Lang-Firsov transformation in detail

Ding Yi
yi.ding@ubbcluj.ro

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Introduction

The Lang-Firsov transformation is a tool which can eliminate the interaction term in electron-photon-interaction system to simplify the calculation. Generally, the form of Lang-Firsov transformation is taken as

$$\tilde{H} = e^S H e^{-S}, \tag{1}$$

$$S = \sum_{i=0}^{\infty} g_i (b_i^\dagger - b_i) a_i^\dagger a_i. \tag{2}$$

Here, g_i is the transformation coefficient, $b_i^\dagger(b_i)$ is the creation(annihilation) operator of photon and $a_i^\dagger(a_i)$ is corresponding creation(annihilation) operator of electron. The system is given as,

$$H = \epsilon_0 a^\dagger a + \lambda(b^\dagger + b) a^\dagger a + \omega b^\dagger b. \tag{3}$$

We take $U = e^{\nu(b^\dagger - b)a^\dagger a}$,

$$\tilde{a} = U a U^\dagger. \tag{4}$$

$$\Rightarrow a = U^\dagger \tilde{a} U. \tag{5}$$

Commutation relation of Fermi operator and Boson operator

$$[a^\dagger a, a] = a^\dagger a a - a a^\dagger a = 0 - a = -a, \tag{6}$$

$$[a^\dagger a, a^\dagger] = a^\dagger a a^\dagger - a^\dagger a^\dagger a = a^\dagger - 0 = a^\dagger, \tag{7}$$

$$[b, b^\dagger] = 1. \tag{8}$$

Baker-Campbell-Hausdorff formula

$$e^{sA} B e^{-sA} = A + s[A, B] + \frac{s^2}{2!}[A, [A, B]] + \frac{s^3}{3!}[A, [A, [A, B]]] + \cdots \tag{9}$$

Details

$$
\begin{aligned}
a &= U^\dagger \tilde{a} U \\
&= e^{-\nu(b^\dagger - b)a^\dagger a} \tilde{a} e^{\nu(b^\dagger - b)a^\dagger a} \\
&= \tilde{a} + -\nu(b^\dagger - b)[a^\dagger a, \tilde{a}] + \frac{(-\nu(b^\dagger - b))^2}{2!}[a^\dagger a, [a^\dagger a, a]] + \cdots \\
&= \tilde{a} + \nu(b^\dagger - b)\tilde{a} + \frac{(-\nu(b^\dagger - b))^2}{2!}\tilde{a} - \frac{(-\nu(b^\dagger - b))^3}{3!}\tilde{a} + \cdots \\
&= \tilde{a} + \nu(b^\dagger - b)\tilde{a} + \frac{(\nu(b^\dagger - b))^2}{2!}\tilde{a} + \frac{(\nu(b^\dagger - b))^3}{3!}\tilde{a} + \cdots \\
&= \tilde{a} e^{\nu(b^\dagger - b)}
\end{aligned} \tag{10}
$$

Detail for Boson operator

$$
\begin{aligned}
b &= U^\dagger \tilde{b} U \\
&= e^{-\nu(b^\dagger - b)a^\dagger a} \tilde{b} e^{\nu(b^\dagger - b)a^\dagger a} \\
&= \tilde{b} - \nu a^\dagger a[b^\dagger - b, \tilde{b}] + \frac{(-\nu a^\dagger a)^2}{2!}[b^\dagger - b, [b^\dagger - b, \tilde{b}]] + \cdots \\
&= \tilde{b} - \nu a^\dagger a(-1) + \frac{(-\nu a^\dagger a)^2}{2!}[b^\dagger - b, -1] + \cdots \\
&= \tilde{b} + \nu a^\dagger a
\end{aligned} \tag{11}
$$

