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Principles of theory of strongly coupled (nonideal) plasmas

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Strongly coupled plasma (SCP) is an electron-ion system where the number of charged particles N_D in the sphere of Debye radius is less than 1. Achieved are values of N_D about 10^{-1}-10^{-2}. Coulomb interaction energy between particles becomes comparable to the value of thermal energy in SCP. The expansions that use the smallness of Coulomb to thermal energy ratio fail for SCP. Non-degenerate SCP is treated in the paper.

Plasma waves and collective degrees of freedom. Plasma waves are the foundation of the SCP theory as for the conventional plasma where $N_D > 1$. The collision mechanism changes when N_D becomes less than 1 because of the change of screening radius from the Debye value to the average interparticle distance [1]. For that reason the maximum value of the damping decrement to plasma frequency ratio does not exceed 0.2 and plasma waves exist in the whole area of SCP parameters [2]. Another plasma characteristic is the number *s* of collective degrees of freedom introduced by Bohm. *s* is proportional to the inverse value of N_D and reaches its maximum for SCP [1]. Therefore, the subsystem of free charges in SCP can be described as a system of the collective variables with relatively small interaction between them. This presentation opens up the way to the development of SCP theory.

Spectra of bound and localized electron states. These states supplement the collective variables. Quasi-classical bound states give another oscillatory mode. Interaction between oscillatory modes of Langmuir plasma waves and electron bound states results in: (a) limitation of the bound state spectrum, (b) repulsion between dispersion curves of plasma waves and bound states and (c) formation of the soft energy gap between spectra of bound and free electrons. The concept developed is checked by the comparison with experimental optical properties of SCP: shift, broadening, merging and absolute intensity of spectral lines and photoionization (recombination) spectra of SCP of diverse chemical species [3].

Transformation of bound and free states spectrum is presented in Fig. 1. The value of J is compared with U in Anderson localization. The value of J fluctuation ($\cong 4J$) is compared with Δ in Lifshits localization. The cases for ideal, nonideal and liquid-metal plasmas differ remarkably because J grows exponentially with N, U grows slowly as $N^{1/4}$, Δ_1 and Δ_2 do not depend on N, the energy ε_{IT} of jump from Δ_1 to Δ_2 grows slowly as $N^{4/15}$.

