

E aqui aparece a primeira ordem da constante de acoplamento. Queremos, como anteriormente, desprezar termos de ordem superior a $|g_{\mathbf{k},\lambda}|^2$. Mas,

$$\left[G_{\mathbf{k},\lambda}^\dagger, H(t) \right] = \left[G_{\mathbf{k},\lambda}^\dagger, H_{at}(t) + H_{int} \right].$$

A ideia aqui é que queremos, depois que encontrarmos $U^\dagger(t) G_{\mathbf{k},\lambda}^\dagger U(t)$, substituir o resultado na equação para $b_{\mathbf{k},\lambda}(t)$ e desprezar ordens superiores a $|g_{\mathbf{k},\lambda}|$, já que precisamos de combinações de um operador de criação multiplicado por um de aniquilação para que o valor do traço junto com a matriz densidade dos fótons seja não nulo. Ainda estamos fazendo a aproximação de segunda ordem nas constantes de acoplamento, pois queremos algo equivalente à nossa equação mestra. Logo, no comutador $\left[G_{\mathbf{k},\lambda}^\dagger, H(t) \right]$ queremos manter apenas primeira ordem em $G_{\mathbf{k},\lambda}^\dagger$ ou $G_{\mathbf{k},\lambda}$. Sendo assim, podemos escrever, para essa finalidade,

$$\begin{aligned} \left[G_{\mathbf{k},\lambda}^\dagger, H(t) \right] &\approx \left[G_{\mathbf{k},\lambda}^\dagger, H_{at}(t) \right] \\ &= \left[G_{\mathbf{k},\lambda}^\dagger, K \right], \end{aligned}$$

já que todos os outros termos em $H_{at}(t)$ comutam com $G_{\mathbf{k},\lambda}^\dagger$. Lembremos que

$$G_{\mathbf{k},\lambda}^\dagger \equiv g_{\mathbf{k},\lambda}^* \exp(-i\mathbf{k} \cdot \mathbf{R}_{CM})$$

e

$$\exp(-i\mathbf{k} \cdot \mathbf{R}_{CM}) = \int d^3r' \int d^3p' f(\mathbf{r}', \mathbf{p}') \exp(-i\mathbf{k} \cdot \mathbf{r}').$$

Logo,

$$\begin{aligned} b_{\mathbf{k},\lambda}(t) &= \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + \int_0^t dt' \exp[-i\omega_{\mathbf{k},\lambda}(t-t')] \\ &\quad \times g_{\mathbf{k},\lambda}^* \int d^3r' \int d^3p' U^\dagger(t') f(\mathbf{r}', \mathbf{p}') U(t') \exp(-i\mathbf{k} \cdot \mathbf{r}') \sigma_{01}(t'), \end{aligned}$$

isto é,

$$\begin{aligned} b_{\mathbf{k},\lambda}(t) &= \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \int_0^t dt' \exp[-i\omega_{\mathbf{k},\lambda}(t-t')] \\ &\quad \times \int d^3r' \int d^3p' F(\mathbf{r}', \mathbf{p}', t') \exp(-i\mathbf{k} \cdot \mathbf{r}') \sigma_{01}(t'). \end{aligned}$$

Se o t_2 é próximo o bastante de t_1 , segue que

$$\begin{aligned} F(\mathbf{r}, \mathbf{p}, t_2) &\approx F\left(\mathbf{r} - \mathbf{p} \frac{t_2 - t_1}{M}, \mathbf{p}, t_1\right) \\ &\approx F(\mathbf{r}, \mathbf{p}, t_1), \end{aligned}$$

supondo que o átomo se desloca muito mais lentamente do que o operador $b_{\mathbf{k},\lambda}(t)$ varia. Então,

$$\begin{aligned} b_{\mathbf{k},\lambda}(t) &\approx \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \int_0^t dt' \exp[-i\omega_{\mathbf{k},\lambda}(t-t')] \\ &\quad \times \int d^3r' \int d^3p' F(\mathbf{r}', \mathbf{p}', t) \exp(-i\mathbf{k} \cdot \mathbf{r}') \sigma_{01}(t'), \end{aligned}$$

ou seja,

$$b_{\mathbf{k},\lambda}(t) \approx \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \int d^3r' \int d^3p' F(\mathbf{r}', \mathbf{p}', t) \exp(-i\mathbf{k} \cdot \mathbf{r}') \\ \times \int_0^t dt' \exp[-i\omega_{\mathbf{k},\lambda}(t-t')] \sigma_{01}(t').$$

Também sabemos que

$$\frac{\partial}{\partial t} \sigma_{01}(t) = \frac{1}{i\hbar} U^\dagger(t) [\sigma_{01}(0), H(t)] U(t).$$

Mas,

$$[\sigma_{01}(0), H(t)] = [\sigma_{01}(0), H_{at}(t) + H_{int}] \\ \approx [\sigma_{01}(0), H_{at}(t)],$$

porque não vamos considerar outro termo proporcional à constante de acoplamento. Logo,

$$[\sigma_{01}(0), H(t)] \approx [\sigma_{01}(0), \hbar\omega_{at}\sigma_{11}(0)] + \left[\sigma_{01}(0), -\hbar\frac{\Omega_{op}^\dagger}{2}\sigma_{10}(0) \exp(-i\omega_L t) \right].$$

