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A new formulation of the dynamical response of many-electron systems and the photoabsorption cross section of small metal clusters

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Abstract. Static polarizabilities and photoabsorption cross sections of clusters Na_7^-, Na_8, Na_{19}^- Na_{20} are calculated, based on the spherical jellium model including the self-interaction correction (SIC) of Perdew and Zunger. To this end, a new formulation of the theory of the linear response is presented, which is suitable for general, self-interaction corrected, many-electron systems. The results obtained display an overall agreement with available experimental data, offering a systematic improvement with respect to the standard TDLDA. Furthermore, the cross sections of the negatively charged clusters are found to be dominated by a broad peak in the visible region, whose line width can be related to the lifetime of the surface plasmon against electron detachment.

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Since the first application of the time-dependent local density approximation (TDLDA) [1, 2], based on the jellium model, to the calculation of the dynamical polarizability of small metal clusters [3], experimental data have become available [4–6] on the photoabsorption cross section of these many-electron systems. This, in turn, has stimulated a wealth of calculations within this and related frameworks [7, 8] which, though successful in describing the general trends of the data, bring to the excitation spectrum the intrinsic flaws already present in the LDA ground state.

The incorporation of self-interaction correction (SIC) [9] in the description of the ground state (GS) properties of small metal clusters [10] has proved very successful, leading, among other features, to: a) potentials which have the correct asymptotic behaviour, b) orbital eigenvalues in fair agreement with the calculated quasiparticle energies [11] and c) electron affinities in good agreement with experimental data [10]. This, in turn, poses the natural question of the physical implications of SIC in the calculation of excitation spectra of many-electron systems. In this paper, we address this question by calculating the dynamical response of small sodium clusters within the spherical jellium model, starting from a GS which is self-interaction corrected in the way proposed by Perdew and Zunger [9]. Under these circumstances, the general formalism developed in [1], based on a mean field potential, is no longer applicable, and a new formulation of the independent-particle susceptibility is used which is suitable for a SIC-corrected ground state (we shall henceforth denote this formalism as SIC-TDLDA). It will be concluded that the SIC-TDLDA leads to static polarizabilities and to line shapes of photoabsorption cross sections in overall agreement with available experimental data, resulting in a systematic improvement with respect to the TDLDA results. Although the model developed in this paper is applied to the study of small metallic aggregates, we feel it is well suited for application in other fields of science, such as atomic physics and surface science, where LDA methods have been widely used [13]. For example, it is well known that LDA does not provide stable ground state solutions for negative ions [14, 15], and using SIC in the determination of properties such as electron affinities has proved very rewarding [16]. By means of SIC-TDLDA, the study of atomic and ionic photoabsorption and photoemission processes, among others, becomes no more difficult than the TDLDA study of rare gas atoms.

The SIC scheme corrects for the self-interacting part of the total LDA mean field potential acting on a "Kohn-Sham"-like single-particle state by subtracting from it a term which depends exclusively on the modulus square of the single particle wave function [9, 17] namely,

$$V_{\mathrm{SIC}}^{(i)}(\mathbf{r}) = V_{\mathrm{MF}}(\mathbf{r}) - e^2 \int \frac{n_i(\mathbf{r}')\,\mathrm{d}\,\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} - V_{xc}[n_i(\mathbf{r})],$$

$$n_i(\mathbf{r}) = |\tilde{\psi}_i^{(i)}(\mathbf{r})|^2, \qquad (1)$$

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where the mean field potential $V_{MF}(\mathbf{r})$ reads

$$V_{MF}(\mathbf{r}) = V_I(\mathbf{r}) + e^2 \int \frac{n(\mathbf{r}')\,d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} + V_{xc}[n(\mathbf{r})],$$

