CEM 993 **Spring 2023**

Assignment No. 5 (20 pts.) **Due Date: April 14, 2023**

1. (4 pts.) Let
$$S[\tilde{\Phi}] = \mathrm{Re}\langle\Psi|\tilde{\Phi}\rangle/\sqrt{\langle\tilde{\Phi}|\tilde{\Phi}\rangle}$$
be the overlap functional used to determine the Brueckner spin-orbitals ($|\tilde{\Phi}\rangle$ is the IPM state, $|\Psi\rangle$ is the exact state). Let $|\tilde{\Phi}\rangle = e^{\hat{C}_1}|\Phi\rangle$ be the trial IPM wave function ($\hat{C}_1$ is the single excitation operator resulting from the use of the Thouless theorem) and let $|\Phi\rangle$ represent the single determinantal state that maximizes $S[\tilde{\Phi}]$. By analyzing the difference $S[\tilde{\Phi}] - S[\Phi]$, show that the first variation of $S[\tilde{\Phi}]$ at $|\tilde{\Phi}\rangle = |\Phi\rangle$, i.e. $\delta S[\Phi]$, equals
$$\delta S[\Phi] = \mathrm{Re}\langle\Psi|\hat{C}_1|\Phi\rangle.$$

2. (2 pts.) As shown in one of our classes, the spectral representation of the reduced resolvent $R^{(0)}$, in terms of the eigenstates and eigenvalues of the unperturbed operator K_0, $|\Phi_n\rangle$ and κ_n, respectively, is
$$R^{(0)} = \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\kappa_0 - \kappa_n}.$$
Use this explicit representation of $R^{(0)}$ to prove that
$$Q(\kappa_0 - K_0)R^{(0)} = Q,$$
where
$$Q = \hat{1} - P \equiv \hat{1} - |\Phi_0\rangle\langle\Phi_0|$$
is a projection operator on the subspace of the Hilbert space orthogonal to the subspace spanned by $|\Phi_0\rangle$.

3. (6 pts.) Use the bracketing technique to derive the formula for the 4th-order correction to the wave function and the 5th-order correction to the energy, $|\Psi_0^{(4)}\rangle$ and $k_0^{(5)}$, respectively, in the Rayleigh-Schrödinger perturbation theory in terms of the perturbation operator W and the reduced resolvent $R^{(0)}$ of the unperturbed operator K_0.

Problems 4–7, combined together, result in a proof of the following operator identity:
$$\begin{aligned} e^{-A}Be^{A} &= B + [B,A] + \frac{1}{2!}[[B,A],A] + \frac{1}{3!}[[[B,A],A],A] + \cdots \\ &= \sum_{n=0}^{\infty} \frac{1}{n!}[\cdots[B,\underbrace{A],\cdots,A]}_{n \text{ times}}, \end{aligned} \tag{1}$$
where A and B are operators and $[\ ,\ ]$ designates the commutator. This identity is essential in various quantum-mechanical considerations, including those relevant to the coupled-cluster theory.

4. (2 pts.) If $f(z)$ is a function of a complex variable z, which can be represented by a power series (Taylor) expansion

$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f(z)}{dz^n}\bigg|_{z=0} z^n, \tag{2}$$

then the corresponding function $f(A)$, where A is an operator, is defined as

$$f(A) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f(z)}{dz^n}\bigg|_{z=0} A^n \tag{3}$$

(as usual, $\dfrac{d^0 f(z)}{dz^0} \equiv f(z)$). For example,

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n. \tag{4}$$

Consider the operator

$$e^{xA} = \sum_{n=0}^{\infty} \frac{1}{n!} x^n A^n, \tag{5}$$

where x is a real variable. Use Eq. (5) to prove that

$$\frac{d}{dx} e^{xA} = A e^{xA}. \tag{6}$$

By the repeated use of Eq. (6) and mathematical induction show that

$$\frac{d^n}{dx^n} e^{xA} = A^n e^{xA}, \quad n = 1, 2, \dots\ . \tag{7}$$

5. (2 pts.) Consider the auxiliary operator quantity

$$F(x) = e^{-xA} B e^{xA}, \tag{8}$$

where x is a real variable and A and B are operators. Note that F(1) represents the left-hand side of Eq. (1). Just like e^{xA} defined by Eq. (5), $F(x)$ is an operator function of x, i.e., it is an operator which simultaneously depends on x. In many respects, operators of this type behave like ordinary functions. For example, the first derivative of the product of two operator functions $G_1(x)$ and $G_2(x)$ with respect to x can be calculated as

