MINISTRY OF EDUCATION AND TRAINING
HANOI PEDAGOGICAL UNIVERSITY 2
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TRAN THI NHAN

STUDY ON SOME MICRODYNAMIC BEHAVIORS OF LIQUID WATER

Major: Theoretical Physics and Mathematical Physics
Code: 9 44 01 03
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SUMMARY OF DOCTORAL THESIS IN PHYSICS

Ha Noi - 2020

INTRODUCTION

1. Motivation

Water is studied by interdisciplinary science, including physics, chemistry, and biology. A great attention of researcher has been paid for water with an impressive accomplishment. However, the nonlinear microdynamics of liquid water and aqueous solutions is not still thoroughly understood, needing a further investigation.

In 1974, using Molecular Dynamics (MD) simulations, it was proposed the coexistence of the fast sound (3050 m/s) and the common sound (1500 m/s) in liquid water. A great number of experimental works whose results supported the coexistence of the two modes. According to the viscoelastic model, neither the forming nor the breaking of the hydrogen bonds can occur as the frequency $\Omega > 1/\tau_F$. Liquid water behaves in its glass-like regime, leading to the propagation of both the modes. The two-mode interaction model proposed that the two branches are originated from splitting of the longitudinal branch due to the interaction between elementary excitations of the linear dispersion mode and those of the dispersionless mode. The dispersion relations with the presence of the coupling coefficient $\beta(Q)$ between each other were suggested on the phenomenological basis. However, the microscopic mechanism responsible for the presence of the fast mode, its spectrum, and the splitting of the two modes remains still insufficiently understood.

The temperature dependence of the water permittivity below 1 MHz with the isopermittivity point at $\omega_{iso} \approx 3000$ Hz was observed. However, there is lacking a theoretical model originated from solid arguments interpreting its dispersion. In addition, the work of S. Li *et.al.* (2014) reported the conductivity dispersion of electrolyte solutions in the range of GHz frequency via combining Debye-Drude theory and experimental data with interesting results. The microscopic mechanism responsible for the dispersion of microwave conductivity needs a further study.

Electrostatics of dilute electrolyte solution is linear and it is carefully studied. However, it exhibits the nonlinear property for concentrated solutions. The microscopic mechanism responsible for the nonlinear electrostatics such as the decrement in the permittivity and the increase in the specific conductivity is being a hot topic for research with different points of view.

As mentioned above, it remains several open topics about the nonlinear dynamics of water systems in relation to the interaction between liquid water and electromagnetic field. In order to take part into further clarification on the microscopic dynamical mechanisms responsible for some complicated microdynamic behaviors of water and aqueous solutions, we select the topic "**Study on some microdynamic behaviors of liquid water**" for this doctoral thesis.

2. Purposes, objectives, and scopes

The thesis only focuses on studying several nonlinear microdynamic behaviors of liquid water and aqueous solutions in relation to the interaction between liquid water and electromagnetic field, specifically as:

- Developing a theoretical model to describe the dispersion of the collective density oscillations of liquid water in the THz region and illuminating their dynamic mechanism.
- Interpreting the dispersion of low-frequency permittivity of

liquid water and pointing out the science behind the isopermittivity point.

- Providing a model for the dispersion in microwave conductivity of electrolyte solutions in GHz range and clarifying its dynamic mechanism.
- Investigating nonlinear electrostatics such as the decrement in the permittivity and the increase in the conductivity of electrolyte solutions.

Our research further contributes to new research results on water dynamics in hope to promote study about chemical and biological interactions.

3. Research methods

We use several methods: combination and customization of theoretical techniques used in solid physics, modeling and numerical calculations, statistics, similarity, data analysis and so on.

4. Thesis outline

Besides the parts of Introduction, Conclusions, and References, the thesis includes:

- **Chapter 1** *Properties and complicated behaviors of water*
- **Chapter 2**: *Some dynamic features of liquid water*
- **Chapter 3**: *Microwave electrodynamics of electrolyte solutions*
- **Chapter 4:** *Nonlinear electrostatics of electrolyte solutions*

Chapter 1

PROPERTIES AND COMPLICATED BEHAVIORS OF WATER

In this chapter, we attempt to outline some fundamental properties and complicated behaviors of water and aqueous solutions in order to find out open topics for research.