A frequência de Rabi, em geral, é muito menor do que ω_{at} e, portanto, podemos aproximar, dentro da escala em que os campos variam,

$$[\sigma_{01}(0), H(t)] \approx \hbar\omega_{at} [\sigma_{01}(0), \sigma_{11}(0)] \\ = \hbar\omega_{at}\sigma_{01}(0).$$

Sendo assim, vem

$$\frac{\partial}{\partial t} \sigma_{01}(t) \approx \frac{1}{i\hbar} U^\dagger(t) \hbar\omega_{at}\sigma_{01}(0) U(t) \\ = -i\omega_{at}\sigma_{01}(t)$$

e, portanto,

$$\sigma_{01}(t') \approx \exp[-i\omega_{at}(t'-t)] \sigma_{01}(t).$$

Logo,

$$b_{\mathbf{k},\lambda}(t) \approx \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \int d^3r' \int d^3p' F(\mathbf{r}', \mathbf{p}', t) \exp(-i\mathbf{k} \cdot \mathbf{r}') \\ \times \int_0^t dt' \exp[-i\omega_{\mathbf{k},\lambda}(t-t')] \exp[-i\omega_{at}(t'-t)] \sigma_{01}(t'),$$

isto é,

$$b_{\mathbf{k},\lambda}(t) \approx \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \int d^3r' \int d^3p' F(\mathbf{r}', \mathbf{p}', t) \sigma_{01}(t) \exp(-i\mathbf{k} \cdot \mathbf{r}') \\ \times \int_0^t dt' \exp[i(\omega_{at} - \omega_{\mathbf{k},\lambda})(t-t)].$$

O que acabamos de fazer é também chamado de aproximação de Weiskopf & Wigner. É equivalente à nossa equação mestra de Born & Markov. Agora usamos o resultado que já utilizamos anteriormente:

$$\int_0^t dt' \exp[i(\omega_{at} - \omega_{\mathbf{k},\lambda})(t - t')] \approx \mathcal{P} \frac{i}{\omega_{at} - \omega_{\mathbf{k},\lambda}} + \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}).$$

Já sabemos que a parte principal vai resultar no Lamb shift que já levamos em conta por hipótese e, assim, utilizar este termo só vai causar o shift de novo, que não queremos. Logo, utilizamos, ao invés,

$$\int_0^t dt' \exp[i(\omega_{at} - \omega_{\mathbf{k},\lambda})(t - t')] \approx \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}).$$

Portanto,

$$\begin{aligned} b_{\mathbf{k},\lambda}(t) &\approx \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \\ &\quad \times \int d^3 r' \int d^3 p' F(\mathbf{r}', \mathbf{p}', t) \sigma_{01}(t) \exp(-i\mathbf{k} \cdot \mathbf{r}'). \end{aligned}$$

O que temos a fazer agora é escrever as equações de movimento para os operadores de Heisenberg e a do operador de Wigner, eliminando os operadores de fótons usando a equação acima que acabamos de obter. Feito isto, teremos um conjunto de equações ópticas de Bloch para a dinâmica interna e uma equação de movimento para o centro de massa. Essas equações estarão acopladas, formando um sistema dinâmico.

Começemos com a dinâmica interna:

$$\frac{\partial}{\partial t} \sigma_{mn}(t) = \frac{1}{i\hbar} U^\dagger(t) [\sigma_{mn}(0), H(t)] U(t).$$

Calculemos

$$\begin{aligned} [\sigma_{mn}(0), H(t)] &= [\sigma_{mn}(0), \hbar\omega_{at}\sigma_{11}(0)] \\ &\quad + \left[\sigma_{mn}(0), -\hbar\frac{\Omega_{op}}{2}\sigma_{01}(0)\exp(i\omega_L t) - \hbar\frac{\Omega_{op}^\dagger}{2}\sigma_{10}(0)\exp(-i\omega_L t) \right] \\ &\quad + \left[\sigma_{mn}(0), -\hbar \sum_{\mathbf{k},\lambda} \left\{ iG_{\mathbf{k},\lambda}\sigma_{10}(0)a_{\mathbf{k},\lambda} - iG_{\mathbf{k},\lambda}^\dagger\sigma_{01}(0)a_{\mathbf{k},\lambda}^\dagger \right\} \right]. \end{aligned}$$

Temos, então, o comutador para cada um dos operadores de Heisenberg específicos:

$$\begin{aligned} [\sigma_{00}(0), H(t)] &= [\sigma_{00}(0), \hbar\omega_{at}\sigma_{11}(0)] \\ &\quad + \left[\sigma_{00}(0), -\hbar\frac{\Omega_{op}}{2}\sigma_{01}(0)\exp(i\omega_L t) - \hbar\frac{\Omega_{op}^\dagger}{2}\sigma_{10}(0)\exp(-i\omega_L t) \right] \\ &\quad + \left[\sigma_{00}(0), -\hbar \sum_{\mathbf{k},\lambda} \left\{ iG_{\mathbf{k},\lambda}\sigma_{10}(0)a_{\mathbf{k},\lambda} - iG_{\mathbf{k},\lambda}^\dagger\sigma_{01}(0)a_{\mathbf{k},\lambda}^\dagger \right\} \right] \\ &= -\hbar\frac{\Omega_{op}}{2}\sigma_{01}(0)\exp(i\omega_L t) + \hbar\frac{\Omega_{op}^\dagger}{2}\sigma_{10}(0)\exp(-i\omega_L t) \\ &\quad + i\hbar \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}\sigma_{10}(0)a_{\mathbf{k},\lambda} + i\hbar \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}^\dagger\sigma_{01}(0)a_{\mathbf{k},\lambda}^\dagger. \end{aligned}$$

