III. VARIATIONAL AND PROJECTOR MONTE CARLO FOR FERMIONS

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A. Fixed-node approximation

Quite generally, the ground state of any (regular) Hamiltonian, is nodeless and symmetric with respect to particle exchange. Thus, all QMC methods described above can be directly applied to obtain the ground state of a system containing N Bosons. This is not the case for Fermions, since the ground state wave function of a Fermi system must be antisymmetric,

$$\Psi_F(\dots,\mathbf{r}_i,\dots,\mathbf{r}_j) = -\Psi_F(\dots,\mathbf{r}_j,\dots,\mathbf{r}_i), \quad \text{for any } i,j$$
(1)

leading to nodes where $\Psi(\mathbf{R}) = 0$. Thus, in general, the ground state of fermions is never the lowest eigenstate of the Hamiltonian of the system. Only in particular situations which we do not address here, e.g. for some particular Hamiltonian in one spatial dimension, it can be degenerate with the Bose ground state.

It is possible to extend the variational principle for the energy to some excited states, $|\Psi_m\rangle$ with $E_m > E_0$, imposing orthogonality of the trial wave function to all lower eigenfunctions, $\langle \Psi_T | \Psi_n \rangle = 0$ for all n with $E_n < E_m$. Since the Fermion ground state wave function is the lowest eigenfunction in the space of anti-symmetric wave functions, orthogonality to states is guaranteed by symmetry. Since VMC based methods are based on sampling $|\Psi_T(\mathbf{R})|^2 \ge 0$, they can be directly applied to Fermions by using antisymmetric trial wave functions which obey Eq. (1).

Fermion sign problem. In contrast to VMC, Projection Monte Carlo methods stochastically sample $\Psi_0(\mathbf{R})$ which now contains negative regions where the wave function cannot be interpreted as probability. Let us try to represent a Fermion wave function, starting with

$$\Psi_T = \Psi_T^+ - \Psi_T^-, \quad \Psi_T^+ \ge 0, \Psi_T^- \ge 0$$
(2)

$$\Psi_T^+ = \frac{1}{2} \left(|\Psi_T| + \Psi_T \right), \quad \Psi_T^- = \frac{1}{2} \left(|\Psi_T| - \Psi_T \right)$$
(3)

and now we will diffuse Ψ_T^{\pm} separately. Using $|\Psi_T|$ for importance sampling, we obtain the mixed distribution

$$f_{\beta}^{\pm}(\mathbf{R}) = |\Psi_{T}(\mathbf{R})|\Psi_{\beta}^{\pm}(\mathbf{R}) \tag{4}$$

However, both Ψ_{β}^{\pm} do have some overlap with the bosonic ground state, Ψ_{B} , of energy E_{B} ,

$$\Psi_{\beta}^{\pm} = \frac{1}{2} \left(c_B e^{-\beta E_B} \Psi_B(\mathbf{R}) \pm c_F e^{-\beta E_F} \Psi_F(\mathbf{R}) + \ldots \right)$$
(5)

$$c_B = \int d\mathbf{R} \Psi_B(\mathbf{R}) |\Psi_T(\mathbf{R})|, \quad c_F = \int d\mathbf{R} \Psi_F(\mathbf{R}) \Psi_T(\mathbf{R})$$
(6)

We can now calculate the expectation value of some operator for the Fermion state as

$$\langle O \rangle = \frac{\int d\mathbf{R}s(\mathbf{R})O(\mathbf{R})(f_{\beta}^{+} - f_{\beta}^{-})}{\int d\mathbf{R}s(\mathbf{R})(f_{\beta}^{+} - f_{\beta}^{-})} = \frac{1}{\bar{s}} \frac{\int d\mathbf{R}s(\mathbf{R})O(\mathbf{R})(f_{\beta}^{+} - f_{\beta}^{-})}{\int d\mathbf{R}(f_{\beta}^{+} + f_{\beta}^{-})}$$
(7)

where $s(\mathbf{R}) \equiv \Psi_T(\mathbf{R})/|\Psi_T(\mathbf{R})| = \pm 1$ and

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$$\bar{s} = \frac{\int d\mathbf{R}s(\mathbf{R})(f_{\beta}^{+} - f_{\beta}^{-})}{\int d\mathbf{R}(f_{\beta}^{+} + f_{\beta}^{-})} = \frac{c_{F}^{2}e^{-\beta E_{F}} + \dots}{c_{B}^{2}e^{-\beta E_{B}} + \dots}$$
(8)