1.1 Anomalous properties of liquid water

It was pointed out that water possesses about 72 different anomalous features. The anomalous properties are rather derived from the unique property of hydrogen bonds, the small size and the polarity of water molecules.

1.2 Dielectric constant of water systems

There are numerous of experimental data about the water dielectric in the range from MHz to THz given by different methods. Several mathematical models have been developed for macroscopic description of the complex permittivity. One of the most well-known semi-empirical models is Debye equation, describing dielectric relaxation not only for liquid water but also for electrolyte solutions as interaction between water molecules is not significant. In fact, there is an interaction among dipoles. Therefore, it is necessary to improve the Debye equation by adding empirical parameters, for examples, models of Cole-Cole, Cole-Davidson, and Havriliak-Negami. The information on the structure and dynamics of the liquid water or aqueous systems could be revealed as the relation between the permittivity and microscopic features is established. The microscopic mechanism responsible for the relaxation of the permittivity of pure water and aqueous solutions is being studied with surprise and interesting results.

1.3 Outstanding microdynamics of liquid water

In liquid water systems, the hydrogen bonding makes particles response collectively with external excitation besides diffusion. The diffusive motion is quite complicated, consisting of reorientation diffusion and self-diffusion.

Liquid water is a plasma of $H^{+\delta}$ cations and $O^{-2\delta}$ anions (δ - reduced electron charge) due to the strong polarity of water molecules. Charge particles in oscillation can radiate an AC Electromagnetic (EM) field. This field can couple with collective density oscillations, resulting in complicated phenomena. Applying plasma, plasmon, Phonon Polariton (PP) theories allows us to further understand dynamic properties of the water systems.

Chapter 2

SOME DYNAMIC FEATURES OF LIQUID WATER

In this chapter, we study the dynamic mechanism responsible for the coexistence of the common sound mode and the fast mode on the basis of PP theory. In addition, a simple model with two separated arguments is developed for interpreting the dispersion of low-frequency water permittivity and illuminating the science behind the appearance of the isopermittivity point. The material presented in this chapter forms the basis of the second and the fourth papers in the list of the author's works related to the thesis.

2.1 Modified PP model

Water dynamics closely relate to the fluctuation of molecules, diffusion, interaction among molecules, breaking and forming hydrogen bonding network. As the frequency of collective density fluctuations is higher than ω_F, traverse phonons emerge. In addition, water is considered as a plasma. The fluctuation of dipoles could radiate a local EM field with frequency ω aboutTHz whose wavelength is approximate 10 μm. The coupling of the traverse mode with the local EM field leads to the appearance of the high-energy mode and the low-energy one whose dispersion satisfies PP theory

$$\Omega_{\pm}^2(Q) = \frac{1}{2}\{\frac{c_0^2}{\varepsilon_{\infty 1}}Q^2 + \omega_{L1}^2 \pm [(\frac{c_0^2}{\varepsilon_{\infty 1}}Q^2 + \omega_{L1}^2)^2 - 4\frac{c_0^2}{\varepsilon_{\infty 1}}Q^2\omega_{T1}^2]^{1/2}\}, \tag{2.1}$$

where $\varepsilon_{\infty 1}$ is the dielectric response of liquid water at high frequency, ω_{L1} and ω_{T1} are the longitudinal and the transverse resonance frequencies, Q is the wave vector, and c_0 is the speed of light in vacuum

2.2 The main results of modified PP model

The modified PP model with the two dispersion relations describes quite well the dispersion of two modes on both the quality and quantitative sides, travelling with $v_f \approx 3050\ m/s$ in the large region of Q and $v_s \approx 1500\ m/s$ as $Q \to 0$, in agreement with experimental data (Fig. 2.1). The spectrum of both the modes is determined from ω_F (Frenkel frequency) to Debye frequency $\omega_D \approx 40$ meV. As a consequence, the wave vector of the spectrum is from Q_F to Q_D (about from 0.4 Å^{-1} to 1.2 Å^{-1} at room temperature). Rising temperature T makes ω_F increase. Therefore, it is predicted that the spectrum range becomes more narrow as increasing T. It is seen that the band gap is located between ω_{T1} and ω_{L1}.

