CPMC: UHF fast update

Shu Fay Ung

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

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

The overlap matrix with the trial wavefunction is

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

Notice that

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

$$\implies \vec{u} = (\psi_T^\sigma)^\dagger_{\bullet i}\,, \quad \vec{v} = \left[\phi^{(n)\sigma}_{i\bullet}\right]^\mathsf{T}, \tag{10}$$

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

$$\mathbf{O}^{(n+1)\sigma} = \mathbf{O}^{(n)\sigma} + n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\vec{u}\otimes\vec{v} \tag{11}$$

$$\longrightarrow \mathbf{O}^{(n)\sigma} + \vec{u}\otimes\vec{v} \tag{12}$$

$$\vec{u} = (\psi_T^\sigma)^\dagger_{\bullet i}\,, \quad \vec{v} = n_{i\sigma}\left(e^{-\Delta\tau U/2+\mathrm{sign}\,(\sigma)\gamma x_i} - 1\right)\left[\phi^{(n)\sigma}_{i\bullet}\right]^\mathsf{T}, \tag{13}$$

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

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

$$\tag{15}$$

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 $\det\mathbf{O}^{(n)\sigma}$,

$$\det\mathbf{O}^{(n+1)\sigma} = \det\left[\mathbf{O}^{(n)\sigma} + \vec{u}\otimes\vec{v}\right] = \left[1 + \vec{v}^\dagger\left(\mathbf{O}^{(n)\sigma}\right)^{-1}\vec{u}\right]\det\mathbf{O}^{(n)\sigma}. \tag{16}$$

[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:

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

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

$$\left[\mathbf{O}^{(n+1)\sigma}\right]^{-1} = \left[\mathbf{O}^{(n)\sigma} + \vec{u} \otimes \vec{v}\right]^{-1} = \left[\mathbf{O}^{(n)\sigma}\right]^{-1} - \frac{\left[\mathbf{O}^{(n)\sigma}\right]^{-1} (\vec{u} \otimes \vec{v}) \left[\mathbf{O}^{(n)\sigma}\right]^{-1}}{1 + \vec{v}^{\dagger}\mathbf{O}^{(n)\sigma}\vec{u}}. \tag{17}$$

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