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Visualizing Quantum Mechanical Phenomena

Preprint SC 99-39 (December 1999)

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Abstract

In this paper we discuss several ways to visualize stationary and non-stationary quantum mechanical systems. We demonstrate an approach for the quantitative interpretation of probability density isovalues which yields a reasonable correlation between isosurfaces for different timesteps. As an intuitive quantity for visualizing the momentum of a quantum system we propose the probability flow density, which can be treated by vector field visualization techniques. Finally, we discuss the visualization of non-stationary systems by a sequence of single timestep images.

1 Introduction

Quantum mechanics deals with models very different from classical mechanics and accordingly requires specific visualization. The objects of classical mechanics are point-like particles which are completely characterized by their positions and momenta. A classical particle could be visualized by a point in 3-space with an arrow attached to this point to indicate its momentum. The evolution in time, i.e. the particle's trajectory, could be represented by a curve in 3-space.

In contrast, quantum mechanics characterizes the state of a system statistically. The state of a quantum mechanical N-particle system is represented by a complex valued wavefunction $\Psi(\vec{x_1}, \dots, \vec{x_N})$ defined on the 3N-dimensional position space. Its absolute square $|\Psi(\vec{x_1}, \dots, \vec{x_N})|^2$ can be interpreted as a probability density. For a single particle system that means we have a real scalar field yielding the probability $P(V)$ for finding the particle in V:

$$P(V) = \int_V |\Psi(\vec{x})|^2 \, d^3x \tag{1}$$

For N particles the probability density cannot be considered as a set of N single particle densities. In classical mechanics positions of different particles can be specified independently, and interdependence does not occur until a force acts between the particles. However, in quantum mechanics only a combined probability density for the positions of all particles together exists.

Thus, a visualization of a quantum mechanical N-particle system has to deal with scalar fields in 3N dimensions. In this paper we will address the single particle case.

There have been some approaches to visualize quantum mechanical systems. Brandt and Dahmen [1] gave an illustrated introduction to quantum mechanics. Abramov et al. [2] proposed to display the probability density by isosurfaces or volume rendering. They treated a three particle system and represented it in different coordinate systems to express its important characteristics in a suitably small number of degrees of freedom.

Pauschenwein and Thaller [3] took stationary states of the hydrogen atom and showed isosurfaces and slices of the probability density color coding the phase of the wavefunction. Further, they displayed the spin structure of a zero-energy state in a magnetic field by vector field visualization.

A special approach for quantum chemistry is to visualize the charge density ρ. Levit [4] shows isosurfaces of $\Delta\rho$ while Stalling [5] visualizes the electric field $\vec{E} = -\nabla\rho$ induced by ρ. Klimenko, Nikitin et al. [6] developed tools for the visualization of topological features of relativistic string dynamics.

In the next section we will briefly describe the two quantum mechanical example systems used subsequently. In section 3 we will discuss the visualization of the positional probability density and then introduce a way for choosing isovalues of the probability density which yields a quantitative interpretation of the isovalues. For non-stationary states this interpretation defines a reasonable correlation between isosurfaces in succeeding time steps. In sections 4 and 5 we discuss methods to visualize the full position and momentum information contained in the wavefunction. In section 6 we demonstrate the use of the probability flow density which is especially useful for representing the dynamics of a stationary state. Finally, we discuss the visualization of non-stationary systems by sequences of isosurfaces and volume renderings in section 7.

2 Quantum mechanical model systems

In the following we discuss several visualization techniques using two quantum mechanical model systems. One system is stationary and describes a particle scattered on a single point interaction described by a δ-shaped potential

$$V(\vec{x}) = \frac{1}{\alpha}\delta(\vec{x}) \tag{2}$$

with interaction strength α. We consider a stationary state for momentum $\vec{p} = \hbar\vec{k}$ given analytically by

$$\psi(\vec{k}, \vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \frac{e^{i|\vec{k}|\cdot|\vec{x}|}}{(4\pi\alpha - i|\vec{k}|)|\vec{x}|}. \tag{3}$$

As discussed in [7] we will see that for suitably chosen $|\vec{k}|$ this system exhibits a vortex in its probability flow density.

