第二量子化　計算

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$$
\begin{aligned}
|\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_N\sigma_N\rangle &= \frac{1}{\sqrt{N!}}\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}_1)\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}_N)\,|\mathrm{vac}\rangle \\
\hat{\psi}_\sigma(\boldsymbol{r})\,|\mathrm{vac}\rangle &= 0 \\
\left[\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}_{\sigma'}(\boldsymbol{r}')\right]_s &= 0 \\
\left[\hat{\psi}^\dagger_\sigma(\boldsymbol{r}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\right]_s &= 0 \\
\left[\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\right]_s &= \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma,\sigma'}
\end{aligned}
$$

を前提として。

$$
\langle\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_N\sigma_N|\boldsymbol{r}'_1\sigma'_1, \ldots, \boldsymbol{r}'_{N'}\sigma'_{N'}\rangle = \frac{\delta_{N,N'}}{N!}\sum_P s^P \delta(\boldsymbol{r}_1-\boldsymbol{r}'_{p_1})\delta_{\sigma_1,\sigma'_{p_1}}\cdots\delta(\boldsymbol{r}_N-\boldsymbol{r}'_{p_N})\delta_{\sigma_N,\sigma'_{p_N}}
$$

を示そう。
まずは $N = N'$ の場合について考える。
$P(i_1, \ldots, i_K)$ は $1, \ldots, N$ が $i_1, \ldots, i_K, 1, \ldots, \underbrace{\quad}_{i_1,\ldots,i_K}, \ldots, N$ になるように並べ替えたときに偶置換で入れ替

える場合は 0, 奇置換で入れ替わる場合は 1 とした値とする。

$$\begin{aligned}
\langle \boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_N\sigma_N|\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_N\sigma'_N\rangle =&\frac{1}{N!}\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_1}(\boldsymbol{r}_1)\hat\psi^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_2}(\boldsymbol{r}_2)\delta(\boldsymbol{r}_1-\boldsymbol{r}'_1)\delta_{\sigma_1,\sigma'_1}\hat\psi^\dagger_{\sigma_2}(\boldsymbol{r}'_2)\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
&+\frac{1}{N!}s\,\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_2}(\boldsymbol{r}_2)\hat\psi^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\hat\psi_{\sigma_1}(\boldsymbol{r}_1)\hat\psi^\dagger_{\sigma_2}(\boldsymbol{r}'_2)\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_2}(\boldsymbol{r}_2)\delta(\boldsymbol{r}_1-\boldsymbol{r}'_1)\delta_{\sigma_1,\sigma'_1}\hat\psi^\dagger_{\sigma_2}(\boldsymbol{r}'_2)\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
&+\frac{1}{N!}s\,\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_2}(\boldsymbol{r}_2)\hat\psi^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\delta(\boldsymbol{r}_1-\boldsymbol{r}'_2)\delta_{\sigma_1,\sigma'_2}\hat\psi^\dagger_{\sigma_3}(\boldsymbol{r}'_3)\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
&+\frac{1}{N!}s^2\,\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_2}(\boldsymbol{r}_2)\hat\psi^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\hat\psi^\dagger_{\sigma_2}(\boldsymbol{r}'_2)\hat\psi_{\sigma_1}(\boldsymbol{r}_1)\hat\psi^\dagger_{\sigma_3}(\boldsymbol{r}_3)\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{i_1}s^{P(i_1)}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{i_1})\delta_{\sigma_1,\sigma'_{i_1}}\\
&\times\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_2}(\boldsymbol{r}_2)\hat\psi^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\underbrace{}_{i_1}\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{i_1\neq i_2}s^{P(i_1,i_2)}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{i_1})\delta_{\sigma_1,\sigma'_{i_1}}\delta(\boldsymbol{r}_2-\boldsymbol{r}'_{i_2})\delta_{\sigma_2,\sigma'_{i_2}}\\
&\times\langle\mathrm{vac}|\,\hat\psi_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat\psi_{\sigma_3}(\boldsymbol{r}_3)\hat\psi^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\underbrace{}_{i_1,i_2}\cdots\hat\psi^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\,|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{P}s^{P}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{p_1})\delta_{\sigma_1,\sigma'_{p_1}}\cdots\delta(\boldsymbol{r}_N-\boldsymbol{r}'_{p_N})\delta_{\sigma_N,\sigma'_{p_N}}\,\langle\mathrm{vac}|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{P}s^{P}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{p_1})\delta_{\sigma_1,\sigma'_{p_1}}\cdots\delta(\boldsymbol{r}_N-\boldsymbol{r}'_{p_N})\delta_{\sigma_N,\sigma'_{p_N}}
\end{aligned}$$

てか、交換子の法則を用いればもっと分かりやすく求まりそう。

$$\left[\hat A,\hat B_1\cdots\hat B_n\right]_{s^n}=\sum_{i=1}^{n}s^{i-1}\hat B_1\cdots\hat B_{i-1}\left[\hat A,\hat B_i\right]_s\hat B_{i+1}\cdots\hat B_n$$

