What is the most important for a nanoscale structure formations in HTSC?, spin, phonon or third way in Coulomb interaction and correlations?

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Abstract. We show that nanoscale superstructures observed in STM experiments in high temperature superconductor (HTSC) such as cuprates in superconducting state [1] are well described by a model of two-dimensional charged boson gas(2DBG). The bosons are located on top of a uniform, structureless, jellium neutralizing background. This model is the most fundamental and clean quantum system where different properties of the formation of the superconducting and insulating states can be studied by changing only one parameter - the boson density $n_0$. At high densities the ground state is always superconducting, that is associated with the Bose-Einstein condensation of the charged bosons which form a superfluid state. Whereas at very low densities bosons localize into a Wigner crystal. Here we show that a dilute amount of impurities with opposite charge to bosons alter dramatically the properties of the system. Any charged impurity induces density oscillations, similar to Friedel oscillations in Fermi liquids. When the density decreases the amplitude of these charge density wave(CDW) oscillations increases. At some critical density there arises the CDW instability. As the result around each impurity a Coulomb bubble(CB) is formed. At such a CB there arises an orthogonality catastrophe associated with the formation of localized states inside CB orthogonal to the fluid of free bosons. The creation of localized states may be accompanied by a formation of local lattice distortions. The phenomenon is very similar to the conventional self-trapping or a formation of electronic strings[2]. The CDW instability arises due to over-screening of the Coulomb interaction. The phenomenon of CB formation is very general. They can be created and become localized around any potential induced by phonons or by individual impurities or both. As the result the quantum system separates into two phases: localized CBs distributed randomly and superfluid bosons forming a homogeneous state. When the density decreases after the formation of CBs the area covered by them increases while the superfluid area decreases. Also with decreasing density the number of Coulomb bubbles grows in a step-like manner. At each such step more remote impurities outside the superconducting plane take part in trapping of CBs and reduce significantly the superfluid density. The insulating state emerges either via creation of an infinite percolating cluster of CBs or due to the Wigner crystallization of the bosonic phase.

1. Introduction
The charged boson fluid represents the most fundamental quantum system where the interplay between the Anderson localization and the Coulomb interaction can be studied. At high densities the fluid is superconducting and at low densities it forms the Wigner crystal. Anderson
localization has been observed in many low dimensional electron systems with disorder and proved to be a genuine phenomenon in the quantum behaviour of electrons. However, when the disorder is not very strong the Coulomb interaction may prevent the localization leading to the existence of a correlated quantum liquid. In the two-dimensional (2D) electron gas the interplay between the electron - electron interaction and disorder has been studied in many experimental and theoretical papers (see, [3] and references inside, for details).

Here we focused on the disorder in the 2D charged boson fluid when its density varies. We investigate the role of single charged impurities embedded into 2D charged boson fluid in a phenomenon, which is similar to Anderson localization. However, there is a strong difference between fermions and bosons. Macroscopic amounts of bosons can condense into the lowest lying state due to the Bose-Einstein condensation (BEC), which creates a long range order into the charged fluid. According to the Landau criterion if the lowest energy collective excitations of the BEC state have a linear or steeper spectrum near the origin or the spectrum has a gap then the fluid is superconducting. The fraction of particles in the condensate depends on the strength of the interaction between them. In the charged fluid the strength increases when the density \(n_0\) of the system decreases or the parameter \(r_s = 1/\sqrt{\pi n_0} r_B\) increases. Here \(r_B\) is the Bohr radius. A single charged impurity induces in its surrounding a charge density wave (CDW) which amplitude depends on the density or on associated \(r_s\) parameter. With increasing \(r_s\) the relative amplitude with respect to the boson density increases. Finally, at some critical density the amplitude at the minimum nearest to the impurity becomes equal to the average boson density. That triggers the CDW instability, which localizes bosons surrounding impurities, decouples them from the rest of the superfluid and therewith forms a Coulomb bubble (CB). As a result the homogeneous boson fluid phase separates into two phases containing localized and freely moving bosons mixed together.

At zero temperature a fraction of the charged boson fluid is in the condensed state. The condensate fraction is largest at the highest densities where \(r_s \rightarrow 0\), decreases monotonically with the density and vanishes at the Wigner crystallisation around \(r_s \approx 60\) [4, 5]. With this Bose-Einstein condensation the superfluid flow of the charged fluid becomes possible and makes them genuine superconductors. The situation is very different when there is a low density of the charged impurities embedded randomly in the boson fluid. In this case we anticipate formation of localized bubbles around impurities. Each bubble will contain a small number bosons. We find that at high densities the lowest energy state has no trapped bosons around the impurity. The first stable bubble appear at the critical \(r_s \approx 3.5\), which traps five particles. When the density decreases further a bubble with six bosons becomes stable. Similarly impurities away from the superconducting plane and weaker impurities become able trap bosons. This process continues until the density of non-localized charge carriers will be so low that a Wigner crystal is formed. We assume here a layered superconducting structure like in high \(T_c\) superconductors, where the superconductivity is coupled with the copper oxide layers, but impurities are scattered randomly in the three-dimensional space.

The charged bosons described above arise as local electron or hole pairs. Good candidates for local pairs could be resonance valence bonds (RVB) or bi-polarons. The BEC of local pairs may be responsible for the superconducting state of the underdoped cuprates. Then the superconductor-insulator (SIT) transition can happen through localized bubble phase as sketched above. A superconductor-insulator crossover which can be ascribed to SIT transition has been observed in underdoped cuprates, such as the superconductor yttrium barium copper oxide (YBCO), the superconductor bismuth strontium calcium copper oxide (BSCCO) and others [6, 7, 8, 9].

We can make an estimation of the critical density for \(La_2CuO_4\) where the dielectric constant \(\varepsilon_0\) has been measured in detail[10] and it is approximately equal to \(\varepsilon_0 \approx 30\). Taking into account this value and that the charge of the local pairs is equal to 2 we may estimate the Bohr radius.
for the charged boson which is equal to \( r_B = 3.5 \) Angstrom. The superconducting-insulator crossover has been observed in \( \text{Lu}_2-x \text{Sr}_x \text{CuO}_4 \) (known as LSCO) at the value \( x \approx 0.06 \). That effectively corresponds to the value \( r_s \approx 8 \) which is in agreement with our calculations. Using many-body theory, now let us describe microscopically, in detail, how the formation of these Coulomb bubbles and the SIT transition occur.

2. Variational theory

The microscopic, variational theory where positively charged, localized, random impurities are embedded into the two-dimensional charged boson gas assumes the Hamiltonian,

\[
H = H_b + H_I = -\sum_{i=1}^{N} \frac{\hbar^2}{2m} \nabla^2_i + \frac{1}{2} \sum_{i,j=1}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{\hbar^2}{2M} \nabla^2_0 - \sum_{i=1}^{N} \frac{e^2}{\varepsilon |\mathbf{r}_0 - \mathbf{r}_i|}.
\]

(1)

We have separated the purely bosonic part \( H_b \) from terms containing the impurity \( H_I \). The number of bosons is \( N \), they have the mass \( m \), charge \( e \) and position \( \mathbf{r}_i \). The impurity is placed at \( \mathbf{r}_0 \) and its kinetic energy is controlled by the mass \( M \). For a localized impurity we let the mass grow to infinity. We also add into the Hamiltonian a structureless, charged jellium, which neutralizes the system. The strength of the Coulomb interaction depends on the dielectric constant \( \varepsilon \). Both the boson mass and dielectric constant depend on the band structure of the material and it is convenient to use the atomic units where all distances are given in units of \( r_0 = r_s r_B \) and energies in Rydbergs.