The other system is non-stationary and describes the photodissociation of an HF-molecule situated in a face centered cubic crystal of Ar-atoms [8]. An excited

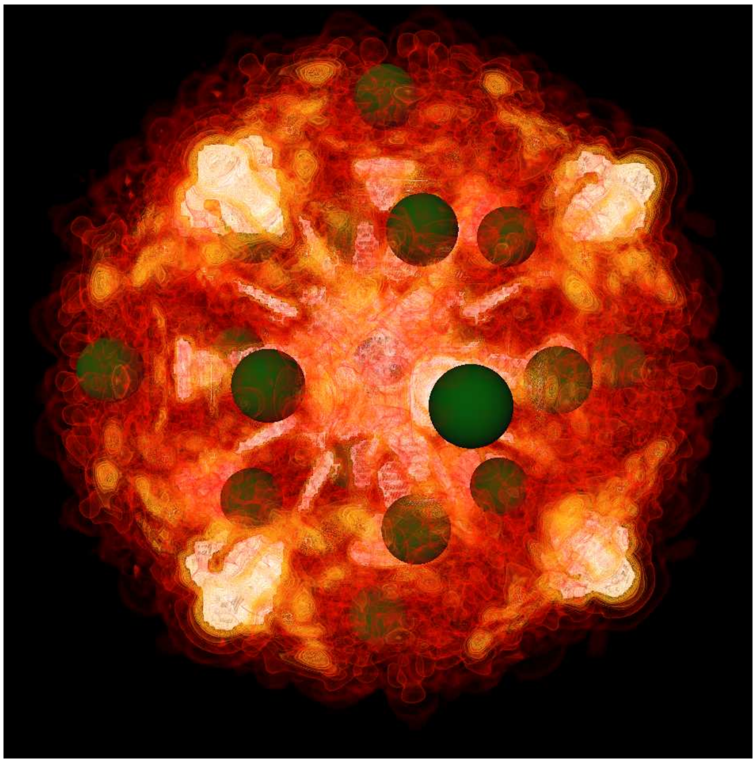

Figure 1: Volume Rendering of the positional probability density (PPD). The opacity has peaks distributed over the density range producing an onion-like shell structure in the image. The color varies from red for small values over yellow to white for large values (cf. color plates).

initial state is assumed for the HF-molecule and its time evolution is numerically determined in a quantum classical calculation. Ar and F are described classically while the proton is treated quantum mechanically. The positions of Ar and F are symbolized in the pictures by green and blue spheres with arbitrary diameter.

3 Positional probability density

As the positional probability density (PPD) $|\Psi(\vec{x})|^2$ is a density field an obvious approach is to visualize it by volume rendering. The advantage of this method is the possibility to consider the whole density field in one qualitative image and thereby to represent its fuzziness. However, with volume rendering it is difficult to recognize the spatial structure of the displayed object. Figure 1 shows the PPD of the photodissociation system visualized by hardware volume rendering using 3D texture hardware [9].
Another technique giving a much better impression of the spatial structure is to compute an isosurface of the PPD. Unfortunately, this approach disregards a great deal of information. An isosurface only shows those points where the field's value