Therefore, we have

$$\bar{s} \sim \exp[-N\beta(E_F - E_B)/N]$$
 (9)

which enters in the normalization of any expectation value of an observable. Assuming a finite gap between the fermionic and bosonic ground state energy per particle, \bar{s} vanishes exponentially in $N\beta \gg 1$. Since $\langle s^2 \rangle = 1$, the variance is one, and the signal to noise ratio prevents any direct sampling involving \bar{s} .

$$\sigma_s^2 = \overline{s^2} - \overline{s}^2 \approx 1 \gg \overline{s} \sim \exp[-N\beta(E_F - E_B)/N]$$
(10)

Therefore the error bar of the sign $\sim \sqrt{\sigma_s^2/P}$ will be always of order $P^{-1/2}$ where P is the number of independent points. But since the signal is exponentially small, we roughly need

$$P \sim \frac{1}{\bar{s}^2} \sim \exp[2N\beta(E_F - E_B)/N] \tag{11}$$

independent samples, increasing exponentially with N and β . This is called **Fermion sign problem**.

Antisymmetry and nodes. Importance sampling DMC was based on the overlap

$$f(\mathbf{R}) = \Psi_T(\mathbf{R})\Psi_0(\mathbf{R}) \tag{12}$$

Let us imaging that we have found a trial wave function with exacly the same positive and negative regions as the Fermion ground state we are looking for, $f(\mathbf{R}) \geq 0$ for $\Psi_0 \in \Psi_F$. In this case, if we impose $f(\mathbf{R}) \geq 0$ during the time evolution in DMC, we expect that DMC converges to the exact Fermion ground state. What happens? Looking at the drifted random walk created by the importance sampling, imposing $f(\mathbf{R}) \geq 0$ for all \mathbf{R} , we reject any move $\mathbf{R} \to \mathbf{R}'$ with $\Psi_T(\mathbf{R})\Psi_T(\mathbf{R}') < 0$. Our population of walkers can be separated into two sets, positive walkers at \mathbf{R}^+ which satisfy $\Psi_T(\mathbf{R}^+) \geq 0$, and negative walkers at \mathbf{R}^- with $\Psi_T(\mathbf{R}^-) < 0$. Postive and negative walkers are separated by the nodal surface \mathbf{S} where $\Psi_T(\mathbf{S}) \equiv 0$, and it is enough to know the exact nodal surface. Note that the nodal surface \mathbf{S} is a hypersphere in Nd - 1 dimensions. For any sufficiently regular antisymmetric trial function, applying the Permutation operator to any positive configuration, we obtain a negative walker, and vice versa. It is therefore sufficient to sample only the positive space as long as we are only interested in physical observables which commutes with the permutation operator.

Fixed-node approximation. Everything above is fine, but we still do not know the nodal surface for almost all fermion problems. Since we have no further idea right now, let us search for the best approximation we can do. In the fixed-node approximation, we simple impose the nodes of a given trial wave function. Once started with positive walkers, our fixed-node DMC algorithm will converges to an eigenfunction of the Hamiltonian

$$H\Psi_{FN}(\mathbf{R}) = E_{FN}\Psi_{FN}(\mathbf{R}), \quad \text{for all } \mathbf{R} \text{ in } \mathbf{R}^+, \text{ the positive region with } \Psi_T(\mathbf{R}) \ge 0$$
(13)

On the nodes **S** of Ψ_T , we also have $\Psi_{FN}(\mathbf{S}) = 0$, and we can continue the wave function to the negative regions, \mathbf{R}^- using permutations $\Psi_{FN}(\mathbf{R}) = (-)^{|P|} \Psi_{FN}(P\mathbf{R})$, where the permutation P can be determined from solving $\Psi_T(\mathbf{R}) = (-)^{|P|} \Psi_T(P\mathbf{R})$ for P. As long as Ψ_T is a sufficiently regular fermionic trial wave function, we can reach all configuration space by this procedure, and the continued Ψ_{FN} is a continuous antisymmetric wave function.