The transformation from hydrodynamics to glass-like regime at frequency ω_F leads to the change in some dynamic parameters that could be estimated. Below Frenkel frequency, shear modulus is not supported. In the glass-like regime, there is the presence of the low- and the high-frequency moduli whose values are determined, $G_m = \rho_d v_s^2$ and $M_m = \rho_d v_f^2$ (ρ_d is the mass density of water,v_f - speed of fast sound and v_s - speed of common

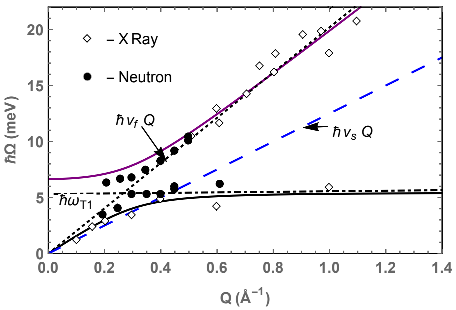

Fig. 2.1. Dispersion of the collective density oscillations model versus Q: The upper solid curve - the fast mode; The lower curve - ordinary one; The dot-dashed - transverse phonons with frequency ω_{T1}; The symbols - experimental data.

one). Therefore, the viscosity at low and high frequencies could be given, $\eta_s = G_m\tau_F$ and $\eta_f = M_m\tau_F$.

According to the model and Lyddane- Sachs-Teller relation, the dielectric constant of liquid water can be estimated $\varepsilon_{\infty 1} = c^2/v_f^2 \approx 5.46$ at approximately 10 THz and $\varepsilon_{01} \approx 8.05$ at about 1 THz. The change in dielectric constant versus frequency represents an electro-acoustic correlation. Indeed, the collective density fluctuations make the distribution of electrons around hydrogen and oxygen atoms periodically distort, resulting in the change of the dielectric constant.

The group and phase velocity corresponding to the high-energy mode of collective density oscillations could be defined $v_{gf}(Q) = \frac{d\Omega_+(Q)}{dQ}$ and $v_{pf}(Q) = \frac{d\Omega_+(Q)}{Q}$ (Fig. 2.2). Because $v_{gf}(Q) = v_{pf}$(Q)≈ 3050 m/s at room conditions, we could infer that the collective density vibrations in the large Q-region and high frequencies could perform the function of information propagation into organics. The phase velocity and the group speed for the low-frequency mode are also given in similar way.

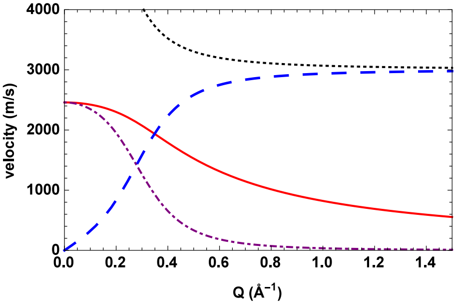

Fig. 2.2. Phase and group speeds - dashed and dotted curves for the high-frequency mode; the solid curves - phase speed and dot-dashed - group speed for the low-frequency mode.

2.3 Microscopic approach for low-frequency dielectric constant

We suggest that the dispersion of the permittivity is in the relation with two separated arguments, in agreement with the common theory about the isosbestic point. The first argument relates to the rotation of dipoles in the direction of electric field, depending on T. Because the thermal noise leads to the difficulty in polarization of dipoles, increasing temperature makes this argument decrease. We propose

$$\varepsilon_{dip}(T) = D_1 exp(\upsilon_1 \frac{T_0 - T_i}{T - T_i}) + \varrho_\infty, \tag{2.2}$$

where ϱ_∞, D_1 and υ_1 are constants, $T_i = 273$ K, and $T_0 = 293$ K is the room temperature. The second argument is in relation to the motion toward the electrodes of ion pairs created from Maxwell-Wagner-Sillars effect, depending on both T and ω

$$\varepsilon_{ion}(\omega, T) = B_{ion}(T) exp[-\beta_{ion}(T)\omega]. \tag{2.3}$$

