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Time-dependent formalism for the decay of ground-state deformed nuclei by proton emission: a numerical challenge

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Abstract

The numerical challenge associated with the time-dependent approach to the general problem of bi-dimensional quantum - tunneling is discussed and methods towards its application to concrete problems are developed.

1 Introduction

The problem of the decay of metastable states is of major importance for the understanding of many physical, chemical or biological processes. A metastable state, or a quasi-stationary state, is defined as a state of local stability which decays with a finite lifetime towards a true stable minimum. When the temperature of the decaying system is low, quantum tunneling is the dominant decay process. An intuitive and precise approach to this phenomenon involves the numerical solution of the time-dependent Schrodinger equation (see [1], [2]).

The different methods that have been developed for solving numerically the TDSE consist of a discretization both in space and time. The mesh size Δx and the time step Δt have to be, respectively, much smaller than the spatial dimension and the time scale of the particular problem to be solved. Since the description of most practical problems involves at least two coordinates (spatial or generalized), we are often faced with a tremendous numerical task : computers with highest speed and largest memories are needed. In the experimentally accessible cases of relatively long - lived isomers (milliseconds or more), there is an additional difficulty : double or even quadruple precision is necessary to calculate extremely small increases $\Delta\rho$ of the tunneling probability during each time step Δt. It is therefore necessary to systematically investigate these difficulties of calculating on large grids, for long times, small decay rates, in order to develop methods to overcome them.

In the next section the most relevant numerical schemes will be reviewed emphasizing their differences.

In the third section the problem of artificial boundary conditions will be tackled through two methods : the **transparent** boundary conditions and the **absorbing** boundary conditions. They have been developed to reduce the reflections of the wave packet on the numerical boundaries with the aim of decreasing the size of the spatial grid used.

In the fourth section the above mentioned formalisms are applied (and compared) to the proton emission from spherical ground - state nuclei. For illustration, the experimentally observed decay of the lowest lying ($Q_p = 0.829MeV$) metastable p - state $2d_{5/2}$ in ^{109}I was chosen .

Although the present work involves for simplicity the one - dimensional TDSE, it was done having in mind the immediate application of the information extracted to the more practical two - dimensional case.

2 Numerical solutions of TDSE

Let us consider the one dimensional TDSE , with a time - independent potential $V(x)$:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{1}$$

where

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{2}$$

The formal solution of (1) can be expressed by:

$$\psi(t+\Delta t) = exp(\frac{-iH\Delta t}{\hbar})\psi(t). \tag{3}$$

Various schemes have been proposed to approximate the exponential function. The simplest one is the Euler scheme (EU) in which $exp(\frac{-iH\Delta t}{\hbar})$ is expanded into a Taylor series and only the leading terms are kept. Thus,

$$\psi(t+\Delta t) = (1 - iH\Delta t/\hbar)\psi(t) + O((H\Delta t)^2). \tag{4}$$

This scheme is an explicit scheme, that is, it does not need matrix inversion, but it has no practical utility, since it is unstable and not unitary. Therefore, others procedures should be used. Among the various schemes which were proposed, Crank-Nicholson (CN), multi-step differencing (MSD) , split-operator method (SO) and Chebyshev method (CH) are the most relevant for our purposes. The main features of these methods will be described in the next subsections.

2.1 Crank - Nicholson method

In this scheme the exponential is approximated by the Cayley transform (i.e., a rational approximation by two polynomials of degree 1) ([3]):

$$\psi(t+\Delta t) = \frac{1 - iH\Delta t/2\hbar}{1 + iH\Delta t/2\hbar}\psi(t) + O((H\Delta t)^3). \tag{5}$$

The spatial interval $[x_{min}, x_{max}]$ is divided in equidistant points with a mesh Δx , resulting the grid $x_{min} = x_1,\ x_2, \ldots, x_M = x_{max}$. We denote by ψ_j^n the solution at the time n and the point x_j. In calculating $H\psi_j^n$ an approximation of the second derivative is needed. In the CN scheme, this is done by the finite difference formula:

$$\frac{\partial^2\psi_j^n}{\partial x^2} = \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2}. \tag{6}$$

According to (5), we can write:

$$(1 + iH\Delta t/2\hbar)\psi_j^{n+1} = (1 - iH\Delta t/2\hbar)\psi_j^n. \tag{7}$$

By using the approximation (6) and denoting $V_j = V(x_j)$ the following system results for determining the values ψ_j^{n+1}:

$$\psi_{j+1}^{n+1}+(\lambda-\mu V_j-2)\psi_j^{n+1}+\psi_{j-1}^{n+1} = -\psi_{j+1}^{n}+(\lambda+\mu V_j+2)\psi_j^{n}-\psi_{j-1}^{n}\ , j = 1, 2, \ldots, M \tag{8}$$

where

$$\lambda = \frac{4im\Delta x^2}{\hbar\Delta t},\ \ \mu = \frac{2m\Delta x^2}{\hbar^2}. \tag{9}$$

The linear system (8) is tridiagonal and can be solved fast and accurately by $L\ U$ decomposition.