The ground-state wave function without impurity contains correlations between pairs of bosons and we make the Jastrow-type variational ansatz

\[
\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = e^{\frac{1}{2} \sum_{i,j=1}^{N} u^{bb}(|\mathbf{r}_i - \mathbf{r}_j|)}
\]

(2)

The correlation function \( u^{bb}(|\mathbf{r}_i, \mathbf{r}_j|) \) is determined by minimizing the total energy,

\[
\frac{\delta}{\delta u^{bb}(\mathbf{r}_i, \mathbf{r}_j)} \frac{\langle \Psi | H_b | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0.
\]

(3)

The wave function of the system with the impurity,

\[
\Psi^I(\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_N) = e^{\frac{1}{2} \sum_{i=1}^{N} u^I(|\mathbf{r}_0, \mathbf{r}_i|)} \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N),
\]

(4)

contains then the impurity-boson correlation function \( u^I(|\mathbf{r}_0, \mathbf{r}_i|) \), which is determined by minimizing the chemical potential of the impurity. In other words the energy gained or lost by adding one impurity particle into the fluid,

\[
\mu^I = E_{N+1} - E_N = \frac{\langle \Psi^I | H_I | \Psi^I \rangle}{\langle \Psi^I | \Psi^I \rangle} - \frac{\langle \Psi | H_I | \Psi \rangle}{\langle \Psi | \Psi \rangle}.
\]

(5)

The solution of this problem in three dimensions has been studied in Ref. [11] and an instability is found at \( r_s \approx 14 \). The new phase is identified as a bound cluster by studying the boson scattering from the effective interaction with the impurity. A similar system of the positron annihilation in three-dimensional electron gas has been discussed in detail by Apaja et al. [12]. They have shown that fermionic corrections, when included in full, give only minor corrections to the purely bosonic results. They find an instability at densities of \( r_s \approx 10 \), which is slightly below the instability seen at the purely bosonic case.

In this paper we show that a similar instability is present also in the two-dimensional charged boson gas with oppositely charged impurities. We show here that this instability leads to a
spontaneous creation of Coulomb bubbles. The Coulomb bubbles form a percolating network and serve as the driving mechanism for the superconducting-insulator transition in that system. The key ingredients of the theory are, along with the correlation functions, the two-particle distribution functions,

\[ \rho^{bb}(\mathbf{r}_1 - \mathbf{r}_2) = n_0^2 g^{bb}(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\int d^2r_2 \ldots d^2r_N |\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2}{\langle \Psi | \Psi \rangle} \]

\[ \rho^{f}(\mathbf{r}_0 - \mathbf{r}_1) = \frac{n_0}{\Omega} g^{f}(\mathbf{r}_0 - \mathbf{r}_1) = \frac{\int d^2r_2 \ldots d^2r_N |\Psi^f(\mathbf{r}_0, \ldots, \mathbf{r}_N)|^2}{\langle \Psi^f | \Psi^f \rangle} \] 

(6)

where \( g^{bb}(\mathbf{r}_1 - \mathbf{r}_2) \) and \( g^{f}(\mathbf{r}_0 - \mathbf{r}_1) \) are the boson-boson and impurity-boson radial distribution functions, respectively, \( \Omega \) is the total volume occupied by the system and \( n_0 \) is the boson density. The Fourier transforms of the distribution functions define the static structure functions,

\[ S^{bb}(k) = 1 + n_0 \int d^2r e^{i\mathbf{k} \cdot \mathbf{r}} [g^{bb}(r) - 1] \]

\[ S^{f}(k) = n_0 \int d^2r e^{i\mathbf{k} \cdot \mathbf{r}} [g^{f}(r) - 1]. \] 

(7)

The additional information needed to solve the Euler equations (3) and in minimizing the chemical potential (5) is the connection between the correlation functions and the physically observable distribution functions. This is provided by the infinite order hypernetted-chain (HNC) equations [13]. These equations are derived by diagrammatic analysis of the radial distribution functions in terms of the two-particle correlation functions. We have also checked that elementary diagrams and triplet correlations give only negligible corrections at density range interesting interesting for this work [14] and thus we will ignore both of them. Within these well tested assumptions we can write the chemical potential of one charged impurity in the form [15, 16]

\[ \mu^I = n_0 \int d^2r \left[ -\frac{e^2}{\varepsilon} \frac{g^f(r) - 1}{r} + \frac{\hbar^2}{2m_{\text{red}}} |\nabla \sqrt{g^f(r)}|^2 \right] + \frac{1}{2} \int \frac{d^2k}{(2\pi)^2} n_0 S^f(k) \tilde{\omega}^I_{\text{ind}}(k) \] 

(8)

where \( m_{\text{red}} = mM/(m+M) \) is the reduced mass. The second term is induced by the many-body effects, where both ring- and ladder-diagrams are summed self-consistently [16]

\[ \tilde{\omega}^I_{\text{ind}}(k) = \frac{\hbar^2 k^2 S^f(k)(S^{bb}(k) - 1)}{4m} \left[ \frac{m}{m_{\text{red}}} S^{bb}(k) + 1 \right]. \] 

(9)

The chemical potential is now a functional of \( \sqrt{g^f(r)} \) and the Euler equation which minimizes \( \mu^I \) can be written as,

\[ -\frac{\hbar^2}{2m_{\text{red}}} \nabla^2 \sqrt{g^f(r)} + \left[ -\frac{e^2}{\varepsilon r} + \omega^I_{\text{ind}}(r) \right] \sqrt{g^f(r)} = 0. \] 

(10)

with the Fourier transform \( \omega^I_{\text{ind}}(r) \) of the induced interaction (9). Equation (3) defines the effective interaction

\[ V_{\text{eff}}(r) = -\frac{e^2}{\varepsilon r} + \omega^I_{\text{ind}}(r) \] 

(11)

experienced by bosons around the impurity in coordinate space. The perfect screening condition at long distances requires that \( 1/r \) tail of the Coulomb interaction is exactly canceled by the
induced potential. Eq. (3) preserves that condition, because in the long wavelength limit
$S^{I}(0) = 1$ and $(S_{bb}^{I}(k))^{2} \rightarrow \varepsilon \hbar^{2} k^{3}/8 \pi m^{2}$.

At short distances the 1/r potential dominates because the induced potential $w_{\text{ind}}^{I}(0) = \text{const.}$
This means that the radial distribution function must satisfy the usual the cusp condition of the
s-state wave function in a hydrogen-like atom,

$$\lim_{r \to 0} \frac{d\log g^{I}(r)}{dr} = -\frac{2}{r_{B}} \frac{m_{\text{red}}}{m},$$ (12)

and far away from the impurity $\lim_{r \to \infty} g^{I}(r) = 1$.

The integral of the effective interaction can be easily calculated by combining the Euler equation and the chemical potential,

$$n_{0} \int_{0}^{\infty} d^{2}r V_{\text{eff}}(r) = -\mu^{I} - \frac{1}{2} \int \frac{d^{2}k}{(2\pi)^{2} n_{0}} S^{I}(k) \bar{w}_{\text{ind}}^{I}(k) > 0.$$(13)

The chemical potential of a single impurity is always negative and dominates over the second
integral, hence making the integral of the effective interaction repulsive. In other words, many-body effects lead to over-screening of the attractive Coulomb interaction of a charged impurity and that makes the superconducting state possible in a two dimensional boson gas even when the impurities are present.

**Figure 1.** (Colour online) a) The radial distribution function $g^{I}(r)$, describing the distribution
of bosons around the impurity for $r_{s}$ values 1., 1.5, 2., 2.5, 3., 3.4 . The impurity is located at
the value $r = 0$.
b) The radial distribution function $g^{I}(r)$ for the same $r_{s}$ values as above, but now the focus is in
the region of the first minimum. One may see that when the value $r_{s} \to 3.4$ the boson density at
the minimum vanishes. This indicates the separation of boson liquid into two sides: the bosons
localised near impurity (CBs) and the rest, superfluid liquid.

