Laser excitation of clusters: observables from electron emission

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Abstract. We give a brief review of the theoretical description of photo-electron spectra (PES) and photo-angular distributions (PAD) and discuss a few selected, typical results. The description is based on time-dependent density-functional theory at the level of the local-density approximation augmented by a self-interaction correction which is crucial for a quantitative assessment of emission processes. Coordinate-space grids are used together with absorbing boundary conditions. We discuss the basic features and trends of PES and PAD for two typical test cases, the clusters Na\(_8\) and C\(_{60}\).

1. Introduction

Photo-induced reactions are key tools to explore the properties of electronic systems as atoms, molecules, and clusters. The basic step are optical absorption measurements which provide information on both, structure and dynamics of clusters, for an overview see \([1, 2, 3, 4]\). More information can be gathered by measuring the properties of electrons emitted through an excitation by electromagnetic fields, particularly by short laser pulses. A first useful indicator is the mere net ionization yield. More specifically, photo-electron spectroscopy (PES) which measures the distribution of the kinetic energy of emitted electrons is a tool of choice as it delivers information, e.g., on the energies of occupied single electron states, for early applications see \([8, 9]\). A further, more involved step is to analyze the photo-electron angular distribution (PAD). Such measurements came up more recently in clusters and are usually combining PAD with PES, then providing double differential cross-sections (energy- and angular-resolved). First measurements dealt with cluster anions: W\(_{N^-}\), \(N = 4 - 11\) \([10, 11]\), Hg\(_{N^-}\), \(N = 3 - 20\) \([12]\), and C\(_{N^-}\), \(N = 10 - 22\) \([13, 14, 15]\). More recent results were published for the C\(_{60}\) cluster \([16]\) and medium sized Na\(_{N^-}\) clusters \([17, 18]\). The latter results nicely demonstrate a dependence of the photo-emission on the electronic ground state wave functions.

The theoretical description of PAD has a long history in atomic physics \([19, 20, 21]\). PAD have also been investigated theoretically in some molecular systems \([24, 25, 26]\). Such early investigations of PAD, and also those for PES on atoms and molecules \([22]\), employ (multi-photon) perturbation theory \([23]\). These perturbative methods require a good knowledge of the continuum states for the outgoing electrons and become extremely inconvenient for systems with low or without any symmetry as it is typically the case for clusters. Particularly for clusters, time-dependent density-functional theory at the level of the local-density approximation (TDLDA)
propagated directly in the time domain has proven to be a robust, reliable, and efficient tool, see e.g. [28, 29, 27]. This approach gives a convenient framework for analyzing electronic emission properties when augmented by a self-interaction correction (SIC) [30] and when using absorbing boundary conditions [31, 32]. Reliable absorption allows a comparatively inexpensive recording of PES during TDLDA propagation [33]. With developing a careful book-keeping of the directions of the absorbed (emitted) electrons, one can develop a direct TDLDA-SIC description of PAD [37]. Angular distributions from free Na clusters with fixed orientation have been studied extensively in [37] and from Na clusters deposited on MgO(001) or Ar(001) substrates in [38]. A fixed cluster orientation is naturally given when depositing the cluster on a substrate. But free clusters usually come along as an isotropic ensemble of cluster orientations. Recently, we have developed efficient schemes for orientation averaging of PAD from TDLDA [39, 40, 41]. This contribution presents and discusses typical results on PES and PAD for small Na clusters and for C_{60}. The aim is to review briefly the most important features and trends.

The paper is outlined as follows: Section 2 summarizes the formal framework, discussing in particular the evaluation of PES and PAD. In section 3, we discuss basic properties and trends on the example of Na clusters. Section 4 shows first results for the C_{60} cluster.

2. Formal framework
Cluster dynamics is described with standard coordinate-space techniques as outlined in detail in [32, 46]. Basis of the description is time-dependent density functional theory at the level of the time-dependent local-density approximation (TDLDA) using the exchange-correlation functional of [47] augmented with an averaged self-interaction correction (SIC) and absorbing boundary conditions. The coupling to the ions is mediated by soft local pseudo-potentials for Na [48] and non-local pseudo-potentials for C [49]. Alternatively, we also consider a soft jellium model for Na_{8}. The ionic background is frozen. This is a legitimate approximation as we consider short laser pulses and direct electron emission which proceeds rather fast. Laser excitation is described by an external classical laser field with a finite temporal envelope \propto \sin(\pi t / T_{\text{pulse}})^2.