$$\frac{d}{dx}(G_1(x)G_2(x)) = \left(\frac{d}{dx}G_1(x)\right) G_2(x) + G_1(x)\left(\frac{d}{dx}G_2(x)\right). \tag{9}$$

We only have to remember that operator functions do not necessarily commute (they are operators), i.e., one has to preserve their original ordering in writing the various expressions of the type of Eq. (9) (note that $G_1(x)$ is always before $G_2(x)$ in Eq. (9)). Show that the first derivative of $F(x)$, Eq. (8), with respect to x can be given the following compact form:

$$\frac{d}{dx} F(x) = e^{-xA}[B, A] e^{xA}. \tag{10}$$

6. (3 pts.) Show that the second derivative of $F(x)$, Eq. (8), can be written as

$$\frac{d^2}{dx^2}F(x) = e^{-xA}[[B, A], A]e^{xA}. \tag{11}$$

Use the mathematical induction to prove that

$$\frac{d^n}{dx^n}F(x) = e^{-xA}[\cdots[B, \underbrace{A], \cdots, A]}_{n \text{ times}} e^{xA}, \quad n = 1, 2, \ldots\ . \tag{12}$$

As usual,

$$\frac{d^0}{dx^0}F(x) = F(x) = e^{-xA}Be^{xA}. \tag{13}$$

7. (1 pt.) We can represent the operator function $F(x)$, Eq. (8), by the following Taylor expansion:

$$F(x) = \sum_{n=0}^{\infty} x^n \frac{1}{n!} \frac{d^n F(x)}{dx^n}\bigg|_{x=0}. \tag{14}$$

In particular, when x in the above equation is set at 1, we obtain,

$$F(1) = e^{-A}Be^{A} = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n F(x)}{dx^n}\bigg|_{x=0}. \tag{15}$$

Use Eqs. (12), (13), and (15) to prove Eq. (1).

SOLUTIONS

1. $$S[\tilde{\Phi}] = \mathrm{Re}\,\langle \Psi | e^{\hat{C}_1} | \Phi \rangle \, \langle \Phi | e^{\hat{C}_1^{\dagger}} e^{\hat{C}_1} | \Phi \rangle^{-\frac{1}{2}}$$

$$S[\tilde{\Phi}] - S[\Phi] =$$

$$= \mathrm{Re}\,\langle \Psi | \left(1 + \hat{C}_1 + O(\hat{C}_1^2)\right) | \Phi \rangle \times$$

$$\times \langle \Phi | \left[1 + \hat{C}_1^{\dagger} + O(\hat{C}_1^{\dagger 2})\right]\left[1 + \hat{C}_1 + O(\hat{C}_1^2)\right] | \Phi \rangle^{-\frac{1}{2}}$$

$$- \mathrm{Re}\,\langle \Psi | \Phi \rangle$$

$$= \left[\mathrm{Re}\,\langle \Psi | \Phi \rangle + \mathrm{Re}\,\langle \Psi | \hat{C}_1 | \Phi \rangle + O(\hat{C}_1^2)\right]$$

$$\times \Big[1 + \overbrace{\langle \Phi | \hat{C}_1^{\dagger} | \Phi \rangle}^{=0} + \overbrace{\langle \Phi | \hat{C}_1 | \Phi \rangle}^{=0}$$

$$+ \; O(\hat{C}_1^2) \Big]^{-\frac{1}{2}} - \mathrm{Re}\,\langle \Psi | \Phi \rangle =$$

