Three-Dimensional Orbital Tomographic Imaging of N_2

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Background

- When atoms or molecules interact with intense laser, **high-order harmonics** are generated, which have high spatial and time resolutions, leading to the generation of **molecular orbital tomography (MOT)**.
- MOT was firstly applied to the imaging of N_2 [1], and then developed to a more general method and extended to more complex symmetric molecules.
- MOT before obtains the **two-dimensional (2D) orbital**, which is the three-dimensional orbital projected onto the plane perpendicular to the laser propagation direction.
- Here we develop a **three-dimensional (3D) MOT** method and successfully applied to the reconstructions of the highest occupied molecular orbital (HOMO) of N_2.

Methods

- The exact 2D orbital is calculated by Firefly program, and the 2D projected orbital is reconstructed based on the transition dipole moment calculated by SLIMP program [2].
- The 2D slice orbital and 3D orbital of N2 are reconstructed with our 3D MOT method.

Results

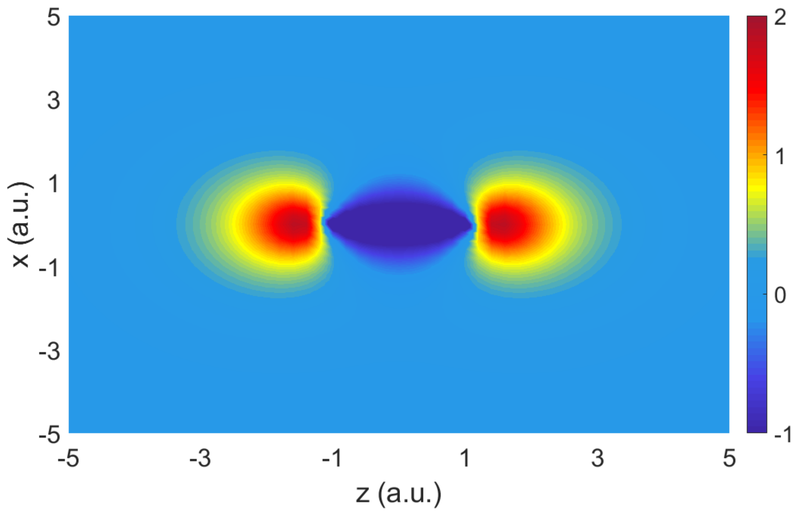

