

Applications of genetic algorithms for inverting positron lifetime spectrum [☆]

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Abstract

Inversion of positron lifetime spectrum is performed via genetic algorithms considering a simulating counting of positron annihilation. Preliminary analysis without the inclusion of noise and for only one run produced large oscillations for the second peak in the inverted spectrum. An alternative strategy was proposed to reduce the oscillations that produced an average error of 0.03%. A maximum error of 40% was considered in the simulated data that produced a random average error of 10% in the counting data. The final inverted spectrum considering this error is in reasonable agreement with the exact result, producing a relative error of 2%. © 2005 Elsevier B.V. All rights reserved.

1. Introduction

Properties of a specified system can be, in principle, extracted from experimental data such as lifetime spectra of positron [1–3]. The inversion strategy based on trial-and-error consists of considering filters and the applications of least-squares methods. Particularly, these types of methods are applied for experimental spectroscopic data [3] or for fitting potential energy functions to describe molecular systems [4–8]. However, the ill-posed condition usually arises in signal processes as investigated by Sellone and Falletti [9] or in spectroscopic data [10] and the inversion procedure may not be consistent, for example, through least-squares methods. Therefore, special techniques are applied to carry out the inversion, for example, singular-value decomposition (SVD) or Tikhonov regularization approaches [11,12]. These types of methods have recently been used to analyze several chemical problems [13–15].

Alternative methodologies based on artificial intelligence have also been used to tackle chemical problems where there are ill-posed conditions [16–18]. Particularly, Hopfield neural network has been recently applied to recover the spherical potential energy function from second virial coefficient experimental data [17] and positron lifetime spectrum [19]. In both cases, the inversions are well characterized as ill-posed problems. The results were quantitative compared against the data assumed as experimental measurements. However, as pointed out in [19] it was necessary to truncate the inverted solution obtained through the Hopfield network due to negative results.

An alternative methodology that has been widely used to optimize several types of problems and particularly very efficient for determining atomic and molecular structures of clusters is called genetic algorithm (GA) [20–24]. Although the genetic algorithm has shown to be very efficient to determine accurately lowest atomic and molecular energies for the best structures found [20,21], it has not been applied for inverting experimental spectra. Alternatively, GAs have recently been used to analyze ill-posed problems. For example, Mera et al. [25] proposed a multi-population GA to analyze

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its efficiency in order to minimize Tikhonov functionals and the results were equivalent to those calculated by Tikhonov. Similarly, Montero used GAs to study optimal control problems [26] and found that GAs are robust tools for global optimization either for linear or non-linear cases.

Particularly, dealing with chemical problems, Elliott et al. [27] showed that the GA methodology can be efficient to optimize the reaction rate parameters. However, the analysis based on GA approach has not been done in the case of dealing with chemical spectroscopic data that can be characterized as ill-posed problems, with especial attention to positron lifetime spectrum. The present work is therefore concerning with the use of genetic algorithms for inverting positron annihilation lifetime spectrum. The analysis is performed considering a simulating counting of positron annihilation with and without noises.

2. Genetic algorithm methodology

Genetic algorithms can be defined as adaptive heuristic search methods based on natural evolutionary processes. Mathematical genetic operators are constructed and the basic operators are mutation, crossover and natural selection. The operations are performed to better estimate the solution of a specified problem and are then evaluated through a specified fitness function. The approach is repeated until a desired convergence is achieved. In general, one requires that GAs can find global minima, however, it may not find the best solution but more often the method comes up with a partially optimal response which is generally accepted as global minimum [21,28]. Therefore, due to the nature of GA approach, it may be efficient to solve problems with rank deficiency as shown for several ill-posed problem studies [25–27,29]. However, the method needs to be tested for chemical problems such as the inversion of positron annihilation lifetime spectrum.

The present work does not intend to introduce a new GA method with new operators as previously proposed [21]. In contrast, it deals with the application of GA to invert the positron lifetime spectrum and hence a simple GA as described by Goldberg [30] is applied. The proposed analysis via GA is performed considering a problem with 16 and 32 data that define the annihilation rate probability and the counting of positron annihilation (assumed as the experimental measurement). The problem therefore consists of optimizing 16 or 32 data via GA. Both cases are ill-posed although a higher rank deficiency is found for 32 data and we will return to this point later. The first step on the application of GA is performed by defining the initial population of 100 individuals. There are several ways for creating an initial population and here a random initialization is done based on the work of Park and Miller [31]. This popula-

tion is binary encoded with 80 bits for the variables to be optimized. Mating is carried out for the selected individuals by adopting the standard stochastic universal sampling as described in the literature [30,32–34]. A rate of 70% is considered and the best individuals are selected for the crossover operation similar to that applied in [21] although a single-cut procedure is employed [35]. A random position of a representative individual of each parent is cut (single) and then mating is carried out to generate new individual. The latter operation is performed to the whole population and then ranked according to the objective function used. A low rate mutation (7%) is used to avoid stagnation or premature convergence. Finally, the new offspring is included in the population considering an elitist strategy and hence best solution can never be lost. This will avoid oscillations in the annihilation rate probability providing a more efficient strategy for inverting the spectrum.

The standard stochastic universal sampling used in this work is written as

$$F(f_i) = \frac{g(f_i)}{\sum_i g(f_i)}, \quad (1)$$

where $g(f)$ defines the objective function given by

$$g(f) = \|\mathbf{Kf} - \mathbf{c}\|_2^2, \quad (2)$$

where $\mathbf{c}$ is the experimental measurement which is modeled according to [19]

$$c(t) = \int_0^{t_{\max}} \left(a_1 e^{-\alpha_1 (\ln(\lambda) - \sigma_1)^2} + a_2 e^{-\alpha_2 (\ln(\lambda) - \sigma_2)^2} \right) e^{-\lambda t} d\lambda, \quad (3)$$

$\mathbf{K}$ is the Kernel that was discretized as in [19] and is defined as a model according to Fredholm integral equation of first order

$$\int_a^b K(t, \lambda) f(\lambda) d\lambda = c(t). \quad (4)$$

Three genetic operators were used, namely, mating, mutation and natural selection. Mutation operator is applied mutating some parents and offsprings. In the offspring mutation process, the original offspring and the offspring mutated are preserved and minimized. The natural selection operator does not permit the increasing of the population and mutation will avoid, in principle, premature convergence (stagnation) into a local minimum. Finally, the best individuals (highest fitness) are selected throughout the natural selection operator which allows the best individuals to generate a new population. In the present GA, the population size is constant during all generations and our natural selection is elitist. This procedure will avoid oscillations in the minimization procedure and can therefore be more efficient at finding global minima. Due to the stochastic nature of GAs, we have introduced the same approach adopted in the classical trajectory methodology, i.e., an average

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