Continuação de relação entre os operadores de Heisenberg e o operador densidade reduzido atômico

Antes de usarmos expansões em termos do operador de Wigner para o centro de massa, vamos ainda ficar com a base da posição $\{|\mathbf{r}\rangle\}$. Podemos combinar as identidades I_{CM} e I_{at} de forma a escrever

$$I_{CM} \otimes I_{at} = \sum_m \int d^3r \; |\mathbf{r}, m\rangle \langle \mathbf{r}, m| \,.$$

Para os fótons, vamos usar letras gregas especificando cada elemento da base:

$$I_B = \sum_\alpha |\alpha\rangle \langle \alpha| \,.$$

Como vimos na aula anterior,

$$\rho_{tot}(t) = U(t)\,\rho_{tot}(0)\,U^\dagger(t) \,.$$

Vamos definir nosso operador densidade atômico aquele operador densidade reduzido onde tomamos o traço só sobre os fótons. Assim,

$$\rho_{at}(t) = \mathrm{Tr}_B\left[U(t)\,\rho_{tot}(0)\,U^\dagger(t)\right] .$$

Só por um momento, agora, vamos considerar uma notação muito menos carregada do que a nossa. Vamos pensar que, como em nosso caso, temos um par de sistemas, um de nosso interesse, inicialmente no estado ρ, e outro que é o banho térmico, digamos, inicialmente no estado η. Dada um operador evolução $U = U(t)$, calculemos o que segue:

$$\begin{aligned}
\mathrm{Tr}_B\left(U\rho\eta U^\dagger\right) &= \sum_{m,n} \mathrm{Tr}_B\left(U|m\rangle\langle m|\rho|n\rangle\langle n|\eta U^\dagger\right) \\
&= \sum_{m,n} \rho_{mn} \mathrm{Tr}_B\left(U|m\rangle\,\eta\,\langle n|U^\dagger\right) \\
&= \sum_{m,n} \rho_{mn} \sum_\alpha \langle\alpha|U|m\rangle\,\eta\,\langle n|U^\dagger|\alpha\rangle \\
&= \sum_{m,n} \rho_{mn} \sum_\alpha \langle\alpha|U|m\rangle \sum_\beta |\beta\rangle\langle\beta|\,\eta \sum_\gamma |\gamma\rangle\langle\gamma|\,\langle n|U^\dagger|\alpha\rangle \\
&= \sum_{m,n}\sum_{\beta,\gamma} \rho_{mn}\eta_{\beta\gamma} \sum_\alpha \langle\alpha|U|m,\beta\rangle\langle n,\gamma|U^\dagger|\alpha\rangle \\
&= \sum_{m,n}\sum_{\beta,\gamma} \rho_{mn}\eta_{\beta\gamma} \sum_{r,s} |r\rangle\langle s| \sum_\alpha \langle r,\alpha|U|m,\beta\rangle\langle n,\gamma|U^\dagger|s,\alpha\rangle \\
&= \sum_{m,n}\sum_{\beta,\gamma} \rho_{mn}\eta_{\beta\gamma} \sum_{r,s} |r\rangle\langle s|\,\langle n,\gamma|U^\dagger \sum_\alpha |s,\alpha\rangle\langle r,\alpha|U|m,\beta\rangle \\
&= \sum_{m,n}\sum_{\beta,\gamma} \rho_{mn}\eta_{\beta\gamma} \sum_{r,s} |r\rangle\langle s|\,\langle n,\gamma|U^\dagger|s\rangle\langle r|U|m,\beta\rangle \\
&= \sum_{m,n}\sum_{\beta,\gamma} \eta_{\beta\gamma} \sum_{r,s} |r\rangle\langle s|\,\rho_{mn}\,\langle n,\gamma|U^\dagger|s\rangle\langle r|U|m,\beta\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{m,n}\sum_{\beta,\gamma}\eta_{\beta\gamma}\sum_{r,s}\left|r\right\rangle\left\langle s\right|\left\langle m\right|\rho\left|n\right\rangle\left\langle n,\gamma\right|U^{\dagger}\left|s\right\rangle\left\langle r\right|U\left|m,\beta\right\rangle \\
&= \sum_{\beta,\gamma}\eta_{\beta\gamma}\sum_{r,s}\left|r\right\rangle\left\langle s\right|\sum_{m}\left\langle m\right|\left(\rho\left\langle\gamma\right|U^{\dagger}\left|s\right\rangle\left\langle r\right|U\left|\beta\right\rangle\right)\left|m\right\rangle \\
&= \sum_{\beta}\sum_{r,s}\left|r\right\rangle\left\langle s\right|\sum_{m}\left\langle m\right|\left(\rho\sum_{\gamma}\eta_{\beta\gamma}\left\langle\gamma\right|U^{\dagger}\left|s\right\rangle\left\langle r\right|U\left|\beta\right\rangle\right)\left|m\right\rangle \\
&= \sum_{\beta}\sum_{r,s}\left|r\right\rangle\left\langle s\right|\sum_{m}\left\langle m\right|\left(\rho\left\langle\beta\right|\eta\sum_{\gamma}\left|\gamma\right\rangle\left\langle\gamma\right|U^{\dagger}\left|s\right\rangle\left\langle r\right|U\left|\beta\right\rangle\right)\left|m\right\rangle \\
&= \sum_{\beta}\sum_{r,s}\left|r\right\rangle\left\langle s\right|\sum_{m}\left\langle m\right|\left(\rho\left\langle\beta\right|\eta U^{\dagger}\left|s\right\rangle\left\langle r\right|U\left|\beta\right\rangle\right)\left|m\right\rangle \\
&= \sum_{r,s}\left|r\right\rangle\left\langle s\right|\sum_{m,\beta}\left\langle m,\beta\right|\left(\rho\eta U^{\dagger}\left|s\right\rangle\left\langle r\right|U\right)\left|m,\beta\right\rangle \\
&= \sum_{r,s}\left|r\right\rangle\left\langle s\right|\mathrm{Tr}\left(\rho\eta U^{\dagger}\left|s\right\rangle\left\langle r\right|U\right) \\
&= \sum_{r,s}\left|r\right\rangle\left\langle s\right|\mathrm{Tr}\left(\rho\eta\sigma_{sr}\right) \\
&= \sum_{r,s}\left|r\right\rangle\left\langle s\right|\mathrm{Tr}\left(\sigma_{sr}\rho\eta\right),
\end{aligned}
$$