Figure 1. The 2D slice HOMO calculated by Firefly program

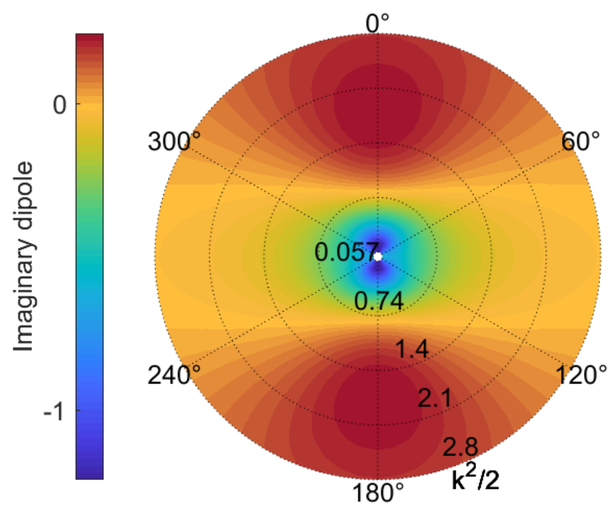

Figure 2. The transition dipole moment calculated by SLIMP program

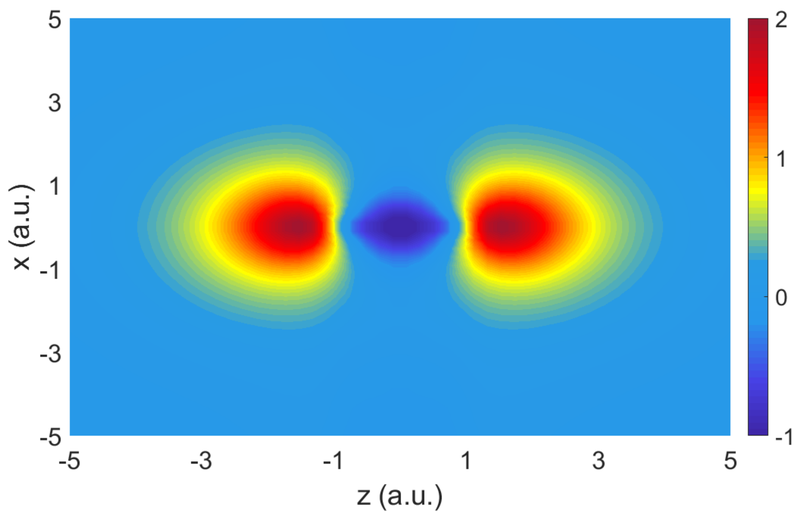

Figure 3. The reconstructed 3D HOMO projected onto a 2D plane

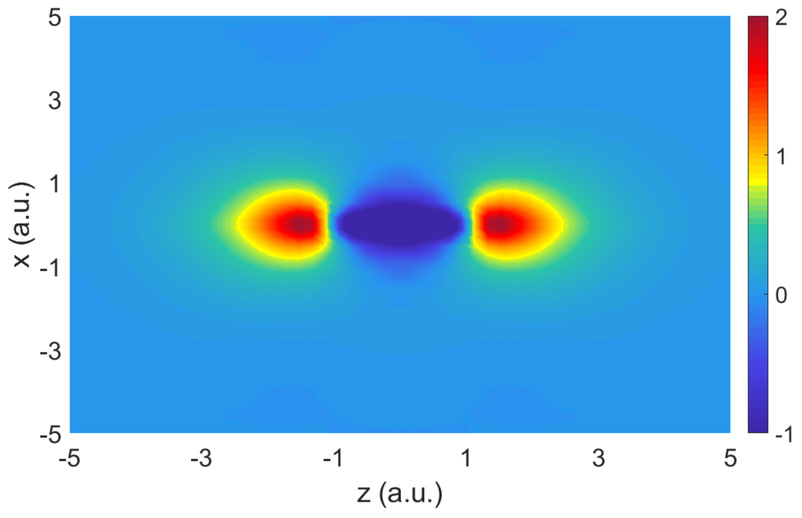

Figure 4. The reconstructed 2D slice HOMO

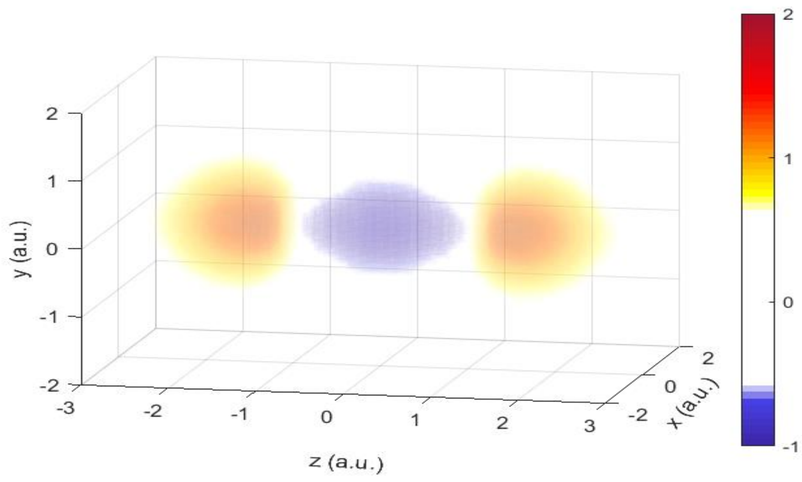

Figure 5. The reconstructed 3D HOMO

References

[1] J. Itatani et al., “Tomographic imaging of molecular orbitals”, Nature, 867-871, 2004.

[2] S. Patchkovskii, Z. Zhao, T. Brabec and D. M. Villeneuve, “High harmonic generation and molecular orbital tomography in multielectron systems: beyond the single active electron approximation”. Physical Review Letters, 123003,2006.

Conclusions

- There are deviations of weights of the projected HOMO onto the 2D plane that the general MOT obtains compared with the exact 2D slice HOMO calculated by Firefly program. Our 3D MOT method, which can reconstruct the 3D HOMO and 2D slice HOMO, reduces the deviations and makes the reconstructions closer to the exact HOMO.