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STRONG COUPLING EFFECTS ON BOUND STATES IN PLASMAS.(U)
AUG 82 G J KALMAN AFOSR-81-0091

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PROGRESS REPORT I.

Grant AFOSR 81-0091

STRONG COUPLING EFFECTS ON

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Progress in three major areas is reported: (1) Kinetics and response of strongly coupled multi-component plasmas. (2) Study of plasma phase transition and determination of the degree of ionization of a dense plasma (3) Generalization of the Thomas-Fermi-Debye-Huckel scheme for strongly coupled plasmas with atoms and ions.

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I. RESEARCH WORK

Research in the report period concentrated on three major areas:

1). The analysis of the kinetics of strongly coupled two-component plasmas.

2). Study of the ionization equilibrium in a strongly coupled plasma medium.

3). Setting up a scheme appropriate for the study of the energy levels and of the ionization potential of atoms and ions in a strongly coupled plasma medium.

1). The kinetics of two- or multi-component strongly coupled plasmas requires generalization of the methods already developed by us[1] for one-component systems. This has been undertaken in a number of publications (A,B,C). Even though there are no bound systems (atoms or ions) in this model, the analysis of the formalism is a necessary prerequisite of the description of media with bound systems. In (A) we analysed the cornerstones of our approximation scheme, the VAA (Velocity Average Approximation) and the NLFDT (Non Linear Fluctuation-Dissipation Theorem). In (B) the dynamical NLFDT was extended to two-component systems. In (C) we calculated the nonlinear response of an electron-ion gas, with the electron-ion interaction and quantum effects modelled through a Deutsch-potential[2].

Publications (D) and (E) deal with the problem of plasma oscillations in strongly coupled systems. Plasma oscillations are expected to reach a high level of excitation ($\sim\gamma$) for strong coupling. The ensuing dynamical perturbation on the bound states becomes substantial and the knowledge and understanding of the precise plasmon spectrum under these circumstances is essential.

2). The standard method for determining the degree of ionization in a plasma medium is through the use of the Saha-equation. However, the Saha-equation, based on a model of a gas composed of independent particles, becomes quite unreliable at high densities. The main effects ignored by the Saha equation treatment are (i) the proximity effect, and (ii) the depression of the ionization potential due to screening. We have developed and analyzed a model which shows the effect of the latter. The influence of the medium on the atom is described through the replacement of the intra-atomic potential by a screened Debye potential where the screening constant $\kappa = (4\pi e^2 n\beta)^{1/2}$ depends on the free electron density. Increasing values of κ cause the disappearance of high-lying bound states, leading to the elimination of the last bound state at $\kappa a \approx 1.1$ (a= Bohr-radius)[3]. Consequently, ionization becomes easier, and the calculated degree of ionization is substantially above the simple Saha result. Moreover, as more electrons become free, the ionization potential is further depressed and an avalanche developes generating a sudden phase-transition-like transition from the weakly ionized to a highly ionized state. We have used the computed tables of Rogers, Gabroske and Harwood[3] to describe the bound states in a screened potential. The Saha equation was modified by using the Larkin correction[4] for the partition function. The resulting rather complex self-consistency condition for the degree of ionization was solved numerically. Detailed computer work on the subject is in the process of completion.

3). There are a number of methods available for the study of the dynamics of an atom or ion immersed in an ionized medium[5]. The Thomas-Fermi (TF) method combines relative simplicity with excellent qualitative descriptive capability. While the TF scheme and its refinement have been employed to the problem on hand, the approaches used are appropriate for weakly coupled situations and not for the case of strong coupling. The scheme we have worked out is intended to include specific strong coupling effects and is described below.

1. The system is considered to consist, for the purpose of the TF equation, of three species:

   (i) N_i classical nuclei of charge Z, (ii) $N_e = N_i X$ hot, classical, "free" electrons, and (iii) $N_b = N_i Y$ ($Y=Z-X$) degenerate bound electrons.

