CPMC: UHF fast update

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At each propagation step, the walker wavefunction is updated by the two-body term as

$$
\begin{aligned}
|\phi^{(n+1)}\rangle &= e^{-\Delta\tau U \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}} |\phi^{(n)}\rangle \\
&= \frac{1}{2}\sum_{x_i\in\{\pm 1\}} e^{(-\Delta\tau U/2+\gamma x_i)\hat{n}_{i\uparrow}} e^{(-\Delta\tau U/2-\gamma x_i)\hat{n}_{i\downarrow}} |\phi^{(n)}\rangle \\
&= \frac{1}{2}\sum_{x_i\in\{\pm 1\}} \left\{ e^{(-\Delta\tau U/2+\gamma x_i)\hat{n}_{i\uparrow}} |\phi^{(n)\uparrow}\rangle \right\} \left\{ e^{(-\Delta\tau U/2-\gamma x_i)\hat{n}_{i\downarrow}} |\phi^{(n)\downarrow}\rangle \right\}, \qquad (1)
\end{aligned}
$$

i.e. each spin sector is propagated independently. We can write

$$
\begin{aligned}
\hat{B}^{i\sigma} &= e^{[-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i]\hat{n}_{i\sigma}} \\
&= \sum_{k=0}^{\infty} [-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i]^k \, \hat{n}_{i\sigma}^k \\
&= 1 + \hat{n}_{i\sigma} \sum_{k=1}^{\infty} [-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i]^k \qquad (2) \\
&= 1 + \hat{n}_{i\sigma} \left(e^{-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i} - 1 \right), \qquad (3)
\end{aligned}
$$

where we defined $\mathrm{sign}(\sigma) = 1(-1)$ if $\sigma = \uparrow (\downarrow)$ and used the identity $\hat{n}_{i\sigma}^k = \hat{n}_{i\sigma}$ in (2). In the site basis $\{|p\rangle\}$, $\hat{B}^{i\sigma}$ is represented by the matrix

$$
\begin{aligned}
\hat{B}^{i\sigma}_{pq} &= \langle p| e^{[-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i]\hat{n}_{i\sigma}} |q\rangle \\
&= \langle p| 1 + \hat{n}_{i\sigma} \left(e^{-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i} - 1 \right) |q\rangle \\
&= \langle p|q\rangle + \langle p|\hat{n}_{i\sigma}|q\rangle \left(e^{-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i} - 1 \right) \\
&= \delta_{pq} + \delta_{pi}\delta_{qi} n_{i\sigma} \left(e^{-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i} - 1 \right), \qquad (4) \\
\implies \mathbf{B}^{i\sigma} &= \mathbf{I} + n_{i\sigma} \left(e^{-\Delta\tau U/2 + \mathrm{sign}\,(\sigma)\gamma x_i} - 1 \right) \underbrace{\hat{e}_i \otimes \hat{e}_i}_{\substack{\text{outer} \\ \text{product}}}, \qquad (5)
\end{aligned}
$$

where $n_{i\sigma}$ is the occupancy of the spin σ orbital at site i and $\hat{e}_i$ is the unit basis vector with the i-th element of value 1 as the only nonzero element[1]. Applying $\hat{B}^{i\sigma}$ to $|\phi^{(n)\sigma}\rangle$ in this basis, we have

$$\begin{aligned}\mathbf{B}^{i\sigma}\phi^{(n)\sigma} &= \left[\mathbf{I} + n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\hat{e}_i \otimes \hat{e}_i\right]\phi^{(n)\sigma} \\ &= \phi^{(n)\sigma} + n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\left(\hat{e}_i \otimes \hat{e}_i\right)\phi^{(n)\sigma}. \qquad (7)\end{aligned}$$

The overlap matrix with the trial wavefunction is

$$\begin{aligned}\mathbf{O}^{(n+1)\sigma} &= \left(\psi_T^\sigma\right)^\dagger \mathbf{B}^{i\sigma}\phi^{(n)\sigma} \\ &= \left(\psi_T^\sigma\right)^\dagger \phi^{(n)\sigma} + n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\left(\psi_T^\sigma\right)^\dagger\left(\hat{e}_i \otimes \hat{e}_i\right)\phi^{(n)\sigma}. \qquad (8)\end{aligned}$$