$$n(\mathbf{r}) = \sum_{i=1}^{N} |\tilde{\psi}_i^{(i)}(\mathbf{r})|^2, \tag{2}$$

N being the total number of valence electrons in the cluster, $V_I(\mathbf{r})$ the jellium potential of $\aleph$ positive ions. $\tilde{\psi}_j^{(i)}(\mathbf{r})$ represents the eigenfunction of orbital potential $V_{SIC}^{(i)}$ with quantum numbers j, and $\tilde{\varepsilon}_j^{(i)}$ is the corresponding eigenvalue. V_{xc} is the LDA for the exchange and correlation for which we retain the functional form of Gunnarsson and Lundqvist [18]. Finally, the single-particle orbitals are solutions of the "Kohn-Sham"-like equations (but with an orbital-dependent potential),

$$\left[\frac{-\hbar^2}{2m}\Delta + V_{SIC}^{(i)}(\mathbf{r})\right]\tilde{\psi}_j^{(i)}(\mathbf{r}) = \tilde{\varepsilon}_j^{(i)}\,\tilde{\psi}_j^{(i)}(\mathbf{r}). \tag{3}$$

The self-consistent solution of (1) to (3) accounts for the GS description of the metal cluster. Because of the orbital dependence of the single-particle potentials, the "Kohn-Sham"-like wave functions are, in principle, non-orthogonal. This has been shown to be unimportant as the ground state properties of finite many-electron systems are concerned [9]. However, it may have significant consequences in the calculation of excited properties, and therefore we solved (3) performing, at each iteration of the self-consistent scheme, a Gramm-Schmidt orthonormalization of all the wave-functions. This ensures we get a self-consistent solution involving orthonormal wave-functions.

We now proceed to the calculation of the independent-particle susceptibility $\chi_0(\mathbf{r}, \mathbf{r}'; \hbar\omega)$ which can be generally written as

$$\chi_0(\mathbf{r}, \mathbf{r}'; \hbar\omega) = \sum_{i,j=1}^{\infty} (f_i - f_j)\frac{\psi_i^*(\mathbf{r})\,\psi_j^*(\mathbf{r}')\,\psi_j(\mathbf{r})\,\psi_i(\mathbf{r}')}{\hbar\omega - (\varepsilon_i - \varepsilon_j) + i\delta}. \tag{4}$$

In the above equation, $\{f_i, f_j\}$ represent the Fermi occupation factors (1 for occupied orbitals and 0 otherwise). Because of the eigenfunction expansion of the single-particle Green's function,

$$G(\mathbf{r}, \mathbf{r}', E) = \sum_{j=1}^{\infty} \frac{\psi_j(\mathbf{r})\,\psi_j(\mathbf{r}')^*}{E - \varepsilon_j + i\delta}, \tag{5}$$

the independent-particle susceptibility can be rewritten as

$$\chi_0(\mathbf{r}, \mathbf{r}'; \hbar\omega) = \sum_{i}^{occ} \psi_i^*(\mathbf{r})\,\psi_i(\mathbf{r}')\,\tilde{G}(\mathbf{r}, \mathbf{r}', \varepsilon_i + \hbar\omega) + \psi_i(\mathbf{r})\,\psi_i^*(\mathbf{r}')\,\tilde{G}^*(\mathbf{r}, \mathbf{r}', \varepsilon_i - \hbar\omega), \tag{6}$$

where,

$$\tilde{G}(\mathbf{r}, \mathbf{r}', \varepsilon_i + \hbar\omega) = \left[G(\mathbf{r}, \mathbf{r}', \varepsilon_i + \hbar\omega) - \sum_{j}^{occ} \frac{\psi_j(\mathbf{r})\,\psi_j(\mathbf{r}')^*}{\varepsilon_i + \hbar\omega - \varepsilon_j + i\delta}\right]. \tag{7}$$