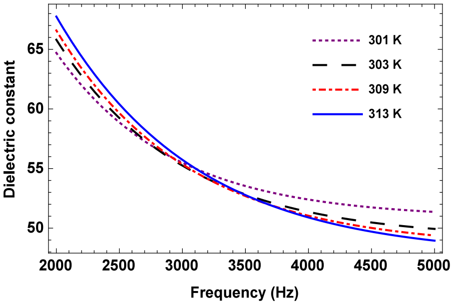

Fig. 2.3. The $\omega-$dependence of $\varepsilon(\omega, T)$ in the model.

In the relationship (2.3), we suggest that

$$B_{ion}(T) = \alpha_{ion} + \theta_{ion} exp[\frac{-\eta_{ion}(T_0 - T_i)}{T - T_i}]$$

$$\beta_{ion}(T) = a_{ion} + b_{ion}\frac{T_0 - T_i}{T - T_i},$$

in which α_{ion}, θ_{ion}, η_{ion}, a_{ion}, and b_{ion} are constants. The appearance of $B_{ion}(T)$ and $\beta_{ion}(T)$ in $\varepsilon_{ion}(\omega, T)$ illustrates the pH reduction upon temperature, leading to the decrease of water dielectric constant.

The dispersion of the low-frequency permittivity is written by

$$\varepsilon(\omega, T) = \varepsilon_{dip}(T) + \varepsilon_{ion}(\omega, T). \tag{2.4}$$

All constants in Eq. 2.4 are given on the basis of the general theory about isosbestic points and experimental data.

2.4 Dynamical mechanism of the isopermittivity point

The dielectric constant $\varepsilon(\omega, T)$ decreases as rising frequency and vice versa at a definite temperature with the existence of the isopermittive point at ω_{iso}, in agreement with experimental results with a small deviation (Fig. 2.3 and 2.4). As increasing T, the first component increases while the second component decreases at frequencies below ω_{iso} or vice versa above ω_{iso}. Thus, both the effects compensate each other, resulting in the isopermittivity point at ω_{iso}.

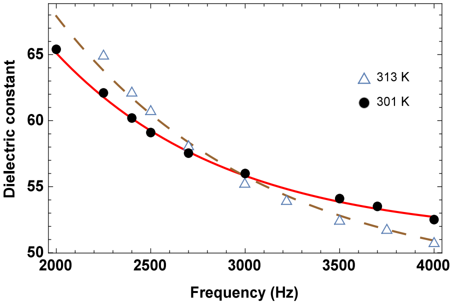

Fig. 2.4. Comparing dielectric dispersion of liquid water in the model at 301K (solid curve) and 313K (dashed one) with experimental data.

2.5 Van't Hoff effect and isopermittive point

At the isopermittivity point, the system is in equilibrium, exhibiting van't Hoff effect $\Delta G_{equil} = -RT\ln K_{equil}$ (ΔG_{equil}-Gibbs free energy variation) where the equilibrium constant $K_{equil} =$

$\varepsilon_{dip}(T)/\varepsilon_{ion}(\omega, T)$. Van't Hoff plot corresponds to the equation

$$y(1/T) = lnK_{equil} = \frac{\Delta G_{equil}}{RT} = \frac{\Delta H_{equil}}{RT} - \frac{\Delta S_{equil}}{R}. \tag{2.5}$$

in which ΔH_{equil} and ΔS_{equil} are respectively the enthalpy and the entropy changes. Because van't Hoff plot is a strange line (Fig. 2.5), ΔH_{equil} does not depend on T, resulting in the isopermittivity point. According to van't Hoff plot, it is pointed out that $\Delta H_{equil} \approx T\Delta S_{equil}$, i.e. $\Delta G_{equil} \approx 0$ at ω_{iso} in the temperature range of 301− 313K. Therefore, the system reaches to the thermal equilibrium state in a narrow range of temperature.

