Pis'ma v ZhETF, vol. 117, iss. 1, pp. 55 – 56

Hubbard bands, Mott transition and deconfinement in strongly correlated systems

V. Yu. Irkhin[1)]

M. N. Mikheev Institute of Metal Physics, 620108 Ekaterinburg, Russia

Ural Federal University, 620002 Ekaterinburg, Russia

Submitted 10 November 2022
Resubmitted 15 November 2022
Accepted 16 November 2022

DOI: 10.31857/S123456782301007X, EDN: nvlwux

The old problem of Mott (metal-insulator) transition is still of interest and importance. Usually this transition occurs in antiferromagnetic phase (Slater scenario), but the situation changes for frustrated systems: only the paramagnetic metallic and insulator state are involved, a spin liquid being formed [1]. The transition into insulator state is related to correlation Hubbard splitting (the Mott scenario). In the Mott state the gap in the spectrum is essentially the charge gap determined by boson excitation branch. Therefore the electrons become fractionalized: the spin degrees of freedoms are determined by neutral fermions (spinons), and charge ones by bosons. The corresponding slave-boson representation was first introduced by Anderson, see [2]. The deconfined spin-liquid state involved includes fractionalization and long-range many-particle quantum entanglement [3]. Generally, description of the correlated paramagnetic phase, which may have a complicated internal structure, is an important problem.

In fact, boson and fermion are coupled by a gauge field, so that the problem of confinement occurs [2]. The transition into the metallic confinement state is described as a Bose condensation, the electron Green's function acquiring the finite residue. On the other hand, in the insulator state the bosons have a gap, so that the spectrum is incoherent (the electron Green's function is a convolution of boson and fermion ones) and includes Hubbard's bands.

New theoretical developments provided a topological point of view for the Mott transition, since spin liquid possesses topological order (see review in [3]). Phase transitions in frustrated systems can be treated in terms of topological excitations (instantons, monopoles, visons, vortices) which play a crucial role for confinement.

A useful analogy is given by the charged Bose liquid in a magnetic field where one has to take into account the gauge invariance. Here, the magnetic field penetrates into the sample as vortex filaments which carry unit flux quanta and can originate and terminate at instantons and anti-instantons [4].

In a pure gauge model, the magnetic monopoles (instantons) – the point singularities of the gauge field – occur, which are non-local excitations of the system, interacting according to the Coulomb law. In the case of compact field, a confinement situation can occur owing to the monopoles. With adding a material field the Higgs effect (occurrence of the gauge boson mass) can result in formation of a new "Coulomb" phase which is essentially a deconfined phase.

The pure gauge model in the space-time dimension $d = 2{+}1$ is always confining at arbitrarily small coupling constant g owing to occurrence of instantons which provide tunneling events. In the presence of a material field, the situation can change due to the Higgs phenomenon. The phase diagram for $d = 3{+}1$ case contains the Higgs-confinement phase and Coulomb (free charge) phase [4]. A crossover between the Higgs and confinement states is also possible. In the Coulomb phase, the gauge field is deconfining and massless, and the Bose field remains disordered.

For $d = 2 + 1$ we have only the confinement phase where the gauge field is massive due to instantons. In the strong coupling (large g) limit the gauge field does not have its own dynamics and provides the constraint of integer boson occupation at each lattice site, resulting in an insulator state. Therefore the confinement phase may be understood as a Bose Mott insulator. This Mott phase turns out to extend to include the entire phase diagram up to the line $g = 0$.

The situation in $d = 2 + 1$ can change in a gapless spin liquids with a large number of gapless fermionic matter fields, e.g., Dirac points [1, 5] where gauge field can become non-compact.

The Kotliar–Ruckenstein representation (see [6]) uses the Bose operators e_i, $p_{i\sigma}$, d_i and Fermi operators $f_{i\sigma}$:

$$c^\dagger_{i\sigma} \to f^\dagger_{i\sigma} z^\dagger_{i\sigma},\ z^\dagger_{i\sigma} = g_{2i\sigma}(p^\dagger_{i\sigma} e_i + d^\dagger_i p_{i-\sigma}) g_{1i\sigma}, \qquad (1)$$

[1)]e-mail: valentin.irkhin@imp.uran.ru

with the constraints

$$\sum_\sigma p^\dagger_{i\sigma}p_{i\sigma}+e^\dagger_i e_i+d^\dagger_i d_i=1,\ \ f^\dagger_{i\sigma}f_{i\sigma}=p^\dagger_{i\sigma}p_{i\sigma}+d^\dagger_i d_i. \quad (2)$$

The critical value for the Mott transition in the Brinkman–Rice approximation reads $U_c = 8\varepsilon$ where $\varepsilon = 2\left|\int_{-\infty}^{\mu} d\omega\omega\rho(\omega)\right|$ the average non-interacting energy, $\rho(\omega)$ the bare density of electron states.