onde Tr representa o traço total, sobre todos os graus de liberdade do sistema todo.

Com esse resultado, podemos escrever que

$$
\begin{aligned}
\rho_{at}(t) &= \mathrm{Tr}_B\left[U(t)\,\rho_{tot}(0)\,U^{\dagger}(t)\right] \\
&= \int d^3r\int d^3r'\sum_{m,n}\left|\mathbf{r},m\right\rangle\left\langle\mathbf{r}',n\right|\mathrm{Tr}\left[U(t)\,\sigma_{nm}(0)\left|\mathbf{r}'\right\rangle\left\langle\mathbf{r}\right|U^{\dagger}(t)\,\rho_{tot}(0)\right] \\
&= \int d^3r\int d^3r'\sum_{m,n}\left|\mathbf{r},m\right\rangle\left\langle\mathbf{r}',n\right|\mathrm{Tr}\left[U(t)\,\sigma_{nm}(0)\,U^{\dagger}(t)\,U(t)\left|\mathbf{r}'\right\rangle\left\langle\mathbf{r}\right|U^{\dagger}(t)\,\rho_{tot}(0)\right] \\
&= \int d^3r\int d^3r'\sum_{m,n}\left|\mathbf{r},m\right\rangle\left\langle\mathbf{r}',n\right|\mathrm{Tr}\left[\sigma_{nm}(t)\,U(t)\left|\mathbf{r}'\right\rangle\left\langle\mathbf{r}\right|U^{\dagger}(t)\,\rho_{tot}(0)\right].
\end{aligned}
$$