Vamos usar a notação

$$\Omega_{op}(t) \equiv U^\dagger(t) \Omega_{op} U(t)$$

e

$$G_{\mathbf{k},\lambda}(t) \equiv U^\dagger(t) G_{\mathbf{k},\lambda} U(t).$$

Então,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{00}(t) &= i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) - i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &\quad + \sigma_{10}(t) \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}(t) b_{\mathbf{k},\lambda}(t) + \sum_{\mathbf{k},\lambda} b_{\mathbf{k},\lambda}^\dagger(t) G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t). \end{aligned}$$

Notemos que aqui, para cada instante t , podemos escrever

$$\begin{aligned} [\sigma_{10}(t) G_{\mathbf{k},\lambda}(t), b_{\mathbf{k},\lambda}(t)] &= U^\dagger(t) [\sigma_{10}(0) G_{\mathbf{k},\lambda}, a_{\mathbf{k},\lambda}] U(t) \\ &= 0 \end{aligned}$$

e

$$\begin{aligned} [b_{\mathbf{k},\lambda}^\dagger(t), G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t)] &= U^\dagger(t) [a_{\mathbf{k},\lambda}^\dagger, G_{\mathbf{k},\lambda}^\dagger \sigma_{01}(0)] U(t) \\ &= 0. \end{aligned}$$

Também podemos reescrever:

$$\begin{aligned} b_{\mathbf{k},\lambda}(t) &\approx \exp(-i\omega_{\mathbf{k},\lambda} t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \\ &\quad \times U^\dagger(t) \int d^3 r' \int d^3 p' f(\mathbf{r}', \mathbf{p}') \sigma_{01}(0) \exp(-i\mathbf{k} \cdot \mathbf{r}') U(t) \\ &= \exp(-i\omega_{\mathbf{k},\lambda} t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) U^\dagger(t) \sigma_{01}(0) \exp(-i\mathbf{k} \cdot \mathbf{R}_{CM}) U(t) \\ &= \exp(-i\omega_{\mathbf{k},\lambda} t) a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{01}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)], \end{aligned}$$

de forma mais compacta. Claramente,

$$b_{\mathbf{k},\lambda}^\dagger(t) \approx \exp(i\omega_{\mathbf{k},\lambda} t) a_{\mathbf{k},\lambda}^\dagger + g_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{10}(t) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)].$$

Como $b_{\mathbf{k},\lambda}(t)$ e $b_{\mathbf{k},\lambda}^\dagger(t)$ envolvem, respectivamente, os operadores $a_{\mathbf{k},\lambda}$ e $a_{\mathbf{k},\lambda}^\dagger$, segue que quando tomarmos o traço sobre os fótons, é melhor escrevermos tudo usando ordenamento normal para os operadores de campo, pois aí estaremos selecionando a ordem tal que os termos envolvendo apenas um $a_{\mathbf{k},\lambda}$ ou $a_{\mathbf{k},\lambda}^\dagger$ serão nulos. Por isso escrevemos, na equação para $\partial \sigma_{00}(t) / \partial t$, o operador $b_{\mathbf{k},\lambda}(t)$ à direita do operador $G_{\mathbf{k},\lambda}(t) \sigma_{10}(t)$ e o operador $b_{\mathbf{k},\lambda}^\dagger(t)$ à esquerda do operador $G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t)$, ou seja, usamos o ordenamento normal.

Para $\sigma_{11}(t)$, obtemos, já em ordem normal,

$$\begin{aligned} [\sigma_{11}(0), H(t)] &= \hbar \frac{\Omega_{op}}{2} \sigma_{01}(0) \exp(i\omega_L t) - \hbar \frac{\Omega_{op}^\dagger}{2} \sigma_{10}(0) \exp(-i\omega_L t) \\ &\quad - i\hbar \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda} \sigma_{10}(0) a_{\mathbf{k},\lambda} - i\hbar \sum_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}^\dagger G_{\mathbf{k},\lambda}^\dagger \sigma_{01}(0). \end{aligned}$$

Logo,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{11}(t) &= -i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) + i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &\quad - \sigma_{10}(t) \sum_{\mathbf{k}, \lambda} G_{\mathbf{k}, \lambda}(t) b_{\mathbf{k}, \lambda}(t) - \sum_{\mathbf{k}, \lambda} b_{\mathbf{k}, \lambda}^\dagger(t) G_{\mathbf{k}, \lambda}^\dagger(t) \sigma_{01}(t). \end{aligned}$$

