PERTURBATIVE FORWARD WALKING IN THE CONTEXT OF THE MIRROR POTENTIAL APPROACH TO THE FERMION PROBLEM

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ABSTRACT

We introduce and discuss a perturbative variant of "forward walking" in Quantum Monte Carlo and develop the theory as applied to many-fermion problems.

The mirror potential approach[1] to the Fermion problem recognizes the fact that a probability density that describes the position of an ensemble of random walkers must be positive and therefore cannot be orthogonal to a symmetric ground state. Any such density, when iterated by the methods of Green's Function Monte Carlo, will converge to that symmetric state. It would be highly desirable to find equations that lead to the Fermion ground state as the asymptotic antisymmetric component, while, at the same time stabilizing the symmetric component. The mirror potential approach starts with the density having a symmetric and antisymmetric component, ψ_S and ψ_A respectively, composing the total density either as

$$\psi^+(x) = \psi_S(x) + \psi_A(x)$$

or as

$$\psi^-(x) = \psi_S(x) - \psi_A(x)$$

with both $\psi^\pm$ positive everywhere. Clearly

$$\psi^-(x) = \psi^+(P_{odd}x),$$

for any odd permutation P_{odd}. In the rest of this paper, we write $P_{odd}x$ symbolically as $-x$.

In order to assure that such a density is maintained asymptotically, we modify the Schrodinger equation

$$H\psi^\pm(x) = E\psi^\pm(x)$$

either by adding a many-body repulsive potential $C(x)\psi^\mp(x)$ (where C is for the moment an arbitrary symmetric function) to the Hamiltonian to get

$$[H + C(x)\psi^\mp(x)]\psi^\pm(x) = E\psi^\pm(x)$$

or subtract the same from the right hand side of the integral equation to get

$$\psi^{\pm}(x) = \int g(x,y)[E_T - C(y)\psi^{\mp}(y)]\psi^{\pm}(y)dy$$

$$\equiv \int g(x,y)r^2(y)\psi^{\pm}(y)dy$$

where $g(x,y)$ is the kernel of H^+ and E_T is some trial energy. These are the mirror equations. We use

$$C(x) = \frac{(E_T - H)\psi_{ST}(x)}{\psi_T^+(x)\psi_T^-(x)} \equiv \frac{U_S(x)}{\psi_T^+(x)\psi_T^+(-x)}$$

that has the property that the symmetric part of the mirror equation is satisfied for any ψ_{ST} when ψ_{AT} is the exact antisymmetric solution. Since the difference, $\psi^+ - \psi^-$ satisfies the Schrodinger equation, we expect that the solution of the mirror equations will converge having the exact antisymmetric component, and a symmetric component close to ψ_{ST}.

From here we use only the equation for ψ^+. We also assume that it is possible to estimate E well enough in the course of the calculation to set $E = E_T$.

For the moment, assume that $r^2(x)$ is known. Recall that $g(x,y)$ is a symmetric function of its arguments. Now define another symmetric kernel,

$$g_s(x,y) = r(x)g(x,y)r(y)$$

and an importance modified kernel:

$$\begin{aligned}\tilde{g}(x,y) &= r^2(x)\psi_T^+(x)g(x,y)/\psi_T^+(y)\\ &= r(x)\psi_T^+(x)g_s(x,y)/r(y)\psi_T^+(y)\end{aligned}$$

Also define a sequence of functions:

$$\begin{aligned}\tilde{g}_0(x,z) &= \delta(x-z)\\ \tilde{g}_1(x,z) &= \int \tilde{g}(x,y)\delta(y-z)dy = \tilde{g}(x,z)\\ \tilde{g}_{n+1}(x,z) &= \int \tilde{g}(x,y)\tilde{g}_n(y,z)dy\\ &= r(x)\psi_T^+(x)\int\cdots\int g_s(x,y_1)\cdots g_s(y_n,y_{n+1})\\ &\quad\times \delta(y_{n+1}-z)dy_1\cdots dy_{n+1}/r(z)\psi_T^+(z)\end{aligned}$$