2. The potential around a chosen nucleus is determined by the Poisson-equation.

   $$\nabla^2 \Psi(x) = 4\pi e^2 \{Z\delta(x) - n_b(x) - n_e(x) + X n_i(x)\}$$

   with

   $$n_b(x) = \int_{\varepsilon_p<0} d^3p\ 1/\{1+\exp\beta(\varepsilon_p-\mu)\}$$

   $$\varepsilon_p = p^2/2m - \Psi(x)$$

   $$n_e(x) = \bar{n}_e\{1+g_{ei}(x)\}$$

   $$n_i(x) = \bar{n}\{1+g_{ii}(x)\}$$

   g_{ei} and g_{ii} are the pair correlation functions for an electron-ion pair or ion-ion pair.

3. For the purpose of the calculation of the correlation functions the system consists of (i) N_i ions of charge X and (ii) N_e hot classical, "free" electrons, interacting through ϕ_{ee},, ϕ_{ii} and ϕ_{ei}, where

   $$\phi_{ee}(x) = e^2/x$$

   $$\phi_{ii}(x) = e^2 Z^2_{eff,i}(x)/x$$

   $$\phi_{ei}(x) = e^2 Z_{eff,e}(x)/x$$

   such that $Z > Z_{eff} > X$

$Z_{eff}(o) = Z$

$Z_{eff}(a) = X$

<u>a</u> being the ion-radius

4. $Z_{eff, i}$ and $Z_{eff, e}$ are to be determined by the integrated charge densities of the <u>bound</u> electrons only.

5. The correlation functions g_{ee} and g_{ei} are now to be determined by using one of the strongly coupled static plasma schemes-either the STLS[6] or TI mean field theories, or HNC.

6. Finally X is to be determined by calculating the free energy of the system and minimizing it with respect to X.

The salient feature of this scheme is that it applies the philosophy of the TF-DH method, but replaces the DH distribution with the correlation functions appropriate for strong coupling. In turn, the correlation functions depend on the effective potentials. A scheme for the STLS and TI methods with an arbitrary set of effective potentials for a two-component system has already been worked out by us[7] and it will be applied here.

Our present approach to the calculation is to start with a constant Z_{eff}, determining g_{ei}, g_{ii} from STLS then solve for Ψ and n_b and then to iterate to find a better Z_{eff}. It will however, be very instructive to analyze the difference in Ψ and n_b between the values provided by the present scheme and by those by the TF-DH scheme as a function of γ even for constant Z_{eff}.

References

1. G. Kalman: Approximation Schemes for Strongly Coupled Plasmas, in Strongly Coupled Plasmas, edited by G. Kalman (Plenum Press, N.Y., 1978), p. 141.

   K.I. Golden: Generalized Response Function Approach to Strongly Coupled Plasmas, in Strongly Coupled Plasmas, edited by G. Kalman (Plenum Press, N.Y., 1978), p. 223.

   K.I. Golden and G. Kalman: Approximation Scheme for Strongly Coupled Plasmas: Dynamical Theory, Phys. Rev. A19, 2112 (1979).

   P. Carini, G. Kalman, and K.I. Golden: Plasmon Dispersion for Strong Coupling, Phys. Lett. 78A, 450 (1980).

2. T. Dunn and A.A. Broyles, Phys. Rev. A157, 156 (1967); M.A. Pokrant, A.A. Broyles and T. Dunn, Phys. Rev. A10, 379 (1974); M.M. Gombert and C. Deutsch, Phys. Lett. 47A, 473 (1974).

3. C.R. Smith, Phys. Rev. 134, A1235 (1964); F.J. Rogers, H.C. Grabroske, Jr., and D.S. Harwood, Phys. Rev. A1, 1577 (1970); J.L. Jackson and L.S. Klein, Phys. Rev. 177, 352 (1969).