Upper bound theorem for fixed-node wave functions. Unfortunately, the first derivatives of the constructed FN wavefunction with respect to \mathbf{r}_i are in general not continuous at the nodal surface. Therefore, we cannot directly apply the variational principle as the underlying expansion in eigenfunctions of the true Hamiltonian is only complete for wavefunctions with continuous first derivatives. However, we can smear out our wave function at a distance ϵ close to the nodes to make them sufficiently smooth to apply the variational theorem, so that the smoothed function provides an upper bound for the energy. This smoothing will increase the absolute value of the curvature $\sim \epsilon^{-1}$ close to the node and the laplacian of the kinetic energy will produce large absolute values, $\sim \varepsilon^{-1}$ However, since the wave function vanishes as ϵ , the kinetic energy contribution of the smoothed wave function close to the nodal region $\sim \int_{\epsilon} \psi \nabla^2 \psi \sim \epsilon$ vanishes. Therefore, the energy of our fixed-node wave function provides a true upper bound to the fermion ground state energy, E_F ,

$$E_F \le E_{FN} = \frac{\int d\mathbf{R} \Psi_{FN}(\mathbf{R}) E_L(\mathbf{R}) \Psi_{FN}(\mathbf{R})}{\int d\mathbf{R} \Psi_{FN}(\mathbf{R}) \Psi_{FN}(\mathbf{R})}$$
(14)

For many-body fermion problems, the fixed-node energies are the most accurate values. The upper bound property further allows us to judge the quality of different trial wave function without relying on comparison with experiment.

Fixed-phase approximation. As a generalization of the fixed-node approach, the fixed-phase approximation is based on a complex trial wave function

$$\Psi_T(\mathbf{R}) = A(\mathbf{R}) \exp[-i\varphi(\mathbf{R})], \quad \text{with positive amplitude } A(\mathbf{R}) \ge 0 \text{ and real phase } \varphi(\mathbf{R})$$
(15)

For any given phase, we can then minimize the energy of the trial wave function for an explicitly given phase, $\varphi(\mathbf{R})$. However, since the phase is only well defined (and behaved) for non-vanishing amplitude, we also have to fix the nodes of the amplitude. An argument similar to that above shows that the fixed-phase wave function provides also an upper bound for the ground state energy in the same symmetry class as Ψ_T . Fixed-phase methods are needed for treating twisted boundary conditions, magnetic field effects, etc.

B. Fermionic Trial Wave Functions

We are interested in describing extended condensed matter, e.g. gas, liquid or solid. As our simulation can only contain a finite number of particles, and the Hamiltonian contains the lon-ranged Coulomb interaction, boundary conditions play an important role for extracting bulk properties. Most common are periodic boundary conditions where wave functions obey

$$\Psi(\dots,\mathbf{r}_i+L,\dots)=\Psi(\dots,\mathbf{r}_i,\dots) \tag{16}$$

but also different conditions are possible.

Slater-Jastrow wave function. Let us consider the simplest model, the electron gas embedded in a uniform positive background charge. To simulate a bulk system, we require translational invariance of the system which we can impose by periodic boundary conditions, Eq. (16). The simplest antisymmetric trial wave function of N (spin-polarized) electrons is a simple Slater determinant

$$D[\varphi_n(\mathbf{r})] \equiv \det_{ni} \varphi_n(\mathbf{r}_i) \tag{17}$$

where $\varphi_n(\mathbf{r}) = \sum_k e^{i\mathbf{k}\cdot\mathbf{r}}\varphi_{n\mathbf{k}}$ is some single particle orbital which must be expressed in Fourier sum over discrete **k**-vector for any finite system. In the high density region of the electron gas $r_s \sim n^{-1/3} \to 0$, the kinetic energy strongly dominates the repulsive Coulomb interaction, and Fourier components with high momentum in the orbitals are punished. The best single particle orbitals we can chose in this region are just based on the lowest N wave vectors, $\mathbf{k}_i, i = 1...N$. and the determinant simplifies

$$D \sim \det_{ni} e^{i\mathbf{k}_n \cdot \mathbf{r}_i}$$
 with $n = 1, \dots N$ (18)

Building a wave function of superpositions of orthogonal Slater determinants, we we would simply recover what's called *Configuration Interaction* methods, and for larger systems, we typically have to increase quite dramatically the number of determinants to reach equal accuracy. To avoid this, we note that any function of the form $u(\mathbf{r}_i - \mathbf{r}_j)$ is automatically translational invariant, therefore we try

$$\Psi_{SJ} = \det_{ni} e^{i\mathbf{k}_n \cdot \mathbf{r}_i} \exp[-U], \quad U = \sum_{i < j} u(\mathbf{r}_i - \mathbf{r}_j)$$
(19)

which is still an antisymmetric function and U is the two-body Jastrow potential. We can now parametrize the **Jastrow** function $u(\mathbf{r})$, e.g. by expanding in a basis set, and optimize the parameters within VMC. However, before doing that, it is worth to examine the asymptotic properties of u one might expect.