This form of the independent-particle susceptibility ensures *explicitly* that the Pauli principle is not violated. Because in TDLDA, the single-particle potentials are orbital-independent, the summations over j in (7) have symmetric signs for $\tilde{G}$ and $\tilde{G}^*$ and therefore they cancel automatically, which results in the standard TDLDA result [1, 3] and amounts to replace $\tilde{G}$ by G in (6). However, in the SIC case, the orbital dependence of the potentials means that the summations over j in (7) do not cancel and therefore the SIC form of the independent-particle susceptibility is written [12] as a function of the (now) orbital-dependent Green's functions $G^{(i)}(\mathbf{r}, \mathbf{r}', \hbar\omega)$ and single-particle wave functions $\tilde{\psi}_j^{(i)}(\mathbf{r})$ as

$$\chi_0((\mathbf{r}, \mathbf{r}'; \hbar\omega) = \sum_{i}^{occ} \tilde{\psi}_i^{(i)*}(\mathbf{r})\,\tilde{\psi}_i^{(i)}(\mathbf{r}')\,\tilde{G}^{(i)}(\mathbf{r}, \mathbf{r}', \tilde{\varepsilon}_i^{(i)} + \hbar\omega) + \sum_{i}^{occ} \tilde{\psi}_i^{(i)}(\mathbf{r})\,\tilde{\psi}_i^{(i)*}(\mathbf{r}')\,\tilde{G}^{(i)*}(\mathbf{r}, \mathbf{r}', \tilde{\varepsilon}_i^{(i)} - \hbar\omega), \tag{8}$$

with $\tilde{G}^{(i)}$ given in terms of $G^{(i)}$ via

$$\tilde{G}^{(i)}(\mathbf{r}, \mathbf{r}', \tilde{\varepsilon}_i^{(i)} + \hbar\omega) = \left[G^{(i)}(\mathbf{r}, \mathbf{r}', \tilde{\varepsilon}_i^{(i)} + \hbar\omega) - \sum_{j}^{occ} \frac{\tilde{\psi}_j^{(i)}(\mathbf{r})\,\tilde{\psi}_j^{(i)*}(\mathbf{r}')}{\tilde{\varepsilon}_i^{(i)} + \hbar\omega - \tilde{\varepsilon}_j^{(i)} + i\delta}\right]. \tag{9}$$

The sums are restricted to the set of single-particle quantum numbers corresponding to occupied orbitals in the GS.

The orbital dependence of both the Green's functions and the wave functions $\tilde{\psi}_j^{(i)}(\mathbf{r})$ reflects the fact that the "virtual orbitals" into which an electron in an occupied state can be promoted under the action of an external perturbation should be self-interaction corrected. To account for this, the virtual orbitals are therefore computed with the potential appropriate for the initial state of the electron [9]. This is the SIC-LDA counterpart of the improved virtual orbitals (IVO) method [19], widely used in physics and chemistry in the framework of the Hartree-Fock approximation. We would like to point out that, by maintaining the definition of the independent-particle susceptibility in terms of the Green's functions, which are determined by standard numerical integration, we perform the infinite sums over the complete sets of states "exactly" [1], being left with a small number of terms to be subtracted.

Once $\chi_0(\mathbf{r}, \mathbf{r}'; \hbar\omega)$ is determined the SIC-TDLDA susceptibility is now calculated as the solution of the following integral equation [3]:

$$\chi(\mathbf{r}, \mathbf{r}'; \hbar\omega) = \chi_0(\mathbf{r}, \mathbf{r}'; \hbar\omega) + \int d\mathbf{r}''\,d\mathbf{r}'''\,\chi_0(\mathbf{r}, \mathbf{r}''; \hbar\omega) \cdot K(\mathbf{r}'', \mathbf{r}''')\,\chi(\mathbf{r}''', \mathbf{r}'; \hbar\omega), \tag{10}$$

where [20]

$$K(\mathbf{r},\mathbf{r}')=\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}+\frac{\mathrm{d}V_{xc}}{\mathrm{d}n}\,\delta(\mathbf{r}-\mathbf{r}'). \tag{11}$$