が成り立つので示す。

$$\begin{aligned}
\sum_{i=1}^{n}s^{i-1}\hat B_1\cdots\hat B_{i-1}\left[\hat A,\hat B_i\right]_s\hat B_{i+1}\cdots\hat B_n=&\sum_{i=1}^{n}s^{i-1}\hat B_1\cdots\hat B_{i-1}\hat A\hat B_i\cdots\hat B_n-\sum_{i=1}^{n}s^{i}\hat B_1\cdots\hat B_i\hat A\hat B_{i+1}\cdots\hat B_n\\
=&\sum_{i=1}^{n}s^{i-1}\hat B_1\cdots\hat B_{i-1}\hat A\hat B_i\cdots\hat B_n-\sum_{i=2}^{n+1}s^{i-1}\hat B_1\cdots\hat B_{i-1}\hat A\hat B_i\cdots\hat B_n\\
=&\hat A\hat B_1\cdots\hat B_n-s^n\hat B_1\cdots\hat B_n\hat A\\
=&\left[\hat A,\hat B_1\cdots\hat B_n\right]_{s^n}
\end{aligned}$$

これを用いて

$$
\begin{aligned}
\langle \boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_N\sigma_N|\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_N\sigma'_N\rangle =&\frac{1}{N!}\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_1}(\boldsymbol{r}_1)\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_1}(\boldsymbol{r}_1)\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)|\mathrm{vac}\rangle\\
&-\frac{1}{N!}s^n\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_2}(\boldsymbol{r}_2)\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\hat{\psi}^\dagger_{\sigma_2}(\boldsymbol{r}'_2)\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\hat{\psi}_{\sigma_1}(\boldsymbol{r}_1)|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_2}(\boldsymbol{r}_2)\left[\hat{\psi}_{\sigma_1}(\boldsymbol{r}_1),\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)\right]_{s^n}|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{i_1}s^{i_1-1}\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_2}(\boldsymbol{r}_2)\\
&\times\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\hat{\psi}^\dagger_{\sigma_{i_1-1}}(\boldsymbol{r}_{i_1-1})\left[\hat{\psi}_{\sigma_1}(\boldsymbol{r}_1),\hat{\psi}^\dagger_{\sigma_{i_1}}(\boldsymbol{r}_{i_1})\right]_s\hat{\psi}^\dagger_{\sigma_{i_1+1}}(\boldsymbol{r}_{i_1+1})\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{i_1}s^{P(i_1)}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{i_1})\delta_{\sigma_1,\sigma'_{i_1}}\\
&\times\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_2}(\boldsymbol{r}_2)\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\underbrace{}_{i_1}\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{i_1\neq i_2}s^{P(i_1,i_2)}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{i_1})\delta_{\sigma_1,\sigma'_{i_1}}\delta(\boldsymbol{r}_2-\boldsymbol{r}'_{i_2})\delta_{\sigma_2,\sigma'_{i_2}}\\
&\times\langle\mathrm{vac}|\hat{\psi}_{\sigma_N}(\boldsymbol{r}_N)\cdots\hat{\psi}_{\sigma_3}(\boldsymbol{r}_3)\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\underbrace{}_{i_1,i_2}\cdots\hat{\psi}^\dagger_{\sigma_N}(\boldsymbol{r}'_N)|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{P}s^{P(i_1,\dots,i_N)}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{p_1})\delta_{\sigma_1,\sigma'_{p_1}}\cdots\delta(\boldsymbol{r}_N-\boldsymbol{r}'_{p_N})\delta_{\sigma_N,\sigma'_{p_N}}\langle\mathrm{vac}|\mathrm{vac}\rangle\\
=&\frac{1}{N!}\sum_{P}s^{P}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{p_1})\delta_{\sigma_1,\sigma'_{p_1}}\cdots\delta(\boldsymbol{r}_N-\boldsymbol{r}'_{p_N})\delta_{\sigma_N,\sigma'_{p_N}}
\end{aligned}
$$

交換子を用いると、計算自体は追いやすいが、なぜ s^P になるかを追いにくくなる。
$N<N'$ については

$$
\begin{aligned}
\langle \boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_N\sigma_N|\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_{N'}\sigma'_{N'}\rangle =&\frac{1}{N!}\sum_{P}s^{P}\delta(\boldsymbol{r}_1-\boldsymbol{r}'_{p_1})\delta_{\sigma_1,\sigma'_{p_1}}\cdots\delta(\boldsymbol{r}_N-\boldsymbol{r}'_{p_N})\delta_{\sigma_N,\sigma'_{p_N}}\\
&\times\langle\mathrm{vac}|\hat{\psi}^\dagger_{\sigma_1}(\boldsymbol{r}'_1)\cdots\underbrace{}_{i_1,\dots,i_N}\cdots\hat{\psi}^\dagger_{\sigma_{N'}}(\boldsymbol{r}'_{N'})|\mathrm{vac}\rangle\\
=&0
\end{aligned}
$$

$N>N'$ も同様にできる。