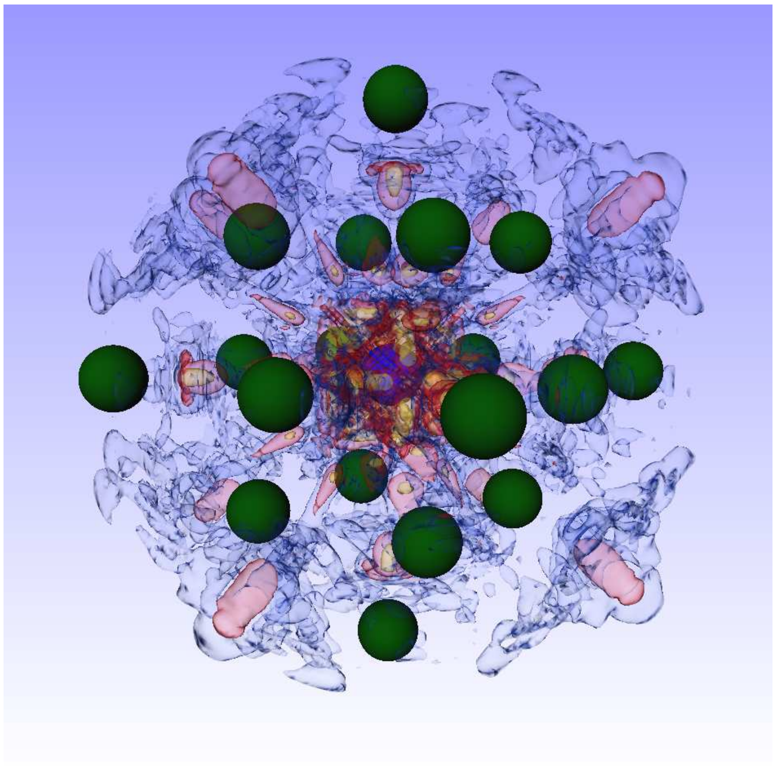

Figure 2: Transparent isosurfaces of the PPD. By a histogram-like analysis the isovalue is chosen such that the probability for finding the particle inside the volume enclosed by the emerging isosurface has a prescribed value p. Here we show three nested isosurfaces with probabilities 25% (yellow), 50% (red), and 75% (yellow) (cf. color plates).

is equal to the isovalue ignoring any other information contained in the field. As a compromise between the two methods we use nested transparent isosurfaces with different isovalues (Figure 2). Thereby we get a richer impression of the field structure without the diffuseness of volume rendering.

An important aspect of using isosurfaces is to use isovalues which allow a quantitative interpretation of the corresponding isosurfaces. Our approach is to choose an isovalue $v(p)$ corresponding to a given value $0 \leq p \leq 1$ such that the particle is with probability p on one side of the emerging isosurface and with probability $1-p$ on the other side. Therefore we first calculate a histogram-like function out of the PPD.

In our case the PPD is given by values v_{ijk} on a uniform cartesian grid. We subdivide the value range of the PPD by choosing values $v_1 < \cdots < v_{N+1}$ such that any value of the PPD lies in the interval $[v_1, v_{N+1}]$. For $l \epsilon \{1, \ldots, N\}$ we compute the sum s_l of all values v_{ijk} which lie in the interval $[v_l, v_{l+1})$. If we multiply s_l by the volume of a grid cell V_{grid}, we get the probability to find the particle at a

position where the PPD has a value in the interval $[v_l, v_{l+1})$. Accordingly the sum over all s_l multiplied by V_{grid} is 1.
We choose a logarithmic distribution of the $v_1, \ldots, v_{N+1}$, i.e. the values satisfy $v_l = C^l v_1$, where C is a suitably chosen constant. This is useful, since the probability for finding a particle at a position with density v increases with decreasing v.
In order to find the isovalue $v(p)$ corresponding to the probability p we define

$$S_l = V_{grid} \cdot \sum_{m=l}^{N} s_m \tag{4}$$

and search for l_p with

$$S_{l_p} > p > S_{l_p+1}. \tag{5}$$

Then the isovalue satisfies $v_{l_p} < v(p) < v_{l_p+1}$. We approximate $v(p)$ by

$$v(p) \approx \frac{S_{l_p} - p}{s_{l_p}} (v_{l_p+1} - v_{l_p}) + v_{l_p}. \tag{6}$$

Using this approach, a well defined statistical interpretation of the isovalue is possible. Moreover, we obtain a correspondence between isosurfaces for successive timesteps, which can thus be combined into animation sequences.

4 Phase

From the mathematical point of view the complementary and up to now unconsidered part of information is the phase $\phi(\vec{x})$ of the wavefunction defined by

$$\Psi(\vec{x}) = \sqrt{\rho(\vec{x})} e^{i\phi(\vec{x})}. \tag{7}$$

The phase distribution of the wavefunction has no relevance for statements about the position of the described particle but contains informations about the momentum of the system. The phase is ambiguous up to a global offset $\Delta\phi$, i.e. $\Psi(\vec{x})$ and $\tilde{\Psi}(\vec{x}) = \Psi(\vec{x}) \cdot e^{i \cdot \Delta\phi}$ describe the same state of a quantum mechanical system. The relevant part of the phase distribution are the spatial phase variations.
The phase distribution is interesting to visualize, since the ratio between phase frequency and geometric dimensions is an indicator for the degree of quantum mechanical behaviour.
The phase distribution in combination with the PPD can be visualized by volume rendering mapping the PPD onto the opacity and the phase onto the color by a color circle. Thereby we use the complete information contained in the complex field.
In case of the photodissociation, the surfaces of equal phase are approximately parts of concentric spheres, which makes it complicated to get a useful visual impression. In the middle of Figure 3 the camera is oriented orthogonally to these