This scheme is unconditionally stable, unitary (conserves the norm) and its accumulated error is proportional to Δt^2.

2.2 Multiple step differencing methods

The multiple step differencing schemes are explicit methods, thus avoiding a linear system solution as is the case with CN method, which is implicit. However, they are only conditionally stable, which imposes restrictions on the time step. The simplest is the second order differencing scheme (MSD2), which is obtained by using the relation (3) for $t + \Delta t$ and $t - \Delta t$ and the expansion of the two exponentials in Taylor series, as follows:

$$\psi(t+\Delta t) - \psi(t-\Delta t) = [\exp(-iH\Delta t/\hbar) - \exp(+iH\Delta t/\hbar)]\psi(t) =$$

$$= -2iH\Delta t/\hbar\psi(t) + O((H\Delta t)^3). \tag{10}$$

To obtain this formula, the Taylor series are truncated after the first 3 terms. Thus, in MSD2 the solution at time $n+1$ is obtained from solutions at times n and $n-1$ by the relation:

$$\psi^{n+1} = -2iH\Delta t/\hbar\psi^n + \psi^{n-1}. \tag{11}$$

The scheme is conditionally stable. The stability condition is:

$$\Delta t < \frac{\hbar}{E_{max}}, \tag{12}$$

where E_{max} is the eigenvalue with largest absolute value of the discrete Hamiltonian operator.

It should be noted also that the norm and energy are not rigorously conserved. In fact, relations of the following form can be deduced:

$$< \psi(t-\Delta t), \psi(t) > \ = \ < \psi(t), \psi(t+\Delta t) > \ = \ constant$$

$$< \psi(t-\Delta t)|H|\psi(t) > \ = \ constant$$

which differ from the standard ones, like

$$< \psi(t+\Delta t), \psi(t+\Delta t) > \;\; = \;\; < \psi(t), \psi(t) > .$$

Because of this particular form of norm and energy conservation, during the propagation an error accumulates in the phase. To minimize the error in the phase, it is customary to choose a time step Δt smaller than the stability limit. So, $\Delta t < \frac{\hbar}{k\Delta E_{grid}}$, where k is $5-10$.

High order differencing schemes can also be obtained. Thus, the 4-th order differencing scheme (MSD4) and the 6-th order differencing schemes have, respectively, the following formulae:

$$\psi(t+2\Delta t) = \psi(t-2\Delta t) - 4iH\Delta t/\hbar[-\frac{1}{3}\psi(t) + \frac{2}{3}(\psi(t+\Delta t) + \psi(t-\Delta t))] + \\ + O((H\Delta t)^5). \tag{13}$$

$$\psi(t+3\Delta t) = \psi(t-3\Delta t) - 6iH\Delta t/\hbar[\frac{13}{10}\psi(t) - \frac{7}{10}(\psi(t+\Delta t) + \psi(t-\Delta t)) + \\ + \frac{11}{20}(\psi(t+2\Delta t) + \psi(t-2\Delta t))] + O((H\Delta t)^7). \tag{14}$$

The schemes MSD4 and MSD6 are more accurate with respect to Δt, but the conditions of stability are also more restrictive, requiring smaller time steps. There is a trade-off between the higher order accuracy and the condition of the stability.

We have to note that unlike the CN scheme, which requires only the usual initial wave function (at $t = 0$), to start MSD schemes we need also auxiliary initial wave functions at $t = \Delta t\ , 2\Delta t\ , \ldots$ These can be prepared by using the Taylor expansion of the time evolution operator

$$\psi(t) = \exp(\frac{-iHt}{\hbar})\psi(0) \approx \sum_{n=0}^{N_{order}} \frac{(-iHt/\hbar)^n}{n!}\psi(0) \tag{15}$$

where N_{order} is the order of MSD.

See ([6]), ([7]).

2.3 Split Operator method

In this method, the exponential operator is approximated by ([6]), ([8]):

$$\exp(\frac{-iH\Delta t}{\hbar}) \approx \exp(\frac{-iK\Delta t}{2\hbar})\exp(\frac{-iV\Delta t}{\hbar})\exp(\frac{-iK\Delta t}{2\hbar}) + O(\Delta t^3) \tag{16}$$

where K is the kinetic energy operator $K = -\frac{\hbar^2}{2m}\Delta$ (Δ is the Laplace operator).