Cusp conditions. Let us assume a particular configuration of the electrons, **R**, where all electrons have roughly the same distance, but two, *i* and *j* become arbitrary close, $r_{ij} \to 0$. Due to the diverging Coulomb repulsion of between *i* and *j*, the effect of the interaction with all other electrons is secondary, and we may write the wave function as $\Psi(\mathbf{R}) = \widetilde{\Psi}(\mathbf{R})\varphi(\mathbf{r}_{ij})$ and assume that $\varphi(\mathbf{r})$ satisfies

$$-\frac{\hbar^2}{m}\nabla^2\varphi(\mathbf{r}) + \frac{e^2}{r}\varphi(\mathbf{r}) = \epsilon\varphi(\mathbf{r}), \quad \text{for } r \to 0$$
⁽²⁰⁾

corresponding to the relative wave function of two particles interacting via the Coulomb repulsion. Assuming spherical symmetry we have

$$-\frac{\hbar^2}{m}\left(\varphi''(r) + \frac{D-1}{r}\varphi'(r)\right) + \frac{e^2}{r}\varphi(r) = \epsilon\varphi(r)$$
(21)

where D is the dimension. Assuming a regular $\varphi(r)$ the coefficient in front of the 1/r must vanish, which implies

$$\frac{\varphi'(r)}{\varphi(r)} = \frac{me^2}{2\hbar^2}, \quad \text{or } \varphi(r) \sim \exp[me^2 r/2\hbar^2], \quad r \to 0$$
(22)

which implies a cusp in the wave function

$$u(r) = -\log\varphi(r) = -Cr, \quad \text{with } C = me^2/2\hbar^2 \text{ for } r \to 0$$
(23)

assuming that $\widetilde{\Psi}(\mathbf{R})$ is more regular for $\mathbf{r}_{ij} \to 0$. The same argument for electron close to a nuclei of charge Z just recovers the hydrogen s orbital behavior $u(\mathbf{r} - \mathbf{R}_p) = me^2 |\mathbf{r} - \mathbf{R}_p|/\hbar^2$.

$$u(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} u_k e^{i\mathbf{k}\cdot\mathbf{r}}, \quad U = \frac{1}{2V} \sum_{\mathbf{k}} u_k \rho_{\mathbf{k}} \rho_{-\mathbf{k}}, \quad \rho_{\mathbf{k}} = \sum_n e^{i\mathbf{k}\cdot\mathbf{r}_n}$$
(24)

Let us again consider the local energy of the Slater-Jastrow wave function

$$E_L = \frac{\hbar^2}{2m} \left[\nabla^2 U - (\nabla U)^2 \right] + V + \text{ parts containing } \nabla D \text{ and } \nabla^2 D$$
(25)

Using the collective coordinates, $\rho_{\mathbf{k}}$, the expression contains the following term in **k**-space

$$-\frac{1}{V}\sum_{\mathbf{k}\neq0}\frac{\hbar^2k^2}{2m}u_k\rho_{\mathbf{k}}\rho_{-\mathbf{k}} + \frac{1}{V^2}\sum_{\mathbf{k}\neq0}\sum_{\mathbf{p}\neq0}u_{\mathbf{k}}u_{\mathbf{p}}\frac{\hbar^2(\mathbf{k}\cdot\mathbf{p})}{2m}\rho_{\mathbf{k}+\mathbf{p}}\rho_{-\mathbf{k}}\rho_{-\mathbf{p}} + \frac{1}{2V}\sum_{\mathbf{k}\neq0}v_k\rho_{\mathbf{k}}\rho_{-\mathbf{k}}$$
(26)

$$=\frac{1}{V}\sum_{\mathbf{k}\neq0}\frac{-\hbar^{2}k^{2}}{2m}u_{k}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}+\frac{1}{V^{2}}\sum_{\mathbf{k}\neq-\mathbf{p}\neq0}u_{\mathbf{k}}u_{\mathbf{p}}\frac{\hbar^{2}(\mathbf{k}\cdot\mathbf{p})}{2m}\rho_{\mathbf{k}+\mathbf{p}}\rho_{-\mathbf{k}}\rho_{-\mathbf{p}}-\frac{n}{V}\sum_{\mathbf{k}\neq0}\frac{\hbar^{2}k^{2}}{2m}u_{k}^{2}+\frac{1}{2V}\sum_{\mathbf{k}\neq0}v_{k}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}$$
(27)