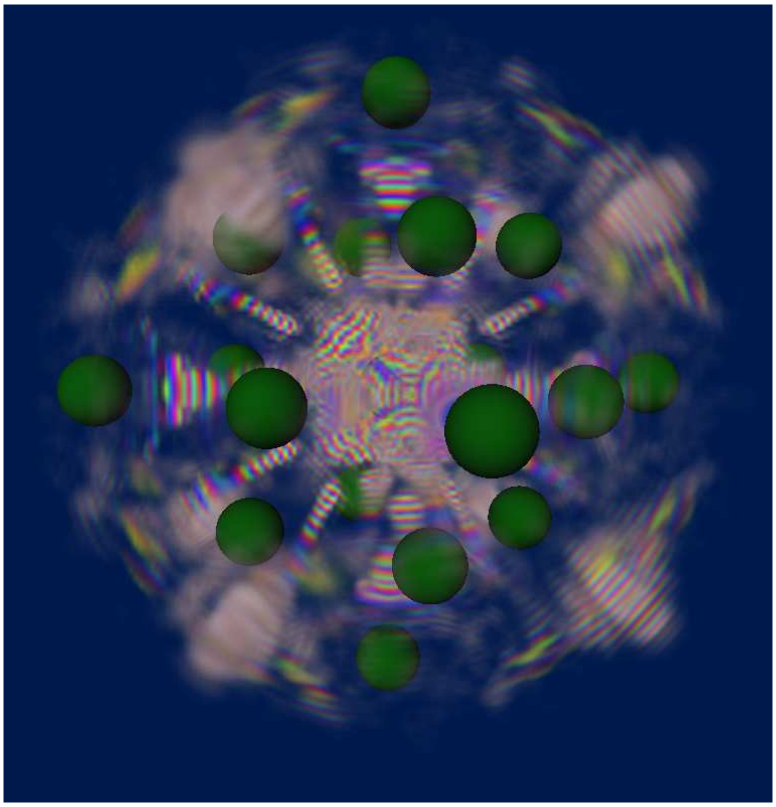

Figure 3: Combined volume rendering of PPD and phase. The viewing direction is partly parallel to the surfaces of equal phase and partly orthogonal, which leads to either rainbow-like or diffuse regions (cf. color plates).

surfaces; all surfaces contribute to the color of a volume rendered pixel, and thus no phase variation is visible. At the top the surfaces are parallel to the viewing direction, mainly one surface contributes to a pixel's color, and a rainbow-like distribution is visible.

5 Momentum probability density

The second part of information contained in the wavefunction, beside the positional probability density, is the momentum probability density. To find this, we take the Fourier transform of $\Psi(\vec{x})$

$$\hat{\Psi}(\vec{p}) = \frac{1}{(2\pi\hbar)^{\frac{2}{3}}} \int e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\Psi(\vec{x})d^3x \tag{8}$$

Its absolute square $|\hat{\Psi}(\vec{p})|^2$ represents the probability density in momentum space. The advantage of the momentum distribution over the phase distribution is its intuitive interpretation as it describes a physical quantity. On the other hand, it is