Similar to [7], the calculation of the boson Green's function yields the spectrum

$$\omega_{a\mathbf{q}} = \frac{1}{2}[\pm U\zeta - (-1)^a\sqrt{U^2\zeta^2 + U(U_c - 4\Sigma(\mathbf{q}))}]. \quad (3)$$

Here $\zeta = (1 - U_c/U)^{1/2}$, we have taken into account the boson self-energy

$$\Sigma(\mathbf{q}) = -2\sum_{\mathbf{k}\sigma} t_{\mathbf{k}-\mathbf{q}}n_{\mathbf{k}\sigma},\ n_{\mathbf{k}\sigma} = \langle f^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle. \quad (4)$$

The dispersion of bosons is influenced by details of fermion spectrum which is determined by the f-system state. Spin degrees of freedom can be treated separately with the Heisenberg Hamiltonian in the f-pseudofermion representation. Under some conditions, one can expect formation of a spin-liquid state where excitation are essentially spinons – neutral fermions.

The mean-field picture of spinon spectrum $E_\mathbf{k}$ can be stabilized in the case of a non-compact gauge field or by gapless Fermi excitations. In the insulator state this spectrum is not influenced by bosons, various spin-liquid phases being obtained [2].

In the absence of considerable $\mathbf{k}$-dependence of $n_{\mathbf{k}\sigma}$ (a localized spin phase without fermion hopping), Σ tends to zero. However, for a spin liquid we have a sharp Fermi surface. Indeed, for Mott insulators the spinon Fermi surface is expected to be preserved even in the insulating phase, so that the Luttinger theorem remains valid. Although, generally speaking, the spinon spectrum form differs from bare electron one, for $q = 0$ we still have $\Sigma(0) = U_c/4$ since the spinon band is half-filled and the chemical potential (the position of the Fermi energy) is fixed.

Thus the spectrum picture in the insulating state is considerably influenced by the spinon spin-liquid spectrum and hidden Fermi surface. This interpretation of spectrum is different from that in [7] where the limit of vanishing renormalized electron bandwidth (i.e., in the Mott phase where the averages e, $d \to 0$) is treated in a Gutzwiller-type approach.

In the nearest-neighbor approximation, after passing in (4) to the coordinate representation one can see that the spectrum of spinons and correction to holon spectrum differ, roughly speaking, only in the replacement of J by t ($\Sigma(\mathbf{q}) \propto E(\mathbf{q})$). In particular, we have for a square lattice

$$\Sigma(\mathbf{q}) = U_c(\cos q_x + \cos q_y)/8,$$
$$\Sigma(\mathbf{q}) = \pm U_c\sqrt{\cos^2 q_x + \cos^2 q_y}/(4\sqrt{2}) \quad (5)$$

for the the uniform RVB phase and π-flux phase (which contains Dirac points), respectively.

In the large-U limit we have

$$\omega_{a\mathbf{q}} = \mathrm{const} - (-1)^a\Sigma(\mathbf{q})/\zeta.$$

It is important that a characteristic scale of spinon energies is small in comparison with that of electron ones, so that the spinon Fermi surface is strongly temperature dependent; this situation is somewhat similar to the case of magnetic order.

The observable electron Green's function is obtained as a convolution of the boson and spinon Green's functions. Then we obtain the upper and lower Hubbard subbands with energies near 0 and U and the width of order of bare bandwidth, the gap between them vanishing at the transition point $U \to U_c$. At some points in the Brillouin zone the interaction with the gauge field owing to constraints can play an important role [2]. The expressions for the Green's functions can be used to calculate the optical conductivity, cf. [7].

Although most theoretical investigations are performed in $d = 2 + 1$, spin- liquid states exists in some three-dimensional systems, e.g., pyrochlores. Even if an instability with respect to magnetic ordering or superconductivity occurs in the ground state, a spin-liquid-like state can occur in an intermediate temperature regime, especially in frustrated systems.

The author is grateful to Yu. N. Skryabin for numerous fruitful discussions.

This is an excerpt of the article “Hubbard bands, Mott transition and deconnement in strongly correlated systems”. Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S002136402260269X

---

1. T. Senthil, Phys. Rev. B **78**, 045109 (2008).
2. P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. **78**, 17 (2006).
3. V. Yu. Irkhin and Yu. N. Skryabin, Phys. Met. Metallogr. **120**, 513 (2019).
4. N. Nagaosa and P. A. Lee, Phys. Rev. B **61**, 9166 (2000).
5. M. Hermele, T. Senthil, M. P. A. Fisher, P. A. Lee, N. Nagaosa, and X.-G. Wen, Phys. Rev. B **70**, 214437 (2004).
6. M. Lavagna, Phys. Rev. B **41**, 142 1990).
7. R. Raimondi and C. Castellani, Phys. Rev. B **48**, 11453(R) (1993).