Também temos:

$$\begin{aligned} [\sigma_{10}(0), H(t)] &= [\sigma_{10}(0), \hbar \omega_{at} \sigma_{11}(0)] \\ &\quad + \left[\sigma_{10}(0), -\hbar \frac{\Omega_{op}}{2} \sigma_{01}(0) \exp(i\omega_L t) - \hbar \frac{\Omega_{op}^\dagger}{2} \sigma_{10}(0) \exp(-i\omega_L t) \right] \\ &\quad + \left[\sigma_{10}(0), -\hbar \sum_{\mathbf{k}, \lambda} \left\{ i G_{\mathbf{k}, \lambda} \sigma_{10}(0) a_{\mathbf{k}, \lambda} - i G_{\mathbf{k}, \lambda}^\dagger \sigma_{01}(0) a_{\mathbf{k}, \lambda}^\dagger \right\} \right] \\ &= -\hbar \omega_{at} \sigma_{10}(0) - \hbar \frac{\Omega_{op}}{2} [\sigma_{11}(0) - \sigma_{00}(0)] \exp(i\omega_L t) \\ &\quad + i \hbar \sum_{\mathbf{k}, \lambda} a_{\mathbf{k}, \lambda}^\dagger G_{\mathbf{k}, \lambda}^\dagger [\sigma_{11}(0) - \sigma_{00}(0)]. \end{aligned}$$

Assim,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{10}(t) &= i \omega_{at} \sigma_{10}(t) + i \frac{\Omega_{op}(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(i\omega_L t) \\ &\quad + \sum_{\mathbf{k}, \lambda} b_{\mathbf{k}, \lambda}^\dagger(t) G_{\mathbf{k}, \lambda}^\dagger(t) [\sigma_{11}(t) - \sigma_{00}(t)] \end{aligned}$$

e, claramente,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{01}(t) &= -i \omega_{at} \sigma_{01}(t) - i \frac{\Omega_{op}(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(-i\omega_L t) \\ &\quad + [\sigma_{11}(t) - \sigma_{00}(t)] \sum_{\mathbf{k}, \lambda} G_{\mathbf{k}, \lambda}(t) b_{\mathbf{k}, \lambda}(t). \end{aligned}$$

Usando a aproximação de Weiskopf & Wigner nas equações de movimento dos operadores de Heisenberg

Já usando

$$b_{\mathbf{k}, \lambda}^\dagger(t) \approx \exp(i\omega_{\mathbf{k}, \lambda} t) a_{\mathbf{k}, \lambda}^\dagger + g_{\mathbf{k}, \lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{10}(t) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)]$$

e, portanto,

$$b_{\mathbf{k}, \lambda}(t) \approx \exp(-i\omega_{\mathbf{k}, \lambda} t) a_{\mathbf{k}, \lambda} + g_{\mathbf{k}, \lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{01}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)],$$

obtemos:

$$\frac{\partial}{\partial t} \sigma_{00}(t) \approx i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) - i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t)$$

$$\begin{aligned}
& +\sigma_{10}(t) \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}(t) \exp(-i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda} \\
& +\sigma_{10}(t) \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) G_{\mathbf{k},\lambda}(t) \sigma_{01}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \\
& + \sum_{\mathbf{k},\lambda} \exp(i\omega_{\mathbf{k},\lambda}t) a_{\mathbf{k},\lambda}^\dagger G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t) \\
& +\sigma_{10}(t) \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t).
\end{aligned}$$

Para já simplificar as contas, vamos tomar como estado inicial dos fótons

$$\rho_B = |vac\rangle \langle vac|,$$

como dissemos. Vamos justificar isto numericamente. Pensemos que o laboratório está a 27°C (é, o ar condicionado está com problemas...), ou seja, $T \approx 300$ K. Neste caso,

$$\frac{k_B T}{h} \approx 6 \times 10^{12} \text{ Hz},$$

mas acontece que

$$\nu_{at} \approx 10^{15} \text{ Hz}$$

e vemos que a nossa hipótese de temperatura nula leva a um erro da ordem de alguns décimos de um por cento. Se o experimento for feito com frequências mais altas e em um ambiente mais frio, a aproximação fica ainda melhor.

Quando tomarmos o traço sobre os fótons da equação acima, porque temos o operador $a_{\mathbf{k},\lambda}$ e $a_{\mathbf{k},\lambda}^\dagger$ nas posições dadas pelo ordenamento normal, o resultado do valor esperado será nulo. Então, de agora em diante, já vamos ignorar esses termos nas equações de movimento. Logo, escrevemos

$$\begin{aligned}
\frac{\partial}{\partial t} \sigma_{00}(t) & \approx i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) - i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\
& +\sigma_{10}(t) \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) G_{\mathbf{k},\lambda}(t) \sigma_{01}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \\
& +\sigma_{10}(t) \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t),
\end{aligned}$$

isto é,

$$\begin{aligned}
\frac{\partial}{\partial t} \sigma_{00}(t) & \approx i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) - i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\
& + \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) G_{\mathbf{k},\lambda}(t) \sigma_{11}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \\
& + \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{11}(t).
\end{aligned}$$

Mas,

$$G_{\mathbf{k},\lambda}(t) \equiv g_{\mathbf{k},\lambda} \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)]$$

e

$$G_{\mathbf{k},\lambda}^\dagger(t) \equiv g_{\mathbf{k},\lambda}^* \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)].$$

Assim,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{00}(t) &\approx i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) - i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &+ \sum_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) |g_{\mathbf{k},\lambda}|^2 \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \sigma_{11}(t) \\ &+ \sum_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) |g_{\mathbf{k},\lambda}|^2 \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \sigma_{11}(t), \end{aligned}$$

ou seja,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{00}(t) &\approx i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) - i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &+ \sum_{\mathbf{k},\lambda} 2\pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) |g_{\mathbf{k},\lambda}|^2 \sigma_{11}(t). \end{aligned}$$