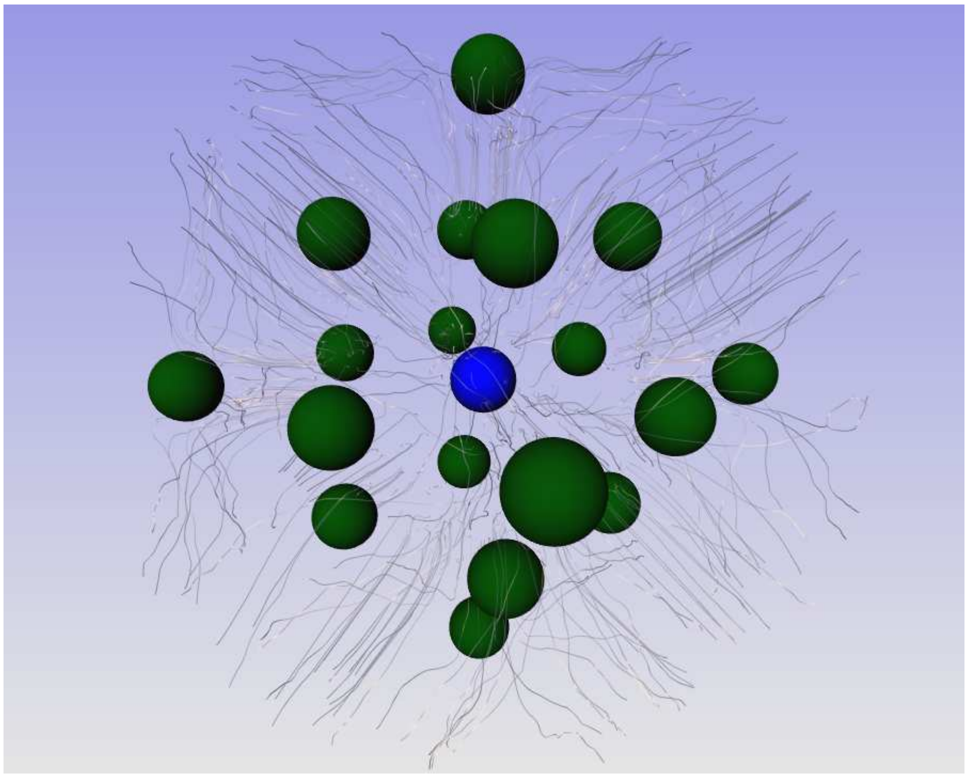

Figure 4: Probability flow density of the photodissociation of HF visualized with illuminated field lines. For better perception of spatial structure long field lines are used. They should not be interpreted as trajectories because the vector field is time dependent.

defined in momentum space and thus cannot be combined in one picture with the positional probability density.

6 Probability flow density

An alternative, which offers both an intuitive interpretation as quantity of physical dynamics and joined presentability with the positional probability density, is the *probability flow density* (PFD), which can be deduced from the preservation of probability. The probability density fulfills an equation of continuity,

$$\frac{\partial}{\partial t} |\psi|^2 + \nabla \vec{j} = 0, \tag{9}$$

where $\vec{j}$ is called PFD and can be computed from the wavefunction ψ:

$$\vec{j} = \frac{\hbar}{2mi} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) = \frac{1}{m} Re \left(\psi^* \frac{\hbar}{i} \nabla \psi \right). \tag{10}$$

