Importance sampling transformation of the imaginary-time Schrödinger equation

For a wave function $\Psi(\mathbf{R},\tau)$ the imaginary-time Schrödinger equation, with some constant energy offset E_{T}, is

$$\left[-\frac{1}{2}\nabla^2_{\mathbf{R}} + V(\mathbf{R}) - E_{\mathrm{T}}\right]\Psi(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau}\Psi(\mathbf{R},\tau). \tag{1}$$

Then, using the mixed distribution

$$f(\mathbf{R},\tau) = \Psi(\mathbf{R},\tau)\Psi_{\mathrm{T}}(\mathbf{R}), \tag{2}$$

for some trial wave function $\Psi_{\mathrm{T}}(\mathbf{R})$, we can transform Eq. (1) into its importance-sampled version by substituting

$$\Psi(\mathbf{R},\tau) = \frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})}, \tag{3}$$

to obtain

$$\left[-\frac{1}{2}\nabla^2_{\mathbf{R}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} + V(\mathbf{R})\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} - E_{\mathrm{T}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})}\right] = -\frac{\partial}{\partial\tau}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})}. \tag{4}$$

The trial wave function $\Psi_{\mathrm{T}}(\mathbf{R})$ is independent of τ, so we can pull this out of the time derivative on the right

$$\left[-\frac{1}{2}\nabla^2_{\mathbf{R}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} + V(\mathbf{R})\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} - E_{\mathrm{T}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})}\right] = -\frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\frac{\partial}{\partial\tau}f(\mathbf{R},\tau), \tag{5}$$

and multiply both by sides by $\Psi_{\mathrm{T}}(\mathbf{R})$ to give

$$\left[-\frac{1}{2}\Psi_{\mathrm{T}}(\mathbf{R})\nabla^2_{\mathbf{R}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} + V(\mathbf{R})f(\mathbf{R},\tau) - E_{\mathrm{T}}f(\mathbf{R},\tau)\right] = -\frac{\partial}{\partial\tau}f(\mathbf{R},\tau). \tag{6}$$

Now, focussing on the Laplacian and using the product rule we find

$$\begin{aligned}
\nabla^2_{\mathbf{R}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} &= \nabla_{\mathbf{R}}\cdot\nabla_{\mathbf{R}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} \\
&= \nabla_{\mathbf{R}}\left[\frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau) - \frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\right] \\
&= \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) - \frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) \\
&+ \frac{2}{\Psi^3_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\Big(\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\Big)^2 - \frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) \\
&- \frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}).
\end{aligned} \tag{7}$$

Collecting like terms and multiplying by $-\frac{1}{2}\Psi_{\mathrm{T}}(\mathbf{R})$ we obtain

$$\begin{aligned} -&\frac{1}{2}\Psi_{\mathrm{T}}(\mathbf{R})\nabla^2_{\mathbf{R}}\frac{f(\mathbf{R},\tau)}{\Psi_{\mathrm{T}}(\mathbf{R})} = -\frac{1}{2}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) + \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) \\ -&\frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\Big(\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\Big)^2 + \frac{1}{2\Psi_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}). \end{aligned} \tag{8}$$

Substituting Eq. (8) into Eq. (6) we now have

$$\begin{aligned} -&\frac{1}{2}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) + \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) - \frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\Big(\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\Big)^2 \\ +&\underbrace{\frac{1}{2\Psi_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) + V(\mathbf{R})f(\mathbf{R},\tau)}_{K} - E_{\mathrm{T}}f(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau}f(\mathbf{R},\tau). \end{aligned} \tag{9}$$

Then, adding $\frac{1}{2}K - \frac{1}{2}K$ gives

$$\begin{aligned} -&\frac{1}{2}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) + \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) \\ +&\left[-\frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\Big(\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\Big)^2 + \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\right] \\ -&\frac{1}{2\Psi_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) + V(\mathbf{R})f(\mathbf{R},\tau) - E_{\mathrm{T}}f(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau}f(\mathbf{R},\tau), \end{aligned} \tag{10}$$

and pulling $f(\mathbf{R},\tau)$ out as a common factor (and swapping the order of the terms in square brackets), we arrive at

$$\begin{aligned} -&\frac{1}{2}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) + \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) \\ +&f(\mathbf{R},\tau)\left[\frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) - \frac{1}{\Psi^2_{\mathrm{T}}(\mathbf{R})}\Big(\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})\Big)^2\right] \\ +&\left(-\frac{1}{2\Psi_{\mathrm{T}}(\mathbf{R})}\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) + V(\mathbf{R}) - E_{\mathrm{T}}\right)f(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau}f(\mathbf{R},\tau). \end{aligned} \tag{11}$$