Since the Fourier transform of the Coulomb potential, $v_k = 4\pi e^2/k^2$ is singular for $k \to 0$, the Jastrow factor u_k must also be singular, and the most singular expressions in the local energy for $k \to 0$ (the last two terms in the expression above) must compensate

$$u_k \to \left(\frac{mv_k}{n\hbar^2 k^2}\right)^{1/2} \sim \frac{1}{k^2}, \quad \text{for } k \to 0$$
 (28)

which corresponds to a 1/r tail in real space. Notice that the Slater determinant does not contain any singular terms in ρ_k in the longrange limit, and the first two terms in (27) are less singular, the second since it involves one more summation. Using this argument we can also see that the structure factor (the Fourier transform of the electronic pair correlation function)

$$S(\mathbf{k}) = \frac{1}{N} \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle \tag{29}$$

is dominated by the Jastrow singularity for $k \to 0$ and we can use $|\Psi| \sim e^{2U}$ in this limit

$$S(\mathbf{k}) \to \frac{1}{N} \frac{\int d\mathbf{R} \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \exp\left[-\frac{1}{V} \sum_{\mathbf{p}} u_p \rho_{\mathbf{p}} \rho_{-\mathbf{p}}\right]}{\int d\mathbf{R} \exp\left[-\frac{1}{V} \sum_{\mathbf{p}} u_p \rho_{\mathbf{p}} \rho_{-\mathbf{p}}\right]} = \frac{1}{N} \frac{\int d\mathbf{R} \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \exp\left[-\frac{u_k}{V} \rho_{\mathbf{k}} \rho_{-\mathbf{k}}\right]}{\int d\mathbf{R} \exp\left[-\frac{u_k}{V} \rho_{\mathbf{k}} \rho_{-\mathbf{k}}\right]}$$
(30)

which is nothing else than a gaussian integration when changing $d\mathbf{R}$ to $d\rho_k$. We get

$$S(k) \to \frac{1}{2nu_k} \sim k^2, \quad \text{for } k \to 0$$
 (31)

Let us for a moment consider the wave function $\rho_{\mathbf{k}}\Psi_0(\mathbf{R})$ which represents a collective (phonon-like) excitation for small k, approaching an exact eigenstate for $k \to 0$ as Feynman argued. The excitation energy of this state, $\varepsilon_k = E_k - E_0$, is given by

$$\varepsilon_k = \frac{\int d\mathbf{R} \Psi_0(\mathbf{R}) \rho_{-\mathbf{k}} H \rho_{\mathbf{k}} \Psi_0(\mathbf{R})}{NS(k)} - E_0 \simeq \frac{k^2}{2mS(k)} = \hbar \omega_p, \quad \text{for } k \to 0$$
(32)

where $\omega_p = (4\pi n e^2/m)^{1/2}$ is the classical plasma frequency. Therefore, the long-range part of the Jastrow factor simply describes plasmon excitations, a simple harmonic oscillator wave function when introducing collective coordinates. This result can be generalized, the long-range part of the Jastrow is responsible for the description of collective long-range excitations in fluids.

Backflow wave functions. How can we improve the variational wave function, in particular the antisymmetric part? For atomic and molecular systems, the orbitals can be optimized, and multideterminant wave function can be introduced. However, for extended systems, in particular for the uniform electron gas, multideterminants are not only costly, but are not size-consistent: increasing the system size at uniform densities, much more determinants are