### 3. Results

We begin by solving the Euler equation (3) for the distribution function positively charged
bosons around a negatively charged impurity embedded into the boson gas and calculating the
chemical potential of the impurity from Eq. (8). We assume that the impurity is localized and set its mass to infinity, $M = \infty$. At high densities the Coulomb attraction of the impurity is completely screened. The screening cloud collected by the impurity or in other words the distribution of particles around the impurity is described by the radial distribution function $g^I(r)$ which is plotted in Fig. 1a in the region of the impurity position, which is at $r = 0$ and in Fig. 1b in the region of the first minimum of this function. The height of the peak in $g^I(r)$ (see, Fig. 1b) increases rapidly with decreasing density or increasing $r_s$ and its width becomes narrower. The minimum (see, Fig. 1b) becomes deeper with increasing $r_s$ and it approaches zero at the instability.

At the same time $S^I(k)$ develops a large peak at about $k = 2.5/r_0$ as shown in Fig. 2a. The normalization sets $g^I(\infty) = 1$ and the perfect screening condition requires that $S^I(0) = 1$. The impurity chemical potential as a function of $r_s$ is shown in Fig. 2b. It has a maximum at about $r_s = 1.1$ and the value at this maximum equal -4.7 Ry is slightly below the binding energy of 4 Ry of the two-dimensional hydrogen atom (with an infinite mass of proton). When $r_s > 1.1$ the absolute value of the chemical potential monotonically increases. When the density decreases the Euler equation (3) has solutions only for $r_s \leq 3.4$. It indicate that at lower densities a CDW instability arises. As the result at $r_s \approx 3.4$ a cluster of self-trapped bosons or the CB is localized around the impurity. The self-trapping arises due to the over-screening of the Coulomb potential from an impurity. This effective Coulomb interaction results between the impurity and bosons consists of the sum of the induced potential $u_{\text{ind}}(r)$ and the bare Coulomb potential. The bound state of bosons in the Coulomb bubble is a result of the Coulomb attraction caused by the impurity and the repulsion by the other bosons in the fluid, which push them towards the impurity.

When a bubble a formed, the method described above must be extended to the quantum system with bound states. The boson-boson correlations remain the same as in the homogeneous fluid, but the bubble is treated as an extended impurity, which contains the charge of the impurity at the origin and the charge density of boson bound into the trap. The response of the
Figure 3. (Colour online) a) The part of the chemical potential associated with the individual impurity alone (presented by red curve with crosses) and the sum of the chemical potential of the bubble with impurity and the binding energy of \( N \) bosons inside the bubble. The curves are numbered by the number of particles \( N \). The total energy for \( N = 3 \) particles bound in a bubble is very close to the energy of homogeneous liquid with the embedded bare impurity (i.e. without a Coulomb bubble). The energy curve associated with \( N = 4 \) particles bound in the bubble begins roughly at \( r_s = 3 \) and it is always located below the red curve. b) The chemical potentials of bubbles with \( N \) bound bosons located inside the bubbles. When the bubble has \( N = 2 \) or \( N = 3 \) particles the value of the chemical potential is positive, which means that such bubble is repelled from the charged quantum boson fluid, i.e. cannot exist inside the charged quantum fluid. When \( r_s \geq 4 \) and \( N \geq 4 \) the associated value of the bubble chemical potential is negative and one gains energy in putting the Coulomb bubble into the charged quantum fluid.

The rest of the bosons is calculated by solving the Euler equation with the bare Coulomb interaction replaced with the combined interaction caused by the impurity and trapped bosons together and modifying in a similar way the chemical potential. The bound state wave function and their binding energy is then calculated from the effective Schrödinger equation

\[
-\frac{\hbar^2}{2m_{\text{red}}} \nabla^2 \phi(r) + \left[ -\frac{e^2}{\varepsilon r} + w_{\text{ind}}(r) \right] \phi(r) = E\phi(r) .
\]

where the induced potential is determined by all bosons in the system. That gives us the charge distribution of bosons \( |\phi(r)|^2 \) around the impurity with the normalization set equal to the number of bound particles

\[
n_0 \int d^2r |\phi(r)|^2 = N
\]

The distribution \( |\phi(r)|^2 \) is then inserted back to the calculation of the CB profile and the system of equations is iterated until self-consistency is reached, which happens within three-four iterations.

The chemical potential of the impurity alone (shown already in the Fig. 2b by red curve with crosses) and the sum of the chemical potential of the bubble and the binding energy of \( N \) bosons inside the bubble are presented in Fig.3a. The curves associated with the sum are numbered
by the number of particles $N$. The total energy for $N = 3$ bound particles is very close to the energy of homogeneous liquid with the embedded bare impurity. The curve associated with bubble having $N = 4$ bosons trapped begins roughly at $r_s = 3$ and is located below the red curve. The chemical potential of the bubble with $N$ bosons trapped into it is presented in Fig. 3b. With $N = 2$ and $N = 3$ its value is positive, which means that the bubble is repelled from the charged boson fluid, i.e. it can not exists there. When $r_s \geq 4$ and $N \geq 4$ the associated value of chemical potential is negative and the system gains energy when the Coulomb bubble is embedded into the charged fluid.

The effective screened potentials for different $r_s$ values are shown in Fig. 4a. The attractive Coulomb potential is overscreened by the induced potential shown in Fig. 4b. This basically plasmon mediated many-body interaction gives an increasing repulsive barrier around the impurity and oscillations in the tail. This barrier is created due to the collective many-body interaction. At $r_s \approx 3.4$ around the impurity the CB is formed. This is due to the Coulomb attraction of bosons to the impurity and their effective repulsion from the rest boson liquid. And this potential is stronger than the repulsive Coulomb interaction between the trapped bosons. As the result the Coulomb bubble consisting of a bound cluster of bosons is formed. These bosons are trapped inside the Coulomb bubble and are separated from the rest boson condensate by the large barrier surrounding the impurity.

The charge distribution around the impurity is given by $e (g_l (r) - 1)$, where $e$ is the charge of bosons. By integrating $e \int_0^r (g_l (r') - 1) d^2 r'$ we can evaluate the amount of charge accumulated around the impurity inside the radius $r$. The results are shown in Fig. 5a for $r_s$ values 1.1, 1.5, 2, 2.5, 3.0 and 3.4. The maximum of the integral is $\approx 5$. This means that five bosons are self-trapped and bound with the impurity within the radius $r \approx 1$ leaving us with a cluster of charge $5 \times e$ (e is the boson charge) where we have set that the impurity has the charge $-e$. The impurity has then effectively changed its sign and the newly formed CB pushes the rest of the bosons away revealing the negative background (i.e. having opposite sign to bosons). That is why due to this depletion area when integrated further the charge is reduced and becomes $e$ at infinity to compensate the charge $-e$ at the origin. This is shown in Fig. 5b where both the
charge distribution and the integrated charge are plotted.

(a) \hspace{1cm} (b)

**Figure 5.** (Colour online) a) The amount of charge around the impurity inside the radius \( r \) for \( r_s \) values 1., 1.5, 2, 2.5, 3, and 3.4, the higher the peak the larger \( r_s \) value. b) The charge distribution (green curve) and the charge inside the sphere of the radius \( r \) from the impurity (red curve) at \( r_s = 3.4 \).