Podemos usar o resultado que não é muito difícil deduzir:

$$
\left|\mathbf{r}'\right\rangle\left\langle\mathbf{r}\right| = \int d^3p\, f\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p}\right)\exp\left[i\frac{\mathbf{p}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}{\hbar}\right].
$$

Então,

$$
U(t)\left|\mathbf{r}'\right\rangle\left\langle\mathbf{r}\right|U^{\dagger}(t) = \int d^3p\, U(t)\, f\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p}\right)U^{\dagger}(t)\exp\left[i\frac{\mathbf{p}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}{\hbar}\right]
$$

e podemos definir um operador de Wigner na representação de Heisenberg como

$$
F(\mathbf{r},\mathbf{p},t) = U(t)\, f(\mathbf{r},\mathbf{p})\, U^{\dagger}(t).
$$

Logo,

$$\begin{aligned}
\rho_{at}(t) &= \int d^3r \int d^3r' \sum_{m,n} |\mathbf{r},m\rangle \langle \mathbf{r}',n| \operatorname{Tr}\left\{\sigma_{nm}(t) \int d^3p\, F\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p},t\right) \exp\left[i\frac{\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}{\hbar}\right] \rho_{tot}(0)\right\} \\
&= \int d^3r \int d^3r' \int d^3p \sum_{m,n} |\mathbf{r},m\rangle \langle \mathbf{r}',n| \exp\left[i\frac{\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}{\hbar}\right] \operatorname{Tr}\left[\sigma_{nm}(t)\, F\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p},t\right) \rho_{tot}(0)\right].
\end{aligned}$$

Assim, a moral da história é que toda a informação que nos interessa a respeito do sistema está em $\rho_{at}(t)$ e basta sabermos encotrar $\sigma_{nm}(t)$ e $F(\mathbf{r},\mathbf{p},t)$ para depois encotrar o valor esperado do produto desses operadores para termos como calcular $\rho_{at}(t)$. Com nossa simplificação em que podemos tomar, aproximadamente,

$$\rho_{CM} = |\psi_{CM}\rangle \langle \psi_{CM}|$$

e

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

o traço que queremos fica

$$\operatorname{Tr}\left[\sigma_{nm}(t)\, F\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p},t\right) \rho_{tot}(0)\right] = \operatorname{Tr}_{at}\left[\left(\langle\psi_{CM}| \otimes \langle vac|\right) \sigma_{nm}(t)\, F\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p},t\right) \left(|\psi_{CM}\rangle \otimes |vac\rangle\right)\right].$$

As equações ópticas de Bloch acopladas ao movimento translacional atômico

Tudo que depender do centro de massa será escrito em termos do operador de Wigner e, portanto, a correspondente versão na representação de Heisenberg será dada em termos de $F(\mathbf{r},\mathbf{p},t)$. O que depender dos graus de liberdate atômicos internos será escrito em termos dos operadores de Heisenberg $\sigma_{nm}(t)$. O foco a seguir é como considerar os operadores dos fótons. Vamos, portanto, definir a versão de Heisenberg dos operadores bosônicos como

$$b_{\mathbf{k},\lambda}(t) \equiv U^\dagger(t)\, a_{\mathbf{k},\lambda} U(t)$$

and

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

Então,

$$\begin{aligned}
\frac{\partial}{\partial t} b_{\mathbf{k},\lambda}(t) &= \frac{1}{i\hbar}\left[b_{\mathbf{k},\lambda}(t), H_H(t)\right] \\
&= \frac{1}{i\hbar} U^\dagger(t)\left[a_{\mathbf{k},\lambda}, H(t)\right] U(t),
\end{aligned}$$

