Does a Bose Gas Have Properties Helpful for Understanding the Nature of High Temperature Super Conductivity?

(How many subsystems should be reflected in the ground state vector of a HTSC?)

Valentin Voroshilov, Physics Department, Boston University, Boston, MA, 02215, USA

Despite intensive experimental and theoretical research the mechanism responsible for high temperature superconductivity is yet not clear. This might be a sign for taking a closer look at the fundamental ideas on which the prospective theory might be based. A set of simple models is considered, leading to a proposal for the ground state vector for the system of electrons in a strong periodic potential. The ground state vector includes terms accounting for pairs of pairs of electrons. The anomalous electron Green function vanishes at the half-filling. The proposed ground state might be used as a basis for the future investigation.

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Nowadays a common opening of a paper on HTSC often sounds like "despite intensive experimental and theoretical research the mechanism responsible for high temperature superconductivity[1] is yet not clear". This might be a sign for taking a closer look at the fundamental ideas on which the prospective theory might be based. The existence of preformed electron pairs[2] points out at a Bose gas as a system playing an important role in the phenomenon. In every textbook on statistical physics[3] one finds expression (1) which relates temperature T, chemical potential μ and the number of non-interacting Bosons N of mass m contained in a box with volume V (the gas is spinless, the Plank's constant, and the Boltzmann's constant are set to unity)

$$n = \frac{N}{V} = \frac{(mT)^{3/2}}{\sqrt{2}\pi}\int_0^\infty \frac{\sqrt{z}dz}{e^{z-a}-1} = \frac{(mT)^{3/2}}{\sqrt{2}\pi}\int_0^\infty \rho(z)dz = \frac{(mT)^{3/2}}{\sqrt{2}\pi}I(a), \quad a = \frac{\mu}{T}. \qquad (1)$$

Above the critical temperature T_c the chemical potential is negative, at critical temperature it becomes zero and remains zero below T_c. Below the critical temperature integral (1) gives the density of bosons with non-zero momenta $n_n = N_n/V$ ("normal" density); the density of the condensate is equal to $n_0 = n - n_n$.

We can ask, however, why does not the chemical potential become positive below the critical temperature but remains being equal to zero? Could normal density n_n be given by integral (1) with $a > 0$?

The standard answer to the later question is "no", because: (a) if chemical potential is positive the integrand in (1) diverges at $z > 0$, and (b) for $a > 0$ the energy density $\rho_\varepsilon(\varepsilon) = \rho(z = \varepsilon/T)$ seems having negative values.

However if for a moment we close the eyes on these issues and analyze the integral, it can be rewritten with the integrand not having any divergence even when $a > 0$

$$a > 0, \qquad I(a) = \int_0^\infty \rho(z)dz, \qquad \rho(z) = \begin{cases} \dfrac{\sqrt{z+a}}{e^z - 1}, z > a \\ \dfrac{\sqrt{a+z} - e^z\sqrt{a-z}}{e^z - 1}, 0 < z < a \end{cases}. \qquad (2)$$

Not every mathematically correct transformation should make a sense from a physical point of view, but for Eq. (2) the natural interpretation would be that below the critical temperature there is a set of possible solutions with normal density $n_n = n_n(T, 0 \le \mu < T)$ and with energy density $\rho_\varepsilon(\varepsilon)$ provided by Eq. (2) (another but more unusual interpretation is that in states with $\mu > 0$

energy levels below some certain value are restricted). If the solution with $\mu = 0$ is only one of many, usually that means that the solution which a system realizes minimizes its free energy (or another appropriate thermodynamic potential).

For an ideal Bose gas we can write its free energy $F = F_0 + F_{\mathrm{n}}$ as the sum of the free energy of the condensate $F_0 = 0$ and the free energy of the subsystem of the bosons with non-zero momenta

$$F_n = \Omega_n + \mu_n N_n, \quad \Omega_n = T\sum_{\vec{p}\neq 0}\{1-\exp(\mu_n - \frac{p^2}{2mT})\}. \tag{3}$$

Condition $\frac{\partial F}{\partial N_n} = 0$ leads to the conclusion $\mu_n = 0$, which gives us the standard result.