Now let $\tilde{g}_\infty(x,z) = \lim_{n\to\infty} \tilde{g}_n(x,z)$. Using a formal expansion of the delta function in eigenfunctions of g_s in the last equation, one sees that

$$\int \tilde{g}_\infty(x,z)dx \propto \frac{\psi^+(z)}{\psi_T^+(z)}.$$

Using $\tilde{g}(x_{n+1},x_n)$ to generate a walk from $z \equiv x_0$ to x_1 to ... to x_n... to estimate $\psi^+(z)/\psi_T^+(z)$ is called "forward walking".[2-5]

As will become clear, we need $\psi^+(z)/\psi_T^+(z) - 1$. So we define

$$\Delta(x,z) = \tilde{g}_\infty(x,z) - \delta(x,z)$$

$$\int \Delta(x,z)dx = \psi^+(z)/\psi_T^+(z) - 1$$

$$\int \Delta(x,y)\tilde{g}(y,z)dy = \tilde{g}_\infty(x,z) - \tilde{g}(x,z)$$

$$\Delta(x,z) = \tilde{g}(x,z) - \delta(x,z) + \int \Delta(x,y)\tilde{g}(y,z)dy$$

Integrating with respect to x, we get the integral equation for perturbative forward walking (PFW),

$$\Delta(z) = \int \tilde{g}(x,z)dx - 1 + \int \Delta(y)\tilde{g}(y,z)dy$$

With,

$$\Delta_0(z) = \int \tilde{g}(x,z)dx - 1 = \int r^2(x)\psi_T^+(x)g(x,z)dx/\psi_T^+(z) - 1$$

we write the integral equation as

$$\Delta(z) = \Delta_0(z) + \int \Delta(y)\tilde{g}(y,z)dy.$$

We now return to deal with the fact that $r^2(x)$ is not known in advance, but must be determined as part of the solution by the relation

$$r^2(x) = E_T - C(x)\psi^-(x) = E_T - C(x)\psi^+(-x)$$

Writing out $\tilde{g}(y,z)$, we find

$$\begin{aligned}\tilde{g}(y,z) &= [E_T - C(y)\psi^+(-y)]\psi_T^+(y)g(y,z)/\psi_T^+(z)\\ &= [E_T\psi_T^+(y) - U_S(y)\psi^+(-y)/\psi_T^+(-y)]g(y,z)/\psi_T^+(z)\end{aligned}$$

Using

$$\psi^+(z)/\psi_T^+(z) = \Delta(z) + 1$$

and

$$U_S(x) = (E_T - H)\psi_{ST}(x)$$

the result is

$$\begin{aligned}\tilde{g}(y,z) &= [E_T\psi_T^+(y) - E_T\psi_{ST}(y) + H\psi_{ST}(y) - U_S(y)\Delta(-y)]g(y,z)/\psi_T^+(z)\\ &= [E_T\psi_{AT}(y) + H\psi_{ST}(y) - U_S(y)\Delta(-y)]g(y,z)/\psi_T^+(z)\\ &\equiv [U_X(y) - U_S(y)\Delta(-y)]g(y,z)/\psi_T^+(z)\end{aligned}$$

Recalling that

$$\begin{aligned}\Delta_0(z) &= \int \tilde{g}(x,z)dx - 1\\ &= \int U_X(x)g(x,z)dx/\psi_T^+(z) - 1 - \int U_S(x)\Delta(-x)g(x,z)dx/\psi_T^+(z)\\ &\equiv \Delta_T(z) - \int U_S(x)\Delta(-x)g(x,z)dx/\psi_T^+(z)\end{aligned}$$

Substituting into the PFW equation, we get

$$\begin{aligned}\Delta(z) = \Delta_T(z) &- \int \Delta(-x)U_S(x)g(x,z)dx/\psi_T^+(z) \\ &+ \int \Delta(x)U_X(x)g(x,z)dx/\psi_T^+(z) \\ &- \int \Delta(x)\Delta(-x)U_S(x)g(x,z)dx/\psi_T^+(z)\end{aligned}$$

Consider now the last term of the last equation – the bilinear term. Both $\Delta(x)\Delta(-x)$ and $U_S(x)$ are symmetric functions. If $S(x)$ is symmetric then $\int S(y)g(y,x)dy$ is also. The bilinear integral (when multiplied back by $\psi_T^+(z)$ to get $\psi^+(z)$) is then symmetric and, in the end contributes nothing to an antisymmetric wave function.