Observables from electron emission will be explained in somewhat more detail. The description of electron emission requires absorbing boundary conditions. These are indicated in
The absorption is performed after each time step as follows: First, we perform a standard time step from \( t \) to \( t + \delta t \), \( \phi(\mathbf{r}, t) \rightarrow \hat{\phi}(\mathbf{r}) \), and then we apply a mask function to the preliminary wavefunction \( \hat{\phi} \) to obtain \( \phi(\mathbf{r}, t + \delta t) = M(\mathbf{r})\hat{\phi}(\mathbf{r}) \) which removes gradually any flow towards the bounds. We use here a spherically symmetric mask profile

\[
M = \cos \left( \frac{|\mathbf{r}| - R_{\text{in}}}{R_{\text{out}} - R_{\text{in}}} \frac{\pi}{2} \right)^{1/8}
\]

(1)

which is active in an absorbing margin \( R_{\text{in}} < |\mathbf{r}| < R_{\text{out}} \). The spherical profile is needed to minimize gridding artifacts when computing angular distributions [37]. A detailed discussion of absorbing bounds and optimal choice of absorption profiles is found in [50].

The absorbing bounds reduce gradually the norm of the wavefunctions. This mimics the dynamical ionization of the system. The net ionization, i.e. the number of escaping electrons can be computed simply from the single-particle norms as \( N_{\text{esc}} = N_{\text{el}}(t = 0) - \sum_{\alpha} (\phi_{\alpha} | \phi_{\alpha}) \). The PES are evaluated for each state separately from the phase oscillations of the single-electron wavefunction at an analyzing point \( r_{\text{meas}} \) near the absorbing bounds, see figure 1 and ref. [33]. The protocol \( \phi_{\alpha}(r_{\text{meas}}, t) \) is Fourier transformed to \( \hat{\phi}_{\alpha}(r_{\text{meas}}, \omega) \) and the spectrum \( P(\omega) \propto |\hat{\phi}_{\alpha}(r_{\text{meas}}, \omega)|^2 \) is translated to a kinetic-energy spectrum of emitted electrons by identifying \( \hbar \omega = \varepsilon_{\text{kin}} \). This simple identification is possible by virtue of the absorbing bounds which manage to leave only outgoing waves in its vicinity (thus establishing a unique relation between frequency and momentum). The case of high laser intensity (not employed here) requires slight modifications of this recipe [51].

The PAD are evaluated in angular bins as indicated in figure 1. We collect all probability which was removed by the absorption step (1) and accumulate it in the bin to which \( r \) belongs. That is done for each wavefunction separately. At the end, we dispose of the PAD for emission from each state and, of course, of the total angular distribution as well.

This procedure yields the PAD for a fixed cluster orientation. Free clusters usually come along in isotropic ensembles of orientations (each direction has equal weight). This requires orientation averaging as outlined in [39, 40]. There are two strategies for that. The first is a brute force numerical sampling of orientations. It was found that one can achieve converged results with about 18-32 appropriately chosen reference orientations. This method, although cumbersome, is applicable in all dynamical regimes. The second strategy employs formally perturbation theory to develop a compact evaluation requiring only six reference orientations. This method is applicable only to one-photon emission. Whatever averaging scheme is used, we end up with a PAD which depends only on one angle, the emission angle \( \vartheta \) relative to the laser polarization axis. The PAD for emission from s.p. state \( i \) can thus be expanded as

\[
\frac{d\sigma}{d\Omega} \propto 1 + \beta_2^{(i)} P_2(\cos \vartheta) + \beta_4^{(i)} P_4(\cos \vartheta) + \beta_6^{(i)} P_6(\cos \vartheta) + \ldots
\]