Similarmente,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{11}(t) &= -i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) + i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &- \sigma_{10}(t) \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}(t) \exp(-i\omega_{\mathbf{k},\lambda} t) a_{\mathbf{k},\lambda} \\ &- \sigma_{10}(t) \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}(t) g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{01}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \\ &- \sum_{\mathbf{k},\lambda} \exp(i\omega_{\mathbf{k},\lambda} t) a_{\mathbf{k},\lambda}^\dagger G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t) \\ &- \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{10}(t) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t), \end{aligned}$$

isto é,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{11}(t) &\approx -i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) + i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &- \sigma_{10}(t) \sum_{\mathbf{k},\lambda} G_{\mathbf{k},\lambda}(t) g_{\mathbf{k},\lambda}^* \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{01}(t) \exp[-i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] \\ &- \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{10}(t) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k},\lambda}^\dagger(t) \sigma_{01}(t) \\ &= -i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) + i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &- \sigma_{10}(t) \sum_{\mathbf{k},\lambda} |g_{\mathbf{k},\lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{01}(t) \\ &- \sum_{\mathbf{k},\lambda} |g_{\mathbf{k},\lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k},\lambda}) \sigma_{10}(t) \sigma_{01}(t), \end{aligned}$$

ou seja,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{11}(t) &\approx -i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) + i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 2\pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{11}(t). \end{aligned}$$

Também,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{10}(t) &= i\omega_{at} \sigma_{10}(t) + i \frac{\Omega_{op}(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(i\omega_L t) \\ &\quad + \sum_{\mathbf{k}, \lambda} \exp(i\omega_{\mathbf{k}, \lambda} t) a_{\mathbf{k}, \lambda}^\dagger G_{\mathbf{k}, \lambda}^\dagger(t) [\sigma_{11}(t) - \sigma_{00}(t)] \\ &\quad + \sum_{\mathbf{k}, \lambda} g_{\mathbf{k}, \lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{10}(t) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k}, \lambda}^\dagger(t) [\sigma_{11}(t) - \sigma_{00}(t)], \end{aligned}$$

isto é,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{10}(t) &\approx i\omega_{at} \sigma_{10}(t) + i \frac{\Omega_{op}(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} g_{\mathbf{k}, \lambda} \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \exp[i\mathbf{k} \cdot \mathbf{R}_{CM}(t)] G_{\mathbf{k}, \lambda}^\dagger(t) \sigma_{10}(t), \end{aligned}$$

ou seja,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{10}(t) &\approx i\omega_{at} \sigma_{10}(t) + i \frac{\Omega_{op}(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{10}(t) \end{aligned}$$

e, obviamente,

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{01}(t) &\approx -i\omega_{at} \sigma_{01}(t) - i \frac{\Omega_{op}^\dagger(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(-i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{01}(t). \end{aligned}$$

Para a dinâmica interna, no entanto, queremos achar o valor esperado de cada elemento de matriz densidade, irrespectivamente do estado do centro de massa. Assim, queremos calcular

$$\begin{aligned} \rho_{mn}(t) &\equiv \int d^3 r \langle \mathbf{r}, m | \rho_{at}(t) | \mathbf{r}, n \rangle \\ &= \int d^3 r \int d^3 r_1 \int d^3 r_2 \langle \mathbf{r} | \mathbf{r}_1 \rangle \langle \mathbf{r}_2 | \mathbf{r} \rangle \int d^3 p \exp \left[i \frac{\mathbf{p} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}{\hbar} \right] \\ &\quad \times \text{Tr} \left\{ U^\dagger(t) \left[f \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \mathbf{p} \right) \otimes |n\rangle \langle m| \otimes \mathbb{I}_B \right] U(t) (\rho_{CM} \otimes \rho \otimes \rho_B) \right\}, \end{aligned}$$

isto é,

$$\begin{aligned}\rho_{mn}(t) &= \int d^3r \int d^3p \text{Tr} \{ U^\dagger(t) [f(\mathbf{r}, \mathbf{p}) \otimes |n\rangle\langle m| \otimes \mathbb{I}_B] U(t) (\rho_{CM} \otimes \rho \otimes \rho_B) \} \\ &= \int d^3r \int d^3p \text{Tr} \{ U^\dagger(t) [f(\mathbf{r}, \mathbf{p}) \sigma_{nm}(0)] U(t) (\rho_{CM} \otimes \rho \otimes \rho_B) \},\end{aligned}$$

ou seja,

$$\rho_{mn}(t) = \int d^3r \int d^3p \text{Tr} \{ [F(\mathbf{r}, \mathbf{p}, t) \sigma_{nm}(t)] (\rho_{CM} \otimes \rho \otimes \rho_B) \},$$

como deve ser mesmo.

