From the Coulomb to Effective Interaction: Application to Bose–Einstein Condensation

S. A. Trigger\textsuperscript{a,b}\*<br>

\textsuperscript{a} Joint Institute for High Temperatures, Russian Academy of Sciences, 13/19 Izhorskaya St., Moscow, 127412 Russia<br>
\textsuperscript{b} Prokhorov General Physics Institute, Russian Academy of Sciences, 38 Vavilova St., Moscow, 119991 Russia; \textsuperscript{*} e-mail: satron@mail.ru

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Abstract—An expression for the short-range effective interaction potential of “quasinuclei” is derived based on the “pure” Coulomb interaction model. This model represents the equilibrium Coulomb system (CS) of interacting electrons and identical nuclei using the adiabatic approximation for nuclei and an arbitrarily strong (in general) interaction for the electronic subsystem (degenerate or nondegenerate). Based on general properties of the Coulomb interaction, it is shown that the Fourier component of the effective pair potential between “quasinuclei” is discontinuous at the wave vector $q = 0$ in the case of the weak interaction between electronic and nuclear subsystems. This discontinuity is important for Bose-condensed systems such as HeII and rarefied alkali-metal gases at temperatures lower than that of the Bose condensation transition when a macroscopic number of quasiparticles with momentum $q = 0$ exist. It is shown that there can be a spectral gap for single-particle excitations, which disappears in the normal state.

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Accurate models describing equilibrium systems of interacting particles are of fundamental importance. The most adequate model of real matter is the quasi-neutral non-relativistic system of electrons and nuclei interacting according to the Coulomb law. In the Coulomb system (CS), matter properties are almost completely controlled by the collective behavior of electrons and nuclei. This approach in statistical physics was primarily developed in the pioneering papers \cite{1–3}. Current concepts of the problem and extended references are given in \cite{4}.

The consideration of the CS is most general since it does not include fitting parameters of the interaction potential. However, even in the simplest case of identical nuclei, there are four independent parameters, i.e., the interaction parameter $\Gamma = e^2 n_e^{1/3} / T$, degeneracy parameters for electrons and nuclei $\lambda_e = \hbar^2 n_e^{2/3} / m_e T$, $\lambda_i = \hbar^2 Z n_e^{2/3} / m_i T$, and the nuclei charge $Z$, which leads to a wide variety of possible states and features for the CS properties. For hydrogen, $Z = 1$ and the situation is simpler (see the diagram introduced in \cite{5}) (see also, e.g., \cite{6}).

In many cases, at relatively low temperatures and densities, the model of “simple” (or “neutral”, or “ordinary”) matter is used, which represents a system of identical composite particles (in fact, quasiparticles for statistical systems, such as, e.g., gas of atoms) interacting with each other via effective short-range interaction potentials. The model of “simple” matter can be considered as a useful approach based on the introduction of quasiparticles (e.g., “atoms” in gases and condensed phases of matter) appropriate for a certain range of thermodynamic parameters \cite{1, 7}. The statistical theory of “simple” matter is based on the assumption that interaction potentials of “atoms” are known in advance (see, e.g., \cite{7}). Although such approach significantly simplifies the description of matter properties, it is associated with considerable ambiguity in the determination of the interaction potential.

A consecutive determination of the effective interaction potential of “atoms” is directly related to the problem of the transition from the CS concept (or the so-called “physical” model of electron-nuclear...
As is known, the quasi-neutrality condition \( n_e = Z_n n_i \) (where \( Z_n \) is the nucleus or point ion charge) provides elimination (cancellation) of diverging terms with zero wave vector \( \sum_{a,b} n_a n_b v_{a,b}(q = 0) \) in the perturbation theory series for a large CS class. Here subscripts \( a, b \) are notations for electrons and nuclei interacting via Coulomb potentials \( v_{a,b}(q) = e_a e_b / q^2 \) (or for electrons and point ions with charge \( Z_n \) in models of electron-ion plasma). However, as shown in [8], the quasi-neutrality condition is insufficient to provide identical results for the canonical ensemble and grand ensemble. The stronger condition

\[
v_{a,b}(q = 0) = 0
\]

is necessary for Coulomb potentials, which provides a self-consistent CS description. To all appearance, condition (1) was used for the first time in [2] when considering thermodynamic properties of a weakly nonideal plasma in the grand ensemble. Condition (1) has a deep physical meaning since there is no physical carrier of the interaction with momentum \( hq = 0 \).