$$= \left[\mathrm{Re}\langle\Psi|\Phi\rangle + \mathrm{Re}\langle\Psi|\hat{C}_1|\Phi\rangle + O(\hat{C}_1^2)\right]$$

$$\times\left[1 + O(\hat{C}_1^2)\right]^{-\frac{1}{2}} - \mathrm{Re}\langle\Psi|\Phi\rangle$$

$$= \left[\mathrm{Re}\langle\Psi|\Phi\rangle + \mathrm{Re}\langle\Psi|\hat{C}_1|\Phi\rangle + O(\hat{C}_1^2)\right]$$

$$\times\left[1 - \tfrac{1}{2}O(\hat{C}_1^2)\right] - \mathrm{Re}\langle\Psi|\Phi\rangle$$

$$= \cancel{\mathrm{Re}\langle\Psi|\Phi\rangle} + \mathrm{Re}\langle\Psi|\hat{C}_1|\Phi\rangle + O(\hat{C}_1^2)$$

$$- \cancel{\mathrm{Re}\langle\Psi|\Phi\rangle} = \mathrm{Re}\langle\Psi|\hat{C}_1|\Phi\rangle +$$

$$+ O(\hat{C}_1^2).$$

Thus,

$\delta S[\Phi] \equiv$ term linear in $\hat{C}_1$ in

$$S[\tilde{\Phi}] - S[\Phi] = \mathrm{Re}\langle\Psi|\hat{C}_1|\Phi\rangle.$$

2.

$$R^{(0)} = \sum_{n \neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0 - \mathcal{E}_n}$$

$$Q(\mathcal{E}_0 - K_0) R^{(0)} = Q \sum_{n \neq 0} \frac{(\mathcal{E}_0 - K_0)|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0 - \mathcal{E}_n}$$

By definition,

$$K_0 |\Phi_n\rangle = \mathcal{E}_n |\Phi_n\rangle .$$

Thus,

$$Q(\mathcal{E}_0 - K_0) R^{(0)} = Q \sum_{n \neq 0} \frac{\cancel{(\mathcal{E}_0 - \mathcal{E}_n)}|\Phi_n\rangle\langle\Phi_n|}{\cancel{\mathcal{E}_0 - \mathcal{E}_n}}$$

$$= Q \sum_{n \neq 0} |\Phi_n\rangle\langle\Phi_n|$$

$$= Q \cdot Q = Q ,$$

since $Q = 1 - P = \sum_{n \neq 0} |\Phi_n\rangle\langle\Phi_n|$ and $Q^2 = Q$.

3.

$$
\begin{aligned}
|\Psi_0^{(4)}\rangle = {} & R^{(0)} W R^{(0)} W R^{(0)} W R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} W R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} W R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} W R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} W R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W \rangle R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W R^{(0)} W R^{(0)} W \rangle R^{(0)} W |\Phi_0\rangle \\
& + R^{(0)} \langle W R^{(0)} \langle W \rangle R^{(0)} W \rangle R^{(0)} W |\Phi_0\rangle
\end{aligned}
$$

$$
\begin{aligned}
&= (R^{(0)}W)^4|\Phi_0\rangle - \langle W\rangle\big[R^{(0)2}WR^{(0)}WR^{(0)}W \\
&\quad + R^{(0)}WR^{(0)2}WR^{(0)}W + R^{(0)}WR^{(0)}WR^{(0)2}W\big]|\Phi_0\rangle \\
&\quad + \langle W\rangle^2\big[R^{(0)3}WR^{(0)}W + R^{(0)2}WR^{(0)2}W \\
&\quad + R^{(0)}WR^{(0)3}W\big]|\Phi_0\rangle \\
&\quad - \langle W\rangle^3 R^{(0)4}W|\Phi_0\rangle \\
&\quad - \langle WR^{(0)}W\rangle\big[R^{(0)2}WR^{(0)}W + R^{(0)}WR^{(0)2}W\big]|\Phi_0\rangle \\
&\quad + 2\langle W\rangle\langle WR^{(0)}W\rangle R^{(0)3}W|\Phi_0\rangle \\
&- \big[\langle WR^{(0)}WR^{(0)}W\rangle - \langle W\rangle\langle WR^{(0)2}W\rangle\big]R^{(0)2}W|\Phi_0\rangle
\end{aligned}
$$

