Quantum Dynamics in Tailored Intense Fields

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## Ultra long-range ab initio calculations

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We propose a generalization of the Bloch state which involves an additional sum over a finer grid in reciprocal space around each k-point. This allows for ab-initio calculations of ultra long-range modulations in the density which may involve millions of unit cells but with an efficiency rivaling that of single unit cell. This is due to a new algorithm developed specifically for solving the particular eigenvalue problem that this ansatz requires. Thus physical effects on the micron length scale, which nevertheless depend on details of the electronic structure on nanometer length scales, can be computed exactly within density functional theory. As a specific example, we will apply our method to treat a tailored spatially extended field in a solid.

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