mathbf{q}, \epsilon)$ are considered to be known and fixed from a fit to the data of inelastic neutron scattering measurement on LiV$_2$O$_4$, as discussed in [2].

The SCR theory offers a phenomenological description for "critical" spin fluctuations in nearly antiferromagnetic itinerant electron systems by taking into account effects of mode-mode coupling between spin fluctuations at $|\mathbf{q}| \sim |\mathbf{Q}_c|$. The location in $\mathbf{q}$-space and the multiplicity of "critical" wave vectors $\mathbf{Q}_c$ are produced by specific properties of the electronic band structure and the topology of the many-sheet Fermi surface (FS) in LiV$_2$O$_4$.

Following the standard notation, the Boltzmann equation (1) can be rewritten in the form $X_{\mathbf{k}} = \sum_{\mathbf{k'}} W_{\mathbf{kk'}} \Phi_{\mathbf{k'}}$. Then the electrical resistivity can be obtained by minimizing a functional

$$\rho[\Phi] = min\left[\frac{\langle \Phi, W\Phi \rangle}{|\langle \Phi, X(E = 1)\rangle|^2}\right]. \tag{5}$$

Here $E = 1$ means the unit electrical field, and the scalar product of two functions $\Phi_{\mathbf{k}}$ and $\Psi_{\mathbf{k}}$ is defined as $\langle \Phi, \Psi \rangle = \sum_{\mathbf{k}} \Phi_{\mathbf{k}} \Psi_{\mathbf{k}}$. In fact, in Eq.(5) the $\mathbf{k}$-integration over the actual FS is implied which follows from the property of the scattering operator $W_{\mathbf{kk'}}$ and the explicit form of $X_{\mathbf{k}} = e(\mathbf{Ev_k})(-df^0_{\mathbf{k}}/d\epsilon_{\mathbf{k}})$. A way to search for a variational solution of Eq.(5) for the deviation function $\Phi_{\mathbf{k}}$ is to expand it in a set of the Fermi-surface harmonics (FSH) $\phi_L(\mathbf{k})$:

$$\Phi_{\mathbf{k}} = \sum_L \eta_L \phi_L(\mathbf{k}), \tag{6}$$

where η_L are variational parameters and L is a convenient composite label that includes numbering of different sheets of the Fermi surface in LiV$_2$O$_4$

Then any matrix element of the scattering operator $W_{LL'} = \langle \phi_L, W\phi_{L'} \rangle$ contains a nearly constant (at low T) term $W^{imp}_{LL'}$ and a T-dependent spin-fluctuation term $W^{sf}_{LL'}$ that can be presented in a factorized form

$$W^{sf}_{LL'} \approx C_{LL'} \mathcal{F}(T), \tag{7}$$

where

$$C_{LL'} = \left(\frac{1}{2\pi}\right)^6 \oint \frac{d^2k}{v_{\mathbf{k}}} \oint \frac{d^2k'}{v_{\mathbf{k'}}} \left[\phi_L(\mathbf{k}) - \phi_L(\mathbf{k'})\right] M^{sf}_{\mathbf{kk'}} \left[\phi_{L'}(\mathbf{k}) - \phi_{L'}(\mathbf{k'})\right], \tag{8}$$
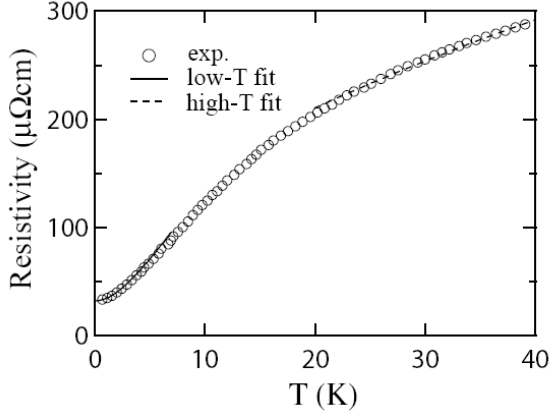
Fig. 1 Theoretical fit to the experimental data (Refs.[7, 8], open circles) for the electrical resistivity $\rho(T)$ in LiV$_2$O$_4$ in different temperature regions.

$$\mathcal{F}(T) = \frac{1}{T} \int\limits_0^\infty d\epsilon \int \frac{d^3q}{(2\pi)^3} \epsilon n(\epsilon)[n(\epsilon) + 1]\mathrm{Im}\chi\left(\mathbf{Q}_c + \mathbf{q}, \epsilon\right), \qquad (9)$$

and the matrix $M_{\mathbf{kk'}}^{sf}$ is defined as $M_{\mathbf{kk'}}^{sf} \simeq 3J_{sf}^2 \sum_{\{\mathbf{Q}_c\}} \delta(\mathbf{k'} - \mathbf{k} - \mathbf{Q}_c)$. The matrix is invariant under simultaneous operations of the lattice point group on both $\mathbf{k}$ and $\mathbf{k'}$, since the manifold $\{\mathbf{Q}_c\}$ is an invariant as well.

Special attention has been paid to two limiting regimes of low- and comparatively high-temperatures ($T < 40$K). In Fig.3, the calculated $\rho(T)$ is compared with physical resistivity $\rho^{\mathrm{exp}}(T)$ reported in [7, 8].

A satisfactory coincidence between the experimental data and calculated results is achieved in both temperature regimes. Our theory provides also the interpolation T-dependent function describing $\rho^{\mathrm{exp}}(T)$ correctly between the low- and high-T limits as well.

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