From Darwin to Sommerfeld: Genetic algorithms and the electron gas

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Abstract

In return for the long-standing contributions of Physics to Biology, now the inverse way is frequently traveled through in order to think about many physics phenomena. In this vein, evolutionary algorithms, particularly genetic algorithms, are being more and more used as a tool to deal with several Physics problems. Here, we show how to apply a genetic algorithm to describe the homogeneous electron gas.

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Several methods, techniques and ideas taken from Physics have been of primary importance for the notable development of Biology in the last sixty years. To agree with this statement is it enough to think about the application of X Ray crystallography to the resolution of protein tertiary and quaternary structures, or the fundamental role that Quantum Mechanics in general and Molecular Physics in particular have played in the establishment of modern (Molecular) Biology, as predicted by Schrödinger[1]. However, since some years ago, the inverse way is also frequently traveled by physicists. Biological methods and concepts, as well as its terminology itself, are more and more used in Physics.

In this context, in the last decades, there has been an increasing interest in algorithms based on the Darwinian evolution principle[2]. Genetic algorithms[3]-[4], evolutionary programming[5],[6], game-playing strategies[7] and genetic programming[8] have found a wide field of applications, not just in Physics but also in other areas where optimization plays an important role, such as financial markets, artificial intelligence, etc. In particular, genetic algorithms tackle even complex problems with surprising efficiency and robustness. In Physics they have been used in calculations that involve from single Schrödinger particles in diverse potentials to astrophysical systems, running through lattice systems, spin glass models, molecules and clusters. The differences among the various evolutionary algorithms can be found not in the basic principles but in the details of the selection, reproduction and mutation procedures.

In general, an evolutionary algorithm is based on three main statements:

a) It is a process that works at the chromosomal level. Each individual is codified as a set of chromosomes.

b) The process follows the Darwinian theory of evolution, say, the survival and reproduction of the fittest in a changing environment.

c) The evolutionary process takes place at the reproduction stage. It is in this stage when mutation and crossover occurs. As a result, the progeny chromosomes can differ from their parents ones.

Starting from a guess initial population, an evolutionary algorithm basically generates consecutive generations (offprints). These are formed by a set of chromosomes, or character (genes) chains, which represent possible solutions to the problem under consideration. At each algorithm step, a fitness function is applied to the whole set of chromosomes of the corresponding generation in order to check the goodness of the codified solution. Then,
according to their fitting capacity, couples of chromosomes, to which the crossover operator will be applied, are chosen. Also, at each step, a mutation operator is applied to a number of randomly chosen chromosomes.

The two most commonly used methods to randomly select the chromosomes are:

i) The roulette wheel algorithm. It consists in building a roulette, so that to each chromosome corresponds a circular sector proportional to its fitness.

ii) The tournament method. After shuffling the population, their chromosomes are made to compete among them in groups of a given size (generally in pairs). The winners will be those chromosomes with highest fitness. If we consider a binary tournament, say the competition is between pairs, the population must be shuffled twice. This technique guarantees copies of the best individual among the parents of the next generation.

After this selection, we proceed with the sexual reproduction or crossing of the chosen individuals. In this stage, the survivors exchange chromosomal material and the resulting chromosomes will codify the individuals of the next generation. The forms of sexual reproduction most commonly used are:

i) With one crossing point. This point is randomly chosen on the chain length, and all the chain portion between the crossing point and the chain end is exchanged.

ii) With two crossing points. The portion to be exchanged is in between two randomly chosen points.

For the algorithm implementation, the crossover normally has an assigned percentage that determines the frequency of its occurrence. This means that not all of the chromosomes will exchange material but some of them will pass intact to the next generation. As a matter of fact, there is a technique, named elitism, in which the fittest individual along several generations does not cross with any of the other ones and keeps intact until an individual fitter than itself appears.

Besides the selection and crossover, there is another operation, mutation, that produces a change in one of the characters or genes of a randomly chosen chromosome. This operation allows to introduce new chromosomal material into the population. As for the crossover, the mutation is handled as a percentage that determines its occurrence frequency. This percentage is, generally, not greater than 5%, quite below the crossover percentage.

Once the selected chromosomes have been crossed and muted, we need some substitution method. Namely, we must choose, among those individuals, which ones will be substituted
for the new progeny. Two main substitution ways are usually considered. In one of them, all modified parents are substituted for the generated new individuals. In this way an individual does never coexist with its parents. In the other one, only the worse fitted individuals of the whole population are substituted, thus allowing the coexistence among parents and progeny.

Since the answer to our problem is almost always unknown, we must establish some criterion to stop the algorithm. We can mention two such criteria: i) the algorithm is run along a maximum number of generations; ii) the algorithm is ended when the population stabilization has been reached, i.e. when all, or most of, the individuals have the same fitness.

In this letter we apply some of the previous ideas in order to calculate the pair distribution function (PDF) of an homogeneous electron gas. For clarity we consider the one-dimensional version of the electron gas, but the method is directly extended to higher dimensions [9].