The bilinear integral contributes to $\Delta(z)$, and we now investigate how such a term is propagated; it has the form $\Delta'(z) = S(z)/\psi_T^+(z)$; substituting this into the linear integrals of the last equation, there results:

$$\begin{aligned}&\int \Delta(-x)U_S(x)g(x,z)dx/\psi_T^+(z) + \int \Delta(x)U_X(x)g(x,z)dx/\psi_T^+(z) \\ &= \int \left\{ \frac{E_T\psi_{AT}(x) + H\psi_{ST}(x)}{\psi_T^+(x)} - \frac{E_T\psi_{ST}(x) - H\psi_{ST}(x)}{\psi_T^+(-x)} \right\} \frac{S(x)g(x,z)dx}{\psi_T^+(z)} \\ &= \int \left\{ H\psi_{ST}(x)\left[\frac{1}{\psi_T^+(x)} + \frac{1}{\psi_T^+(-x)}\right] + E_T\left[\frac{\psi_{AT}(x)}{\psi_{ST}+\psi_{AT}} - \frac{\psi_{ST}(x)}{\psi_{ST}-\psi_{AT}}\right]\right\} \\ &\qquad\qquad\qquad\qquad \times \frac{S(x)g(x,z)dx}{\psi_T^+(z)}\end{aligned}$$

The first bracketed expression is clearly symmetric. The second is

$$\begin{aligned}\frac{\psi_{AT}}{\psi_{ST}+\psi_{AT}} - \frac{\psi_{ST}}{\psi_{ST}-\psi_{AT}} &= \frac{\psi_{AT}(\psi_{ST}-\psi_{AT}) - \psi_{ST}(\psi_{ST}+\psi_{AT})}{\psi_{ST}^2 - \psi_{AT}^2} \\ &= -\frac{\psi_{ST}^2 + \psi_{AT}^2}{\psi_{ST}^2 - \psi_{AT}^2}\end{aligned}$$

which is also symmetric. Hence terms of the form $S(z)/\psi_T^+(z)$ generate others of the same form and may be omitted. In other words, the bilinear term in the integral equation can be ignored. The resulting linear perturbative mirror equation (LPM) is

$$\Delta(z) = \Delta_T(z) + \int [\Delta(x)U_X(x) - \Delta(-x)U_S(x)]g(x,z)dx/\psi_T^+(z).$$

We now consider the equations for a pair of walkers at z and $-z$ together. Since $\Delta(z) = \psi^+(z)/\psi_T^+(z) - 1$, it is appropriate to take the combination

$$\begin{aligned}\Delta_A(z) &= \psi_T^+(z)\Delta(z) - \psi_T^+(-z)\Delta(-z) \\ &= \psi^+(z) - \psi_T^+(z) - \psi^+(-z) + \psi_T^+(-z) \\ &= 2[\psi_A(z) - \psi_{AT}(z)]\end{aligned}$$

Using the LPM equation above, we see that

$$\begin{aligned}
\Delta_A(z) &= \Delta_T(z)\psi_T^+(z) - \Delta_T(-z)\psi_T^+(-z) \\
&\quad + \int [\Delta(x)U_X(x) - \Delta(-x)U_S(x)]g(x,z)dx \\
&\quad - \int [\Delta(x)U_X(x) - \Delta(-x)U_S(x)]g(x,-z)dx \\
&= \Delta_{AT}(z) + \int [\Delta(x)U_X(x) - \Delta(-x)U_S(x)]g(x,z)dx \\
&\quad - \int [\Delta(-x)U_X(-x) - \Delta(x)U_S(-x)]g(x,z)dx \\
&= \Delta_{AT} + \int \{\Delta(x)[U_X(x) + U_S(-x)] - \Delta(-x)[U_S(x) + U_X(-x)]\}g(x,z)dx
\end{aligned}$$