(2)

where \( P_l \) is a Legendre polynomial of order \( l \). The parameter of the leading term, \( \beta_2^{(i)} \), is called the anisotropy parameter. The same expansion applies to the total PAD \( d\sigma/d\Omega \) with the expansion coefficients \( \beta_2, \ldots \), i.e. without index \( (i) \). One-photon processes have only the \( P_2 \) term and vanishing \( \beta_{2n} \) for \( n \geq 2 \). In that case, the values of the anisotropy \( \beta_2^{(i)} \) and \( \beta_2 \) range between \(-1 \) and \( 2 \): \( \beta_2^{(i)} = 2 \) corresponds to a \( \cos^2 \vartheta \)-shape which is aligned with the laser polarization thus having its maxima at \( \vartheta = 0 \) and \( 180^\circ \), \( \beta_2^{(i)} = -1 \) yields a \( \sin^2 \vartheta \)-shape perpendicular to the laser polarization with a maximum at \( \vartheta = 90^\circ \), and \( \beta_2^{(i)} = 0 \) stands for a strictly isotropic distribution. The expansion becomes richer if more photons are involved. One can have finite values for any \( \beta_{2n} \) and \( \beta_2 > 2 \) becomes possible.
Na$_8$ \( \omega_{\text{las}} = 4.5 \) eV, FWHM=33 fs

\[
\beta_2 = 2, \quad \beta_4 = 1.0 \\
I = 10^{13} \text{W/cm}^2, \quad N_{\text{esc}} = 2.2 \\
\beta_2 = 0.6, \quad \beta_4 = 0.0
\]

\[
l = 10^{11} \text{W/cm}^2, \quad N_{\text{esc}} = 0.2
\]

Figure 2. Left panel: PAD for Na$_8$ with spherical jellium background excited with a laser of frequency \( \omega_{\text{las}} = 4.5 \) eV, pulse length of FWHM=33 fs, and varying intensity as indicated. The anisotropy parameter was approximately \( \beta_2 = 2 \) in all cases. The next higher anisotropy parameter \( \beta_4 \) varies as indicated. Right panel: PES for the same test case and weak laser intensity \( I = 10^{10} \text{W/cm}^2 \). Compared are the PES along laser polarization axis (red) with PES orthogonal to it (green). The peaks correspond to different photon numbers \( \nu \) and states (1s or 1p) as indicated.

3. Basic properties

The basic features of PES for clusters have been collected in a series of papers \cite{33, 34, 35, 36} and of PAD in \cite{37, 38, 39, 40, 41}. We summarize them briefly here. PES for one-photon processes provide a direct map of the ground state s.p. spectra as has been used since long in experiments \cite{8, 9}. This requires a laser frequency which is larger than the span of the s.p. spectra to be measured and sufficiently gentle excitation to avoid perturbation of the ground state under investigation. Larger intensities blur the signal from PES. Lower frequencies lead quickly into the regime of multi-photon ionization (MPI) where one can spot the multiple copies of PES peaks each one standing for a certain photon number \( \nu \). The envelope of this multiple peak structure shows exponential decrease with kinetic energy \( E_{\text{kin}} \) of the outgoing electrons. Using larger intensities in the MPI regime again smoothes the signal to pure exponential decrease which can easily be misinterpreted as thermal emission \cite{36}.

PAD show also different pattern in the different dynamical regimes. We illustrate that here for Na$_8$ as typical test case. The left panel of figure 2 shows the PAD for varying laser intensity. (An orientation averaging is not necessary for jellium background.) The lowest intensity (blue line) shows nearly perfectly the typical pattern of emission in the one-photon regime where the anisotropy \( \beta_2 \) alone characterizes the profile and where all higher \( \beta_{2n} \) vanish. In fact, the \( \beta_2 \approx 2 \) demonstrates a case of maximum alignment with the laser polarization. Increasing intensity leads to increasing forward/backward emission and enhances the contribution from \( \beta_4 \) and higher moments. It is interesting to relate that to the total ionization yield. A value of \( N_{\text{esc}} \approx 1 \) is found to define the transition region between the frequency dominated perturbative regime below and the field dominated non-linear regime above \cite{33}.