Equipped with this experience we will consider the ideal Bose gas composed of a subsystem with bosons with non-zero momenta, and a subsystem of bosons with momentum $\vec{\eta} \neq 0$.

Free energy $F = F_\eta + F_{\mathrm{n}}$ now is equal to the sum of the free energy of the moving bosons $F_\eta = \frac{\eta^2}{2m} N_\eta$ and the free energy of the subsystem of the bosons with non-zero momenta given by Eq. (3). Since $N_\eta + N_n = N$ (the total number of bosons), we can write the free energy of the system as $F = \Omega_n + \mu_n N_n + \frac{\eta^2}{2m}(N - N_n)$ and minimize it with respect to N_n. Condition $\frac{\partial F}{\partial N_n} = 0$ leads now to the conclusion $\mu_n = \frac{\eta^2}{2m} > 0$. It has been seen that the fact that a chemical potential is positive does not necessary lead to contradictions (a Bose condensate in cold atoms might be the right system to test this deduction).

Finally, we can try to take a look at the boson-like Cooper pairs existing in HTSC even above the critical temperature as if it is an ideal Bose gas. Based on the previous consideration we conclude that the simplest model should include three ideal subsystems (contained in a box with volume

V), namely, not paired electrons (N_F fermions with mass *m*), electron pairs not included into the condensate (N_B bosons with mass 2*m*), and electron pairs composing the moving condensate (N_η bosons with mass 2*m* and momentum $\vec{\eta} \neq 0$). Since the total number of electrons in the system $N = N_F + 2N_B + 2N_\eta$ does not change, we write Eq. (4) for free energy of this ideal "gas"

$$F = \Omega_F + \mu_F N_F + \Omega_B + \mu_B N_B + \frac{\eta^2}{8m}(N - N_F - 2N_B). \tag{4}$$

Setting $\frac{\partial F}{\partial N_F} = \frac{\partial F}{\partial N_B} = 0$ we find

$$N_\eta = \frac{N}{2} - \sum_{\vec{p}} \{\exp(\tfrac{1}{2mT}(p^2 - \eta^2/4)) + 1\}^{-1} - \sum_{\vec{p}} \{\exp(\tfrac{1}{4mT}(p^2 - \eta^2)) - 1\}^{-1}. \tag{5}$$

In particular, if we set $\eta = 0$ and $N_\eta = 0$ we find critical temperature

$$T_c = \left(\frac{N}{V}\frac{\pi^2}{\sqrt{2}mB}\right)^{\frac{3}{2}}, \quad B = \int_0^\infty \frac{\sqrt{x}dx}{\sinh(x)} \approx 2.99. \tag{6}$$

With electron density[4] $N/V = 10^{21}$ cm^{-3}, Eq. (6) gives $T_c \approx 10^3$ K. However, the system has only one critical temperature.

The theory of HTSC should be based on a Hamiltonian of a system of interacting electrons, and the speculations above cannot be used for analyzing properties of HTSC, but give us an idea which can be useful for developing the correspondent theory, i.e. the idea of the three thermodynamically coupled subsystems, the presence of which should be reflected in either the Hamiltonian or the ground state of the system.

Recently[5] Hamiltonian (7) was introduced on the assumption that in a strong periodic potential pairs are formed by electrons with the same group velocity (which resonates with the view that in HTSC properties of electrons in a momentum space are closely connected with their properties in a real space[6]).

$$H = \sum_{p\sigma} (\varepsilon_p - \mu) a^+_{p\sigma} a_{p\sigma} - \frac{W}{N} V^+ V, \qquad V^+ = \sum_{\substack{\vec{p} \\ \varepsilon_F < \varepsilon_p < -\varepsilon_F}} a^+_{p\uparrow} a^+_{p*\downarrow}, \quad \varepsilon_p = -t(\cos p_x + \cos p_y). \tag{7}$$