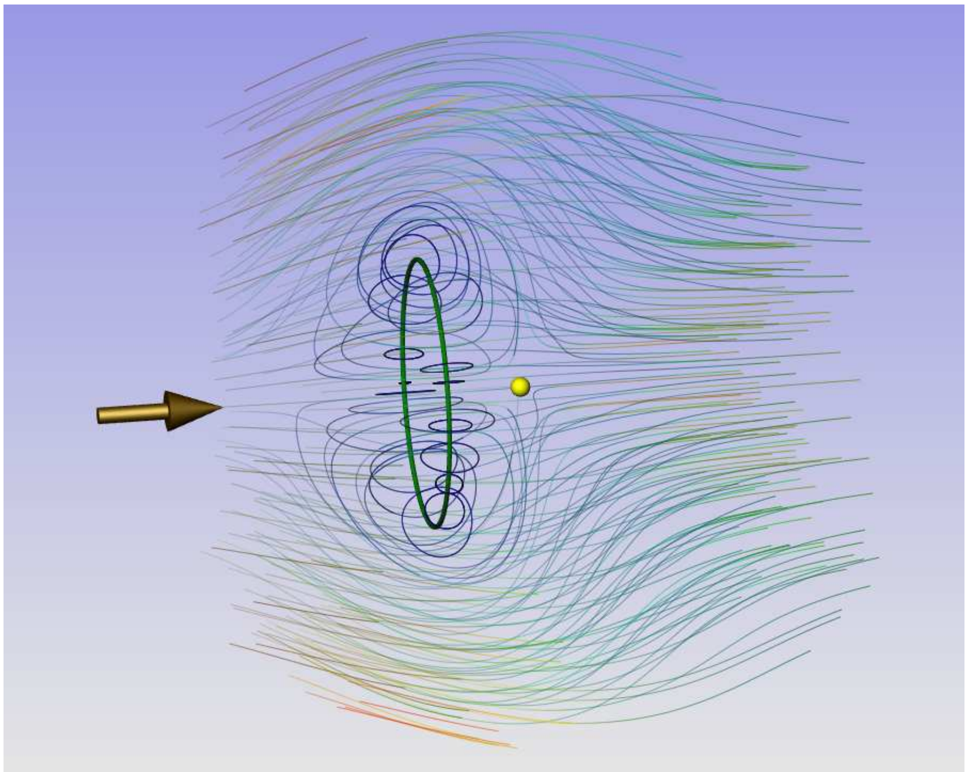

Figure 5: Probability flow density of a particle scattered by a point interaction visualized with illuminated field lines. The arrow indicates the incoming direction of the particle and the yellow sphere marks the position of the point interaction. The PFD exhibits a circular vortex whose core is emphasized by the green circle. The probability flows around the circle in the incoming direction and back through the circle in the opposite direction. The color of the field lines indicates the magnitude of the PFD varying from blue for small values over green and yellow to red for large values (cf. color plates).

The PFD is a vector field describing the dynamics of the wavefunction. We computed the PFD for the proton wavefunction at several timesteps and visualized it by illuminated lines [10].

For a good spatial impression it is necessary to use long field lines, but regarding the non-stationarity of the system and the vectorfield long field lines are misleading (Figure 4). The vector field in a single timestep is just a snapshot and can strongly change in the time that an imaginary particle would need to follow the field line.

In the stationary case the use of long field lines is reasonable and expressive. We took a stationary state of a particle scattered by a point interaction. For a suitably chosen momentum of the scattered particle and strength of the interaction the PFD exhibits a circular vortex centered around the collision axis (Figure 5).

7 Animation

So far we have only treated single timesteps. Having visualized the PPD by an isosurface it would be desirable to define a surface enclosing a certain part of the PPD and then to let the surface evolve driven by the probability flow density of the wavefunction. Thereby one could observe the dynamics of the enclosed part of the "probability fluid".

Displaying a sequence of isosurfaces for a constant probability p we can approximate such a physically evolving surface as long as the wavefunction is compressed or decompressed homogeneously enough. This is a basic problem of animating isosurfaces. As soon as the wavefunction is subject to local compression and decompression, e.g. in case of collisions, new parts of the surface can appear unexpectedly out of nowhere. On the other hand choosing an isovalue which covers all interesting parts of the wavefunction in one timestep leads to visual clutter in other timesteps.

The left column of Figure 6 shows snapshots of such an animation sequence for photodissociating HF. As described above we show three nested isosurfaces enclosing 25%, 50%, and 75% of the probability.

The initial state, which is not displayed, is a rotationally excited eigenstate of HF. It consists of six wavepackets located on the positive and negative branches of the x-, y- and z-axis. Further, there are twelve wavepackets with lower probability density between them. In the top image, after 5.8 fs, the wavefunction has expanded. All wavepackets have moved away from the center. In the middle image, after 12.2 fs, the main axis packets are colliding with the neighbor atoms. After this collision the wavepackets are partly scattered back to the center. The 75% isosurface begins to cover a kind of "corona" which has been invisible up to now. In the bottom image, after 21.4 fs, the low density packets, which had nearly disappeared, are visible again and are still moving away from the center.

Alternatively, we generated an animation sequence with volume rendering. The right column of Figure 6 shows snapshots from this sequence at the same moments as in the isosurface case. While the images are more diffuse than those with isosurfaces, all information is used that is available from the probability density. Respectively we can see that the "corona" has been there all the time but with a density too small for the used isovalue.

8 Conclusion

We have demonstrated a method for the quantitative interpretation of isovalues of the positional probability density. Thereby we proposed a reasonable way to generate corresponding isosurfaces for different timesteps. For intuitive visualization of quantum mechanical dynamics we have introduced the display of the probability flow density by field lines.