4. The semi-quantitative picture of the Coulomb bubble formation

In order to understand how Coulomb bubbles are formed let us consider the distribution of bosons around an impurity calculated at the critical value \( r_s = 3.4 \) when the instability leading to the formation of Coulomb bubbles arises. It is represented by the impurity-boson correlation function \( g_I(r) \) shown as the red curve in Fig.6. After the instability when the Coulomb bubble is formed and the part of the bosons, which were located around the impurity, was dropped from the condensate the distribution of the condensate bosons around the Coulomb bubble was practically not changed (see, the black curve on the Fig.6. The black curve coincides with the red curve, when \( r > r_0 \)). Taking into account the neutralizing charge background, the total charge distribution is given by the green curve, see, the Fig. 6. One may see that at the value \( r > 2.8r_0 \) the system is charge neutral. Together with the charge of the impurity such charge distribution forms an attractive potential in which bosons are trapped. The number of the trapped bosons depends, of course, on how large is the potential well. More bosons will form larger potential well in which they will be self-trapped. In the present case this number of the self-trapped bosons is determined by the integral from the impurity boson correlation function \( \int_0^r g_I(r)dr \), provided that \( r < R \), where \( R \) is the radius of the Coulomb bubble. This integral is effectively the charge accumulated around the impurity and it is presented by the blue curve on the Fig. 6. One sees from this curve that this accumulated charge increases monotonically with the distance from impurity and then saturate forming a step. The value of the integral, at which this step arises, indicates on how many particles have been self-trapped in the Coulomb bubble. Here the step arises at the value about 5.4 show by the line in Fig. 6, and it indicates that 5 particles have been self-trapped in the Coulomb bubble. The green curve gives the charge distribution seen by these five particles. That comes from the jellium background of negative charge distribution. The integrated jellium charge with the impurity is, of course, equal to the number of bound bosons, which is 5 here, because the system is charge neutral. At large values of \( r_s \) the distribution of the total charge around the impurity is more step-like. This observation allows us to introduce the semi-qualitative model for the Coulomb bubble formation.
The number of trapped charges must be an integer number and the system has to adjust itself into the formation of bound states. After a bound state of $N$ bosons is formed its binding energy increases monotonically when $r_s$ increases. At somewhat larger $r_s$ than the critical value here a bubble with $N+1$ bosons becomes also bound with lower energy as shown in Fig. 3. Thus the formation of bubbles is a first order phase transition.

We have assumed above that bosons bound in the bubble retain their bosonic character. That may not be realistic if the size of hole- (electron-)pair is of the order of Bohr radius or larger. In such a case the trapped pairs must be treated as fermions with opposite spins. Because of the Pauli principle only one pair can occupy one bosonic state. However, the degeneracy of the hole
(electron) bands will allow more pairs up to the degeneracy factor to occupy the lowest state and the rest of the pair must find a higher lying bound state. The next state (2s state in hydrogen notation) becomes bound at $r_s \approx 12$ and then the bubble can trap more pairs.

4.1. Coulomb bubble in homogeneous charged liquid

Let us consider a homogeneous charged boson liquid with the density $n_0$. It is embedded on the neutralising background (Jellium background model). There are two different situations, when the Coulomb bubble is formed in homogeneous liquid and when the Coulomb bubble is formed around single impurities.

Let us assume that there in the charged liquid arises a bubble of the radius $R$. Let us estimate the energy of this bubble. Inside the bubble there is homogeneous charge distribution having a sign opposite to the sign of boson charges due to the neutralising background. Therefore due to this background inside the sphere of the radius $r$ there is a charge $-e_0 n_0 4\pi r^3/3$, where $e_0$ is the charge of bosons. This background charge produces the potential $U(r)$, which attracts and traps bosons into the bubble having the form:

$$U(R) = \frac{e_0 n_0 R^2}{6}$$

(16)

From this expression one sees that at the formation of the bubble the background charge is responsible for the surface energy. Inside the bubble each boson has also a kinetic energy equal to

$$E_k = \frac{\hbar^2}{8mR^2}$$

(17)

The total energy for the bubble with a single boson trapped will be equal to $E_1(R) = E_k + e_0 U(R)$:

$$E_1(R) = \frac{\hbar^2}{8mR^2} + \frac{e_0^2 n_0 R^2}{6e_0}$$

(18)

One sees that this expression has a minimum and therefore the bubble binding energy may be obtained by minimising this expression with respect to the bubble radius $R$. If the binding energy is lower than the energy of correlated liquid there an electronic phase separation will arise. However the single boson bubble is indistinguishable from the correlated liquid, it is just a convenient frame to view the Coulomb bubble. However the Coulomb bubble may trap more, ie $M$ particles. The energy of such multi-boson bubbles is equal to

$$E(M) = ME_1(R) + E_c(M, R)$$

(19)

where the second term is the energy of the Coulomb interaction existing between bosons self-trapped into the bubble. Obviously that $E_c(M, R)$ is always positive when $M > 1$, that is the multi-boson bubble although stable will have the energy higher than the single boson bubble. In summary we show here that due to the surface energy the bubble may trap more than one boson and such state will be locally stable. However due to the electron-phonon interaction taken into account one may show[2, 18, 19] that in some cases of the strong or intermediate electron-phonon interaction the multi-boson bubble will have the energy per boson lower than the single boson bubble (see, the next sections, below).

Now let us take into account the electro-neutrality condition of the Coulomb bubble. This means that to make the bubble of the radius $R$ charge-neutral one needs $M$ charged bosons, where

$$M = e_I + e_0 n_0 \frac{4}{3} \pi R^3$$

(20)
Taken into account this condition of the electrical neutrality by expressing the radius $R$ as the function of the number of particles $M$ and the energy of the Coulomb boson-boson interaction inside the bubble estimated in Hartree approximation $E_{Hartree} = \frac{M(M-1)c^2_{\text{b}}}{\epsilon_0 R}$, we obtain finally the energy of the Coulomb bubble, $E_M = E(R)/M$ in the form

$$E_M = \frac{1}{r_s^2(M - 1)^{2/3}} - \frac{1}{r_s(M - 1)^{1/3}} + \frac{M}{r_s(M - 1)^{1/3}} + \frac{(M - 1)^{2/3}}{8\pi r_s}$$

(21)

Here we have used atomic units, where the energy is expressed in $Ry = \frac{e^2}{2\epsilon_0\hbar^2}$

4.2. Coulomb bubbles induced by impurities.

The situation is drastically changed when there are charged impurities. In this case both the energetical and structural properties of the Coulomb bubbles are different. Let us assume that there is a single impurity there located in the point $r = 0$ and there around the impurity arises a spherical bubble of the radius $R$. Let us estimate the energy of this bubble. Without trapped bosons inside the bubble there is a homogeneous background charge distribution having a sign opposite to the sign of boson charges. This is the neutralising background which produces a surface energy of the bubble $U(R) = \frac{\pi n_0 R^2}{6}$. Together with the impurity this background charge produces the electrical potential $U(r)$, which attracts and traps bosons into the bubble:

$$U(r) = \frac{e_b n_0 r^2}{6} - \frac{e_I}{\epsilon_0 r}$$

(22)

where $e_I$ is the charge of the impurity.

There are two different types of states in such a bubble. The first type is when the bosons trapped may form a bound state with the impurity. The binding energy of a single boson with the impurity is equal to the conventional $Ry$, while for $M$ bosons in the same state it will be equal to $M Ry$.