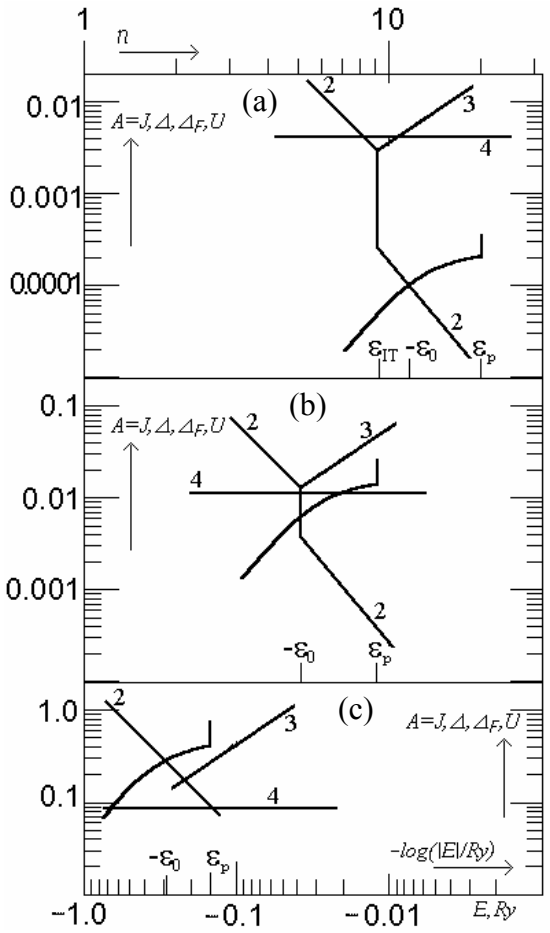

Fig. 1. Schematic illustrations of the relation between characteristic energies for three examples ($T \cong 1$ eV, $N = 2n_e$) of different cases: *a* – ideal plasma ($N \sim 10^{16}$ cm^{-3}), *b* – nonideal plasma ($N \sim 10^{18}$ cm^{-3}), *c* – liquid-metal plasma ($N \sim 10^{21}$ cm^{-3}). Horizontal axis presents the values of the principle quantum number n (upper horizontal) and the corresponding hydrogen-like energies (lower horizontal) of the isolated atom $E_n = -Ry/n^2$, Ry is the Rydberg constant. Vertical axis presents the values of $4J$ (line 1), Δ (step-wise dependence 2), Δ_F (line 3) and U (horizontal 4). J is the averaged value of the overlapping integral $J^{nlm}{}_{n'l'm'}(R)$ between neighboring ions, where n, l and m (n', l' and m') are principal, orbital and magnetic quantum numbers of the first (second) ion, $R = |r_1 - r_2|$, r_1 and r_2 are ion radius-vectors; the dependence $J_n(R) \equiv J^{n00}{}_{n00}(R)$ is found numerically; the dependencies $J(E_n)$ correspond to inter-ionic distances R for different values of N. Δ is the spacing of atomic energy levels; $\Delta = \Delta_1 = 2Ry\, n^{-3}$ for small Stark splitting; $\Delta = \Delta_2 \cong Ry\, n^{-4}$ for large Stark splitting; $\Delta(n)$ jumps from $\Delta_1(n)$ to $\Delta_2(n)$ at $\Delta_1(n) = \Delta_F$; it corresponds to the Inglis-Teller formula. $\Delta_F \cong 3ea_0Fn^2 \cong 13e^2a_0n^2N^{2/3}$ is the Holtzmark splitting which is valid for both ideal and non-ideal plasmas as Monte Carlo calculations showed. F is an average microfield. $U \cong e^{3/2}(NT)^{1/4}$ is a fluctuation of the potential energy

a – The intersection of $\Delta_1(E_n)$ with $\Delta_F(E_n)$ corresponds to the Inglis-Teller merging at $E_n = \varepsilon_{IT}$, since ε_{IT} is less than $|\varepsilon_0|$; the energy ε_0 corresponds to the intersection of $4J(E_n)$ with $\Delta(E_n)$. The electron states are one-centered (atomic) for $E_n < \varepsilon_0$, as electrons are localized both to Anderson ($J < U$) and Lifshits ($4J < \Delta$) criteria. The overlapping of Stark components results in the Inglis-Teller continuum, which is formed by individual atoms.

b – the intersection ε_0 of $4J(E_n)$ with $\Delta(E_n)$ occurs on the vertical part of the $\Delta(E_n)$ dependence. The energy ε_0 substitutes ($-\varepsilon_{IT}$). The Inglis-Teller continuum disappears. The non-overlapping discrete atomic states survive to the left side from ε_0. The region to the right side from ε_0, where $U > J > \Delta/4$, is formed by multi-centered quantum states of electrons localized in long-wavelength fluctuation of micropotential. This region corresponds to the soft gap in optical spectra. $J(E_n)$ tends to infinity at a certain energy ε_p. The states in the interval $\varepsilon_p < E < \varepsilon_f$ can be treated as multi-centered classical states localized in the fluctuation of

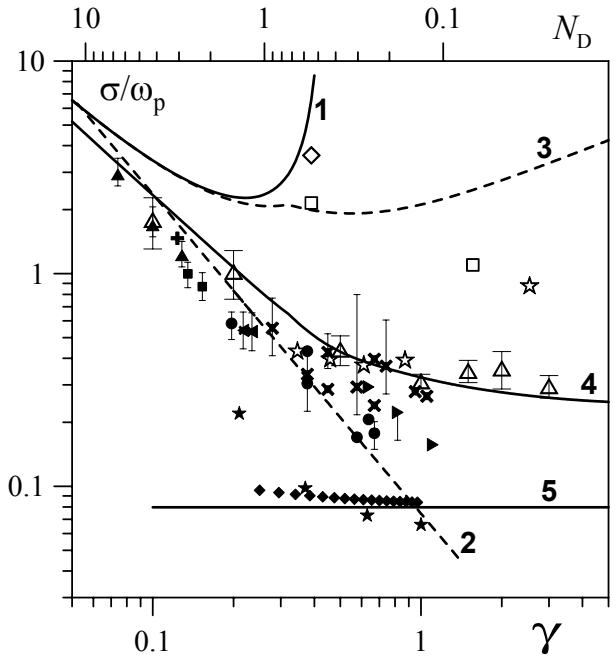

Fig 2. Static electrical conductivity versus nonideality parameter. Filled symbols are different experimental data; empty symbols are MD results: rhombus and squares – [4], triangles – our results, asterisks – Apfelbaum E.M., Ivanov M.F., 2001. Theoretical curves: 1 – Spitzer formula, 2 – the same with fixed Coulomb logarithm ($L_e = 3$), 3 – the same with $\Lambda_e = (\Lambda^2 + 1)^{1/2}/2$, 4 – [5] where the scattering of electrons by plasma waves is taken into account, 5 – $\sigma = \omega_p/4\pi$.

micropotential. Using the one-electron density of states is not valid in SCP. States $E > \varepsilon_f$ describe infinite free motion. The values of ε_p and ε_f can be estimated from the percolation theory. The border between the cases *a* and *b* corresponds to $N \cong 0.5\times10^{18}$ cm^{-3}. It coincides with the border between ideal and nonideal plasmas at $T \cong 1$ eV

c – the intersection ε_0 of $4J(E_n)$ with $\Delta(E_n)$ occurs on the $\Delta_1(E_n)$ part of the $\Delta(E_n)$ dependence at $N > 0.5\times10^{21}$ cm^{-3}. It means that delocalization takes place both to Anderson and Lifshits criteria. The whole region $(-\varepsilon_0) < E < \varepsilon_f$ is a precursor of the valence zone.

