Many-body quantum dynamics by means of the time-dependent density functional based reduced density matrix theory

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We evaluate the density matrix of an arbitrary quantum mechanical system in terms of the quantities pertinent to the solution of the time-dependent density functional theory (TDDFT) problem. Our theory utilizes the adiabatic connection perturbation method of Görling and Levy [1, 2], from which the expansion of the many-body density matrix in powers of the coupling constant λ naturally arises. We then find the reduced density matrix $\rho_\lambda(\mathbf{r}, \mathbf{r}', t)$, which, by construction, has the λ-independent diagonal elements $\rho_\lambda(\mathbf{r}, \mathbf{r}, t) = n(\mathbf{r}, t)$, $n(\mathbf{r}, t)$ being the particle density. The off-diagonal elements of $\rho_\lambda(\mathbf{r}, \mathbf{r}', t)$ contribute importantly to the processes unaccessible via the density, directly or by the use of the known TDDFT functionals. Of those, we consider the momentum-resolved photoemission, doing this to the first order in λ, i.e., on the level of the exact exchange theory. In illustrative calculations of photoemission from the quasi-two-dimensional electron gas and isolated atoms, we find quantitatively strong and conceptually far-reaching differences with the independent-particle Fermi's golden rule formula [3].

[1] Görling A and Levy M 1994 *Phys. Rev. A* **50** 196–204
[2] Görling A 1997 *Phys. Rev. A* **55** 2630–2639
[3] Nazarov V U 2019 *Phys. Rev. Lett.* **123** 095302