Then the total energy of the Coulomb bubble with the charge complex consisting of the $M$ bosons bound with impurity and located inside the bubble is equal to

$$E(R) = M[-Ry + \frac{e_b^2 n_0 R^2}{6\epsilon_0} + \frac{M(M-1)c^2_{\text{b}}}{\epsilon_0 R}]$$

(23)

where number particles $M$ depends on $R$, see, eq.(20). Expressing $R$ via $M$ we obtain the final expression for $E_M = E(R)/M$ in the form:

$$E_M = -1 - \frac{1}{r_s(M - 1)^{1/3}} + \frac{M}{r_s(M - 1)^{1/3}} + \frac{(M - 1)^{2/3}}{8\pi r_s}$$

(24)

For the second type of states when the trapped bosons are unbound from impurity the total energy will be equal to:

$$E(R) = M[\frac{k^2}{8\pi R^2} + \frac{e_b^2 n_0 R^2}{6\epsilon_0} - \frac{e_I e_b}{\epsilon_0 R} + \frac{M(M-1)c^2_{\text{b}}}{\epsilon_0 R}]$$

(25)

In the limit of the low density we see from this expression that the surface energy is vanishing and for a single boson we recover the conventional hydrogen bound states of the boson with the impurity, ie in this limit the first and the second types of states coincide. By minimising the bubble energy with respect to the bubble radius $R$ we obtain that there are bound states of bosons here. At the density when this energy will be lower than the energy of the homogeneous correlated boson liquid per single particle, this single boson will be trapped by the impurity.
forming the bound state similar to that as an electron bound in the hydrogen atom. If we will use
atomic units such as \( m = 1, \ h = 2\pi \) and \( e_b = e_I = 1, \ e_0 = 1 \) we obtain that the energy \( E_1 \) will be
negative and the hydrogen type bound state will be definitely formed when \( n_0 < n_c = 0.0052658 \).
Such critical density corresponds to \( r_{sc} = (3/(4\pi n_c))^{1/3} = 3.57 \) (if we would have here a quasi-
2D system then the critical value would be equal to \( r_{sc} = 1/\sqrt[3]{\pi n_c} = 7.77 \)). However such single
boson state may arise even at significantly higher density or smaller \( r_s \) than \( r_{sc} \) when we will
compare the bubble energy \( E_1 \) with the energy of the charged boson liquid. These numbers
indicate obviously that such bound states will be formed on impurities located in the charged
boson liquid at the values of \( r_s \) significantly smaller than those values corresponding to the
Wigner crystallisation.

In summary we have shown here that due to the surface energy the bubble may trap more than
one boson and such state will be locally stable. Now let us make estimation of the dependence
of the energy of the Coulomb bubble for realistic physical parameters of the HTSC such as
LSCO, ie \( m = 2, \ h = 2\pi, \ e_b = e_I = 1 \) and \( e_0 = 30 \). Then we obtain the following dependence
presented on the Fig. 7, which is very striking. The Coulomb bubble has a minimum when the

![Figure 7](image_url)

**Figure 7.** The dependence of the energy of the Coulomb bubble on the number of particles self-
trapped estimated at the following physical parameters: \( r_s = 7.14, \ m = 2, \ h = 2\pi, \ e_b = e_I = 1 \) and \( e_0 = 30 \).

number of particles trapped inside is about 2 or 3 particles. The state of the bubble having
4 and 5 particles has very close energy as well. The present qualitative consideration has not
taken into account the correlation effects. But if the correlation effects would be taken into
account as above we have obtained that the Coulomb bubble will have the minimal energy when the number of particles self-trapped inside is equal to 5. In some sense these bubbles are very similar to electronic strings, discussed earlier (see, for details the review[18]), and which have been experimentally detected in Ref.[19]. Similar to those electronic strings our qualitative consideration also shows that there in real system may exist the bubbles with different number of bosons self-trapped, i.e. at the chosen values of the parameters this number of bosons inside the CB may vary here from 2 to 6 particles.

4.3. Two-dimensional Coulomb pancakes

Until now we have studied the formation of the CBs in 3D system. Now let us consider quasi-two-dimensional systems. In this case the Coulomb bubbles has the shape of the pancake and the charge neutrality condition has the form

\[ M = e_f + e_b n_0 \pi R^2 \]  

(26)

Then the total energy of the pancake-bubble is equal to

\[ E(R) = M \left( \frac{\hbar^2}{8mR^2} + \frac{e_b^2 n_0 R}{2e_0} - \frac{e_f e_b}{e_0^2 R^2} + \frac{M(M-1)e_b^2}{e_0 R} \right) \]  

(27)

where the boson density \( n_0 \) is now the density of the quasi 2D system (say, like hole density on CuO plane in the HTSC case). Doing exactly the same, i.e. expressing the number of particles in terms of the bubble radius or vice versa we estimate the total energy of the pancake-bubble as the function of the number of particles trapped. Now let us make an estimation of the dependence of the energy of the Coulomb bubble per particle for realistic physical parameters of the HTSC, taking, for example, the LSCO, i.e. \( m = 2, h = 2 \pi, e_b = e_f = 1 \) and \( e_0 = 30 \). Then we obtain the following energy-particle dependence presented on the Fig. 8. There the minimum of the total energy corresponds to \( M = 5 \) particles. However in this case it is convenient to express this dependence of the total energy on \( M \) explicitly. Then \( R = ((M - e_f)/(n_0 \pi e_b))^{1/2} \). Then, with the use of the parameters as above and expressing the radius as a number of particles trapped, \( R = ((M - 1)/(n_0 \pi))^{1/2} \), we obtain the final expression for the total energy \( E \) as the function of the number of particles \( M \) in the form

\[ E/M = \frac{1}{(M - 1)r_s^2} + \frac{(M - 2)}{\sqrt{(M - 1)r_s}} + \frac{\sqrt{(M - 1)}}{(2\pi r_s)} \]  

(28)

The present expression has been obtained when we have assumed that bosons are not forming the bound state with an impurity, but just self-trapped inside the pancake-bubble. However, there is a subtle issue here. Besides the case when free bosons are trapped in the pancake-bubble by a surface energy there may arise another situation, i.e. when bosons are trapped in the pancake-bubble and are forming also a bound state with the impurity. Indeed, as our microscopic calculations show this is precisely the situation which arises in the strongly-correlated charged system. In this case, the binding energy of each boson with impurity is equal to \(-4R_y\). If there are \( M \) bound bosons then the total binding energy will be equal to \( MR_y \). If we will count the energy from vacuum then the binding energy of \( M \) bosons with the impurity is equal to \(-4R_y(M-1)/M\). Taking into account the surface energy and the Coulomb interaction in the Hartree approximation we obtain the final expression for the energy per trapped particle in the form

\[ E/M = -4\frac{(M - 1)}{M} + 2\frac{\sqrt{(M - 1)}}{Mr_s} + \frac{1.17\sqrt{(M - 1)}}{r_s} \]  

(29)

This energy dependence has a single minimum. When the value of \( r_s = 3.2 \) this dependence is presented on the Fig. 9. One may see there that the minimum corresponds to the number of
Figure 8. The dependence of the energy of the Coulomb pancake-bubble on the number of particles self-trapped trapped in quasi-two dimensional system estimated at the following physical parameters: the boson density \( n_0 = 0.0052658 \), the effective mass \( m = 2 \), \( h = 2\pi \), the charge of bosons and impurities \( e_b = e_I = 1 \) and the dielectric constant \( \epsilon_0 = 30 \).

particles \( M = 5 \). This is exactly what we found in our microscopic calculations. When the value of the parameter \( r_s \) increases the number of particles trapped into the pancake-bubble and the binding energy of these self-trapped bosons increase.