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need to reach the same accuracy. In order to avoid this problem, we search for a functional form which introduces many-body correlations into a single determinant. This is possible, if we allow for new generalized coordinates, \mathbf{q} , inside the arguments of the orbitals in the determinant

$$D = \det_{ni} \varphi_n(\mathbf{q}_i), \quad \mathbf{q}_i(\mathbf{R}) = \mathbf{r}_i + \mathbf{d}_i(\mathbf{R}), \quad \mathbf{d}_i = \sum_j \nabla_i y(\mathbf{r}_i - \mathbf{r}_j)$$
(33)

where y(r) is the backflow potential. Notice its form in Fourier space

$$\mathbf{q}_j = \mathbf{r}_j + \frac{i}{V} \sum_{\mathbf{k}} \mathbf{k} y_k e^{i\mathbf{k}\cdot\mathbf{r}_j} \rho_{-\mathbf{k}}$$
(34)

Originally, it was introduced by Feynman to improve the description of excitations in liquid He, however, from the discussion of the Jastrow factor above, we see that backflow describes the coupling between single particle excitations in the determinant and collective excitations described by $\rho_{\mathbf{k}}$. Although the calculation of the local energy using backflow scales as N^3 , the gain in energy and variance often compensates the increasing cost of back-flow calculations.

General structure. One can obtain the general structure of a many body wave function by looking at the structure of the local energy. Let us start with a simple wave function given by a product of single particle states, the antisymmetrization for fermions can be done later

$$\Psi_1 = \prod_i \phi_i(\mathbf{r}_i) \tag{35}$$

We see that the local energy of this wave function

$$\frac{H\Psi_1}{\Psi_1} = -\sum_i \frac{\nabla_i^2 \phi}{2m\phi} + V \tag{36}$$

contains a single particle term and a two-particle term $V = \sum_{i < j} v_{ij}$, the interaction. Whereas the single particle term can in principle be optimized by varying the single particle wave functions ϕ contained in Ψ_1 , traces of the two-body potential will always remain. In order to have a chance to reach a an eigenstate with constant energy, we have to extend the wave function and use a Slater-Jastrow form

$$\Psi_2 = \prod_i \phi_i(\mathbf{r}_i) e^{-U} \tag{37}$$

where $U = \sum_{i < j} u_{ij}$. Now we look at the local energy of Ψ_2

$$\frac{H\Psi_2}{\Psi_2} = -\frac{1}{2m} \sum_i \left(\frac{\nabla_i^2 \phi}{\phi} - \frac{\nabla_i \phi}{\phi} \nabla_i U - \nabla_i^2 U + (\nabla_i U)^2 \right) + V \tag{38}$$

Now we can identify single particle terms, $(\nabla^2 \phi)/\phi$, two particle terms, $\nabla^2 U$ and V, and we can optimize the functions in ϕ and u to make them vanish. However, the local energy contains also a mixed term $(\nabla \phi)(\nabla U)/\phi$ and a three-body term $(\nabla U)^2$. The mixed term necessites the introduction of backflow in the single particle functions and to eliminate $(\nabla U)^2$ in the local energy we need a three-body term of the same structure. It is clear that we can continue with this structure, and basically all kind of many-body correlations compatible with the symmetries will be contained in the wave function, and we should rather look at the possibilities what kind of many-body potentials can be calculated efficiently.

General Many-body Correlation. One can generalize the structure of Jastrow and backflow potential and introduce higher order many-body correlations by introducing vector and tensor function

$$\mathbf{v}_{i}^{\alpha} = \sum_{j} \nabla_{i\alpha} v(\mathbf{r}_{i} - \mathbf{r}_{j}), \quad \mathbf{w}_{i}^{\alpha\beta} = \sum_{j} \nabla_{i\alpha} \nabla_{i\beta} w(\mathbf{r}_{i} - \mathbf{r}_{j}), \quad etc...$$
(39)

and notice that we have to construct a scalar, e.g. $\sum_{i\alpha} \mathbf{v}_i^{\alpha} \mathbf{v}_i^{\alpha}$, in order to include 3 or higher body effects in the Jastrow correlations, and a vector, e.g. $\sum_{\beta} \mathbf{w}_i^{\alpha\beta} \mathbf{v}_i^{\beta}$, in order to build a three-body backflow. Of course all functions of the new potentials have to be parametrized and optimized.

