# On the general mapping between effective two-electron interaction and Jastrow factors.

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This section presents the basics of the transcorrelation for electron-positron wave function

## I. E-POSITRON JASTROW FACTOR

We assume that we have a Jastrow factor $j(\mathbf{r}_i, \mathbf{r}_p)$ where $\mathbf{r}_i$ is the position of the $i$-th electron and $\mathbf{r}_p$ is the position of the positron. We want to compute the similarity transformation of the following Hamiltonian

$$H_{ep} = -\frac{1}{2}\Big(\Delta_{\mathbf{r}_p} + \sum_{i=1}^{N}(\Delta_{\mathbf{r}_i} + v_{ne}(\mathbf{r}_i))\Big) + \sum_{i>j}\frac{1}{r_{ij}} - \sum_{i}\frac{1}{r_{ip}}, \quad (1)$$

with the $N$-electron Jastrow factor

$$\begin{aligned} J(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, \mathbf{r}_p) &= \sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p) \\ &= J(\{\mathbf{r}_i\}, \mathbf{r}_p) \end{aligned} \quad (2)$$

One can then use the usual Baker-Campbell-Hausdorff (BCH) expansion of the similarity transformation

$$e^{-J} H e^{H} = H + [H, J] + \frac{1}{2!}[[H, J], J] + \frac{1}{3!}[[[H, J], J], J] + \dots, \quad (3)$$

but because there is only a second order derivative operator in $H_{ep}$, it naturally terminates at second order

$$\begin{aligned} \tilde{H}_{ep}[j] &= e^{J(\{\mathbf{r}_i\},\mathbf{r}_p)} H_{ep} e^{J(\{\mathbf{r}_i\},\mathbf{r}_p)} \\ &= H_{ep} + [H_{ep}, J(\{\mathbf{r}_i\}, \mathbf{r}_p)] + \frac{1}{2}\Big[[H_{ep}, J(\{\mathbf{r}_i\}, \mathbf{r}_p)], J(\{\mathbf{r}_i\}, \mathbf{r}_p)\Big]. \end{aligned} \quad (4)$$

Actually, as $J(\{\mathbf{r}_i\}, \mathbf{r}_p)$ is a scalar function, the only part of $H_{ep}$ that does not commute is the Laplacian. One can then write

$$\tilde{H}_{ep}[j] = H + [\hat{T}, J(\{\mathbf{r}_i\}, \mathbf{r}_p)] + \frac{1}{2}\Big[[\hat{T}, J(\{\mathbf{r}_i\}, \mathbf{r}_p)], \quad (5)$$

where $\hat{T}$ is the total kinetic energy

$$\begin{aligned} \hat{T} &= -\frac{1}{2}(\Delta_{\mathbf{r}_p} + \sum_{j=1}^{N}\Delta_{\mathbf{r}_j}) \\ &= \hat{T}_p + \hat{T}_e. \end{aligned} \quad (6)$$

Let us compute the first-order commutator

$$[\hat{T}, J(\{\mathbf{r}_i\}, \mathbf{r}_p)] = [\hat{T}_p, J(\{\mathbf{r}_i\}, \mathbf{r}_p)] + [\hat{T}_e, J(\{\mathbf{r}_i\}, \mathbf{r}_p)]. \quad (7)$$

We begin by the electronic part by applying the commutator to a general electron-positron wave function $\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)$

$$\begin{aligned} &-2 \times [\hat{T}_e, J(\{\mathbf{r}_i\}, \mathbf{r}_p)]\phi(\{\mathbf{r}_i\}, \mathbf{r}_p) = \\ &\underbrace{\sum_{j=1}^{N}\Delta_{\mathbf{r}_j}\Big(\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p)\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)\Big)}_{=A} - \underbrace{\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p)\sum_{j=1}^{N}\Delta_{\mathbf{r}_j}\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)}_{=B}. \end{aligned} \quad (8)$$

The term $B$ can be split into three terms according to the $x$, $y$ and $z$ components of the Laplacian

$$B = B_x + B_y + B_z \quad (9)$$

where $B_x$ is simply

$$B_x = (\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p))[\sum_{j=1}^{N}\frac{\partial^2}{\partial {x_j}^2}\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)]. \quad (10)$$