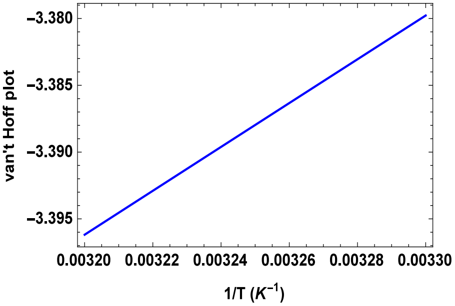

Fig. 2.5. Van't Hoff plot in the model.

Chapter 3

MICROWAVE ELECTRODYNAMICS OF ELECTROLYTE SOLUTIONS

Firstly, the plasmon frequency for electrolyte solutions is given by using jellium theory. Then, the dispersion of microwave conductivity of the solution is built by combining jellium and Drude theories. Finally, the validity of the model is assessed. The material presented in this chapter forms the basis of the first paper in the list of the author's works related to the thesis.

3.1 Plasmon frequency of electrolyte solutions

Jellium theory is applied to determine plasmon frequency of electrolyte solutions. The plasmon frequency is the solution of two Lagrange functions for anion and cation in the long wavelength limit

$$\omega_{pso}^2 = \sum_i \frac{N_i z_i^2 e^2}{\epsilon_0 m_i}, \tag{3.1}$$

where ionic species is labeled by i with the density N_i, charge $z_i e$ (z_i is the reduced effective electron charge and e is electron charge), and mass m_i, ϵ_0 is the electric constant.

For NaCl solution, a representative electrolyte solution, with the density of cation N_{ion}, the plasmon frequency is

$$\omega_p^2 = \frac{N_{ion}e^2}{m^*\epsilon_0}, \tag{3.2}$$

with m^* - the effective mass of ions, $\omega_p \approx 10^{12}$ Hz.

3.2 Microwave conductivity in Drude-jellium model

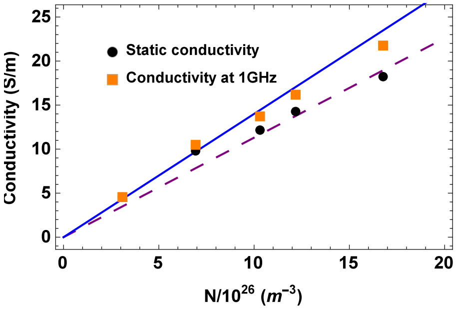

Fig. 3.1. σ^0_{max} at 1 GHz of NaCl solution in Drude-jellium model versus the number of ions is shown by the solid line, in agreement with experimental data (symbols). The dashing line - static conductivity.

Because the dissociated ions play the role as free electrons, it is suitable to apply Drude model for metal permittivity for description of the permittivity of electrolyte solutions $\varepsilon_D(\omega) = \varepsilon''_D(\omega) = j\sigma^0_m/(\epsilon_0\omega)$, in which the frequency of field ω is much smaller than the damping constant γ_0. The static conductivity of NaCl solution is

$$\sigma^0_{solu} = \frac{N_{ion}e^2}{\gamma_0 m^*}. \tag{3.3}$$

At a couple of GHz, the absence of diffusion motion makes the damping constant lower, symbolized γ_i, the conductivity of the solution in low-frequency range is given by

$$\sigma_{max}^{0} = \frac{N_{ion}e^2}{\gamma_i m^*}. \tag{3.4}$$

In comparison with experimental data (Fig. 3.1), we have $\gamma_i \approx 0.78 \times 10^{14}\ \mathrm{s}^{-1} \approx 0.8\gamma_0$.

Ions can't response to EM field at enough higher frequency ω_C, called cutoff frequency, due to their large mass. Because of the thermal fluctuations, the number of ions being responsible for the conductivity of solution gradually decreases versus frequency. We suggest that it obeys logistic statistic. The dispersion of the microwave conductivity is thus expressed by

$$\sigma_{solu}(\omega) = \frac{N_{ion}e^2}{\gamma_i m^*}\frac{1}{1 + exp[\alpha_L(\omega - \omega_c)]}, \tag{3.5}$$

where $\alpha_L = 8.38h/k_B T_0$ (k_B is Boltzmann constant) is the steepness of the curve.