Thermodynamics and conductivity. The smallness of the thermal de Broglie wavelength to average inter-particle distance ratio is used to obtain the thermodynamic functions and equation of state of SCP. The pseudopotential model is used together with the plasma wave and bound state contributions. Plasma waves contribute to the effective electron collision frequency and, therefore, influence a number of SCP properties, for example, electrical conductivity (Fig. 2).

Stochasticity of particle trajectories. The inherent feature of MD system is the Lyapunov instability, i.e. divergence of particle trajectories [6]. Due to this divergence there appears a dynamic memory time t_m that limits the time interval when a solution of the Cauchy problem is valid for MD numerical integration. For times greater than t_m MD trajectory ``forgets" its initial conditions and ceases to correlate with the hypothetical Newtonian trajectory with the same initial conditions. The value of t_m depends on the Lyapunov expo-

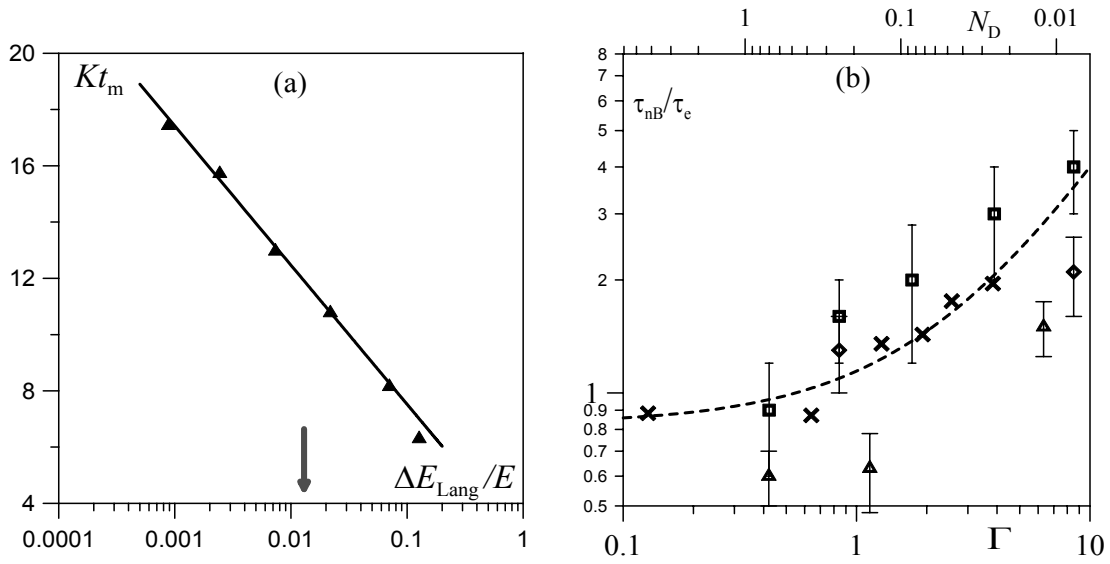

Fig 3. (a) Dependence of $K\,t_m$ on the fluctuation of the total energy caused by the additional Langevin forces. The arrow corresponds to the vibration of ions in water electrolyte.

(b) The value of τ_{nB} depending on the nonideality parameter for different initial conditions: $T_i(0) = 0$, crystal — circles, $T_i(0) = 0$, quasirandom — squares, $T_e(0) = 0$ — rhombus, $T_e(0) = T_i(0) = 0$ — triangles. Crosses correspond to t_m, dashed line is drawn to guide the eye. $\Gamma = 1.28$.

nent K and a noise that initiates the trajectory divergence. Such noise could be simulated e.g. by additional Langevin forces which result in fluctuation of the total energy E_{Lang} (Fig.3, a).

The distinguishing feature of relaxation in two-temperature SCP [7] is a nonexponential stage of the relaxation for $t < t_{nB}$ that precedes the exponential one. The value of τ_{nB} depends on the initial conditions but stays comparable with t_m (Fig.3, b). The next stage of relaxation is the exponential one (see [2]).

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