5. Electron phonon interaction and Coulomb bubbles, microscopic many-body approach
In continuum isotropic approximation the local lattice distortions are usually described by the deformation vector \( \mathbf{u} \) so that each electron inside the crystal is interacting with the local lattice deformation as

\[
H_{\text{int}} = D \text{div}(\mathbf{r})
\]

(30)

where \( D \) is the deformation potential. Obviously, any deformation forms a potential which is in some sense reminds the potential of impurity. Therefore, we expect that there (into the impurity chemical potential) will be a contribution from the local lattice distortion in the from (see, Ref.[2], for details):

\[
\delta\mu = \int \Psi^* H_{\text{int}} \Psi d\mathbf{r}
\]

(31)

Taking into account the boson states localized in the vicinity of the impurity with the use of the electron-impurity correlation function we obtain the contribution from the lattice distortions, which has the form:
Figure 9. The dependence of the total energy of the Coulomb pancake-bubble per/particle $E/M = (E(R) - E_{\text{reference}})/M$ on the number of particles $M$ self-trapped in quasi-two dimensional system. The energy has been expressed in atomic units (ie, in the $Ry$) and estimated at the value of the parameter $r_s = 3.2$. In order to compare with vacuum we chosen the reference energy as equal to the binding energy of a single boson with the charge $e_b = 1$ bound with the single charged impurity in two-dimensions, ie $E_{\text{reference}} = -4Ry$.

$$\delta \mu = D \int (g^l(r) - 1) \text{div} u(r) \, dr$$  \hspace{1cm} (32)$$

Taken into account also the elastic energy of the lattice we have the complete expression for the impurity chemical potential in the form:

$$\mu_{\text{imp}} = \mu_0 + \delta \mu + \frac{K}{2} \int (\text{div} u)^2 \, dr$$  \hspace{1cm} (33)$$

where $K$ is an elastic modulus of the crystal lattice. By a minimization of the total impurity chemical potential with respect to the lattice deformations we have obtained the final contribution from the crystal lattice in the form:

$$\mu_{\text{imp}} = \mu_0 - \frac{D^2}{2K} \int (g^l(r) - 1)^2 \, dr$$  \hspace{1cm} (34)$$

Thus the electron phonon interaction contributes by an extra negative term into the equations. Because of that the local lattice distortions may also stimulate the localization of bosons into the Coulomb bubbles since this lowers the total energy or the impurity chemical potential.

6. Electron-phonon interaction and Coulomb bubbles, qualitative models
In this section we would like to show that due to the electron-phonon interaction taken into account [2, 18, 19] the binding energy of the boson bubbles will become stronger. To describe
these multi-boson (electron) bubbles we employ a Hartree (Hartree-Fock, in the case of fermions) approximation and consider the lattice effects in adiabatic approximation. In the present section we use the discrete lattice, the transition to a continuum limit is straightforward, i.e. by replacing the discrete index $n$ describing the lattice site by a continuum coordinate $r$. First we have to find relevant single particle wave functions. The discrete Schrödinger equations describing a single electron (hole) interacting with a lattice deformation, $\nabla \cdot \vec{u}_n$, in a tight-binding model on a hypercubic lattice has the form:

$$\frac{\hbar^2}{2m} \hat{\Delta} \psi_{np} + D \nabla \cdot \vec{u}_n \psi_{np} + U_n \psi_{np} = E \psi_{np} \tag{35}$$

where $\hat{\Delta}$ is the Laplacian operator and $\psi_{np}$ is the wave function of the $p-$th self-trapped boson (electron or hole) on the $n$-th lattice site, the value $D$ is the constant of deformation potential created by the deformation $\nabla \cdot \vec{u}_n$, and $U_n$ is the additional self-trapping potential from impurity and the neutralising background as described in the previous section, see equation(22).

With the use of the single particle solutions of the Schrödinger equation(35) and the Ritz variational principle we may build up the Hartree many-body wave function and estimate the total energy of the $M$ self-trapped bosons (electrons or holes) including the Coulomb energy and the energy of lattice degrees of freedom:

$$E_s = \sum_{n,p=1}^{M} \left( \frac{\hbar^2}{2m} \psi_{np}^* \hat{\Delta} \psi_{np} + D \nabla \cdot \vec{u}_n | \psi_{np} |^2 \right) + \sum_{n} \left[ \frac{K}{2} (\nabla \cdot \vec{u}_n)^2 + \frac{M_n}{2} \vec{u}_n^2 \right] + E_c, \tag{36}$$

where $K$ is a bulk elastic modulus, $M_n$ is the atomic mass, the index $n$ indicates a summation to be carried out over all lattice sites of the hypercubic lattice and $E_c$ is the Coulomb energy, which includes the energy of the boson-boson, boson impurity and boson background interactions.

Eqs. (35) may be obtained by a minimization of $E_S$ with respect to the boson (electron or hole) wave function $\psi_{np}$ provided that the wave function for the $p$-th trapped particle satisfies the normalization condition: $\sum_n | \psi_{np} |^2 = 1$. With the use of the adiabatic approximation and a minimization of $E_S$ with respect to the deformation $\nabla \cdot \vec{u}_n$ we obtain the system of discrete (or continuum) equations describing deformations created by $M$ self-trapped bosons (electrons or holes) in an isotropic elastic medium:

$$\nabla \cdot \vec{u}_n = -\frac{D}{K} \sum_{p=1}^{M} | \psi_{np} |^2 \tag{37}$$

where the index $p$ indicates a summation carried over all $M$ trapped bosons (electrons or holes). This deformation is purely due to $M$ bosons (electrons or holes) trapped by this potential. The overall potential $D \nabla \cdot \vec{u}$ is actually a superposition of individual potentials created by the individual particles.

With the use of this equation the deformation $\nabla \cdot \vec{u}_n$ can be easily excluded from the eq.(36). When the kinetic energy of the lattice (which is limited by Debye frequencies $\omega_D$) is much smaller than the energy of static deformation associated with the Coulomb bubble, which is here of the order of $MD^2/K$, we may use adiabatic approximation. It is clear that at large number of self-trapped particles $M$ the validity of this approximation is improved. Let us first for a simplicity neglect the Hartree(-Fock) term, then we get the adiabatic potential $A$ of the lattice in the form:

$$A = \frac{\hbar^2}{2m} \sum_{np} \psi_{np}^* \hat{\Delta} \psi_{np} - \frac{D^2}{2K} \sum_{npq} | \psi_{np} |^2 | \psi_{nq} |^2 \tag{38}$$
The first sum in $A$ represents the sum of single particle boson (electron or hole) energies. The extremal points (minima and maxima) of $A$ are determined with the aid of the following nonlinear Schrödinger equations:

$$\frac{\hbar^2}{2m} \hat{\Delta} \psi_{np} - \frac{D^2}{K} \psi_{np} \sum_{q=1}^{M} | \psi_{nq} |^2 = E \psi_{np}$$  \hspace{1cm} (39)

It is important to note that the overall deformatonal potential is a positive superposition of individual potentials of all $M$ bosons (electrons or holes) trapped by the deformation well.

In the Hartree approximation where all bosons trapped are descried by the same wave function the expression for deformation is simplified

$$\nabla \cdot \vec{u} = - \frac{MD}{K} | \psi_n |^2,$$

and so the adiabatic potential does:

$$A_{\text{Hartree}} = - \frac{\hbar^2 M}{2m} \sum_n \psi^* \hat{\Delta} \psi_n - \frac{M^2 D^2}{2K} \sum_n | \psi_n |^2 | \psi_n |^2$$  \hspace{1cm} (41)

Then with the single particle variational wave function such as $\psi_n \sim \exp(-n/R)$ or other one associated with the localized state (all such variational wave functions give very similar results which differ by numerical constants) one may estimate the total energy of the Coulomb bubble when the lattice deformations are taken into account. The semi-quantitative expression for the total energy of the Coulomb bubble $E(R) = E_{M}(R)$ has the form:

$$E(R) = M \left[ \frac{\hbar^2}{8mR^2} + \frac{e_b^2 n_0 R^2}{6\epsilon_0} - \frac{\epsilon_f \epsilon_b}{\epsilon_0 R} \right] + M \left[ (M-1)\frac{e_b^2}{\epsilon_0 R} - \frac{cM}{R^3} \right]$$  \hspace{1cm} (42)

where the coupling constant with lattice deformations $c$, is defined as $c = \frac{D^2}{K} \sum_n | \psi_n |^2 | \psi_n |^2$ and the energy of the Coulomb boson-boson interaction inside the bubble was estimated in electrostatic approximation.