For the future several tasks remain. One is the visualization of the real evolution

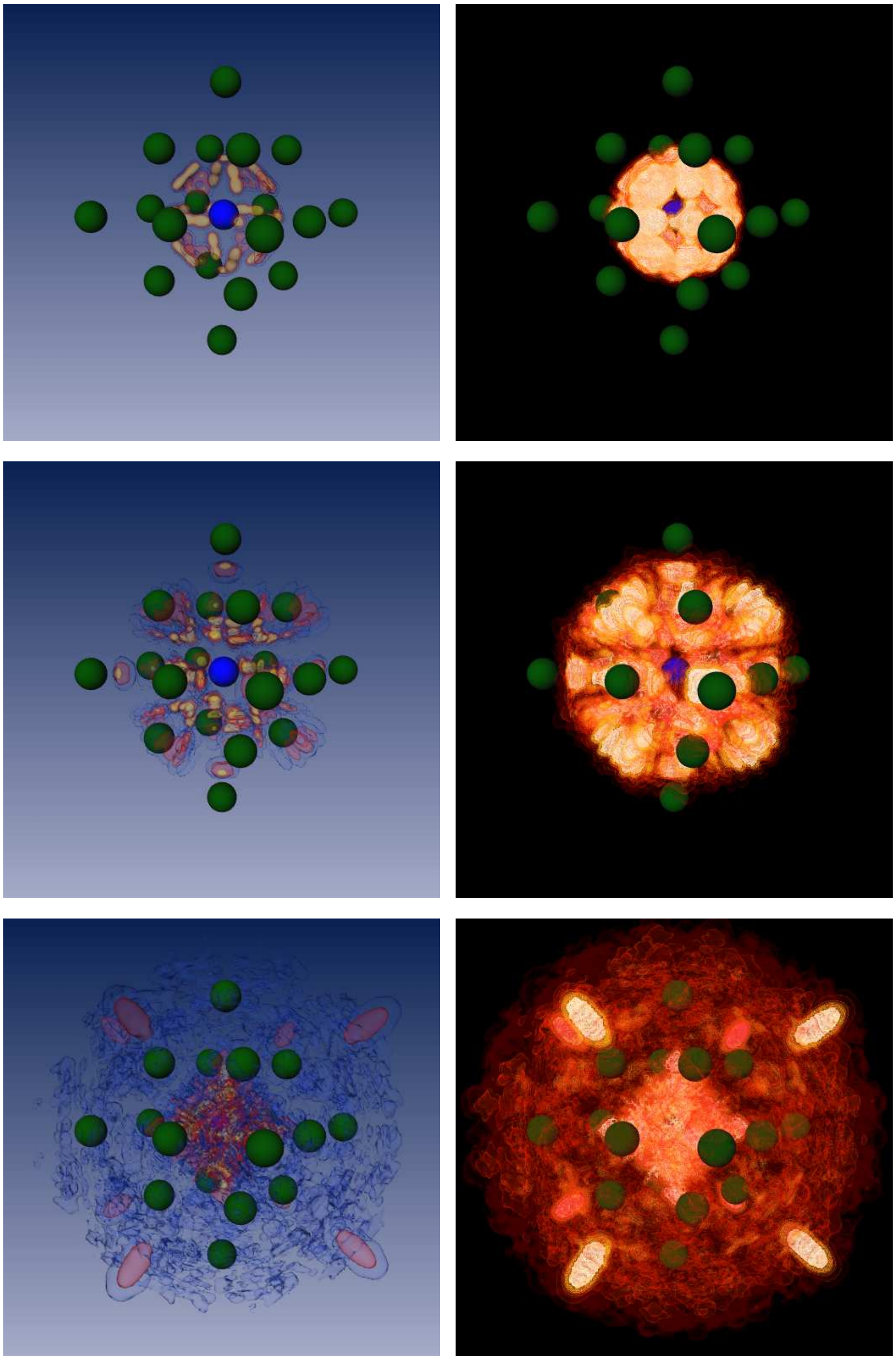

Figure 6: Snapshots from the animation sequences of the photodissociation. At 5.8 fs (top), 12.2 fs (middle), and 21.4 fs (bottom) the left column shows nested transparent isosurfaces of the PPD covering 25% (yellow), 50% (red), and 75% (blue) of the probability. The right column shows volume rendering of the PPD at the same timesteps.

of an initial volume of "probability fluid" with flow surfaces [11]. Another one is to visualize the probability flow density of non-stationary systems by streaklines instead of field lines.

9 Acknowledgements

We would like to thank Martin Holz and Burkhard Schmidt from the ZIB for kindly providing the data of the HF photodissociation. Thanks also to Peter Nettesheim from the ZIB for constant interest, enthusiasm and useful discussions.

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