Let us now proceed with the term $A$ which can also be divided into three terms

$$A = A_x + A_y + A_z, \quad (11)$$

and let us take for example the $A_x$ term

$$A_x = \sum_{j=1}^{N}\frac{\partial^2}{\partial {x_j}^2}\Big(\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p)\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)\Big). \quad (12)$$

and therefore the term $\sum_{i=1}^{N}$ in $A_x$ reduces to $i = j$

$$\begin{aligned} A_x = \sum_{j=1}^{N}\frac{\partial}{\partial x_j}\Big([\frac{\partial}{\partial x_j}\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p)]\phi(\{\mathbf{r}_i\}, \mathbf{r}_p) \\ + (\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p))[\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)]\Big), \end{aligned} \quad (13)$$

but one can notice that

$$\frac{\partial}{\partial x_j} j(\mathbf{r}_i, \mathbf{r}_p) = 0 \quad \text{if } i \neq j, \quad (14)$$

and therefore

$$[\frac{\partial}{\partial x_j}\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p)]\phi(\{\mathbf{r}_i\}, \mathbf{r}_p) = [\frac{\partial}{\partial x_j} j(\mathbf{r}_j, \mathbf{r}_p)]\phi(\{\mathbf{r}_i\}, \mathbf{r}_p) \quad (15)$$

and therefore

$$\begin{aligned} A_x = \sum_{j=1}^{N}\frac{\partial}{\partial x_j}\Big([\frac{\partial}{\partial x_j} j(\mathbf{r}_j, \mathbf{r}_p)]\phi(\{\mathbf{r}_i\}, \mathbf{r}_p) \\ + (\sum_{i=1}^{N} j(\mathbf{r}_i, \mathbf{r}_p))[\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\}, \mathbf{r}_p)]\Big) \end{aligned} \quad (16)$$

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, or again

$$
\begin{aligned}
A_x = &\sum_{j=1}^{N}\Big([\frac{\partial^2}{\partial {x_j}^2} j(\mathbf{r}_j,\mathbf{r}_p)]\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&+[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)][\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)]\\
&+[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)][\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)]\\
&+(\sum_{i=1}^{N} j(\mathbf{r}_i,\mathbf{r}_p))[\frac{\partial^2}{\partial {x_j}^2}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)]\Big) \qquad (17)\\
= B_x + &\sum_{j=1}^{N}\Big([\frac{\partial^2}{\partial {x_j}^2} j(\mathbf{r}_j,\mathbf{r}_p)]\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&+2[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)][\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)]\Big)
\end{aligned}
$$

Therefore, by doing $A_x - B_x$, there only remains

$$
\begin{aligned}
A_x - B_x = &\sum_{j=1}^{N}\Big([\frac{\partial^2}{\partial {x_j}^2} j(\mathbf{r}_j,\mathbf{r}_p)]\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&+2[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)][\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)]\Big),
\end{aligned} \qquad (18)
$$

and we can then conclude that the commutator can be written as

$$
\begin{aligned}
&[\hat{T}_e, J(\{\mathbf{r}_i\},\mathbf{r}_p)]\phi(\{\mathbf{r}_i\},\mathbf{r}_p) =\\
&-\frac{1}{2}\sum_{j=1}^{N}\Big((\Delta_{\mathbf{r}_j} j(\mathbf{r}_j,\mathbf{r}_p)) + 2\nabla_{\mathbf{r}_j} j(\mathbf{r}_j,\mathbf{r}_p)\cdot\nabla_{\mathbf{r}_j}\Big)\phi(\{\mathbf{r}_i\},\mathbf{r}_p),
\end{aligned} \qquad (19)
$$

or that we can write symbolically

$$
[\hat{T}_e, J(\{\mathbf{r}_i\},\mathbf{r}_p)] = -\frac{1}{2}\sum_{j=1}^{N}\Big((\Delta_{\mathbf{r}_j} j(\mathbf{r}_j,\mathbf{r}_p)) + 2\nabla_{\mathbf{r}_j} j(\mathbf{r}_j,\mathbf{r}_p)\cdot\nabla_{\mathbf{r}_j}\Big). \qquad (20)
$$

Similarly, if one considers the commutator involvin $\hat{T}_p$ one obtains

$$
[\hat{T}_p, J(\{\mathbf{r}_i\},\mathbf{r}_p)] = -\frac{1}{2}\Big((\Delta_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p))+2[\sum_{i=1}^{N}\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)]\cdot\nabla_{\mathbf{r}_p}\Big). \qquad (21)
$$