onde

$$H_H(t) \equiv U^\dagger(t)\, H(t)\, U(t).$$

É evidente que

$$\begin{aligned}
\left[a_{\mathbf{k},\lambda}, H(t)\right] &= \left[a_{\mathbf{k},\lambda}, H_B + H_{int}\right] \\
&= \left[a_{\mathbf{k},\lambda}, \hbar \sum_{\mathbf{k}',\lambda'} \omega_{\mathbf{k}',\lambda'} a^{\dagger}_{\mathbf{k}',\lambda'} a_{\mathbf{k}',\lambda'}\right] \\
&\quad -i\hbar \left[a_{\mathbf{k},\lambda}, \sum_{\mathbf{k}',\lambda'} G_{\mathbf{k}',\lambda'} \sigma_{10}(0)\, a_{\mathbf{k}',\lambda'}\right] \\
&\quad +i\hbar \left[a_{\mathbf{k},\lambda}, \sum_{\mathbf{k}',\lambda'} G^{\dagger}_{\mathbf{k}',\lambda'} \sigma_{01}(0)\, a^{\dagger}_{\mathbf{k}',\lambda'}\right],
\end{aligned}$$

ou seja,

$$\begin{aligned}
\left[a_{\mathbf{k},\lambda}, H(t)\right] &= \hbar \sum_{\mathbf{k}',\lambda'} \omega_{\mathbf{k}',\lambda'} \left[a_{\mathbf{k},\lambda}, a^{\dagger}_{\mathbf{k}',\lambda'}\right] a_{\mathbf{k}',\lambda'} \\
&\quad +i\hbar \sum_{\mathbf{k}',\lambda'} G^{\dagger}_{\mathbf{k}',\lambda'} \sigma_{01}(0) \left[a_{\mathbf{k},\lambda}, a^{\dagger}_{\mathbf{k}',\lambda'}\right].
\end{aligned}$$

Mas,

$$\left[a_{\mathbf{k},\lambda}, a^{\dagger}_{\mathbf{k}',\lambda'}\right] = \delta_{\mathbf{k}',\mathbf{k}} \delta_{\lambda',\lambda}$$

e, então,

$$\left[a_{\mathbf{k},\lambda}, H(t)\right] = \hbar\omega_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + i\hbar G^{\dagger}_{\mathbf{k},\lambda} \sigma_{01}(0).$$

Logo,

$$\begin{aligned}
\frac{\partial}{\partial t} b_{\mathbf{k},\lambda}(t) &= \frac{1}{i\hbar} U^{\dagger}(t) \left(\hbar\omega_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}\right) U(t) \\
&\quad + \frac{1}{i\hbar} U^{\dagger}(t) \left[i\hbar G^{\dagger}_{\mathbf{k},\lambda} \sigma_{01}(0)\right] U(t),
\end{aligned}$$

isto é,

$$\begin{aligned}
\frac{\partial}{\partial t} b_{\mathbf{k},\lambda}(t) &= -i\omega_{\mathbf{k},\lambda} b_{\mathbf{k},\lambda}(t) \\
&\quad + U^{\dagger}(t)\, G^{\dagger}_{\mathbf{k},\lambda} U(t)\, U^{\dagger}(t)\, \sigma_{01}(0)\, U(t),
\end{aligned}$$

ou seja,

$$\frac{\partial}{\partial t} b_{\mathbf{k},\lambda}(t) = -i\omega_{\mathbf{k},\lambda} b_{\mathbf{k},\lambda}(t) + \left[U^{\dagger}(t)\, G^{\dagger}_{\mathbf{k},\lambda} U(t)\right] \sigma_{01}(t).$$

Podemos reescrever esta mesma equação assim:

$$\frac{\partial}{\partial t} \left[\exp\left(i\omega_{\mathbf{k},\lambda} t\right) b_{\mathbf{k},\lambda}(t)\right] = \exp\left(i\omega_{\mathbf{k},\lambda} t\right) \left[U^{\dagger}(t)\, G^{\dagger}_{\mathbf{k},\lambda} U(t)\right] \sigma_{01}(t).$$

Portanto,

$$b_{\mathbf{k},\lambda}(t) = \exp\left(-i\omega_{\mathbf{k},\lambda} t\right) a_{\mathbf{k},\lambda} + \int_0^t dt' \, \exp\left[-i\omega_{\mathbf{k},\lambda}(t-t')\right] \left[U^{\dagger}(t')\, G^{\dagger}_{\mathbf{k},\lambda} U(t')\right] \sigma_{01}(t').$$