In Eq. (7) the first term represents kinetic energy of electrons in a 2D square lattice in tight-binding approximation; t > 0 is a hopping integral; the lattice constant is set to unity; all momenta lie in the first Brillouin zone $-\pi < p_{x,y} < \pi$; μ is a chemical potential introduced in the Hamiltonian as a Lagrange multiplier; $a^+_{p\sigma}$ and $a_{p\sigma}$ are creation and annihilation operators for an electron with momentum $\boldsymbol{p} = (p_x, p_y)$ and spin component σ ($\sigma = \uparrow, \downarrow$); N is the number of sites; $-W < 0$ is a coupling constant for paired electrons, $\boldsymbol{p^*} = (\pi \cdot sgn(p_x) - p_x, \pi \cdot sgn(p_y) - p_y)$ ($sgn(p_{x,y})$ is the signum function); the summation runs over the first Brillouin zone, and we assume that the Fermi level $\varepsilon_F < 0$.

Hamiltonian (7) does not reflect directly the presence of the three subsystems; the second term gives the same input for electron pairs not included into the condensate, as well as for pairs in the condensate. To reflect on the presence of the subsystems formed by electron pairs we will include additional terms in the ground state vector of the system. Creation/annihilation of "a boson" (an electron pair) is described by two electron creation/annihilation operators. When bosons form a condensate, the anomalous Green function for two bosons, which is the average of two bosonic creation/annihilation operators, is not zero anymore. This is a reflection of the fact that the ground state vector for a Bose gas also includes pairs of bosons with opposite momenta[7]. If indeed we can treat electron pairs as bosons, the ground sate vector should include terms with four electron creation operators. Based on this view we write Eq. 8 for the ground state vector

$$|E_0> = \prod_{\substack{\vec{p} \\ \varepsilon_F < \varepsilon_p < 0}} \{u_p + v_p a^+_{p\uparrow} a^+_{p*\downarrow} + v_p a^+_{-p\downarrow} a^+_{-p*\uparrow} + w_p a^+_{p\uparrow} a^+_{p*\downarrow} a^+_{-p\downarrow} a^+_{-p*\uparrow}\} \prod_{\substack{\vec{p},\sigma \\ \varepsilon_p < \varepsilon_F}} a^+_{p\sigma} |\mathrm{vac}>. \tag{8}$$

This vector can be seen as describing the state when in addition to a condensate electron pairs form a correlated state if traveling in opposite directions (of course, a similar term could be added to a BCS ground state vector); the last term differs Eq. 8 from BCS ground state vector and from models proposed for studying BCS-BEC crossover[8].

In Eq. (8) functions u, v, w are real; $u_p^2 + 2v_p^2 + w_p^2 = 1$ ($\langle E_0 || E_0 \rangle = 1$); $u_p = u_{p*} = u_{-p} = u_{-p*}$, etc. The number of electrons is equal to $N_e = \langle E_0 | \sum_{p\sigma} a^+_{p\sigma} a_{p\sigma} | E_0 \rangle$; this equation leads to another condition on parameters u, v, and w

$$u_p^2 + w_p^2 = \frac{1}{2}\frac{N_e - 2N_F}{N - 2N_F}, \qquad N_F = \sum_{\vec{p},\, \varepsilon_p < \varepsilon_F} 1 \ . \tag{9}$$

After calculating $E_0 = \langle E_0 | H | E_0 \rangle$ and minimizing it with respect to parameter u_p (we can choose v_p and w_p as dependent parameters) we find that u_p, v_p, and w_p are in fact constants, and obey the third condition $(w+u)(v^2 - wu) = 0$. The solution $w + u = 0$ exists only at the half-filling when $N_e = N$. At this point of the analysis the actual values of the parameters are not important; the new fact is that some of the parameters might be negative. It leads to an important result; if we calculate the anomalous Green function for two electrons $\langle E_0 | a^+_{p\uparrow} a^+_{p*\downarrow} | E_0 \rangle = v(u + w)$ it can be equal to zero, but only at the half-filling. This property of the system is in an agreement with the absence of superconductivity in cuprates at the half-filling.

Clearly, the speculations offered above do not prove the validity of the assumptions on which Hamiltonian (7) and ground state vector (8) have been written. Only the theory based on a more realistic Hamiltonian and covering all temperatures could be used for comparison with experimental data. Development of the correspondent theory is a work in a progress.

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