Some transformation formulas

$$
a = \tilde{a} e^{\nu(\tilde{b}^\dagger - \tilde{b})};\ a^\dagger = \tilde{a}^\dagger e^{-(\nu(\tilde{b}^\dagger - \tilde{b}))}, \tag{12}
$$

$$
b = \tilde{b} + \nu \tilde{a}^\dagger \tilde{a};\ b^\dagger = \tilde{b}^\dagger + \nu \tilde{a}^\dagger \tilde{a} \tag{13}
$$

New Hamiltonian after Lang-Firsov transformation (take $\nu = -\frac{\lambda}{\omega}$)

$$
\begin{aligned}
\tilde{H}_{\text{molecule}} &= \epsilon_0 a^\dagger a + \lambda(b^\dagger + b)a^\dagger a + \omega b^\dagger b, \\
&= \epsilon_0 \tilde{a}^\dagger e^{-(\nu(\tilde{b}^\dagger - \tilde{b}))} \tilde{a} e^{\nu(\tilde{b}^\dagger - \tilde{b})} + \lambda(\tilde{b}^\dagger + \nu\tilde{a}^\dagger\tilde{a} + \tilde{b} + \nu\tilde{a}^\dagger\tilde{a})\tilde{a}^\dagger e^{-(\nu(\tilde{b}^\dagger - \tilde{b}))}\tilde{a} e^{\nu(\tilde{b}^\dagger - \tilde{b})} + \omega(\tilde{b}^\dagger + \nu\tilde{a}^\dagger\tilde{a})(\tilde{b} + \nu\tilde{a}^\dagger\tilde{a}), \\
&= \epsilon_0 \tilde{a}^\dagger\tilde{a} + \lambda(\tilde{b}^\dagger + \tilde{b} + 2\nu\tilde{a}^\dagger\tilde{a})\tilde{a}^\dagger\tilde{a} + \omega(\tilde{b}^\dagger\tilde{b} + \nu^2\tilde{a}^\dagger\tilde{a}\tilde{a}^\dagger\tilde{a} + \nu\tilde{b}^\dagger\tilde{a}^\dagger\tilde{a} + \nu\tilde{b}\tilde{a}^\dagger\tilde{a}) \\
&= \epsilon_0 \tilde{a}^\dagger\tilde{a} + \lambda(\tilde{b}^\dagger + \tilde{b} + 2\nu\tilde{a}^\dagger\tilde{a})\tilde{a}^\dagger\tilde{a} + \omega(\tilde{b}^\dagger\tilde{b} + \nu^2\tilde{a}^\dagger\tilde{a} + \nu\tilde{b}^\dagger\tilde{a}^\dagger\tilde{a} + \nu\tilde{b}\tilde{a}^\dagger\tilde{a}) \\
&= \tilde{a}^\dagger\tilde{a}(\epsilon_0 + \lambda(\tilde{b}^\dagger + \tilde{b} + 2\nu) + \omega(\nu^2 + \nu\tilde{b}^\dagger + \nu\tilde{b})) + \omega\tilde{b}^\dagger\tilde{b} \\
&= \tilde{a}^\dagger\tilde{a}(\epsilon_0 + \lambda(\tilde{b}^\dagger + \tilde{b} - 2\frac{\lambda}{\omega}) + \omega((-\frac{\lambda}{\omega})^2 - \frac{\lambda}{\omega}\tilde{b}^\dagger - \frac{\lambda}{\omega}\tilde{b})) + \omega\tilde{b}^\dagger\tilde{b} \\
&= \tilde{a}^\dagger\tilde{a}(\epsilon_0 + \lambda\tilde{b}^\dagger + \lambda\tilde{b} - 2\frac{\lambda^2}{\omega} + \frac{\lambda^2}{\omega} - \lambda\tilde{b}^\dagger - \lambda\tilde{b}) + \omega\tilde{b}^\dagger\tilde{b} \\
&= \tilde{a}^\dagger\tilde{a}(\epsilon_0 - \frac{\lambda^2}{\omega}) + \omega\tilde{b}^\dagger\tilde{b}
\end{aligned} \tag{14}
$$

References