An angular momentum representation is adequate for our problem, due to the spherical symmetry of the clusters we are considering. Under these conditions, the response is diagonal in angular momentum, meaning that we can express the polarizability of the system with the help of the dipole ($L=1$) component of the susceptibility. We refer the interested reader to [3, 12] for mathematical details. For an external perturbation of the form $-eE_0 z\exp(-\mathrm{i}\omega t)$, the dynamic polarizability can be written as

$$\alpha(\hbar\omega)=-e^2\frac{4\pi}{3}\int_0^{+\infty}\mathrm{d}r\,r^3\int_0^{+\infty}\mathrm{d}r'\,r'^3\,\chi_{L=1}(r,r',\hbar\omega). \tag{12}$$

Finally, the photoabsorption cross section $\sigma(\hbar\omega)$ is simply related to the imaginary part of the polarizability by $\sigma(\hbar\omega)=(4\pi\omega/c)\,\mathrm{Im}[\alpha(\hbar\omega)]$. This equation completes our formalism.

The static and dynamic polarizabilities were calculated for neutral and negatively charged jellium spheres with 8 and 20 valence electrons, with a jellium density corresponding to bulk sodium, that is, a Wigner-Seitz radius of $4\,a_0$ ($a_0=0.529$ Å). For the neutral clusters, the integrated charge in the jellium background was 8 and 20, whereas for the negatively charged clusters was 7 and 19. In Table 1 we collect the results for the static polarizabilities. To allow for direct comparison, both the experimental values taken from [21] and the TDLDA results are tabulated as well. Only experimental values are presented for the neutral clusters since we are not aware of any experimental determination for negatively charged clusters. The SIC-TDLDA results show a systematic improvement with respect to TDLDA [22], in better agreement with the experimental values.

In Fig. 1 the results of the SIC-TDLDA dynamical response are depicted with solid lines; dashed lines show the corresponding TDLDA results. The vertical arrows indicate our estimate (taken from the analysis of the experimental data) for the most probable position of the measured plasmon peaks [5, 6, 24]. Besides the overall red-shift of the SIC-TDLDA line shape with respect to the corresponding TDLDA line, which is simply related to the increase of the static polarizability (see Table 1), the SIC-TDLDA collective response extends over a wider energy spectrum than the TDLDA. Indeed, for

Table 1. Static polarizabilities of Na_7^-, Na_8, Na_{19}^- and Na_{20} in units of $R_0^3=\aleph r_s^3$ as calculated with TDLDA and SIC-TDLDA. EXP stands for the experimental values taken from [21]

N	$\aleph$	TDLDA	SIC-TDLDA	EXP
8	7	2.19	2.44	
8	8	1.41	1.52	1.72 ± 0.03
20	19	1.62	1.80	
20	20	1.34	1.46	1.58 ± 0.04

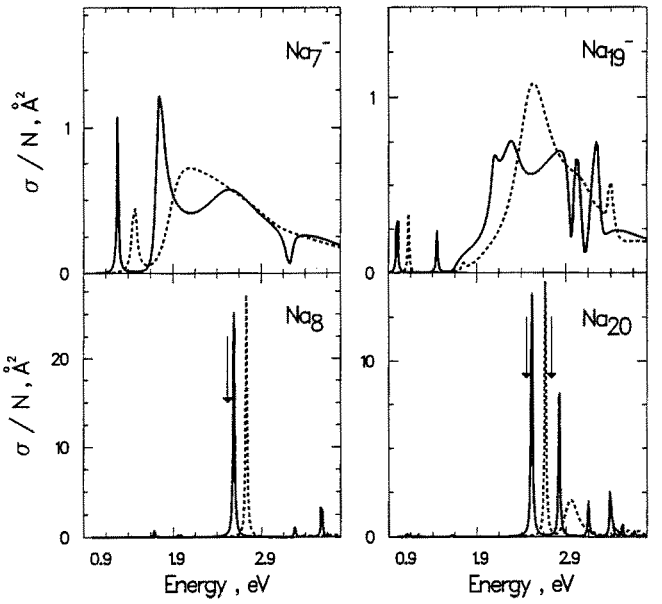

Fig. 1. Photoabsorption cross sections per ion (atom) for Na_7^-, Na_8, Na_{19}^- and Na_{20} in Å^2, calculated making use of the SIC-TDLDA (full lines) and TDLDA (dashed lines). In all cases the value used for the infinitesimal delta (cf. (4) and [3]) was 10 meV. The difference in the resulting line widths reflects the finite lifetime of Na_7^- and Na_{19}^- against electron detachment

