Note of TDDFT

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1 backgrounds

The solution of the time-dependent Schrödinger equation is

$$\Psi(t) = \hat{U}(t, t_0)\Psi_0 \tag{1}$$

the time evolution operator $\hat{U}(t, t_0)$ has two properties, compostion property and unitary

$$\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0) \tag{2}$$

$$\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = 1 \tag{3}$$

If the Hamiltonian is independent of time, the operator is

$$\hat{U}(t, t_0) = e^{-i\hat{H}(t-t_0)} \tag{4}$$

For time-dependent perturbation theory

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t) \tag{5}$$

$$\hat{U}(t, t_0) = e^{-i\hat{H}(t-t_0)}\hat{U}_1(t, t_0) \tag{6}$$

from the time-dependent SE we can derive

$$i \tag{7}$$

$$hatU(t, t_0) = e^{-i\hat{H}(t-t_0)}\hat{U}_1(t, t_0) \tag{8}$$