3.3 Results and discussions

Logistic function describes quite well the dispersion of microwave conductivity of electrolyte solutions, in agreement with experimental data for different concentrations (Fig. 3.2). Moreover, it is able to infer the diffusion coefficient

$$D_d = \frac{k_B T}{m^* \gamma_i}. \tag{3.6}$$

expressing its linear dependence on T like Stokes–Einstein equation.

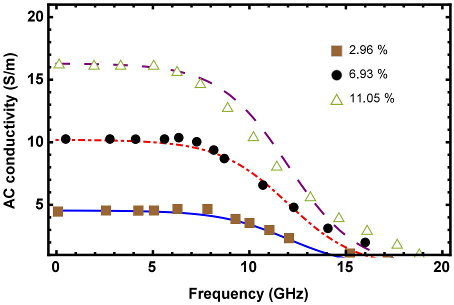

Fig. 3.2. The microwave conductivity in Drude-jellium model for NaCl solution with concentrations of 2.96 %, 6.93 %, and 11.05 % is represented by the solid line, dot-dashed line, and dashing line, respectively, in comparison with data (symbols).

The influence of water background on the motion of ions could be a reason that makes the cutoff frequency much smaller than the plasmon frequency ($\omega_C = 10^{-2}\omega_p$). Therefore, we recommend further extending the model by taking into account influence of water background.

Chapter 4

NONLINEAR ELECTROSTATICS OF ELECTROLYTE SOLUTIONS

A statistic model is built to interpret the nonlinear decrement of dielectric constant that is useful to see more obviously the decrement in the Debye screening length versus concentration. In addition, a simple model depicting the nonlinear increase in specific conductivity is given via considering the property of the local electric field. The material presented in this chapter forms the basis of the third paper in the list of the author's works and a manuscript, in preparation for Communications in Physics.

4.1 Statistic model for the static permittivity of electrolyte solutions

The orientation polarization of the pure liquid water in the direction of electric field is expressed as

$$P = N_0\overline{\mu}_F, \tag{4.1}$$

in which N_0 is the dipole density and $\bar{\mu}_F$ is the average water dipole moment. However, for an electrolyte solution with concentration c

$$P(c, E) = N^*\overline{\mu}_F, \tag{4.2}$$

where $N^* = N_0\{1 - \gamma(c)\}$. $\gamma(c)$ is the correction function because of the dilution of dipole density by non-polar ions and the influence of the local electric field on the rotational polarization of dipoles, obeying the Langevin statistic that is familiar in use to treat the paramagnetism of solid materials, $\gamma(c) = L(\alpha c)$ (α is in relation to the ionic size).

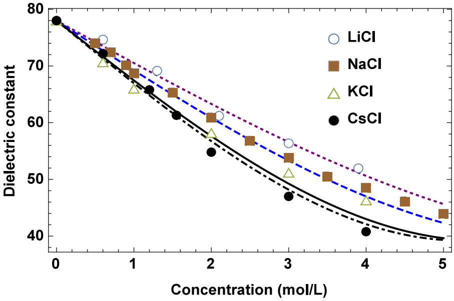

Fig. 4.1. The $c-$ dependence of the static permittivity for electrolyte solutions at 298K in the model, in agreement with experimental data (symbols).

The dielectric constant of solutions is given by

$$\varepsilon_s(c) = \varepsilon_d + \frac{1}{\epsilon_0}\frac{P(c,E)}{E}, \tag{4.3}$$

in which ε_d is the dielectric part originated from the other effects. Therefore

$$\varepsilon_s(c) = \varepsilon_w\{1 - \frac{\alpha c}{3} + \frac{(\alpha c)^3}{45} - \frac{(\alpha c)^5}{945} + ..\}, \tag{4.4}$$

where ε_w is the dielectric constant of pure water. The model exhibits the nonlinear decrement in the permittivity for different electrolyte solutions with concentration below 5 mol/L although it is in the simple mathematical form, in agreement with experimental data (Fig. 4.1). Moreover, the parameter α in relation to the ionic size is extracted.