both Na_8 and Na_{20} (for which the peak(s) occur below the continuum threshold) one can observe the emergence of small humps in the ultraviolet (UV) part of the absorption spectra. This in turn implies a reduction of total strength in the visible region, which occurs without any significant change in the fragmentation pattern of the collective mode. While the small UV humps are directly related to the physically correct Coulomb tail of the SIC-LDA potentials, which now acomodate an infinite number of bound states, the reason for the preservation of the originally calculated TDLDA fragmentation pattern is mainly due to the fact that although the tails of the SIC-TDLDA potentials decrease less steeply than in the TDLDA, the average depth of the former potentials is systematically lowered with respect to the latter, the overall result being a sizeable reduction of the orbital eigenvalues with small changes in the single-particle wave functions [12]. Since the occupied orbital wave functions remain well localized, their overlap with the unoccupied loosely bound states (Rydberg states), most sensitive to the asymptotic behaviour of the potential, remains small, leading to small redistributions of the total strength. Note, however, that the situation may change for the cases in which appreciable strength is concentrated in the UV region. In these cases, and in this region of the spectrum, one may expect the SIC-TDLDA line shapes to be quite different from their TDLDA counterparts.

The situation is different for the negatively charged clusters, for which the overall depth of the single-particle potentials is very small. Their tail is now essentially governed by exchange and correlation, due to the near cancellation of the Coulomb terms, leading to an exponential increase to zero and resulting in a finite, small

number of bound states. The cross section is therefore dominated by transitions which promote the electron into the continuum, where it has a finite probability to leave the cluster. Indeed, and below this threshold, the cross sections display a few isolated peaks which exhaust a very small fraction (4% for Na_7^- and 2% for Na_{19}^-) of the Thomas-Reiche-Kuhn (TRK) sum rule. Since, in SIC-TDLDA the continuum is treated "exactly", the line width of the photoabsorption cross section is directly related to the lifetime of the surface plasmon against electron detachment. The full width at half maximum (FWHM) of the main humps in Fig. 1 for Na_7^- and Na_{19}^- is of the order of 1 eV, in itself roughly a factor of three larger than the experimental FWHM for Na_8 (cf. Fig. 2). Note as well that the line shapes for Na_7^- and Na_{19}^-, predicted by the SIC-TDLDA are quite different from the corresponding ones in TDLDA, showing the importance of correcting for self-interaction.

A direct comparison of the SIC-TDLDA spectra of Fig. 1 with experiment is not adequate. Indeed, experimental data on neutral clusters (see dots in Fig. 2) reveal an absorption spectrum clearly dominated by one or few peaks displaying a finite, sizeable line width, which has been explained to arise mostly from the coupling