The formula for $k_0^{(5)}$ could be obtained in a similar way by inserting brackets into the principal term

$$\langle W R^{(0)} W R^{(0)} W R^{(0)} W R^{(0)} W \rangle$$

or by closing $|\Psi_0^{(4)}\rangle$ with $\langle \Phi_0 | W$, since

$$k_0^{(5)} = \langle \Phi_0 | W | \Psi_0^{(4)} \rangle .$$

We obtain,

$$
\begin{aligned}
k_0^{(5)} = {} & \langle W (R^{(0)} W)^4 \rangle - \langle W \rangle \Big[\langle W R^{(0)2} W R^{(0)} W R^{(0)} W \rangle \\
& + \langle W R^{(0)} W R^{(0)2} W R^{(0)} W \rangle + \langle W R^{(0)} W R^{(0)} W R^{(0)2} W \rangle \Big] \\
& + \langle W \rangle^2 \Big[\langle W R^{(0)3} W R^{(0)} W \rangle + \langle W R^{(0)2} W R^{(0)2} W \rangle \\
& + \langle W R^{(0)} W R^{(0)3} W \rangle \Big] \\
& - \langle W \rangle^3 \langle W R^{(0)4} W \rangle \\
& - \langle W R^{(0)} W \rangle \Big[\langle W R^{(0)2} W R^{(0)} W \rangle + \langle W R^{(0)} W R^{(0)2} W \rangle \Big] \\
& + 2 \langle W \rangle \langle W R^{(0)} W \rangle \langle W R^{(0)3} W \rangle \\
& - \Big[\langle W R^{(0)} W R^{(0)} W - \langle W \rangle \langle W R^{(0)2} W \rangle \Big] \langle W R^{(0)2} W \rangle .
\end{aligned}
$$

PROBLEMS 4-7

4.

$$e^{xA} = \sum_{n=0}^{\infty} \frac{1}{n!} x^n A^n$$

$$\frac{d}{dx} e^{xA} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dx} x^n\right) A^n$$

$$= \sum_{n=1}^{\infty} \frac{1}{n!} n x^{n-1} A^n$$

$$= A \sum_{n=1}^{\infty} \frac{1}{(n-1)!} x^{n-1} A^{n-1}$$

$$\stackrel{n-1=k}{=} A \sum_{k=0}^{\infty} \frac{1}{k!} x^k A^k = \underline{\underline{A e^{xA}}} \Leftarrow (6)$$

Eq. (7) reduces to Eq. (6) for $n=1$.
For $n=2$, we obtain

$$\frac{d^2}{dx^2} e^{xA} = \frac{d}{dx}\left(A e^{xA}\right) = A \frac{d}{dx}\left(e^{xA}\right)$$

$$= A\left(A e^{xA}\right) = A^2 e^{xA}, \text{ which}$$

is Eq. (7) written for $n=2$.

In general, we can use the mathematical induction. Let us assume that Eq. (7) is true for some n. Let us consider the case with n replaced by $n+1$. We obtain

$$\frac{d^{n+1}}{dx^{n+1}}\left(e^{xA}\right) = \frac{d}{dx}\left(\frac{d^n}{dx^n} e^{xA}\right) \overset{\text{Eq.(7)}}{=} \frac{d}{dx}\left(A^n e^{xA}\right)$$

$$= A^n \frac{d}{dx}\left(e^{xA}\right) \underset{\text{Eq.(6)}}{=} A^n A e^{xA}$$

$$= \underline{\underline{A^{n+1} e^{xA}}},$$

which is Eq. (7) written for n replaced by $n+1$.

