1 Kvantová teorie kmitání

1.1 Příklad [1, 18, část 1.3.3]

Dosaďte

$$\hat{Q}_i^I(\lambda) = e^{\frac{i}{\hbar}\hat{H}_S\lambda}\hat{Q}_i^S e^{-\frac{i}{\hbar}\hat{H}_S\lambda} = e^{i\omega_i\lambda}\hat{Q}_i^S \tag{1.1}$$

do

$$\begin{aligned}\hat{\varrho}_S^I(t) - \hat{\varrho}_S^I(t_0) = &- i\sum_i \left\langle \hat{F}_i\right\rangle_R \int_{t_0}^t \mathrm{d}t_1 \left[\hat{Q}_i^I(t_1-t_0), \hat{\varrho}_S^I(t_0)\right] - \sum_{i,j}\int_0^{t-t_0}\mathrm{d}\xi\left(\int_0^{t-t_0-\xi}\mathrm{d}\tau\left(\left(\hat{Q}_i^I(\tau+\xi)\hat{Q}_j^I(\xi)\hat{\varrho}_S^I(t_0)-\right.\right.\right.\\ &\left.\left.\left.-\hat{Q}_j^I(\xi)\hat{\varrho}_S^I(t_0)\hat{Q}_i^I(\tau+\xi)\right)\left\langle \hat{F}_i(\tau)\hat{F}_j\right\rangle_R - \left(\hat{Q}_i^I(\tau+\xi)\hat{\varrho}_S^I(t_0)\hat{Q}_j^I(\xi) - \hat{\varrho}_S^I(t_0)\hat{Q}_j^I(\xi)\hat{Q}_i^I(\tau+\xi)\right)\left\langle \hat{F}_j\hat{F}_i(\tau)\right\rangle_R\right)\right).\end{aligned} \tag{1.2}$$

Řešení. Výraz na pravé straně (1.2) nejprve rozdělíme

$$\begin{aligned}\hat{\varrho}_S^I(t) - \hat{\varrho}_S^I(t_0) = &- i\sum_i \left\langle \hat{F}_i\right\rangle_R \underbrace{\int_{t_0}^t \mathrm{d}t_1 \left[\hat{Q}_i^I(t_1-t_0), \hat{\varrho}_S^I(t_0)\right]}_{=A} - \\ &-\sum_{i,j}\underbrace{\int_0^{t-t_0}\mathrm{d}\xi\left(\int_0^{t-t_0-\xi}\mathrm{d}\tau\left(\left(\hat{Q}_i^I(\tau+\xi)\hat{Q}_j^I(\xi)\hat{\varrho}_S^I(t_0) - \hat{Q}_j^I(\xi)\hat{\varrho}_S^I(t_0)\hat{Q}_i^I(\tau+\xi)\right)\left\langle \hat{F}_i(\tau)\hat{F}_j\right\rangle_R\right)\right)}_{=B} - \\ &-\sum_{i,j}\underbrace{\int_0^{t-t_0}\mathrm{d}\xi\left(\int_0^{t-t_0-\xi}\mathrm{d}\tau\left(\left(\hat{Q}_i^I(\tau+\xi)\hat{\varrho}_S^I(t_0)\hat{Q}_j^I(\xi) - \hat{\varrho}_S^I(t_0)\hat{Q}_j^I(\xi)\hat{Q}_i^I(\tau+\xi)\right)\left\langle \hat{F}_j\hat{F}_i(\tau)\right\rangle_R\right)\right)}_{=C}.\end{aligned}$$

Dosadíme (1.1) a provedeme úpravu

- funkci $e^{i\omega_i(t_1-t_0)}$ vytkneme před komutátor, členy nezávislé na t_1 vytkneme před integrál a provedeme substituci

$$A = \int_{t_0}^t \mathrm{d}t_1\left[e^{i\omega_i(t_1-t_0)}\hat{Q}_i^S, \hat{\varrho}_S^I(t_0)\right] = \left[\hat{Q}_i^S, \hat{\varrho}_S^I(t_0)\right]\int_{t_0}^t \mathrm{d}t_1 e^{i\omega_i(t_1-t_0)} = \left|\begin{matrix} t_1 - t_0 = \xi \\ \mathrm{d}t_1 = \mathrm{d}\xi\end{matrix}\right| = \left[\hat{Q}_i^S, \hat{\varrho}_S^I(t_0)\right]\int_0^{t-t_0}\mathrm{d}\xi e^{i\omega_i\xi}.$$

$$B = \int_0^{t-t_0}\mathrm{d}\xi\left(\int_0^{t-t_0-\xi}\mathrm{d}\tau\left(\left(e^{i\omega_i(\tau+\xi)}\hat{Q}_i^S e^{i\omega_j\xi}\hat{Q}_j^S\hat{\varrho}_S^I(t_0) - e^{i\omega_j\xi}\hat{Q}_j^S\hat{\varrho}_S^I(t_0)e^{i\omega_i(\tau+\xi)}\hat{Q}_i^S\right)\left\langle \hat{F}_i(\tau)\hat{F}_j\right\rangle_R\right)\right) = \dots$$