In these commutators, there is a purely scalar part which is either $\Delta_{\mathbf{r}_j} j(\mathbf{r}_j,\mathbf{r}_p)$ or $\Delta_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)$ which necessary commutes with the scalar function $J(\{\mathbf{r}_i\},\mathbf{r}_p)$. Therefore, to compute the second-order commutator, that we divide into two parts involving the first commutator of $\hat{T}_e$ and that of $\hat{T}_p$,

$$
\begin{aligned}
\frac{1}{2}\Big[[H_{ep}, J(\{\mathbf{r}_i\},\mathbf{r}_p)], J(\{\mathbf{r}_i\},\mathbf{r}_p)\Big] =&\frac{1}{2}\underbrace{\Big[[\hat{T}_e, J(\{\mathbf{r}_i\},\mathbf{r}_p)], J(\{\mathbf{r}_i\},\mathbf{r}_p)\Big]}_{=C_x+C_y+C_z}\\
&+\frac{1}{2}\underbrace{\Big[[\hat{T}_p, J(\{\mathbf{r}_i\},\mathbf{r}_p)], J(\{\mathbf{r}_i\},\mathbf{r}_p)\Big]}_{=D_x+D_y+D_z}
\end{aligned} \qquad (22)
$$

only the terms in either $\nabla_{\mathbf{r}_j}$ and r $\nabla_{\mathbf{r}_p}$ are not going to commute with $J(\{\mathbf{r}_i\},\mathbf{r}_p)$. Let us begin $C_x$

$$
\begin{aligned}
C_x = &-\frac{1}{2}\Big[\sum_{j=1}^{N}\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)\frac{\partial}{\partial x_j},\sum_{i=1}^{N} j(\mathbf{r}_i,\mathbf{r}_p)\Big]\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&= -\frac{1}{2}\sum_{j=1}^{N}[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)](\sum_{i=1}^{N}[\frac{\partial}{\partial x_j} j(\mathbf{r}_i,\mathbf{r}_p)])\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&-\frac{1}{2}\sum_{j=1}^{N}[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)](\sum_{i=1}^{N} j(\mathbf{r}_i,\mathbf{r}_p))\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&+\frac{1}{2}\sum_{j=1}^{N}[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)](\sum_{i=1}^{N} j(\mathbf{r}_i,\mathbf{r}_p))\frac{\partial}{\partial x_j}\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&= -\frac{1}{2}\sum_{j=1}^{N}[\frac{\partial}{\partial x_j} j(\mathbf{r}_j,\mathbf{r}_p)]^2\phi(\{\mathbf{r}_i\},\mathbf{r}_p).
\end{aligned} \qquad (23)
$$

Therefore we can conclude that

$$
\frac{1}{2}\Big[[\hat{T}_e, J(\{\mathbf{r}_i\},\mathbf{r}_p)], J(\{\mathbf{r}_i\},\mathbf{r}_p)\Big] = -\sum_{j=1}^{N}\frac{1}{2}[\nabla_{\mathbf{r}_j} j(\mathbf{r}_j,\mathbf{r}_p)]^2. \qquad (24)
$$

We then compute the term $D$

$$
\begin{aligned}
D = &-\frac{1}{2}\Big[[\sum_{i=1}^{N}\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)]\cdot\nabla_{\mathbf{r}_p},\sum_{j=1}^{N} j(\mathbf{r}_j,\mathbf{r}_p)\Big]\phi(\{\mathbf{r}_i\},\mathbf{r}_p)\\
&= -\frac{1}{2}\sum_{i=1}^{N}[\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)]^2 - \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq j}\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)\cdot\nabla_{\mathbf{r}_p} j(\mathbf{r}_j,\mathbf{r}_p).
\end{aligned} \qquad (25)
$$

We can therefore write the total second-order commutator as

$$
\begin{aligned}
&\frac{1}{2}\Big[[\hat{T}, J(\{\mathbf{r}_i\},\mathbf{r}_p)], J(\{\mathbf{r}_i\},\mathbf{r}_p)\Big] =\\
&-\frac{1}{2}\sum_{i=1}^{N}\Big[[\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)]^2 + [\nabla_{\mathbf{r}_i} j(\mathbf{r}_i,\mathbf{r}_p)]^2\Big]\\
&-\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}[\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)]\cdot[\nabla_{\mathbf{r}_p} j(\mathbf{r}_j,\mathbf{r}_p)].
\end{aligned} \qquad (26)
$$

We can therefore write the total transcorrelated Hamiltonian as

$$
\begin{aligned}
\tilde{H}_{ep} = H &- \frac{1}{2}\sum_{i=1}^{N}(\Delta_{\mathbf{r}_i} j(\mathbf{r}_i,\mathbf{r}_p) + \Delta_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p))\\
&-\sum_{i=1}^{N}(\nabla_{\mathbf{r}_i} j(\mathbf{r}_i,\mathbf{r}_p)\cdot\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p))\\
&-\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}[\nabla_{\mathbf{r}_p} j(\mathbf{r}_i,\mathbf{r}_p)]\cdot[\nabla_{\mathbf{r}_p} j(\mathbf{r}_j,\mathbf{r}_p)].
\end{aligned} \qquad (27)
$$