Geminals/ Pairing wave functions. Determinants are a special case of a Pfaffian, an antisymmetric function of paris

$$P = \mathcal{A}\phi(\mathbf{r}_1; \mathbf{r}_2)\phi(\mathbf{r}_3; \mathbf{r}_4)\dots\phi(\mathbf{r}_{N-1}; \mathbf{r}_N)$$
(40)

In the case of a spin-singlet pairing where the two electrons inside a pair have different spin, it reduces to a pairing determinant, or geminal,

$$S = \det_{ij} \phi(\mathbf{r}_{i\uparrow}; \mathbf{r}_{j\downarrow}) \tag{41}$$

In the case where $\phi(r)$ involves exactly N/2 orbitals, the geminals reduces to the Slater determinants of these orbitals, otherwise they may introduce stronger spin correlations and also describe a superconducting ground state.

C. Variational Path Integral and Reptation Monte Carlo

Sampling the DMC wavefunction, three sources of systematic bias are important:

- short time discretization \rightarrow extrapolation $\tau \rightarrow 0$
- population bias \rightarrow extrapolation $\overline{N_w} \rightarrow \infty$
- mixed estimator bias for observables different from energy

The following Projector Monte Carlo methods avoid the last two sources of systematic errors. They are based on the path-integral representation of Eq. (??) for fixed β , and introduce a finite projection time which necessites the explicit extrapolation $\beta \to \infty$.

Variational Path Integral. Since we have an explicit expression for $\Psi_{\beta}(\mathbf{R})$ in terms of high dimensional integrals with a non-negative integrand, we can simply try to sample $|\Psi_{\beta/2}(\mathbf{R})|^2$, but now in a configuration space $\mathcal{R} \equiv {\mathbf{R}_0, \mathbf{R}_1, \cdots, \mathbf{R}_M}$ which is M + 1 times bigger than just $\mathbf{R} \equiv \mathbf{R}_{M/2}$

$$\langle O \rangle_{\beta/2} = \langle O(\mathbf{R}_{M/2}) \rangle_{\pi} = \int d\mathbf{R}_0 \dots \int d\mathbf{R}_M O(\mathbf{R}_{M/2}) \pi(\mathcal{R}),$$
 (42)

$$\pi(\mathcal{R}) = \Psi_T(\mathbf{R}_0) \exp\left[-\sum_{t=0}^M S(\mathbf{R}_t; \mathbf{R}_{t+1})\right] \Psi_T(\mathbf{R}_M)$$
(43)

where $S(\mathbf{R}, \mathbf{R}') = \log G(\mathbf{R}, \mathbf{R}'; \beta/M)$. However, in contrast to simple VMC moves, updates which change the whole configuration space \mathcal{R} will be most likely rejected, and we have to create new moves in order to equilibrate the (M + 1)N particles in the simulation. I will not discuss typical moves as they are in general borrowed from finite temperature Path-Integral calculations beyond the scope of this lecture.

Reptation Monte Carlo. A particular update in Variational Path Integral is given by simple shifting the old configurations \mathcal{R} in the time directions, e.g.

$$\mathcal{R}' = \{\mathbf{R}'_0, \dots, \mathbf{R}'_M\} \quad \text{with} \quad \mathbf{R}'_0 \equiv \mathbf{R}_1, \mathbf{R}'_1 \equiv \mathbf{R}_2, \dots, \mathbf{R}'_{M-1} \equiv \mathbf{R}_M$$
(44)

together with a new proposition for \mathbf{R}_M based on the drifted random walk used in DMC, $G_D(\mathbf{R}_M \to \mathbf{R}'_M; \tau)$. The inverse move is realized by the shift in the opposite direction which involves a drivted random walk $\mathbf{R}'_0 \equiv \mathbf{R}_1 \to \mathbf{R}_0$. Choosing randomly the direction before any move, the Metropolis acceptance probability then writes

$$p = \min\left\{1, \frac{\pi(\mathcal{R}')}{\pi(\mathcal{R})} \frac{G_D(\mathbf{R}_1 \to \mathbf{R}_0, \tau)}{G_D(\mathbf{R}_M \to \mathbf{R}'_M; \tau)}\right\}$$
(45)