- členy nezávislé na ξ a τ vytkneme před integrál

$$\ldots = \left(\hat{Q}_i^S \hat{Q}_j^S \hat{\varrho}_S^I(t_0) - \hat{Q}_j^S \hat{\varrho}_S^I(t_0) \hat{Q}_i^S\right) \int_0^{t-t_0} \mathrm{d}\xi \left(\int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\mathrm{e}^{\mathrm{i}\omega_i \tau} \mathrm{e}^{\mathrm{i}(\omega_i+\omega_j)\xi} \left\langle \hat{F}_i(\tau) \hat{F}_j \right\rangle_R \right) \right) = \ldots$$

- odseparujeme integrály

$$\ldots = \left(\hat{Q}_i^S \hat{Q}_j^S \hat{\varrho}_S^I(t_0) - \hat{Q}_j^S \hat{\varrho}_S^I(t_0) \hat{Q}_i^S\right) \int_0^{t-t_0} \mathrm{d}\xi \mathrm{e}^{\mathrm{i}(\omega_i+\omega_j)\xi} \int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\mathrm{e}^{\mathrm{i}\omega_i \tau} \left\langle \hat{F}_i(\tau) \hat{F}_j \right\rangle_R \right).$$

- obdobně

$$\begin{aligned} C &= \int_0^{t-t_0} \mathrm{d}\xi \left(\int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\left(\mathrm{e}^{\mathrm{i}\omega_i(\tau+\xi)} \hat{Q}_i^S \hat{\varrho}_S^I(t_0) \mathrm{e}^{\mathrm{i}\omega_j \xi} \hat{Q}_j^I - \hat{\varrho}_S^I(t_0) \mathrm{e}^{\mathrm{i}\omega_j \xi} \hat{Q}_j^S \mathrm{e}^{\mathrm{i}\omega_i(\tau+\xi)} \hat{Q}_i^S \right) \left\langle \hat{F}_j \hat{F}_i(\tau) \right\rangle_R \right) \right) \\ &= \left(\hat{Q}_i^S \hat{\varrho}_S^I(t_0) \hat{Q}_j^I - \hat{\varrho}_S^I(t_0) \hat{Q}_j^S \hat{Q}_i^S \right) \int_0^{t-t_0} \mathrm{d}\xi \left(\int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\mathrm{e}^{\mathrm{i}\omega_i \tau} \mathrm{e}^{\mathrm{i}(\omega_i+\omega_j)\xi} \left\langle \hat{F}_j \hat{F}_i(\tau) \right\rangle_R \right) \right) \\ &= \left(\hat{Q}_i^S \hat{\varrho}_S^I(t_0) \hat{Q}_j^I - \hat{\varrho}_S^I(t_0) \hat{Q}_j^S \hat{Q}_i^S \right) \int_0^{t-t_0} \mathrm{d}\xi \mathrm{e}^{\mathrm{i}(\omega_i+\omega_j)\xi} \int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\mathrm{e}^{\mathrm{i}\omega_i \tau} \left\langle \hat{F}_j \hat{F}_i(\tau) \right\rangle_R \right). \end{aligned}$$

Dohromady

$$\begin{aligned} \hat{\varrho}_S^I(t) - \hat{\varrho}_S^I(t_0) = &- \mathrm{i} \sum_i \left\langle \hat{F}_i \right\rangle_R \left[\hat{Q}_i^S, \hat{\varrho}_S^I(t_0) \right] \int_0^{t-t_0} \mathrm{d}\xi \mathrm{e}^{\mathrm{i}\omega_i \xi} - \sum_{i,j} \left(\hat{Q}_i^S \hat{Q}_j^S \hat{\varrho}_S^I(t_0) - \hat{Q}_j^S \hat{\varrho}_S^I(t_0) \hat{Q}_i^S\right) \int_0^{t-t_0} \mathrm{d}\xi \mathrm{e}^{\mathrm{i}(\omega_i+\omega_j)\xi} \int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\mathrm{e}^{\mathrm{i}\omega_i \tau} \left\langle \hat{F}_i(\tau) \hat{F}_j \right\rangle_R \right) - \\ &- \sum_{i,j} \left(\hat{Q}_i^S \hat{\varrho}_S^I(t_0) \hat{Q}_j^I - \hat{\varrho}_S^I(t_0) \hat{Q}_j^S \hat{Q}_i^S \right) \int_0^{t-t_0} \mathrm{d}\xi \mathrm{e}^{\mathrm{i}(\omega_i+\omega_j)\xi} \int_0^{t-t_0-\xi} \mathrm{d}\tau \left(\mathrm{e}^{\mathrm{i}\omega_i \tau} \left\langle \hat{F}_j \hat{F}_i(\tau) \right\rangle_R \right). \end{aligned}$$

Reference

[1] M. Vrbová, J. Šulc: *Interakce rezonančního záření s látkou* (Nakladatelství ČVUT, 2006)

[2] conVERTER - převody jednotek
http://www.converter.cz/