Depending on the strength of the electron-phonon interaction $c$ the energy of the Coulomb bubble as a function of its radius $R$ and the number of particles self-trapped $M$ may have two minima. One of them is associated with the collapsed state. The minimum of this state having the smallest radius is not well defined in the continuum approximation. To estimate its position properly one have to go beyond the continuum approximation. This state is characterized by small radius and very strong local lattice distortions which can lead sometimes to the spontaneous defect creation[17]. The second broad minimum is well defined and corresponds to more extended state of the CB, which may trap many particles. These two types of states are separated by the self trapped barrier and due to this barrier may coexist with each other. Here for an illustration we present the dependence of the total energy of the Coulomb bubble $E$ on its radius $R$ at different number of particles $M = 3, 4$ and 5 calculated at the value $r_s = 3.57$ on the Fig. 10a and at the value $r_s = 7.14$ on the Fig. 10b. We can not say much about the collapsed state since the continuum approximation is breaking down at small distances, however the second extended state of CB and the self-trapped barrier are well described. However, here we have to take into account also the charge neutrality because each CB is screened by boson liquid and at large distance from the CB centre it is charge neutral. Now let us take into account this charge neutrality of the system (where number particles $M$ depends on $R$, see, eq.(20)), the energy of the local lattice distortions created around CB (se, eq.(42) and calculate the dependence of the energy of the Coulomb bubble on the number of the self-trapped bosons.
Figure 10. a) The dependence of the total energy of the Coulomb bubble $E$ on its radius $R$ at different number of particles $M = 3, 4$ and 5 and at the value $r_s = 3.57$ expressed in atomic units. The curve with the highest maximum corresponds to 5 self-trapped particles $M = 5$, this maximum separate the two states of the bubble, with $R \sim 12.5r_B$ and the collapsed state, at $R \to 0$. Such two states of the bubble exist also for the bubble with 4 trapped particles (the middle curve, $M = 4$). However, the bubble with 3 particles may exist only in the collapsed state, see the lowest curve, where $M = 3$ and there the maximum and the minimum, existing for $M = 4, 5$, disappear. b) The same energy as in a) but at $r_s = 7.14$. Here, besides the collapsed state associated with $R \to 0$ the maximum and the minimum exist for $M = 2, 3, 4$, and 5 particles. The energy is measured in boson Rydberg, while the bubble radius $R$ - in Bohr radius $r_B$. The value of the electron-phonon constant has been taken as $c = 10Ry$.

for realistic physical parameters of the HTSCs such as LSCO, ie $m = 2$, $h = 2\pi$, $e_b = e_I = 1$ and $\epsilon_0 = 30$. We have also taken the density such that the value $r_s = 15.54$. Then, we obtain the
following dependence of the CB energy on the number of particles $M$ presented on the Figure 11.

![Graph showing the dependence of CB energy on the number of particles](image)

**Figure 11.** The dependence of the total energy of the Coulomb bubble (measured in $R_y$) including the energy of the local lattice distortions on the number of particles self-trapped estimated at the following physical parameters: $r_s = 15.54$, $m = 2$, $h = 2\pi$, $e_b = e_f = 1$ and $e_0 = 30$ of the HTSCs such as LSCO. The upper, middle and lower curve correspond to the electron-phonon coupling $c = 1$, $c = 2$ and $c = 3$, respectively.

The three curves presented on the Figure 11 were calculated for each single value of electron-phonon coupling equal to $c = 1$, $c = 2$ and $c = 3$, respectively. Here the value of the coupling $c$ is measured in boson $R_y$. One sees that on the Figure for each curve there are always two minima. One of them is associated with the collapsed state, where the number of particles is always one (the type of the hydrogen impurity state). The second minimum is associated with the many-particle Coulomb bubble, which may exist even without electron-phonon interaction taken into account. In such a minimum the number of particles trapped inside the Coulomb bubble strongly depends on the electron-phonon coupling. This number of the trapped bosons increases when the value of the coupling $c$ increases. So, when the value of the coupling, $c = 1$, the number of particles trapped in the bubble is about 5. But when the value $c = 3$, the number of particles trapped in the bubble is about 30. One may notice also that many states of the bubble having different number of particles have very close energies as well, see the Fig. 11.

7. **CBs formation obtained in the framework of the Gross-Pitaevskii equation**

The dependence of the total energy of the Coulomb bubble on the number of particles may be also obtained with the use of the nonlinear equations, i.e. These equations are similar to those presented in previous section, where we have discussed the role of the electron-phonon interaction. As above we use here the discrete lattice. The discrete time-independent GP equation describing the boson condensate has the form:

$$
-\frac{\hbar^2}{2m} \Delta \psi_n + \phi_n \psi_n + g|\psi_n|^2 \psi_n = \mu \psi_n
$$

(43)
where $\hat{\Delta}$ is the Laplacian operator and $\psi_n$ is the condensate wave function and $\mu$ and $\phi_n$ are the chemical and electrical potentials of the condensate on the n-th lattice site. The chemical potential $\mu$ is found from the condition that the total number of particles $N$ in the condensate is related to the wave function by the eq.

$$N = \sum_n |\psi_n|^2$$  \hfill (44)

The GP equation has the form of the Schroedinger equation discussed in the previous section with the addition of an interaction term, where the coupling constant, $g$, is proportional to the scattering length of two interacting bosons $a_s$:

$$g = \frac{\hbar^2 a_s}{\pi n}$$  \hfill (45)

The electrical potential $\phi_n$ includes the additional self-trapping potential from a charged impurity and the neutralising background as described in the previous sections, see equation (22). The total energy density of the condensate has the form:

$$E_{GP} = -\frac{\hbar^2}{2m} \psi_n^* \hat{\Delta} \psi_n + \phi_n |\psi_n|^2 + \frac{g|\psi_n|^4}{4}$$  \hfill (46)

Then with the use of the variational function we may estimate the energy of the CB formed around an impurity in this condensate of interacting bosons. In the qualitative estimation it has the form similar to those expressions obtained above.

$$E(R) = M\left[\frac{\hbar^2}{8mR^2} + \frac{\epsilon_b^2 n_0 R^2}{6\epsilon_0} - \frac{\epsilon_l \epsilon_b}{\epsilon_0 R} + \frac{gM}{R^3}\right]$$  \hfill (47)

where $M$ is the number of particles in the CB which is related to the CB radius due to the charge neutrality condition, see eq. (20). Now if we take the scattering length $a_s \sim \tau_B$ and for all other parameters use the same values as in previous sections we obtain that the Coulomb bubble with $M \sim 2 - 3$ particles trapped around the impurity corresponds to an absolute minimum of the total energy.