Let us consider the Sommerfeld-Pauli model of metallic solids [10] in 1D, namely $N$ electrons of mass $m$ moving along a segment of the axis $x$ of length $L$. The position of the $i$th electron is denoted with $x_i$ ($i = 1, 2, ..., N$). Electrons $i$ and $j$ interact one with the other through a pair potential $v(x_{ij}) = (x_{ij}^2 + \delta^2)^{-1/2}$. This pair potential is often used to model a quantum wire of width $\delta$. The system Hamiltonian then reads:

$$H = \sum_i^N -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i<j}^N v(x_{ij}).$$

(1)

For the $N$-body wave function we use the trial form [11]

$$\Psi(\vec{x}) = \exp\left[ -\sum_{i<j}^N u(x_{ij}) + \sum_{i<j}^N w(x_{ij}) \right],$$

(2)

where $\vec{x} \equiv (x_1, x_2, ..., x_N)$ denotes the system configuration and

$$w(x) = \ln g_0(x) - \frac{1}{2\pi\rho} \int dk e^{-ikx} \frac{[\tilde{S}_0(k) - 1]^2}{\tilde{S}_0(k)}.$$  

(3)

Here $\rho = N/L$ is the system number density and $g_0(x)$ is the ideal ($v(x) \equiv 0$) electron gas pair distribution function with its Fourier transform $\tilde{S}_0(k)$, the structure factor.

To apply the algorithm, we take $M$ distances $y_1 = 0, y_2 = d, ..., y_M = (M-1)d$ so that, for any $i,j$, the function $u(x_{ij})$ is represented by the random string $u(x_{ij} = y_1), u(x_{ij} = y_2),..., u(x_{ij} = y_M)$, where each $u(x_{ij} = y_k)$ is a random real number $\gamma_{ij}^k \in [0,1]$.
(rounded to an established number \( n \) of decimals): \( u(x_{ij} = y_k) = \gamma_{ij}^k \). Our initial population is then formed by \( N_p \) random replicas of each of the \( N(N-1)/2 \) strings. In this work we have taken \( N = 100, M = 99, n = 3 \) and \( N_p = 100 \).

Given a string \( \gamma_{ij}^1, \gamma_{ij}^2, ..., \gamma_{ij}^M \), the encoding consists in replacing the sequence of real numbers \( \gamma_{ij}^k \in [0, 1] \) by a single natural number obtained by putting their decimal parts one next to the other. For example, taking \( n = 3 \): the string 0.137, 0.935, ..., 0.466 gives 137935...466. In genetic terms, the encoding produces the chromosomal structures of the parents (strings). The inverse process is called decoding.

For the parents population, the energy of the \( \alpha \)-th replica (\( \alpha = 1, 2, ..., N_p \)) is given by

\[
E_\alpha = \frac{\langle \Psi_\alpha | H | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle},
\]

where for the mean kinetic energy we use the Jackson-Feenberg formulae\[12\].

In order to calculate the fitness of the replica \( \alpha \), we previously need to estimate the energy error: \( \epsilon_\alpha = |(H - E_\alpha) \Psi_\alpha| \) and define the fitness function as \( f_\alpha = e^{-\epsilon_\alpha} \). A solution is reached when \( f_\alpha \approx 1 \).

The calculation proceeds by dividing the population of \( N_p \) replicas into \( N_p/2 \) couples. The couples are randomly chosen by using the roulette wheel algorithm\[? \]. This is done by defining the sums \( F = \sum_{\alpha=1}^{N_p} f_\alpha \) and \( S_\beta = \sum_{\alpha=1}^{\beta} f_\alpha \) (\( \beta = 1, 2, ..., N_p \)). Then, a random number \( r \in [0, F] \) is generated and the unique index \( \delta \) such that \( S_{\delta-1} \leq r \leq S_\delta \) is picked up.

Once the first generation of replicas (parents) has been generated and divided into couples, the second generation (offspring) can be generated by applying the crossover operator between the members of each one. Sometimes, some of the members of the new replicas generation can be changed by applying the mutation operator.

Given a couple of replicas, the crossover operator is defined by generating a new random number \( c \in [0, 1] \) which is compared with a pre-established crossover probability \( p \in [0, 1] \). If \( c \leq p \), the crossover operator acts by interchanging all the digits from the \( s \)-th position to the end of the replica between the members of the couple. Here \( s \) is a random integer such that \( 1 \leq s \leq nM \). for example if the couple is

\[
153280472...337
768325399...069
\]
and \( s = 4 \), the new offspring couple will be

\[
153225399...069
\]
To apply the mutation operator we first randomly select those offsprings that will mutate. Then, for each of these offsprings, a gene (a digit) randomly chosen is changed by a random integer number $\ell \in [0, 9]$.

The algorithm was stopped after $2 \times 10^4$ generations. Then, the PDF at the distances $y_1, y_2, ..., y_M$ is calculated

$$g(x) = \frac{N(N-1)}{\rho^2} \int dx_2 dx_4 ... dx_N |\Psi(x_1, x_2, ... x_N)|^2 \int dx_1 dx_2 ... dx_N |\Psi(x_1, x_2, ... x_N)|^2.$$

The so-calculated PDF's were compared with those obtained from Fermi hypernetted chain (FHNC) and Monte Carlo (MC) variational approaches with good agreement for different values of the relevant parameters (Figs. 1-3). FHNC and MC probably are the two most reliable methods available to calculate the electron gas correlations.

Taking into account the good agreement among the curves, and the above mentioned efficiency and robustness of the genetic algorithm, we conclude that the application of this kind of algorithms to many-body problems deserves some attention from physicists in order to achieve a better understanding of the involved physical subtleties.

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Figure Captions

Figure 1. The pair distribution function for the 1D homogenous electron gas with Wigner-Seitz radius $r_s=1$ and screening parameter $\delta=1$.

Figure 2. Same as Fig. 1 for $r_s=1$ and $\delta=2$.

Figure 3. Same as Fig. 1 for $r_s=4.5$ and $\delta=1$. 
Fig. 1 Stoico et al.
Fig. 2 Stoico et al.

$r_s = 1$
$\delta = 2$

g(r)
Fig. 3 Stoico et al.

$r_s = 4.5$

$\delta = 1$

$g(r)$

$r$

GA

FHNC

MC