4.2 Debye screening length

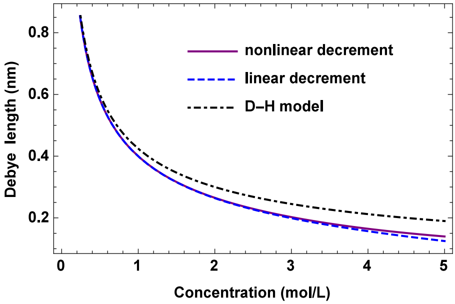

Fig. 4.2. Debye screening length versus the concentration of NaCl solution at 298K in D-H theory, in the model with the linear decrement and nonlinear decrement.

The inverse Debye screening length is determined by

$$K = \sqrt{\frac{4\pi e^2 N_A}{\varepsilon_s \epsilon_0 k_B T} \sum_i c_i z_i^2}, \tag{4.5}$$

where N_A is Avogadro's number. According to the statistical model

$$K^2(c) = \frac{K_0^2}{1 - \frac{\alpha c}{3} + \frac{(\alpha c)^3}{45} - \frac{(\alpha c)^5}{945} + ..}, \tag{4.6}$$

where $K_0 = \sqrt{\frac{4\pi e^2 N_A}{\varepsilon_w \epsilon_0 k_B T} \sum_i c_i z_i^2}$.

Taking into account the linear decrement in static permittivity, the difference in the Debye screening length between this model and the original Debye-Hückel (D-H) theory is quite large for concentrated solutions (Fig. 4.2).

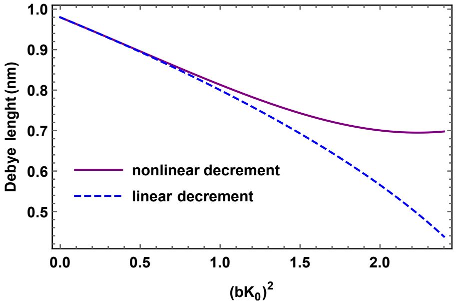

Fig. 4.3. The dependence of the Debye length on $(bK_0)^2$ according to the nonlinear and linear decrement of the static permittivity.

In 2015, it was calculated the activity coefficient of electrolyte solutions according to the linear decrement in static permittivity in the function of K_0

$$\varepsilon_s = \varepsilon_w f(K_0). \tag{4.7}$$

Providing the simple and explicit form of $f(K_0)$ could simplify calculations in this work and improve the agreement between theoretical results and experimental data. It is easy to give

$$f(K_0) = 1 - \frac{(bK_0)^2}{3} + \frac{(bK_0)^6}{45} - \frac{(bK_0)^{10}}{945} + ..' \tag{4.8}$$

where $(bK_0)^2 = \alpha c$ (b - mean radius of ions) without any fitting parameter.

K could be presented in the function of K_0

$$K^2 = \frac{K_0^2}{1 - \frac{(bK_0)^2}{3} + \frac{(bK_0)^6}{45} - \frac{(bK_0)^{10}}{945} + .}. \qquad (4.9)$$

There is a significant difference of the Debye lengths between these two ways according to the linear and the nonlinear decrements in static permittivity (Fig. 4.3). Possibly, it is the reason for a deviation with the experimental data on activity coefficients in the previous work.

4.3 Simple model for static specific conductivity

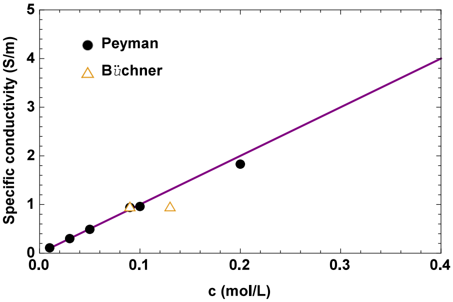

Fig. 4.4. The specific conductivity of dilute NaCl solution versus c in the model (line) in comparison with experimental data.

The static conductivity is a linear function of concentration for dilute electrolyte solutions but a nonlinear one for concentrated solutions. For dilute solutions, the own field radiated by free ions covers a small part of the whole space, i.e. in weak regime. Inversely, the own field covers almost the whole space for concentrated solutions, resulting in strong interaction regime. According to several experimental evidences, the transformation from the weak to the strong regimes of the local electric field happens at about 0.4 mol/L.