Então, nossas equações acima para os operadores de Heisenberg não são suficientes ainda para termos os elementos da matriz densidade reduzida da dinâmica interna do átomo. Vamos, portanto, considerar as equações de movimento para os produtos $U^\dagger(t) f(\mathbf{r}, \mathbf{p}) \sigma_{mn} U(t)$. Sendo assim,

$$\begin{aligned}\frac{\partial}{\partial t} U^\dagger(t) f(\mathbf{r}, \mathbf{p}) \sigma_{mn} U(t) &= \frac{1}{i\hbar} U^\dagger(t) [f(\mathbf{r}, \mathbf{p}) \sigma_{mn}, H(t)] U(t) \\ &= \frac{1}{i\hbar} U^\dagger(t) [f(\mathbf{r}, \mathbf{p}), H(t)] \sigma_{mn} U(t) \\ &\quad + \frac{1}{i\hbar} U^\dagger(t) f(\mathbf{r}, \mathbf{p}) [\sigma_{mn}, H(t)] U(t),\end{aligned}$$

isto é,

$$\begin{aligned}\frac{\partial}{\partial t} U^\dagger(t) f(\mathbf{r}, \mathbf{p}) \sigma_{mn} U(t) &= \frac{1}{i\hbar} U^\dagger(t) [f(\mathbf{r}, \mathbf{p}), K] \sigma_{mn} U(t) \\ &\quad + \frac{1}{i\hbar} U^\dagger(t) [f(\mathbf{r}, \mathbf{p}), V(\mathbf{R}_{CM}, t)] \sigma_{mn} U(t) \\ &\quad + F(\mathbf{r}, \mathbf{p}, t) \frac{\partial}{\partial t} \sigma_{mn}(t),\end{aligned}$$

onde

$$\begin{aligned}V(\mathbf{R}_{CM}, t) &\equiv H_{at}(t) - K + H_{int} \\ &= \hbar\omega_{at}\sigma_{11}(0) - \hbar\frac{\Omega_{op}}{2}\sigma_{01}(0)\exp(i\omega_L t) - \hbar\frac{\Omega_{op}^\dagger}{2}\sigma_{10}(0)\exp(-i\omega_L t) \\ &\quad - \hbar \sum_{\mathbf{k}, \lambda} \left\{ iG_{\mathbf{k}, \lambda} \sigma_{10}(0) a_{\mathbf{k}, \lambda} - ia_{\mathbf{k}, \lambda}^\dagger G_{\mathbf{k}, \lambda}^\dagger \sigma_{01}(0) \right\}.\end{aligned}$$

Já sabemos que, após uma generalização para três dimensões, a aproximação semi-clássica em que tratamos o movimento atômico como clássico é traduzida por

$$[f(\mathbf{r}, \mathbf{p}), V(\mathbf{R}_{CM}, t)] \approx i\hbar [\nabla V(\mathbf{r}, t)] \cdot \nabla_{\mathbf{p}} f(\mathbf{r}, \mathbf{p}).$$

Também sabemos que

$$\begin{aligned}[f(\mathbf{r}, \mathbf{p}), K] &= \left[f(\mathbf{r}, \mathbf{p}), \frac{\mathbf{P}_{CM}^2}{2M} \right] \\ &= -i\hbar \frac{\mathbf{P}}{M} \cdot \nabla f(\mathbf{r}, \mathbf{p}).\end{aligned}$$

Vemos, portanto, que

$$\begin{aligned}\frac{1}{i\hbar}U^\dagger(t)[f(\mathbf{r}, \mathbf{p}), K]\sigma_{mn}U(t) &= -U^\dagger(t)\frac{\mathbf{p}}{M}\cdot\nabla f(\mathbf{r}, \mathbf{p})\sigma_{mn}U(t) \\ &= -\frac{\mathbf{p}}{M}\cdot\nabla[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)]\end{aligned}$$

e

$$\begin{aligned}\frac{1}{i\hbar}U^\dagger(t)[f(\mathbf{r}, \mathbf{p}), V(\mathbf{R}_{CM}, t)]\sigma_{mn}U(t) &\approx U^\dagger(t)[\nabla V(\mathbf{r}, t)]\cdot\nabla_{\mathbf{p}}f(\mathbf{r}, \mathbf{p})\sigma_{mn}U(t) \\ &= [\nabla V(\mathbf{r}, t)]\cdot\nabla_{\mathbf{p}}[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)].\end{aligned}$$

Logo,

$$\begin{aligned}\frac{\partial}{\partial t}[F(\mathbf{r}, \mathbf{p}, t)\sigma_{mn}(t)] &= -\frac{\mathbf{p}}{M}\cdot\nabla[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)] \\ &\quad + [\nabla V(\mathbf{r}, t)]\cdot\nabla_{\mathbf{p}}[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)] \\ &\quad + F(\mathbf{r}, \mathbf{p}, t)\frac{\partial}{\partial t}\sigma_{mn}(t).\end{aligned}$$

Como

$$\rho_{mn}(t) = \int d^3r \int d^3p \text{Tr}\{[F(\mathbf{r}, \mathbf{p}, t)\sigma_{nm}(t)](\rho_{CM} \otimes \rho \otimes \rho_B)\},$$

segue que

$$\frac{\partial}{\partial t}\rho_{nm}(t) = \int d^3r \int d^3p \text{Tr}\left\{[F(\mathbf{r}, \mathbf{p}, t)\frac{\partial}{\partial t}\sigma_{mn}(t)](\rho_{CM} \otimes \rho \otimes \rho_B)\right\},$$

pois

$$\begin{aligned}\int d^3r \int d^3p \text{Tr}\left\{\left[\frac{\mathbf{p}}{M}\cdot\nabla[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)]\right](\rho_{CM} \otimes \rho \otimes \rho_B)\right\} &= \\ \int d^3p \frac{\mathbf{p}}{M}\cdot\int d^3r \nabla \text{Tr}\{[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)](\rho_{CM} \otimes \rho \otimes \rho_B)\} &= 0\end{aligned}$$