We have used the fact the $g(x,z) = g(-x,-z)$. Substituting

$$\begin{aligned}
U_S(x) &= E_T\psi_{ST}(x) - H\psi_{ST}(x) \\
U_X(x) &= E_T\psi_{AT}(x) + H\psi_{ST}(x),
\end{aligned}$$

the result is

$$\begin{aligned}
\Delta_A(z) &= \Delta_{AT}(z) + E_T\int\{\Delta(x)\psi_T^+(x) - \Delta(-x)\psi_T^+(-x)\}g(x,z)dx \\
&= \Delta_{AT}(z) + E_T\int \Delta_A(x)g(x,z)dx
\end{aligned}$$

This seems a remarkable result: we have recovered the linear forward walking fermion equation.

However, by itself, it is not at all the answer to the Fermion sign problem. To see that, let us consider the most elementary Monte Carlo implementation. That would be to start a walker at $z = x_0$, then walk successively to $x_1, x_2, \ldots$, sampling each successive step from $g(x_{n+1}, x_n)$.

The estimator for $\Delta_A(z)$ is simply $\sum \Delta_{AT}(x_n)$. But in the walk defined here, with a trial eigenvalue E_T appropriate for a fermion system, the population will grow exponentially with a symmetric distribution. Of course, $\Delta_{AT}(z)$ is an antisymmetric function so that the successive terms in the estimator have expected values that go to zero exponentially.

In addition, $\Delta_{AT}(z)$ is orthogonal to symmetric solutions of the Schrodinger equation and to antisymmetric solutions with $E = E_T$. To see this, recall the definition:

$$\Delta_{AT}(z) = \Delta_T(z)\psi_T^+(z) - \Delta_T(-z)\psi_T^+(-z)$$

and

$$\Delta_T(z)\psi_T^+(z) = \int U_X(x)g(x,z)dx - \psi_T^+(z)$$

Thus,

$$\begin{aligned}
\Delta_{AT}(z) &= \int [U_X(x) - U_X(-x)]g(x,z)dx - [\psi_T^+(z) - \psi_T^+(-z)] \\
&= \int 2E_T\psi_{AT}(z)g(x,z)dx - 2\psi_{AT}(x)
\end{aligned}$$

$$\int \Delta_{AT}(z)\psi(z)dz = \int\int 2E_T\psi_{AT}(x)g(x,z)\psi(z)dxdz - \int 2\psi_{AT}(z)\psi(z)dz$$

The technical issue that confronts us now is whether one can estimate these successive terms with a variance that grows smaller at least as fast as the square of the expected value with finite total computational work for all terms. We believe that this can be done, indeed that it is straightforward. One key will be to preserve the orthogonality noted above in the estimators. Another is the asymptotic term consists of an antisymmetric function averaged with respect to a symmetric density. For the latter, z and $-z$ occur with equal probability; if we can arrange a pair of walks for which the corresponding pairs of walker positions x and y converge toward opposite points, say, w and $-w$. For the case considered here, this is possible by purely geometric means. In one dimension, one follows the random walk until it touches the origin. Future steps can be paired symmetrically about the origin; such paired walkers contribute zero to our estimator. In more than one dimension, the same technique can be applied one dimension at a time (or with respect to a series of orthogonal hyperplanes). After each first passage crossing, future walks are reflected with respect to the plane just crossed. After crossing all possible planes, the walkers are at w and $-w$. Note that this construction does not depend on the knowledge of a nodal surface for the wave function.

It would appear, however, that linearization has been a step backward. If we recall that the mirror potential, the essence of the bilinear equation, was introduced to cancel the growth of the symmetric component of the distribution of walkers, we should not be surprised that keeping only the linear part of the integral equation leads again to the issue of the growth of the same symmetric part.

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