5. $$\frac{d}{dx}F(x) = \frac{d}{dx}\left(e^{-xA} B e^{xA}\right)$$

$$\overset{\text{Eq.(9)}}{=} \frac{d}{dx}\left(e^{-xA}\right) B e^{xA}$$

$$+ e^{-xA} B \frac{d}{dx}\left(e^{xA}\right)$$

$$\overset{\text{Eq.(6)}}{=} -A e^{-xA} B e^{xA} + e^{-xA} B A e^{xA}.$$

Since A and e^{-xA} commute, we obtain

$$\frac{d}{dx}F(x) = -e^{-xA} A B e^{xA}$$

$$+ e^{-xA} B A e^{xA} = e^{-xA}(BA - AB)e^{xA}$$

$$= \underline{\underline{e^{-xA}[B, A]e^{xA}}}. \Leftarrow (10)$$

6.

$$\frac{d^2}{dx^2}F(x) = \frac{d}{dx}\left(\frac{d}{dx}F(x)\right)$$

$$\underset{\text{Eq.(10)}}{=} \frac{d}{dx}\left(e^{-xA}[B,A]e^{xA}\right)$$

$$\underset{\text{Eq.(9)}}{=} \frac{d}{dx}\left(e^{-xA}\right)[B,A]e^{xA}$$

$$+ \; e^{-xA}[B,A]\frac{d}{dx}\left(e^{xA}\right)$$

$$\underset{\text{Eq.(6)}}{=} -e^{-xA}A[B,A]e^{xA}$$

$$+ \; e^{-xA}[B,A]Ae^{xA}$$

$$= e^{-xA}\left([B,A]A - A[B,A]\right)e^{xA}$$

$$= \underline{\underline{e^{-xA}[[B,A],A]e^{xA}}} . \leftarrow (11)$$

We now move to Eq. (12). Let us assume that Eq. (12) is true for n and let us consider Eq. (12) with n replaced by n+1. We obtain

$$\frac{d^{n+1}}{dx^{n+1}} F(x) = \frac{d}{dx}\left(\frac{d^n}{dx^n} F(x)\right)$$

$$\stackrel{\text{Eq.(12)}}{=} \frac{d}{dx}\left(e^{-xA}\,\underbrace{[\ldots[B,A],\ldots,A]}_{n\text{ times}}\,e^{xA}\right)$$

$$\stackrel{\text{Eq.(9)}}{=} \frac{d}{dx}\left(e^{-xA}\right)\underbrace{[\ldots[B,A],\ldots,A]}_{n\text{ times}}\,e^{xA}$$

$$+\, e^{-xA}\underbrace{[\ldots[B,A],\ldots,A]}_{n\text{ times}}\,\frac{d}{dx}\left(e^{xA}\right)$$

$$\stackrel{\text{Eq.(6)}}{=} -e^{-xA} A\,\underbrace{[\ldots[B,A],\ldots,A]}_{n\text{ times}}\,e^{xA}$$

$$+\, e^{-xA}\underbrace{[\ldots[B,A],\ldots,A]}_{n\text{ times}}\,A\,e^{xA}$$

$$= e^{-xA}\Big([\ldots[B,A],\underbrace{\ldots,A]}_{n\text{ times}}\,A - A\,[\ldots[B,A],\underbrace{\ldots,A]}_{n\text{ times}}\Big)e^{xA}$$

$$= e^{-xA}\,[\ldots[B,A],\underbrace{\ldots,A]}_{n+1\text{ times}}\,e^{xA} \Leftarrow (12) \text{ for } (n+1).$$

7.

$$\frac{d^0}{dx^0}F(x)\Big|_{x=0} = F(0) = B.$$

$$\frac{d^n}{dx^n}F(x)\Big|_{x=0} \overset{\text{Eq.(12)}}{=} [\ldots[B,A],\underbrace{\ldots,A]}_{n\text{ times}}$$

for $n \geq 1$, since $e^{\pm xA} = \hat{1}$ for $x = 0$ ($\hat{1}$ is the unit operator).

Substituting the above expressions into Eq. (15), we obtain

$$\boxed{F(1) = e^{-A}Be^{A} = \sum_{n=0}^{\infty}\frac{1}{n!}[\ldots[B,A],\underbrace{\ldots,A]}_{n\text{ times}}}\,.$$

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