Further use of the importance sampling propagator, Eq. (??), in the statistical weight of the path, we have

$$\pi(\mathcal{R}) = \Psi_T(\mathbf{R}_0) \prod_{i=1}^M G(\mathbf{R}_{i-1}, \mathbf{R}_i; \tau) \Psi_T(\mathbf{R}_M)$$
(46)

$$= \Psi_T^2(\mathbf{R}_0) \prod_{i=1}^M G_T(\mathbf{R}_{i-1} \to \mathbf{R}_i; \tau)$$
(47)

so that

$$\frac{\pi(\mathcal{R}')}{\pi(\mathcal{R})} = \frac{\Psi_T(\mathbf{R}_1)}{\Psi_T(\mathbf{R}_0)G(\mathbf{R}_0, \mathbf{R}_1; \tau)} \frac{G(\mathbf{R}_M, \mathbf{R}'_M; \tau)\Psi_T(\mathbf{R}'_M)}{\Psi_T(\mathbf{R}_M)} = \frac{G_T(\mathbf{R}_M \to \mathbf{R}'_M; \tau)}{G_T(\mathbf{R}_0 \to \mathbf{R}_1; \tau)} \frac{|\Psi_T(\mathbf{R}'_M)|^2}{\Psi_T(\mathbf{R}_M)|^2}$$
(48)

Inserting the explicit expression of the DMC propagator, Eq. (??), the acceptance ratio finally simplifies

$$p = \min\left\{1, \frac{\Psi_T^2(\mathbf{R}'_M)}{\Psi_T^2(\mathbf{R}_M)} \frac{\exp\left(-\tau [E_L(\mathbf{R}'_M) + E_L(\mathbf{R}_M)]/2\right)}{\exp\left(-\tau [E_L(\mathbf{R}_1) + E_L(\mathbf{R}_0)]/2\right)}\right\}$$
(49)

D. Many-body propagator

Zero-temperature DMC propagator. Whereas the primitive approximation may contain singularities, e.g. for systems with Coulomb or hard core interactions, importance sampling based on Ψ_T eliminates this problem. If we are mainly interested in ground state properties, we can also use the expression of the importance sampling propagator used in DMC, Eq. (??), and use Eq. (??) to obtain

$$G(\mathbf{R}, \mathbf{R}'; \tau) = \frac{1}{\Psi_T(\mathbf{R})} G_T(\mathbf{R}' \to \mathbf{R}; \tau) \Psi_T(\mathbf{R}')$$
(50)

Note that the propagator, G, is not any more symmetric with respect to interchanging **R** and **R'**, however, within the order of the approximation, we can conserve this important property by explicit symmetrization, either

$$G(\mathbf{R}', \mathbf{R}, \tau) \approx \left[G_T(\mathbf{R}', \mathbf{R}; \tau)G_T(\mathbf{R}, \mathbf{R}'; \tau)\right]^{1/2}$$
(51)

or

$$G(\mathbf{R}', \mathbf{R}, \tau) \approx \min\left[\Psi_T(\mathbf{R}')G_T(\mathbf{R}', \mathbf{R}; \tau)\Psi_T^{-1}(\mathbf{R}), \Psi_T(\mathbf{R})G_T(\mathbf{R}, \mathbf{R}'; \tau)\Psi_T^{-1}(\mathbf{R}')\right]$$
(52)

together with the explicit expression, Eq. (??).

Pair product approximation. Better approximations for the potential energy can be found, e. g. by considering the effective pair potential, u_p , given by the solution of the two-particle problem

$$e^{-u_p(\mathbf{r}_i,\mathbf{r}_j;\mathbf{r}'_i,\mathbf{r}'_j;\tau)} \equiv \frac{\langle \mathbf{r}_i \mathbf{r}_j | e^{-\tau (T_2+V_2)} | \mathbf{r}'_i, \mathbf{r}'_j \rangle}{\langle \mathbf{r}_i \mathbf{r}_j | e^{-\tau T_2} | \mathbf{r}'_i, \mathbf{r}'_j \rangle}$$
(53)

and the whole propagator is then approximated by

$$G(\mathbf{R}, \mathbf{R}'; \tau) \approx G_0(\mathbf{R}, \mathbf{R}'; \tau) e^{-\tau [U_N(\mathbf{R}) + U_N(\mathbf{R}')]/2} e^{-\sum_{i < j} u_p(\mathbf{r}_i, \mathbf{r}_j; \mathbf{r}'_i, \mathbf{r}'_j; \tau)}$$
(54)

where T_2 is the kinetic energy and V_2 the interatomic potential. This propagator is frequently employed in finite temperature path-integral Monte Carlo calculations. As the time-step error is small, less discretization points M are needed, however, the parametrization of $u_p(\mathbf{r}, \mathbf{r}'; \tau)$ for a given interaction potential v as a function of the relative coordinates \mathbf{r} and \mathbf{r}' is a majeur complication.