The determination of the explicit form of the interaction potential between charged particles (Coulomb law) as a function of the distance between them in the field theory is based on the Fourier transform of the Maxwell equations. According to the field theory, the Coulomb potential controls the electrostatic interaction of charged particles; therefore, to determine the Fourier transform of the Coulomb interaction potential, the Poisson equation is used, which yields the following result for \( q \neq 0 \)

\[
v_{a,b}(q) = \frac{4\pi e_a e_b}{q^2}.
\]

In this case, the value of \( v_{a,b}(q = 0) \), according to the Poisson equation, remains indeterminate. At first sight, such indeterminacy is insignificant since, according to the classical field theory, it does not affect the physically measured values. Furthermore, taking into account Eq. (2), it is easy to determine the Coulomb law using the integral Fourier transform

\[
v_{a,b}(r) = \int \frac{d^3 q}{(2\pi)^3} \exp(iqr)v_{a,b}(q) = \frac{e_a e_b}{r}.
\]

In this case, condition (1) does not affect the form of the Coulomb interaction potential (3) in \( r \) space; however, it plays an important role for Bose-condensed systems where condensation occurs to the state with \( q = 0 \). However, as shown in [8] (see also [9]), Eq. (1) cannot be rigorously justified by the classical theory and requires consideration based on quantum electrodynamics. When constructing the statistical theory for the non-relativistic quantum CS, instead of integral Fourier transform (2) for the Coulomb potential, the Fourier series should be used,

\[
v_{a,b}(r) = \frac{1}{V} \sum_q \exp(iqr)v_{a,b}(q) = \frac{e_a e_b}{r}.
\]

Currently, in calculating the value of \( v_{a,b}(q = 0) \), it is mostly accepted to proceed from that the potential \( v_{a,b}(r) \) is known in the sense that its value is experimentally determined by the Coulomb law. In this case, according to the definition of the Fourier transform for the potential \( v_{a,b}(r) \) (3),

\[
v_{a,b}(q = 0) = \int_V d^3 r v_{a,b}(r), \quad \lim_{V \to \infty} V^{-1} v_{a,b}(q = 0) = 0,
\]

since the integral in (5) diverges as \( V^{2/3} \). On this basis, when determining the thermodynamic properties of a weakly nonideal plasma in [2] and charged Bose gas [10], the statement \( v_{a,b}(q = 0) = 0 \) was formulated from intuitive considerations taking into account the quasi-neutrality condition \( \sum_{a,b} n_a n_b v_{a,b}(q = 0) \) in the thermodynamic limit.

Following to [9], to solve the problem of the value of \( v_{a,b}(q = 0) = 0 \), we turn to the results of the quantum field theory, according to which charged particles interact with each other via the quantized electromagnetic field. In statistical quantum electrodynamics [11], we can speak of consistency of the Green function for the quantized electromagnetic field \( D_{\mu,\nu}(k) \) \((\mu, \nu = 0, 1, 2, 3; k = (\omega/c, \mathbf{q})\) and the interaction potentials between charged particles. In this case, the discrete momentum representation
should be used (see (4)) \[9\]. In this case, the potential 4-vector corresponding to the quantized electromagnetic field does not contain the term with \(q = 0\). Hence, the wave vector \(q\) in the Green function \(D_{\mu,\nu}(k)\) cannot be zero since there is no physical substance which would be the carrier of the interaction which results in the zero momentum transfer.

In the presence of an ensemble of charged particles, the Green function of the quantized electromagnetic field \(D_{\mu,\nu}(k) = 4\pi/k^2\epsilon\ell(k)\), where \(\epsilon\ell(k)\) is the longitudinal permittivity of the system of charged particles, describes the screened Coulomb interaction \[1\]. Thus, according to quantum statistics in electrodynamics, the statement (1) for \(v_{a,b}(q = 0)\) is satisfied in the sense that the Coulomb interaction potentials \(v_{a,b}(r)\) can be written as the Fourier series (4) which does not contain the term with \(q = 0\). Relation (1) and the quasineutrality condition were recently discussed in detail in \[5\] based on \[8\] and \[9\].