8. **Coulomb bubbles made of electrons and holes**

It is interesting to note that similar Coulomb bubbles may arise in strongly correlated fermionic liquids, i.e. the bubbles are consisting of electrons and holes and are embedded in correlated fermionic liquid. The bosonic bubble can be also transformed into the bubble made of fermions when many bosons are self-trapped into the single bubble. This happens because bosons are usually made of two fermions (electrons and holes) and when many bosons are trapped at the same bubble their Coulomb interaction exceeds the binding energy of electrons and holes forming bosons. Then at the formation of the fermionic bubble we have to take into account the Pauli principle. Doing calculations similar to those presented in the previous section (see, eq.(energy-bubble-boson)) we obtain that the total energy of the fermionic CB is equal to:

$$E(R) = \frac{\hbar^2 M^{5/3}}{8m_h R^2} + M\left[\frac{\epsilon_b^2 n_0 R^2}{6\epsilon_0} - \frac{\epsilon_l \epsilon_b}{\epsilon_0 R} \right] + \frac{M(M-1)\epsilon_b^2}{\epsilon_0 R}$$  \hfill (48)

where $M$ is the number of particles in the fermionic CB and $m_h$ is the effective of the fermions (electron or holes) trapped in the CB. The number of particles trapped $M$ is related to the CB radius via the charge neutrality condition, see eq. (20). The first term in the expression for energy, eq.(48) is the kinetic energy of electrons or holes estimated with the Pauli principle taken into account.
Figure 12. The dependence of the energy of the Coulomb bubble (per particle trapped) \( E/M \) made of fermions (ie made of electrons or holes) on the number of particles self-trapped \( M \) estimated at the following physical parameters: \( r_s = 7.14 \), \( m_h = 2 \), \( h = 2\pi \), \( e_b = e_I = 1 \) and \( \epsilon_0 = 30 \).

From the Fig.12 one may notice that at the realistic parameters of cuprates the optimal number of fermions trapped in the CB is equal to 5. Also, the extended type of bosonic and fermionic CBs are very similar. The difference arises for CBs in which the bosons or fermions are bound on the impurity forming the collapsed state.

9. Summary
Thus, we described the following phenomenon of electronic phase separation(EPS) which arises with decreasing of the boson density \( n_0 \) or with increasing \( r_s \) parameter. The EPS arises due to a relative increase of the amplitude of the impurity induced CDW oscillations with respect to the boson density. With decreasing density the amplitude of this oscillation increases. At some critical density or \( r_s \approx 3.2 \) the amplitude of the first ripple, which has the highest amplitude among all other ripples of the CDW induced by given single impurity, will be equal to the boson density \(-n_0\). At this moment the instability arises. As the result this first ripple will be decoupled from the rest of the bosonic liquid forming an island around the impurity - the Coulomb bubble. At such critical value of \( r_s \) such Coulomb bubbles are formed around each single impurity. Then, there with the formation of many CBs the electronic phase separation arises. After that each island with impurity inside acts on the rest boson fluid effectively as a "new impurity" inducing around a charge density wave, like a single impurity at higher density. Due to a formation of such bubbles the boson density will be further decreased and will be equal to \( N_{new} = n_0 - MN_i \), where \( N_i \) is the density of impurities. The number \( M \) arises because \( M \) bosons are self-trapped around the single impurity.

At the next increasing value of \( r_s \) or decreasing density the amplitude of this CDW increases. The weaker impurities, which have lower charge or far remote position may take part in the EPS. Then at some next other critical value around these "new impurities" the new Coulomb bubbles
may be formed. For HTSC such impurities may have a position which is far remote from the superconducting CuO plane. The new Coulomb bubbles are formed in CuO plane, ie on some distance from these impurities. This new stage of EPS may be considered as a formation of a second shell of Coulomb bubbles with localized bosons around spots in CuO plane which are associated with impurities having far remote positions away from the CuO plane. With the next increasing value of \( r_s \) we may expect a formation of more shells with Coulomb bubbles having localized bosons from even more remote impurities. Note that all these CBs are formed in CuO plane.

The formation of this multi-shell structure in the network of Coulomb bubbles with increasing \( r_s \) is associated with a phenomenon of superconductor-insulator transition (SIT) which is going here via a EPS. There at the phase transition arise two phases. One is a superfluid quantum liquid of charged bosons. The second phase consists of boson bubbles (CBs) localized in CuO plane and associated with impurities around. The bubbles are seeds of the insulating state. The diameter of the bubbles slowly increases \( \sim r_s \) when the \( r_s \) increases while the number of particles in each bubble is fixed due to a large Coulomb charging energy. However the number of bubbles increases in steps. Each of these steps is associated with the formation of the new shell of charged Coulomb bubbles. Obviously when the radius of these bubbles will be significantly smaller than the distance between impurities the flow of bosons through the system will be superfluid. However when the distance between impurities will be equal to the bubble’s diameter there a full localization of bosons will arise and the new insulating phase, where all bosons are localized, emerges. Such a state will be not superconducting anymore although some superconducting islands may still exist due to inhomogeneous distribution of impurities and therefore - of CBs. The radius of superconducting islands will be increasing with temperature. The superconducting phase vanishes at the SIT via a proliferation of bubbles, which size increases with \( r_s \), which are localized in some spots associated with impurities around and which number increases by steps, when the boson density monotonically decreases. This is, of course, a quantum phase transition, which at the first stage has a first order character, ie there are nucleus of the new insulating state in the form of CBs. However, at the second stage such a transition reminds the percolation phase transition, ie, the insulating state is formed by a formation of infinite cluster of CBs. It is important that the main role here is played by the Coulomb interaction, namely by the over-screening effect. The role of interaction rises with increasing \( r_s \). There arises an overscreening. With over screening these Coulomb bubbles with localized bosons are formed. With increasing \( r_s \) more and more shells of Coulomb bubbles are formed and the localized states of these Coulomb bubbles proliferate into the superconducting state. As the result of such a percolation of the CBs there a superconductor-insulator phase transition arises.

The results obtained may be relevant to recent findings of the superconducting-insulating crossover by Ando et al [6, 7, 8, 9] in novel HTSC. It was found that metallic behavior has been already observed at 1% doping. Moreover the value of the in-plane resistivity \( \rho_{ab} \) at 1% of the doping is too high for two dimensional metal, ie \( \rho_{ab} \approx 300 \Omega \). That is probably related to a formation of the local pairs in this very underdoped regime[20], where the superconducting state is associated with Bose-Einstein condensation (BEC) of these pairs which are positively charged bosons. There are, of course, localized, negatively charged oxygen impurities. From this point of view we have a system which consists of exactly localized point impurities in the charged boson liquid. There the density of the bosons is controlled by doping. With decreasing doping the bosons are eventually localized around oxygen impurities as described in the present paper. Such a localization is not homogeneous in space and forms a density wave structure of the superconducting condensate stimulated by randomly distributed impurities.

Probably, such nanoscale structures of the superconducting condensate associated with CBs which are induced by oxygen impurities has been observed in experiments by Davis et
al[1, 21, 22]. They have studied the superconductor BSCCO samples with a scanning tunneling microscope (STM) having a very narrow tip, just a few atoms wide. Their measurements reported in detail in the Ref.[1] reveal that the source of the disorder is caused by oxygen ”dopant” atoms. The dopant oxygen atoms nestle between the copper-and-oxygen (CuO) planes and carry some negative charge $-2e$. The dopants leave behind positively charged ”holes” that are pairing and carry a supercurrent along CuO planes. When a large negative voltage from tip to surface has been applied, the current shot up in specific locations (spots), which are less than a nanometer wide. Our estimation for the diameter of the Coulomb bubbles in the experiments [1] is about 2nm. The more spots were found in samples with more oxygen doping, indicating that each such point is marking the location of an oxygen atom or a negatively charged impurity within superfluid positively charged boson gas. Moreover, the superconducting gap measured with STM by Davis et al vanishes near each oxygen dopant. This was a clear evidence that each oxygen atom damages the superconductivity in its neighborhood. The results by Davis et al[1, 21, 22] are in complete agreement with our theory. Indeed, according to our theory the superfluid density, which may be also associated with the amplitude of the superconducting gap, vanishes in the vicinity of the charged impurities associated here with these oxygen dopant atoms. These charged impurities induce Coulomb bubbles and therewith all complicated pattern in the form of nanoscale superstructures as described in the present paper.

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