The right panel of figure 2 shows the photo-electron spectrum (PES) for the same test case. The calculated s.p. energies are: \( \epsilon_{1s} = -5.44 \) eV (twofold degenerated) \( \epsilon_{1p} = -4.08 \) eV (sixfold degenerated). The observed peaks match perfectly with the well-known relation \( \epsilon_{\text{out}} = \epsilon_i + \nu \omega_{\text{las}} \) for a \( \nu \)-photon process (here \( \nu = 1, 2, \) and 3). The laser frequency is just too small to move all
occupied states above threshold. Thus we see from the one-photon process only the map of the 1p state. On the other hand, the choice of parameters allows to display also the multi-photon processes. The figure shows the PES parallel and perpendicular to the laser polarization. Yields in both directions are about the same for $\nu = 1$. However the yield in perpendicular direction drops dramatically with increasing photon number. This demonstrates, here in the case of fixed laser field strength, that emission becomes the more forward directed the more photons are involved.

The impact of the ionic background structure is demonstrated in figure 3 for the case of emission from the 1p states in Na$_8$. We compare results for the anisotropy parameter $\beta_2^{(1p)}$ as function of laser frequency $\omega_{\text{las}}$ produced using detailed ionic background with those produced using soft spherical jellium. For the jellium model we used a Wigner-Seitz radius $r_s = 3.65\, a_0$ and surface thickness $\sigma = 1\, a_0$). Both models deliver about the same IP (jellium: IP$_{\text{jell}} = 4.22\, \text{eV}$; ionic background: IP$_{\text{ion}} = 4.28\, \text{eV}$) in accordance with the empirical value. The general pattern from both models differ very much. For the jellium models, the asymmetry parameter $\beta_2^{(1p)}$ explores almost the full range of possible values between $-1$ and 2. It stays mostly near the maximum possible $\beta_2 = 2$ and dives occasionally down to nearly -1 in a steep and sharp minimum. It is to be noted that these deep minima are correlated with minima in the total yield $N_{\text{esc}}(\omega_{\text{las}})$ as function of $\omega_{\text{las}}$. The ionic background, in contrary, produces a very smooth trend which stays around $\beta_2^{(1p)} = 1.7$ over the whole range of frequencies shown. Particularly, the sharp minima with negative values observed in the jellium models disappear as soon as ionic structure is taken into account. For most frequencies, however, the jellium models overestimate the asymmetry parameter which was already found earlier [40]. The ionic perturbations rescatter the electronic waves and so produce a sizable isotropic component which reduces the forward/backward orientation in cases where $\beta_2^{(1p)}$ was nearly 2 for jellium. The steep minima in the jellium case are due to particular interference effects which are only possible in the highly symmetric situation of a spherical jellium. (The same interference effect is also responsible for the corresponding minima in $N_{\text{esc}}(\omega_{\text{las}})$.) The ionic structure destroys these interferences very efficiently such that the trends with frequency become very smooth. It is to be remarked that already a small deformation of the jellium background suffices to suppress the steep minima in $N_{\text{esc}}(\omega_{\text{las}})$ which, again, is due to reduced wavefunction interferences.

![Figure 3. Angular anisotropy $\beta_2^{(1p)}$ for emission from the 1p states of Na$_8$ with full ionic (red) or spherical jellium (green) background as function of laser frequency $\omega_{\text{las}}$. The laser pulse length was FWHM= 60 fs. The intensity was varied with frequency to stay in a low emission regime with $N_{\text{esc}} = 10^{-4} - 10^{-1}$. The limiting values $\beta_2^{(1p)} = -1$ and 2 are indicated by faint dashed lines.](image-url)
**C\textsubscript{60}, varying laser intensities, low frequency \(\omega = 1.55\) eV (<IP)**

![Graph showing PES yield and s.p. energy distribution for C\textsubscript{60}](image)

**Figure 4.** Left panel: PES for C\textsubscript{60} produced with a laser pulse of low frequency \(\omega_{\text{las}} = 1.55\) eV, pulse length FWHM=33 fs and intensity near of order of 10\(^{10}\)W/cm\(^2\) fine tuned to deliver the indicated ionization \(N_{\text{esc}}\). The various peaks correspond to different photon numbers \(\nu\). Some of them are indicated. Right panel: The distribution of occupied s.p. states (black) and the actual depletion of these states (green).