Hence, the problem of the effect of relation (1) on the form of the effective potential arises, which is essential for the consideration of Bose-condensed systems of composite bosons with zero momentum.

Let us consider a simple model of the effective potential for the case of the weak Coulomb interaction between electronic and nuclear subsystems. Due to the mass difference \(m_e \ll M_n\), where \(m_e\) and \(M_n\) are the electron and nucleus masses, respectively) we use the adiabatic approximation. As is known, the Fourier transform of the effective potential \(v_{n,n}^{\text{eff}}\) between ions (or nuclei) can be written as

\[
v_{n,n}^{\text{eff}}(q) = v_{n,n}(q) + v_{e,n}^2(q) \frac{\Pi_e(q)}{\epsilon\ell(q)},
\]

where \(\Pi_e(q)\) is the polarization function of the electron liquid with arbitrary strong interaction \(v_{e,n} = -4\pi Z_n e^2/q^2\) and \(v_{n,n} = 4\pi Z_n^2 e^2/q^2\). According to relation (1), we have \(v_{n,n}^{\text{eff}}(q = 0) = 0\), since \(\Pi_e(q = 0)\) is finite. At the same time, for \(q \to 0\), from Eq. (6), we come to the nonzero value of \(v_{n,n}^{\text{eff}}(q \to 0)\),

\[
v_{n,n}^{\text{eff}}(q \to 0) = -\frac{Z_n^2}{\Pi_e(q = 0)}.
\]

Taking into account that the long-wavelength limit of the polarization function is related to the screening length \(R_{sc}\) as \(\Pi_e(q = 0) = -1/(4\pi e^2 R_{sc}^2)\), we find a discontinuity at the point \(q = 0\) for the effective potential of nuclei, which is written as

\[
\Delta = v_{n,n}^{\text{eff}}(q \to 0) - v_{n,n}^{\text{eff}}(q = 0) = Z_n^2 4\pi e^2 R_{sc}^2.
\]

For a degenerate electronic subsystem with weak interaction, the screening length is \(R_{sc} = 1/k_{TF} = (\varepsilon_F/6\pi n_e e^2)^{1/2}\), where \(\varepsilon_F\) is the Fermi energy. For the typical electron density in metals \(n_e \simeq 5 \cdot 10^{22} = 7.5 \cdot 10^{-3}/a_0^3\), the screening length is \(R_{sc} \simeq 1.3 \cdot 10^{-8} \text{ cm} \simeq 2.4 a_0\) and screening is very efficient. The characteristic value of \(\Delta \simeq Z_n^2 \cdot 30.1 \cdot e^2 a_0^2\) and the characteristic spectral gap energy \(E_\Delta\) can be estimated as \(E_\Delta \geq \gamma n_e \cdot \Delta \simeq 0.4 \gamma Z_n^2 R_g\), where \(\gamma = n_e/n_n\) is the ratio of the number of particles \(n_e\) (in the nucleus model under consideration) in the condensate to the total number of particles (nuclei) \(n_n\). The appearance of the gap in the single-particle excitation spectrum was predicted in \[12\], \[13\]. According to this prediction, single-particle excitations and phonon-roton collective excitations are different in systems where a Bose–Einstein condensate exists. The existence of the gap between the condensate and excited states of quasiparticles can provide superfluidity at a sufficiently low condensate flow velocity, and the corresponding Landau superfluidity criterion leads to the disappearance of the superfluid motion at \(n_e \to 0\). The strong electron–nuclear interaction causing the existence of atoms will be considered elsewhere based on the Coulomb model of matter.

It was shown that the Fourier component of the effective pair potential between “quasineuclei” is a discontinuous function at the wave vector \(q = 0\), which leads to the existence of the gap in the single-particle excitation spectrum for Bose-condensed systems.

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