Notice that

$$\begin{aligned}\left(\psi_T^\sigma\right)^\dagger\left(\hat{e}_i \otimes \hat{e}_i\right)\phi^{(n)\sigma} &= \left(\psi_T^\sigma\right)^\dagger\left(\hat{e}_i\hat{e}_i^\intercal\right)\phi^{(n)\sigma} \\ &= \left[\left(\psi_T^\sigma\right)^\dagger\hat{e}_i\right]\left[\hat{e}_i^\intercal\phi^{(n)\sigma}\right] \\ &= \left(\psi_T^\sigma\right)^\dagger_{\bullet i}\left[\phi^{(n)\sigma}_{i\bullet}\right] \\ &= \vec{u}^\sigma\left(\vec{v}^\sigma\right)^\intercal = \vec{u}^\sigma \otimes \vec{v}^\sigma \qquad (9) \\ \implies \vec{u}^\sigma = \left(\psi_T^\sigma\right)^\dagger_{\bullet i}, \quad \vec{v}^\sigma &= \left[\phi^{(n)\sigma}_{i\bullet}\right]^\intercal, \qquad (10)\end{aligned}$$

where $\left(\psi_T^\sigma\right)^\dagger_{\bullet i}$ denotes the i-th column of $\left(\psi_T^\sigma\right)^\dagger$ and $\phi^{(n)\sigma}_{i\bullet}$ denotes the i-th row of $\phi^{(n)\sigma}$. We can then write (8) as

$$\begin{aligned}\mathbf{O}^{(n+1)\sigma} &= \mathbf{O}^{(n)\sigma} + n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\vec{u}^\sigma \otimes \vec{v}^\sigma \qquad (11) \\ &\longrightarrow \mathbf{O}^{(n)\sigma} + \vec{u}^\sigma \otimes \vec{v}^\sigma \qquad (12) \\ \vec{u}^\sigma &= \left(\psi_T^\sigma\right)^\dagger_{\bullet i}, \quad \vec{v}^\sigma = n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\left[\phi^{(n)\sigma}_{i\bullet}\right]^\intercal, \qquad (13)\end{aligned}$$

absorbing the prefactor in (11) into $\vec{v}$. To implement importance sampling of the auxiliary fields, we need the overlap ratio

$$\frac{O^{(n+1)}}{O^{(n)}} = \frac{\langle\psi_T|\hat{B}^i|\phi^{(n)}\rangle}{\langle\psi_T|\phi^{(n)}\rangle} = \frac{\langle\psi_T^\uparrow|\hat{B}^{i\uparrow}|\phi^{(n)\uparrow}\rangle\,\langle\psi_T^\downarrow|\hat{B}^{i\downarrow}|\phi^{(n)\downarrow}\rangle}{\langle\psi_T^\uparrow|\phi^{(n)\uparrow}\rangle\,\langle\psi_T^\downarrow|\phi^{(n)\downarrow}\rangle} = \frac{\det\mathbf{O}^{(n+1)\uparrow}}{\det\mathbf{O}^{(n)\uparrow}} \cdot \frac{\det\mathbf{O}^{(n+1)\downarrow}}{\det\mathbf{O}^{(n)\downarrow}}, \qquad (14)$$

(15)

which naively necessitates determinant calculations that scale as $\mathcal{O}(N^3)$ in the number of orbitals N. Fortunately, the form of the overlap matrix update in (12) allows us to leverage the *matrix determinant lemma* in updating $\det\mathbf{O}^{(n+1)\sigma}$ from $\det\mathbf{O}^{(n)\sigma}$,

$$\begin{aligned}\det\mathbf{O}^{(n+1)\sigma} = \det\left[\mathbf{O}^{(n)\sigma} + \vec{u}\otimes\vec{v}\right] &= \left[1 + \vec{v}^\dagger\left(\mathbf{O}^{(n)\sigma}\right)^{-1}\vec{u}\right]\det\mathbf{O}^{(n)\sigma} \qquad (16) \\ \implies \frac{\det\mathbf{O}^{(n+1)\sigma}}{\det\mathbf{O}^{(n)\sigma}} &= \left[1 + \vec{v}^\dagger\left(\mathbf{O}^{(n)\sigma}\right)^{-1}\vec{u}\right]. \qquad (17)\end{aligned}$$

[1] The outer product $\hat{e}_i \otimes \hat{e}_i$ has the only nonzero matrix element at the i-th position on the diagonal:

$$\hat{e}_i \otimes \hat{e}_i = \mathrm{diag}\,[0,\ldots,0,\underbrace{1}_{i^{\mathrm{th}}},0,\ldots,0] \qquad (6)$$

This requires the propagation of the inverse overlap matrix, which can also be updated from the previous time step using the *Sherman-Morrison formula*:

$$\left[\mathbf{O}^{(n+1)\sigma}\right]^{-1} = \left[\mathbf{O}^{(n)\sigma} + \vec{u}^{\sigma} \otimes \vec{v}^{\sigma}\right]^{-1} = \left[\mathbf{O}^{(n)\sigma}\right]^{-1} - \frac{\left[\mathbf{O}^{(n)\sigma}\right]^{-1} \left(\vec{u}^{\sigma} \otimes \vec{v}^{\sigma}\right) \left[\mathbf{O}^{(n)\sigma}\right]^{-1}}{1 + \left(\vec{v}^{\sigma}\right)^{\dagger} \mathbf{O}^{(n)\sigma} \vec{u}^{\sigma}}. \tag{18}$$

Both updates improve the scaling to $\mathcal{O}(N^2)$ from the matrix multiplications involved.