

# Electron-nuclear motion in femtoscale: coherence, decoherence and anti-alignment

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We study the impact of the nuclear motion in the properties of electronic wave packets, that is, coherent superpositions of electronic states. We propose several schemes to manipulate the charge distribution of a molecule, exemplified by the creation of electron dipoles. We perform numerical simulations solving the time-dependent Schrödinger equation in a grid for the nuclear and electronic coordinates to a maximum of two dimensions [1], or by designing a mean-field Ehrenfest approach for the electron and nuclear motion, where the dynamics of the electronic degrees of freedom are propagated in a grid [2].

We consider homonuclear diatomic cations, that is, molecules with no permanent dipole but charge transfer resonances. We argue that to create and manipulate large dipoles any working control mechanism needs i) to break the symmetry of the system and ii) to sustain highly correlated electronic and nuclear motion. The vibrational motions leads to strong decoherence except when the electron dipole moves in femtosecond timescale, in a way that is highly correlated to the nuclear motion. This correlated electron-nuclear motion is possible in the excited electronic state as long as the molecular axis remains aligned with the field polarization, allowing the creation of huge dipoles oscillating in the far infrared [1]. Initially, one would suspect that the requirement of alignment is not surprising and hardly too demanding, as laser-induced alignment is well studied in the ground state. We show, however, that the charge resonant state responsible for the large dipole induces anti-alignment in the excited state, beating the control mechanism, as the molecule rotates perpendicular to the field and the bond breaks [3].

## References

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