Appendix C

Generalization of the QGA for higher dimensions

Now let us extend the Quantum Genetic Algorithm in order to treat quantum systems in two dimensions. We perform calculations on a finite region Ω where we discretize the real space $\Omega \equiv \{(x,y), 0 \leq x \leq d, 0 \leq y \leq d\}$. We assume that the external potential outside Ω is infinitely high.

Let us consider, for example, a two-particle system described by a wave function $\Psi_{HF}(\vec{r}_1, \vec{r}_2)$, with $\vec{r} = (x,y)$, which is the Slater determinant consisting of orthogonal and normalized one particle wave functions $\psi_\nu(\vec{r})$, $\nu = 1,2$. This means that the optimized Ψ_{HF} will represent the exact ground-state wave function for the case of noninteracting particles, whereas for the interacting case Ψ_{HF} will correspond to the Hartree-Fock approximation to the ground-state wave function.

As in the one dimensional case, an initial population of trial two-body wave functions $\{\Psi_i\}, i = 1, .., N_{pop}$ is chosen randomly. For this purpose, we construct each Ψ_i , using a Gaussian-like one-particle wave functions of the form

$$\psi_\nu(x,y) = A_\nu \ \exp\{-(x-\bar{x}_\nu)^2/\sigma_{X,\nu}^2 - (y-\bar{y}_\nu)^2/\sigma_{Y,\nu}^2\} \ x\,(d-x)\,y\,(d-y), \tag{C.1}$$

with $\nu = 1,2$ and random values for $\bar{x}_\nu$, $\bar{y}_\nu$ and for $\sigma_{X,\nu}$, $\sigma_{Y,\nu}$ for each wave function. The amplitude A_ν is calculated from the normalization condition $\int\int |\psi_j(x,y)|^2 dxdy = 1$, and its sign is chosen randomly.

Note, that defined in such way the wave functions $\psi_j(x,y)$ fulfill zero condition on the boundary $\partial\Omega$:

$$\psi_\nu(x,y)\Big|_{\partial\Omega} = 0. \tag{C.2}$$

The constructed initial population $\{\Psi_i\}$ corresponds to the initial generation. Now, the fitness of each individual Ψ_i of the population is determined by the evaluating of the energy functional

$$E_i = E[\psi_i] \equiv \int_\Omega \Psi_i^*(\vec{r}_1, \vec{r}_2)\hat{H}(\vec{r}_1, \vec{r}_2)\Psi_i(\vec{r}_1, \vec{r}_2)d\vec{r}_1 d\vec{r}_2, \tag{C.3}$$

where $\hat{H}$ is the Hamiltonian of the corresponding problem. This means that the expectation value of the energy for a given individual is a measure of its fitness, and we apply the QGA to minimize the energy. By virtue of the variational principle, when the QGA finds the global minimum, it corresponds to the ground state of $\hat{H}$ in the Hartree-Fock approximation.

Now we define the smooth crossover in two dimensions. For two randomly chosen single-particle "parent" functions $\psi_{i\nu}^{(old)}(x,y)$ and $\psi_{l,\mu}^{(old)}(x,y)$ $(i,l=1,..,N_{pop};\, \mu,\nu=1,2)$, one can construct two new functions $\psi_{i\nu}^{(new)}(x,y)$, $\psi_{l\mu}^{(new)}(x,y)$ as

$$\psi_{i\nu}^{(new)}(x,y) = \psi_{i\nu}^{(old)}(x,y)\; St(x,y) + \psi_{l\mu}^{(old)}(x,y)\; (1 - St(x.y)) \quad \text{(C.4)}$$

$$\psi_{l\mu}^{(new)}(x,y) = \psi_{l\mu}^{(old)}(x,y)\; St(x,y) + \psi_{i\nu}^{(old)}(x,y)\; (1 - St(x,y)), \quad \text{(C.5)}$$

where $St(x,y)$ is a 2D smooth step function which produces the crossover operation. We define this function as: $St(x,y) = (1 + \tanh((ax + by + c)/k_c^2))/2$, where a, b, c are chosen randomly, so that the line $ax+by+c=0$ cuts Ω into two pieces. k_c is a parameter which allows to control the sharpness of the crossover operation.

In the same manner we modify the mutation operation for random "parent" $\psi_{i\nu}^{(old)}(x,y)$ as

$$\psi_{i\nu}^{(new)}(x,y) = \psi_{i\nu}^{(old)}(x,y) + \psi_r(x,y), \quad \text{(C.6)}$$

where $\psi_r(x,y)$ is a random mutation function. We choose $\psi_r(x,y)$ as a Gaussian-like function $\psi_r(x,y) = A_r\; \exp(-(x_r-x)^2/R_x^2 - (y_r-y)^2/R_y^2)\, x(d-x)y(d-y)$ with random values for x_r, y_r, R_x, R_y and A_r. Note, that application of the defined above mutation operation does not violate boundary conditions.

As usual, for each iteration of the QGA procedure we randomly perform copy, crossover and mutation operations. After each application of a genetic operation the new-created functions should be normalized and orthogonalized. Then, the fitness of the individuals is evaluated and the fittest individuals are selected. The procedure is repeated until convergence of the fitness function (the energy of the system) to a minimal value is reached. Inside the box Ω one can consider different kinds of external potentials. If the size of the box is large enough, boundary effects become negligible.