e

$$\begin{aligned}\int d^3r \int d^3p \text{Tr}\{[\nabla V(\mathbf{r}, t)]\cdot\nabla_{\mathbf{p}}[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)](\rho_{CM} \otimes \rho \otimes \rho_B)\} &= \\ \int d^3r [\nabla V(\mathbf{r}, t)]\cdot\int d^3p \nabla_{\mathbf{p}} \text{Tr}\{[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)](\rho_{CM} \otimes \rho \otimes \rho_B)\} &= 0,\end{aligned}$$

supondo que

$$\text{Tr}\{[F(\mathbf{r}, \mathbf{p})\sigma_{mn}(t)](\rho_{CM} \otimes \rho \otimes \rho_B)\} \rightarrow 0,$$

para distâncias e momenta muito grandes. Usando

$$\begin{aligned}\frac{\partial}{\partial t}\sigma_{00}(t) &\approx i\frac{\Omega_{op}(t)}{2}\sigma_{01}(t)\exp(i\omega_L t) - i\frac{\Omega_{op}^\dagger(t)}{2}\sigma_{10}(t)\exp(-i\omega_L t) \\ &\quad + \sum_{\mathbf{k}, \lambda} 2\pi\delta(\omega_{at} - \omega_{\mathbf{k}, \lambda})|g_{\mathbf{k}, \lambda}|^2\sigma_{11}(t),\end{aligned}$$

é fácil ver que, assim,

$$\begin{aligned} \frac{\partial}{\partial t} \rho_{00}(t) &\approx i \frac{\Omega_L(\mathbf{r}_{cl}(t))}{2} \rho_{10}(t) \exp(i\omega_L t) - i \frac{\Omega_L^*(\mathbf{r}_{cl}(t))}{2} \rho_{01}(t) \exp(-i\omega_L t) \\ &\quad + \sum_{\mathbf{k}, \lambda} 2\pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) |g_{\mathbf{k}, \lambda}|^2 \rho_{11}(t), \end{aligned}$$

supondo, é claro, que temos uma pacote de ondas atômico muito localizado e que, portanto,

$$\begin{aligned} \text{Tr} \{ [\Omega_{op}(t) F(\mathbf{r}, \mathbf{p}, t) \sigma_{mn}(t)] (\rho_{CM} \otimes \rho \otimes \rho_B) \} &\approx \\ \Omega_L(\mathbf{r}_{cl}(t)) \text{Tr} \{ [F(\mathbf{r}, \mathbf{p}, t) \sigma_{mn}(t)] (\rho_{CM} \otimes \rho \otimes \rho_B) \} &= \Omega_L(\mathbf{r}_{cl}(t)) \rho_{nm}(t). \end{aligned}$$

Analogamente, de

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{11}(t) &\approx -i \frac{\Omega_{op}(t)}{2} \sigma_{01}(t) \exp(i\omega_L t) + i \frac{\Omega_{op}^\dagger(t)}{2} \sigma_{10}(t) \exp(-i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 2\pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{11}(t), \end{aligned}$$

segue que

$$\begin{aligned} \frac{\partial}{\partial t} \rho_{11}(t) &\approx -i \frac{\Omega_L(\mathbf{r}_{cl}(t))}{2} \rho_{10}(t) \exp(i\omega_L t) + i \frac{\Omega_L^*(\mathbf{r}_{cl}(t))}{2} \rho_{01}(t) \exp(-i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 2\pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \rho_{11}(t) \end{aligned}$$

e de

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_{10}(t) &\approx i\omega_{at} \sigma_{10}(t) + i \frac{\Omega_{op}(t)}{2} [\sigma_{11}(t) - \sigma_{00}(t)] \exp(i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \sigma_{10}(t) \end{aligned}$$

segue que

$$\begin{aligned} \frac{\partial}{\partial t} \rho_{01}(t) &\approx i\omega_{at} \rho_{01}(t) + i \frac{\Omega_L(\mathbf{r}_{cl}(t))}{2} [\rho_{11}(t) - \rho_{00}(t)] \exp(i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \rho_{01}(t). \end{aligned}$$

É evidente também que

$$\begin{aligned} \frac{\partial}{\partial t} \rho_{10}(t) &\approx -i\omega_{at} \rho_{10}(t) - i \frac{\Omega_L^*(\mathbf{r}_{cl}(t))}{2} [\rho_{11}(t) - \rho_{00}(t)] \exp(-i\omega_L t) \\ &\quad - \sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \rho_{10}(t). \end{aligned}$$

Agora podemos ver que, fazendo o limite do contínuo,

$$\sum_{\mathbf{k}, \lambda} |g_{\mathbf{k}, \lambda}|^2 \pi \delta(\omega_{at} - \omega_{\mathbf{k}, \lambda}) \rightarrow \sum_{\lambda} \int \frac{V d^3 k}{(2\pi)^3} \frac{2\pi\omega}{\hbar V} |\hat{\mathbf{e}}_{\mathbf{k}, \lambda} \cdot \mathbf{d}_{10}|^2 \pi \delta(\omega_{at} - \omega)$$