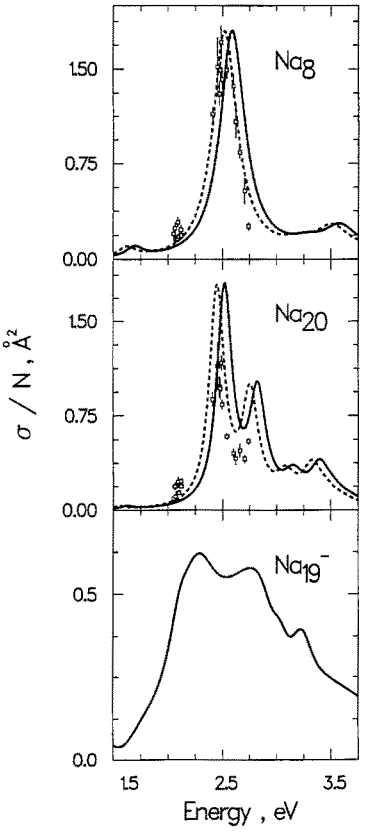

Fig. 2. Experimental values for the photoabsorption cross section per atom for Na_8 and Na_{20}, in $Å^2$, taken from [6]. The results of the present SIC-TDLDA calculation correspond to the full drawn curves. These were obtained from the results in Fig. 1 by the folding procedure discussed in the text, using damping ratios of 0.1 and 0.06 for Na_8 and for Na_{19}^- and Na_{20}, respectively. The dashed curves correspond to red-shifting the SIC-TDLDA results for the neutral clusters by 3% so as to bring the calculated plasmon peaks to their most probable positions

of the surface plasmon to quantal and thermal fluctuations of the cluster [8, 25, 26]. Although this is not included in the SIC-TDLDA, it may be simulated by folding the SIC-TDLDA cross sections with normalized Lorentzian functions, including damping ratios resulting from the above mentioned coupling. In keeping with the findings of [25], appropriate to the cluster temperatures at which experimental measurements were carried out, we used the values $\Gamma/\hbar\omega = 0.1$, 0.06 for Na_8 and Na_{20} respectively. The folded results are displayed in Fig. 2 with solid curves whereas the experimental data, taken from the absolute photoabsorption cross section measurements of [6], are shown with dots. As becomes clear from Fig. 1, SIC-TDLDA results are still $\approx 3\%$ blue-shifted with respect to the experimental peaks. For comparing the folded SIC-TDLDA line shapes with the experimental results, we purposely shifted the dynamical response by 3%, the resulting curves being displayed with dashed lines. While the overall features of the data seem to emerge from the present formalism, we note that the SIC-TDLDA predicts a sizeable accummulation of strength in a region of the absorption spectrum not yet measured. It would be interesting to resolve this part of the spectrum experimentally, in order to confirm whether or not the sum rule strength which seems to be missing in present-day experimental results, is indeed to be found in the UV region of the spectrum, as predicted by the SIC-TDLDA. Note, in passing, that in all cases our curves exhaust the TRK sum rule, whereas (in the case of Na_8, for which the area subtended by the experimental points can be reasonably estimated) the experimental energy window spans $\approx 55\%$ of the TRK sum rule.

For the negatively charged clusters the damping mechanism mentioned above will act to smooth the associated photoabsorption cross sections. Furthermore this mechanism, for these clusters, is expected to have the same order of magnitude as for the neutral ones (cf., e.g., the estimates in [27]). In keeping with this discussion, we folded the cross section for Na_{19}^- making use of a damping ratio of 0.06, the result being displayed in Fig. 2. The line width is now approximately 4 to 5 times larger than the overall width for the associated neutral cluster.

To summarize, a new formalism has been introduced for the study of excitations in many-electron systems. It uses the LDA and starts from a GS which is SIC corrected. It was applied specifically to spherical, neutral and negatively charged metal clusters. Comparison with available experimental data favours this model with respect to the TDLDA. Moreover, we were now able to provide non-trivial predictions for the photoabsorption cross section of negatively charged clusters. Because the surface plasmon is embedded in a continuum of single particle states to which it couples within the SIC-TDLDA, we were able to single out the contribution to the total line width arizing from the probability for electron detachment. This mechanism was found to significantly reduce the lifetime of the surface plasmon as compared to the neutral case. The model considered is general, and we think it can be successfully applied in

other areas where LDA methods have been used. The SIC-TDLDA provides a simple and convenient framework which requires very little extra computational effort and yet yields a theory which remedies many of the unpleasant features intrinsic to the TDLDA. In view of the results obtained, and since the jellium model should work better for larger clusters, we feel that the cluster sizes treated in the present paper constituted the most stringent tests of the model, providing additional grounds for its general validity.

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