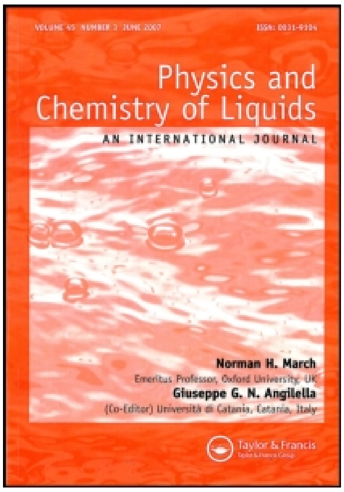

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Inhomogeneous electron liquid due to encapsulated atoms in C_{60} compounds: dynamic polarisability induced in the outer C_{60} shell

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LETTER

Inhomogeneous electron liquid due to encapsulated atoms in C_{60} compounds: dynamic polarisability induced in the outer C_{60} shell

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The work of Amusia and Baltenkov (Phys. Lett. A **360**, 294, (2006)) on the possibility of considering the fullerene shell C_{60} as a conducting sphere is briefly reviewed.

Keywords: endohedral fullerene compounds; dynamical polarisability; inhomogeneous electron liquids

Following the work of Connerade and Solov'yov [1] using classical electrodynamics, it was shown by Amusia *et al.* [2] and Amusia and Baltenkov [3], within a quantum-mechanical framework, that the photoionisation cross-section $\sigma_{C_{60}}(\omega)$ of endohedral atoms – taking into account the dipole collective excitations of C_{60} electrons – is a product of two dynamical factors. Thus, one can define a dimensionless factor $F(\omega)$ as a function of frequency ω given by

$$F(\omega) = \frac{\sigma_{C_{60}}(\omega)}{\sigma_A(\omega)} = \left[1 - \frac{\alpha_d(\omega)}{R^3}\right]^2. \tag{1}$$

Here, $\sigma_A(\omega)$ denotes the photoionisation cross-section of the free (endohedral) central atom A in $A@C_{60}$, while $\alpha_d(\omega)$ is the dynamical polarisability of the outer C_{60} shell. Finally, R in Equation (1) is the radius of the fullerene ion shell.

To relate Equation (1) directly to electric fields, one can calculate the effective electric field, say $\mathbf{E}_{\text{eff}}(\omega)$, at the centre of the fullerene C_{60} when an electric field $\mathbf{E}(\omega)$ is applied. Following Amusia and Baltenkov [4], one can calculate the frequency dependence of the ratio, $\eta(\omega)$ say, defined by

$$\eta(\omega) = \frac{\mathbf{E}_{\text{eff}}(\omega)}{\mathbf{E}(\omega)}. \tag{2}$$

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In [4], $\eta(0)$ is estimated as approximately equal to 2. This is in marked contrast to a model of C_{60} as a hollow conducting sphere for which $\eta(0)$ would be zero in this static limit. As set out by Amusia and Baltenkov [4], Equations (1) and (2) are then related by

$$F(\omega) = \eta(\omega)^2. \tag{3}$$

As stressed in [4] (see also [5]), the real part of the dynamical polarisability of C_{60} introduced in Equation (1) can be calculated from experimental measurements of the photoionisation cross-section of C_{60}, denoted below by $\sigma(\omega)$. The relation is [4]

$$\mathrm{Re}\,\alpha_{\mathrm{d}}(\omega) = \frac{c}{2\pi^2}\int_I^{\infty} \frac{\sigma(\omega')}{\omega'^2 - \omega^2}\,\mathrm{d}\omega', \tag{4}$$

where c is the velocity of light and I denotes the ionisation potential of C_{60}. Since the imaginary part $\mathrm{Im}\,\alpha_{\mathrm{d}}(\omega)$ tends to zero in the static limit $\omega \to 0$, one has from Equation (4) that

$$\alpha_{\mathrm{d}}(0) = \frac{c}{2\pi^2}\int_I^{\infty} \frac{\sigma(\omega)}{\omega^2}\,\mathrm{d}\omega. \tag{5}$$

Amusia and Baltenkov [4] have used the experimental photoabsorption cross-section for C_{60} given in [6] and [7] to plot in their Figure 2 the real part $\mathrm{Re}\,\alpha_{\mathrm{d}}(\omega)$ as a function of ω. It is noteworthy that some, though not all as elaborated upon, with a little explained further, of the structural features of their plot of $\mathrm{Re}\,\alpha_{\mathrm{d}}(\omega)$ are reflected in the treatment of Anderson and Bonderup [8]. Thus, returning to Figure 2 in [4], the first maximum and second minimum of $\mathrm{Re}\,\alpha_{\mathrm{d}}(\omega)$ are at correct frequencies from [8] but at higher frequencies the shapes in [4] and [8] disagree. It seems worthy of emphasis that in Figure 2 in [4], derived from the experimental photoabsorption cross-section for C_{60}, the first three peaks lie at $\omega = 3.4$, 9.8 and 15.6 eV, suggesting a 'quantum' of energy of about 5 eV. There may also be a 'ripple', though no further maximum, in Figure 2 in [4] near 20 eV. No such features are to be found from the treatment in [8].

Returning to the static polarisability $\alpha_{\mathrm{d}}(0)$, experimental values for the C_{60} molecule, as far as we are aware, have been obtained mainly for fullerene films, and are within the range of 540 ± 20 a.u. These values are evidently substantially lower than Amusia and Baltenkov's [4] value of about 850 a.u. in their Figure 2. Therefore, further, we return to some simple models relating to $\alpha_{\mathrm{d}}(0)$ and to some earlier bounds proposed for (large) spherical C cages by Amovilli and March [9].

Benedict *et al.* [10], in their early work, proposed an approximate screened polarisability formula for $\alpha_{\mathrm{d}}(0)$ for large spherical C cages. This has the form

$$\alpha_{\mathrm{d}}(0) = \frac{\alpha_{\mathrm{us}}(0)}{1 + \alpha_{\mathrm{us}}(0)/R^3}, \tag{6}$$

where, for the C cages, R is the ion radius (6.72 a.u. for C_{60}) while $\alpha_{\mathrm{us}}(0)$ is an 'unscreened' polarisability.

We anticipate that, if we divide both sides of Equation (6) by R^3 then, for large enough cages, $\alpha_{\mathrm{d}}(0)/R^3$ will tend to a constant, as polarisability is well known to correlate strongly with molecular volume. Estimates made in [9] indicate that the constant will be about 3/4, and thus from Equation (6) $\alpha_{\mathrm{us}}(0) \approx 4\alpha_{\mathrm{d}}(0)$ for really large spherical cages. It will be of interest to refine these semiquantitative estimates as experimental data utilised by Amusia and Baltenkov [4] for C_{60} become available.

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