The terms in square brackets are now just a product rule expansion of $\nabla_{\mathbf{R}}(\Psi^{-1}_{\mathrm{T}}(\mathbf{R})\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}))$ and we multiply the potential term $V(\mathbf{R})$ by $\Psi_{\mathrm{T}}(\mathbf{R})/\Psi_{\mathrm{T}}(\mathbf{R})$ to find

$$\begin{aligned} -&\frac{1}{2}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) + \frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\nabla_{\mathbf{R}}f(\mathbf{R},\tau)\cdot\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) + f(\mathbf{R},\tau)\nabla_{\mathbf{R}}\left(\frac{\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})}{\Psi_{\mathrm{T}}(\mathbf{R})}\right) \\ +&\left(-\frac{1}{2\Psi_{\mathrm{T}}(\mathbf{R})}\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) + V(\mathbf{R})\frac{\Psi_{\mathrm{T}}(\mathbf{R})}{\Psi_{\mathrm{T}}(\mathbf{R})} - E_{\mathrm{T}}\right)f(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau}f(\mathbf{R},\tau). \end{aligned} \tag{12}$$

Now, the second and third terms on the first line are just another product rule expansion, and we can pull a factor of $\Psi^{-1}_{\mathrm{T}}(\mathbf{R})$ from the first two terms on the second line to give

$$\begin{aligned} -&\frac{1}{2}\nabla^2_{\mathbf{R}}f(\mathbf{R},\tau) + \nabla_{\mathbf{R}}\cdot\left[\frac{\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})}{\Psi_{\mathrm{T}}(\mathbf{R})}f(\mathbf{R},\tau)\right] \\ +&\left(\frac{1}{\Psi_{\mathrm{T}}(\mathbf{R})}\Big[\underbrace{-\frac{1}{2}\nabla^2_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R}) + V(\mathbf{R})\Psi_{\mathrm{T}}(\mathbf{R})}_{\hat{H}\Psi_{\mathrm{T}}(\mathbf{R})}\Big] - E_{\mathrm{T}}\right)f(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau}f(\mathbf{R},\tau), \end{aligned} \tag{13}$$

and we recognise that the square brackets on the second line are now just the Hamiltonian $\hat{H}$ acting on $\Psi_{\mathrm{T}}(\mathbf{R})$, so

$$\begin{aligned} -\frac{1}{2}\nabla^2_{\mathbf{R}} f(\mathbf{R},\tau) + \nabla_{\mathbf{R}} \cdot \Bigg[\underbrace{\frac{\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})}{\Psi_{\mathrm{T}}(\mathbf{R})}}_{\mathbf{V}(\mathbf{R})} f(\mathbf{R},\tau) \Bigg] \quad &+ \quad \Bigg(\underbrace{\frac{\hat{H}\Psi_{\mathrm{T}}(\mathbf{R})}{\Psi_{\mathrm{T}}(\mathbf{R})}}_{E_{\mathrm{L}}(\mathbf{R})} - E_{\mathrm{T}} \Bigg) f(\mathbf{R},\tau) \\ &= \quad -\frac{\partial}{\partial\tau} f(\mathbf{R},\tau). \end{aligned} \tag{14}$$

Finally, by substituting the drift velocity $\mathbf{V}(\mathbf{R}) = \Psi_{\mathrm{T}}^{-1}(\mathbf{R})\nabla_{\mathbf{R}}\Psi_{\mathrm{T}}(\mathbf{R})$ and the local energy $E_{\mathrm{L}}(\mathbf{R}) = \Psi_{\mathrm{T}}^{-1}\hat{H}\Psi_{\mathrm{T}}(\mathbf{R})$, we arrive at the final result

$$-\frac{1}{2}\nabla^2_{\mathbf{R}} f(\mathbf{R},\tau) + \nabla_{\mathbf{R}} \cdot [\mathbf{V}(\mathbf{R}) f(\mathbf{R},\tau)] + (E_{\mathrm{L}}(\mathbf{R}) - E_{\mathrm{T}}) f(\mathbf{R},\tau) = -\frac{\partial}{\partial\tau} f(\mathbf{R},\tau), \tag{15}$$

which is the importance-sampled imaginary-time Schrödinger equation.