4. **C\textsubscript{60}**

The C\textsubscript{60} cluster consists of 60 C atoms arranged in a highly symmetric configuration of what is called a fullerene [42]. The electrons from the 1\(s\) shell of C are considered as being core electrons kept frozen by means of a pseudo-potential during TDLDA calculations. The four electrons from the 1\(p\) shell of the C atom constitute the 240 dynamically active electrons of C\textsubscript{60}. The typically strong binding of C material yields a high ionization potential (IP) of 7.58 eV [43]. The binding is partially metallic with the consequence that one observes a pronounced plasmon resonance [44] which resides around 20 eV, i.e. far above the continuum threshold and which is thus strongly fragmented due to the high density of 1\(ph\) states. The spectral span of the occupied valence states is also rather large ranging over about 20 eV from -27 eV up to the IP [16]. To resolve the s.p. spectrum by a one-photon process, one takes a photon with frequency just above the lowest bound state. We have tested that with TDLDA and find that a laser pulse with \(\omega_{\text{las}} = 33\) eV reproduces the s.p. spectrum nicely including the occupancy weight. A particularity of C\textsubscript{60} is that the HOMO is well separated from the rest of the occupied states. This gives the next bound state, called HOMO-1, particular importance. It lies 1.8 eV below the HOMO.

The left panel of figure 4 shows PES produced with a low frequency laser with \(\omega_{\text{las}} = 1.55\) eV being far below the ionization threshold. It requires at least \(\nu = 6\) photons to move an electron from the HOMO to the continuum. The intense excitation (red line) shows a basically smooth decrease. One is not surprised as one would expect that the broad span of s.p. energies overlays completely the narrow energy difference of 1.55 eV between the multi-photon steps. However, the lower intensity (green line) resolves very clearly various photon orders as indicated. One wonders how that could come about. The explanation is found in the right panel of the figure. Here we show the upper part of the s.p. spectrum, once as it is (black line) and once weighted with the actual depletion, that is \(N_{\text{esc},i}\) taken state-wise, from the laser pulse (green line) with the same low intensity as used for the green line in the left panel. It is obvious that the low-frequency pulse removes electrons preferably from the Fermi surface and that deeper lying states are not touched at all. It is a general feature of all molecular systems that low frequency pulses...
ionize preferably from the Fermi surface while high frequency pulses remove all states with about equal weight [45]. For the particular case here, it has the consequence that the PES emission pattern become rather transparent allowing to resolve the multi-photon steps seen in the left panel (green line). The present case is particularly favorable because the energy difference between HOMO and HOMO-1 is close to the laser frequency such that signals from these two emitting states overlap strongly in the PES (to the extend that the $\nu + 1$ photon signal from the HOMO-1 approximately coincides with the $\nu$ photon signal from the HOMO). The feature that the signal is blurred for higher intensity (red line) stems from the gradual Coulomb down-shift of the spectra during ionization, the same effect as was already figured out for the much simpler Na clusters [33].

5. Conclusions
We have reviewed the theoretical description of photo-electron spectra (PES) and photo-angular distributions (PAD). The numerical evaluation relies on a Cartesian coordinate-space grid with absorbing boundary conditions cutting a dynamically active sphere into the 3D grid. PAD are simply computed from gathering the lost particles in angular segments. PES are obtained from recording the time evolution of each wavefunction at a few selected measuring points near the absorbing bounds. Both techniques add only a small overhead to the underlying TDLDA propagation thus allowing large scale studies. Free clusters require orientation averaging for the PAD which amounts to run several TDLDA calculations in parallel, six different computation in the one-photon regime up to 32 for violent excitations.

We have discussed the basic features of electron emission for two typical test cases, the clusters Na$_8$ and C$_{60}$. The outcome for PES and PAD depends very much on the dynamical conditions set mainly by laser frequency and intensity. The regime of one-photon processes (low intensity, frequency larger than the lowest bound state) is particularly clean thus allowing a detailed analysis of the single particle states in the cluster ground state. Higher intensities and/or lower frequencies lead into the regime of multi-photon ionization. At the lower end of intensities, one stays still in the frequency dominated regime where one can count photons and sees them acting, e.g., in the repeated peaks of PES or in the increasing forward/backward emission with increasing photon number. Higher intensities lead to the field dominated regime where the electrons are soaked off strongly forward/backward along the laser polarization rather independent of laser frequency and cluster structure. The PES become smooth exponential curves with little information content. The results for C$_{60}$ are particularly interesting as several measurements on this large cluster are to be expected in near future. Accordingly, more calculations for C$_{60}$ are underway.

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