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**"LONG-WAVELENGTH BEHAVIOUR OF CHARGE-CHARGE STRUCTURE
FACTOR IN INSULATING AND METALLIC GROUND STATE OF
CONDENSED HYDROGEN UNDER PRESSURE"**

M. A. Amato, D. M. Ceperley and N. H. March

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UNIVERSIDADE DE BRASÍLIA

DEPARTAMENTO DE FÍSICA

70910 Brasília DF

Fone (061) 274 0022 R. 2190 e 2188 Telex (061) 2730 UNBS

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Long-wavelength behaviour of charge-charge structure factor in
insulating and metallic ground state of condensed hydrogen under
pressure.

by

M.A. Amato^{*†}, D.M. Ceperley[‡] and N.H. March^{*}

^{*}Theoretical Chemistry Department

University of Oxford

5, South Parks Road

Oxford OX1 3UB

England.

[‡]National Centre for Supercomputing Application

University of Illinois at Urbana - Champaign

Champaign - Illinois 61820

USA

Using the quantum Monte Carlo charge-charge structure factor $S_{-qq}(k)$ data of Ceperley and Alder [Phys. Rev. B36,2092 (1987)], it is argued that (i) in the metallic phase the small k expansion is non-analytic at order k^5 , reflecting plasmon dispersion effects, while in the insulating phase the non-analyticity occurs at $O(k^3)$, due to van der Waals interaction between the protons.

calculations of the ground state of condensed hydrogen at $T=0$. They avoided the Born-Oppenheimer approximation by solving the quantum many-body problem simultaneously both for the electron and proton degrees of freedom. Using different trial functions and several different crystal structures, the transition between (the explored) molecular and atomic phases was found to take place at a pressure of 3.0 ± 0.4 Mbar.

The purpose of this report is to examine further the small angle behaviour of the charge-charge (qq) structure factor $S_{qq}(k)$ in this two-component system of protons (p) and electrons (e). By analogy with a one-one molten salt² such as KCl, one can write

$$S_{qq}(k) = S_{ee}(k) + S_{pp}(k) - 2S_{ep}(k) \quad (1)$$

and plainly the small angle behaviour of $S_{qq}(k)$ at least in principle, has contributions from each of the three partial structures displayed in eqn.(1).

We next consider the small angle or long wavelength form of $S_{qq}(k)$ in the metallic (M) and insulating (I) phases of condensed hydrogen in turn. To begin with the metallic phase, we appeal to the work of Holas and March³ on the electron-electron structure factor $S_{ee}^0(k)$ in the ground-state of homogeneous jellium. These workers demonstrate that the small k expansion has the form, in the dense metallic electron liquid regime of jellium,

$$S_{ee}^0(k) = \frac{1}{k^2} \left[\frac{1}{2} \left(\frac{1}{k} \right)^2 + \dots \right] \quad (2)$$

the non-analyticity at $k=0$ is a consequence of the long range nature of the interaction around $k=0$ corresponding to a non-terminating inverse power series expansion of the dielectric function in the electron-electron interaction strength. This is in complete contrast to

the behaviour of the structure factor in a simple one-component system, however.

... to contribute a higher-order term to the dielectric function.

Though, of course, the work of Ceperley and Alder¹ is concerned with electrons and (granular) protons, we do not expect proton-proton effects to affect qualitatively the long wavelength behaviour of $S_{ee}^M(k)$ in eqn.(1). Thus, we anticipate that $S_{qq}^M(k)$ in eqn.(1) will have a small k expansion of the form

$$S_{qq}^M(k) = q_2^M k^2 + q_4^M k^4 + q_5^M k^5 + \dots \quad (3)$$

and hence that the quantity $\Gamma(k)$ plotted versus k in Fig. 11 of ref.1, which is proportional to $\Gamma(k)/k^2$, will have the expansion

$$\Gamma^M(k) = \Gamma^M(0) + \gamma_2^M k^2 + \gamma_3^M k^3 + \dots \quad (4)$$

This form of $\Gamma^M(k)$ has been fitted to the data of Ceperley and Alder¹, taking $\Gamma^M(0) = 1$ corresponding to an infinite dielectric constant, i.e. to the assumed metallic state. The value of γ_2^M can be compared with the result for q_5^M estimated from the jellium study of Holas and March³.