$$\begin{aligned}
&= \int \frac{k^2 dk}{(2\pi)^2} \frac{\omega}{\hbar} \pi \delta(\omega_{at} - \omega) \int_0^{2\pi} d\varphi_{\mathbf{k}} \int_0^\pi d\theta_{\mathbf{k}} \sin\theta_{\mathbf{k}} \sum_{\lambda} |\hat{\mathbf{e}}_{\mathbf{k},\lambda} \cdot \mathbf{d}_{10}|^2 \\
&= \int \frac{\omega^3 d\omega}{(2\pi)^2} \frac{1}{\hbar c^3} \pi \delta(\omega_{at} - \omega) \frac{8\pi}{3} |\mathbf{d}_{10}|^2 \\
&= \frac{2\omega_{at}^3}{3\hbar c^3} |\mathbf{d}_{10}|^2,
\end{aligned}$$

onde usamos

$$\int_0^{2\pi} d\varphi_{\mathbf{k}} \int_0^\pi d\theta_{\mathbf{k}} \sin\theta_{\mathbf{k}} \sum_{\lambda} |\hat{\mathbf{e}}_{\mathbf{k},\lambda} \cdot \mathbf{d}_{10}|^2 = \frac{8\pi}{3} |\mathbf{d}_{10}|^2.$$

Vamos definir agora

$$\Gamma \equiv \frac{2\omega_{at}^3}{3\hbar c^3} |\mathbf{d}_{10}|^2.$$

O mais comum é definirmos, ao invés,

$$\begin{aligned}
\gamma &\equiv 2\Gamma \\
&= \frac{4\omega_{at}^3}{3\hbar c^3} |\mathbf{d}_{10}|^2.
\end{aligned}$$

Para podermos ter também a trajetória $\mathbf{r}_{cl}(t)$ que aparece nas equações de movimento para a dinâmica interna atômica, procedemos como segue. Consideremos que a distribuição inicial é muito localizada e que vai permanecer localizada. Calculemos

$$\begin{aligned}
\frac{\partial}{\partial t} \mathbf{R}_{CM}(t) &= \frac{1}{i\hbar} U^\dagger(t) [\mathbf{R}_{CM}, H(t)] U(t) \\
&= \frac{1}{i\hbar} U^\dagger(t) [\mathbf{R}_{CM}, K] U(t).
\end{aligned}$$

Usando novamente

$$[f(\mathbf{r}, \mathbf{p}), K] = -i\hbar \frac{\mathbf{p}}{M} \cdot \nabla f(\mathbf{r}, \mathbf{p}),$$

obtemos

$$\frac{d}{dt} \mathbf{r}_{cl}(t) = - \int d^3r \int d^3p \mathbf{r} \frac{\mathbf{p}}{M} \cdot \nabla \text{Tr}[F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)],$$

onde

$$\int d^3r \int d^3p \mathbf{r} \text{Tr}[F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)] = \mathbf{r}_{cl}(t)$$

e, como está evidente, $\text{Tr}[F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)]$ é a nossa função de Wigner generalizada para matriz densidade e não ket inicial. Então, efetivamente, já podemos usar

$$\text{Tr}[F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)] \rightarrow 0,$$

para distâncias e momenta muito grandes, como já usamos acima. Logo,

$$\int d^3r \int d^3p \mathbf{r} \frac{\mathbf{p}}{M} \cdot \nabla \text{Tr} [F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)] = \\ - \int d^3r \int d^3p \text{Tr} [F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)] \frac{\mathbf{p}}{M}$$

e, assim,

$$\int d^3r \int d^3p \mathbf{r} \frac{\mathbf{p}}{M} \cdot \nabla \text{Tr} [F(\mathbf{r}, \mathbf{p}, t) (\rho_{CM} \otimes \rho \otimes \rho_B)] = - \frac{\mathbf{p}_{cl}(t)}{M}.$$

Portanto,

$$\frac{d}{dt} \mathbf{r}_{cl}(t) = \frac{\mathbf{p}_{cl}(t)}{M},$$

isto é,

$$\mathbf{p}_{cl}(t) = M \frac{d}{dt} \mathbf{r}_{cl}(t).$$

Então, tomando o valor esperado da equação de movimento para $F(\mathbf{r}, \mathbf{p}, t)$, depois multiplicando por \mathbf{p} e finalmente integrando sobre todo o espaço de fases, obtemos:

$$\frac{\partial}{\partial t} \mathbf{p}_{cl}(t) \approx \frac{\hbar}{2} [\nabla \Omega_L(\mathbf{r}_{cl}(t))] \rho_{10}(t) \exp(i\omega_L t) \\ + \frac{\hbar}{2} [\nabla \Omega_L^*(\mathbf{r}_{cl}(t))] \rho_{01}(t) \exp(-i\omega_L t),$$

que é a força que o laser vai fazer sobre o átomo.

Quando queremos apenas a força de pressão de radiação, escrevemos

$$\Omega_L(\mathbf{r}_{cl}(t)) = \Omega_0 \exp[-i\mathbf{k}_L \cdot \mathbf{r}_{cl}(t)],$$

com Ω_0 constante na região em que o átomo se move. Quando queremos que também haja força dipolar elétrica agindo, usamos também uma dependência espacial para Ω_0 , isto é, $\Omega_0 = \Omega_0[\mathbf{r}_{cl}(t)]$. Os desaceleradores e armadilhas ópticos utilizam essas forças para desacelerar e localizar espacialmente a amostra atômica, além de campos magnetostáticos externos para poder modificar a frequência de ressonância do átomo através do efeito Zeeman.