Below 0.4 mol/L, the viscosity of the solution is similar to that of pure water, η_0. The mobility b_i of ion type i th with concentration c_i is given by $b_i = z_i e/6\pi\eta_0 r_i$, where r_i are the radius of the ion. Because free ions behave as free electrons in metals, the conductivity versus concentration is given

$$\sigma^0_{dilu}(c) = \sum_i \frac{N_A c_i z_i^2 e^2}{6\pi\eta_0 r_i}. \tag{4.10}$$

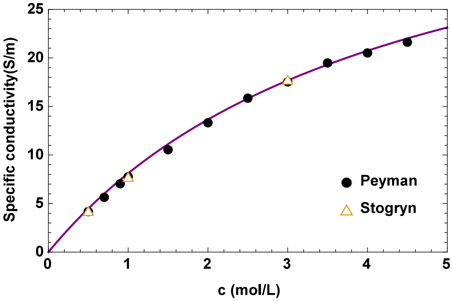

Fig. 4.5. The specific conductivity of concentrated NaCl solution versus c in the model (curve) in comparison with experimental data.

Above 0.4 mol/L, the viscosity of solution η depends on c, $\eta = \eta_0(1 + C\sqrt{c} + Dc)$ (C and D are constants). The specific conductivity $\sigma^0_{solu}(c)$ is thus written by

$$\sigma^0_{solu}(c) = \sum_i \frac{N_A c_i z_i^2 e^2}{6\pi r_i \eta_0 (1 + C\sqrt{c_i} + Dc_i)}. \tag{4.11}$$

This function exhibits the nonlinear feature of the static conductivity (Fig. 4.5), in agreement with experimental observation.

CONCLUSIONS

In this thesis, we focused on studying about several microdynamic behaviors of water systems with following results:

- Modified PP model was developed for interpreting the dispersion of collective density oscillations in liquid water, pointing out the spectrum range and the wave vector region, and estimating some water critical electrodynamic parameters.
- Giving a model with two separated arguments for describing the dispersion of the water permittivity at low frequencies and illuminating the mechanism responsible for the existence of isopermittivity point on the basis of electrodynamics as well as thermodynamics.
- Combining jellium and Drude theories for a description of the microwave conductivity dispersion and further illumination about the microscopic mechanism of electrodynamics of electrolyte solutions
- A statistic model is given for description of the nonlinear decrement in the permittivity of electrolyte solutions by customizing the Langevin statistics. According to the model, the Debye screening length is calculated more carefully. Thus, the deviation between theoretical results and experimental data about the activity coefficient in the previous work is explained.
- A simple model is built to describe the nonlinear reliance of conductivity versus concentration by taking into account the regime transformation of the own field radiated by ions.

FURTHER RESEARCH DIRECTIONS

Applying PP theory to research collective density oscillations of the other liquids and thermodynamic features of water; Investigation into the interaction in biological and chemical materials; Study on electrostatics of electrolyte aqueous solutions upon temperature.

THESIS-RELATED PUBLICATIONS

1. Tran Thi Nhan, Luong Thi Theu, Le Tuan and Nguyen Ai Viet (2018), "Drude-jellium model for the microwave conductivity of electrolyte solutions", *J. Phys.: Conference Series* **1034**(1), 012 006.

2. Tran Thi Nhan, Le Tuan and Nguyen Ai Viet (2019), "Modified phonon polariton model for collective density oscillations in liquid water", *J. Mol. Liq.* **279**, 164-170.

3. Tran Thi Nhan and Le Tuan (2019), "Specific conductivity of electrolyte solutions versus the concentration", *Journal of Science of HNUE* **64**(3), 61-77.

4. Tran Thi Nhan and Le Tuan (2019), "Microscopic approach for water dielectric constant at low frequencies", online publication in *Phys. Chem. Liq.* DOI: 10.1080/00319104.2019.1675156.

5. Tran Thi Nhan and Le Tuan (2019), "Debye Screening length and the non-linear decrement in static permittivity of electrolyte solutions", in publication process of *Communications in Physics.*