Turning to the insulator, we would expect, at least for the atomic insulating phase that the arguments paralleling those of Enderby, Gaskell and March⁴ would lead to a non-analyticity in the proton-proton structure factor $S_{pp}^I(k)$ at $O(k^3)$, arising from the van der Waals interaction between the protons decaying at large r as r^{-6} in the non-relativistic framework that is our concern here. Thus, although the work of ref.4 was for a classical liquid, we anticipate by analogy that the small k expansion of $S_{qq}^I(k)$ will not, in contrast to the metal case (3), have its leading non-analyticity at order k^3 , yielding for $\Gamma(k)$ in the insulating phase the small k form

This is already plotted then in suitable form in Figs. 12 of ref. 1 and the slopes for mean interelectronic spacing r_s/a_0 , with $a_0 = \hbar^2/me^2$ corresponding to values 3, 2.2 and 2.0 are readily shown to be proportional to the electron density $n^{-1/3}$, which is understandable (roughly) from the density factor exhibited in ref. 4. However, that this argument is oversimplistic is shown by the fact that the slope of $\Gamma(k)$ vs k decrease again at $r_s = 1.61$ (cf Fig. 12 of ref. 1), and we have no satisfactory explanation of that at the present time. Nor is it possible, presently, to check the magnitude of the coefficient γ_1^I of the linear term in k in eqn. (5), since we do not, to date, have the quantum-mechanical generalization of the classical limit treated in ref. 4.

In summary, we find that the quantum Monte Carlo data of Ceperley and Alder are consistent with the small k expansions of the charge-charge structure factor $S_{qq}(k)$ in eqn. (3) and, for $\Gamma(k) = S_{qq}/k^2$ in eqn. (5), for metallic and insulating phases respectively. More first-principles theory is called for, before it can be asserted, however that the plausible forms (3) and (4) for the metallic phase, and eqn. (5) for the insulating phase have been derived.

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Permanent address Departamento de Fisica, Universidade de Brasilia, 70.910 Brasilia DF Brasil.

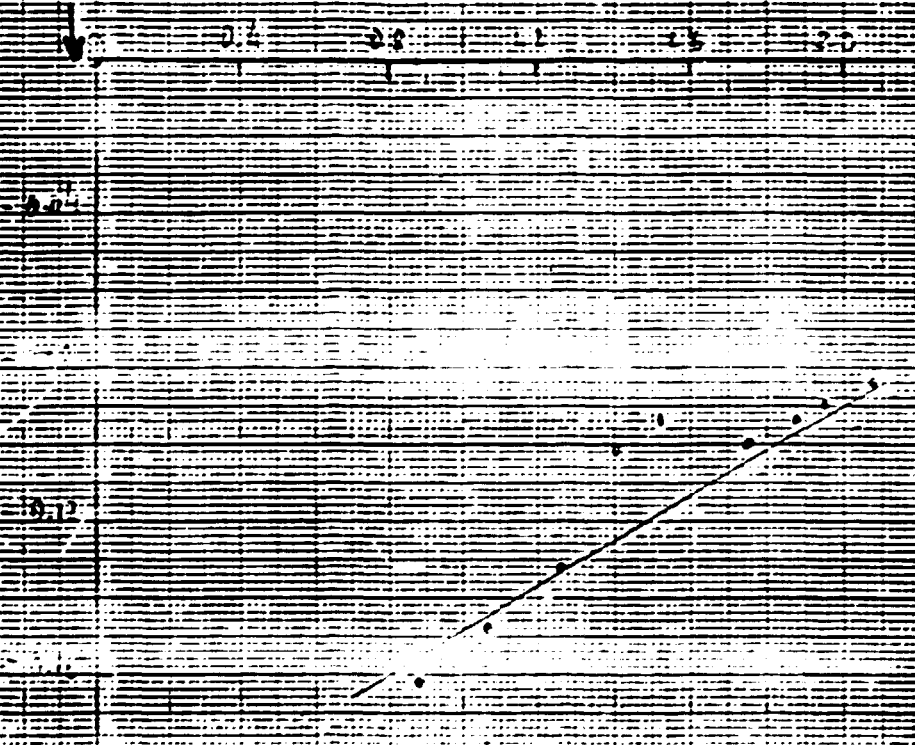
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Figure 1. Solid line is a quadratic plus cubic form (4), neglecting higher terms, of the ϵ_{eff} vs k data of Ceperley and Alder for the atomic metal at $r_s = 1.31a_0$. Working with dimensionless quantity ka as independent variable, the reduced values for τ_2^M and τ_3^M were -0.2055 and 0.0606 respectively.

$$\underline{\underline{\Gamma_3 = 1.31 a_0}}$$

$$\frac{r(x) - r(b)}{x^2} \rightarrow k_3$$



$$r(x) = r(b) + k_2(x - b) + k_3(x - b)^2$$

$$\text{or } r(x) = r(b) + k_2(x - b) + \frac{k_3}{2}(x - b)^2$$

$$\begin{cases} k_2 = -0.2055 \\ k_3 = 0.0606 \end{cases}$$