4. See, e.g., W. Ebeling, W.D. Kraeft and D. Kremp: "Theory of Bound States and Ionization Equilibrium in Plasmas and Solids" (Akademie Verlag, Berlin, 1976).

5. See, e.g., the March 1982 issue of the J. of Quantitative Spectroscopy and Radiative Transfer.

6. K.S. Singwi, M.P. Tosi, R.H. Land and A. Sjolander, Phys. Rev. 176, 589 (1968); K.S. Singwi, A. Sjolander, M.P. Tosi and R.H. Land, Solid State Commun. 7, 1503 (1969); K.S. Singwi, A. Sjolander, M.P. Tosi and R.H. Land, Phys. Rev. B1, 1044 (1970); D.L. Price, K.S. Singwi and M.P. Tosi, Phys. Rev. B2, 2983 (1970); Wei-Mei Shyu, K.S. Singwi and M.P. Tosi, Phys. Rev. B3, 237 (1970).

7. K.I. Golden and G. Kalman: Approximation Schemes for Strongly Coupled Two-Component Plasmas, Phys. Rev. A14, 1802 (1976).

II. PUBLICATIONS AND PRESENTATIONS

(August 1, 1981 through July 31, 1982)

A. K.I. Golden and G. Kalman: Plasma Response Functions, Fluctuation-Dissipation Relations and the Velocity Average Approximation, accepted for publication in the Annals of Physics (N.Y.).

B. K.I. Golden and Lu De-xin: Dynamical Three-Point Correlation and Quadratic Response Functions in Binary Ionic Mixture Plasmas, accepted for publication in the Journal of Statistical Physics.

C. K.I. Golden, G. Kalman and Lu De-xin: RPA Calculations of Nonlinear Response in Electron - Ion Plasmas, to be submitted to Physics Letters A.

D. P. Carini, G. Kalman and K.I. Golden: Exact Dynamical Polarizability for One Component Classical Plasmas, accepted for publication in Physical Review A.

E. G. Kalman and K.I. Golden: Correlational Correction to Plasmon Dispersion Rebuttal of a Reply by Ichimaru, Totsuji, Tange and Pines, International Centre for Theoretical Physics Report, IC/81/175.

G. Kalman and K.I. Golden: Correlational Correction to Plasmon Dispersion: Rebuttal of a Reply by Ichimaru, Totsuji, Tange and Pines, submitted to Physical Review A.

F. G. Kalman: Nonlinear Response Functions and Collective Modes in a Strongly Coupled Plasma, Statistical Mechanics of Ionic Matter, Los Houches, April 1982, unpublished.

G. G. Kalman and K.I. Golden: Lectures on Strongly Coupled Plasmas, Workshop on Condensed Matter, International Centre for Theoretical Physics Trieste, August 1982-unpublished.

The works listed below were sponsored by an earlier AFOSR Grant; they appeared, however, during the present report period.

H. P. Bakshi, R. Calinon, K.I. Golden, G. Kalman and D. Merlini: Particle Correlations in the Strongly Coupled Two Dimensional One-Component Plasma, Phys. Rev. A23, 1915 (1981).

I. K.I. Golden and G. Kalman: Moment Expansion of the Kinetic Equation and its Application to Strongly Coupled Plasmas, accepted for publication in Physical Review A.

J. G. Kalman: Recent Progress in the Understanding of Strongly Coupled Coulomb Systems, Lecture Notes in Physics V142, Springer-Verlag, New York, 1981.

Dr. G. Kalman was invited lecturer at NATO Workshop on the Statistical Mechanics of Ionic Matter, Les Houches, April 1982; Dr. G. Kalman and Dr. K. Golden were invited lecturers and Research Leaders at the Workshop on Condensed Matter, International Centre for Theoretical Physics, Trieste, August 1982; Dr. K. Golden is invited lecturer at various institutions in the People's Republic of China.

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