One step in propagation consists from an evaluation of the kinetic operator on a half of time step, a multiplication by exponential containing the potential and a new evaluation of the kinetic operator on a half time step.

Thus, the solution at $t + \Delta t$ is obtained by the relation:

$$\psi(t + \Delta t) = \exp(\frac{-iK\Delta t}{2\hbar}) \exp(\frac{-iV\Delta t}{\hbar}) \exp(\frac{-iK\Delta t}{2\hbar})\psi(t). \tag{17}$$

By taking into account the expression of K we can write:

$$\frac{-iK}{\hbar} = -i(-\frac{\hbar^2}{2m}\Delta)/\hbar = \frac{i\hbar}{2m}\Delta. \tag{18}$$

In order to see how one step is effectively done, let us denote: $D = \frac{i\hbar}{2m}\Delta$ and $U = -\frac{iV}{\hbar}$.

Then, eq.(17) can be written:

$$\psi(t + \Delta t) = \exp(\frac{\Delta t D}{2}) \exp(U\Delta t) \exp(\frac{\Delta t D}{2})\psi(t). \tag{19}$$

We take separately the factor $\exp(\frac{\Delta t D}{2})\psi(t)$, which we shall denote by $\bar{\psi}$.

$$\bar{\psi}(t + \Delta t) = \exp(\frac{\Delta t D}{2})\psi(t) = \exp(\frac{\Delta t D}{2})\mathbf{F}^{(-1)}(\mathbf{F}\psi(\mathbf{t})), \tag{20}$$

where $\mathbf{F}$ and $\mathbf{F}^{(-1)}$ are the Fourier transform and its inverse.

Then

$$\bar{\psi}(t + \Delta t) =$$

$$= \int_{-\infty}^{\infty} \exp(-\frac{\Delta t i\hbar\pi^2\omega^2}{m})[\int_{-\infty}^{\infty} \psi(t, x') \exp(2\pi i\omega x')dx'] \exp(-2\pi i\omega x)d\omega. \tag{21}$$

The above Fourier transforms are approximated by discrete transforms. For doing this, we suppose that the function ψ either decays to zero for large $|x|$ values. In these conditions, the infinite interval $(-\infty, +\infty)$ is reduced to a finite interval $[-X, X]$. This interval is divided in an uniform mesh:

$$-X = x_0 < x_1 < \ldots < x_{M-1} = X$$

with $M = 2^p$. Let Δx be the step of the spatial mesh. We define also a set of discrete frequencies as follows:

$$\omega_s = \begin{cases} \frac{s}{M\Delta x} & \text{for } s = 0, 1, \ldots, M/2 \\ \\ \frac{s-M}{M\Delta x} & \text{for } s = M/2 + 1, \ldots, M - 1 \end{cases}. \tag{22}$$

So, the frequency step is $\Delta\omega = \frac{1}{M\Delta x}$.

Let us denote by $\bar{\psi}_k^n$ the function $\bar{\psi}$ at the point x_k and the moment $t = n\Delta t$. We have:

$$\bar{\psi}_k^n = \Delta x \Delta\omega \sum_{s=0}^{M-1} \exp(-\frac{\Delta t i\hbar\pi^2\omega_s^2}{m})[\sum_{r=0}^{M-1} \exp(2\pi i\omega_s x_r)\psi_r^{n-1}] \exp(-2\pi\omega_s x_k) \quad (23)$$

$$= \frac{1}{M} \sum_{s=0}^{M-1} (W^{-1})^{ks} \exp(-\frac{\Delta t i\hbar\pi^2\omega_s^2}{m}) R_s,$$

where

$$W = \exp(\frac{2\pi i}{M}), \qquad R_s = \sum_{r=0}^{M-1} W^{sr}\psi_r^{n-1}$$

Thus, $\bar{\psi}_k^n$ is obtained by a direct transformation (getting R_s), a multiplication by the factor $\exp(-\frac{\Delta t i\hbar\pi^2\omega_s^2}{m})$ and an inverse transformation.

Now, the components ψ_k^n of $\psi(t_n, x)$ $(t_n = n\Delta t)$ are obtained by a multiplication of $\bar{\psi}_k^n$ with the factor $\exp(U(x_k))\Delta t$ and a new application of the operator $\exp(\frac{\Delta t D}{2})$.

Concluding, the SO method consists of a free particle propagation over a half - time increment, a phase change from the action of the potential applied over the whole time increment and an additional free particle propagation over a half - time increment.

In order to speed up the calculation of the Fourier transforms, the Fast Fourier Transform is used ([9]).

The SO method is efficient provided the wavefunction is of finite support, i.e., outside an interval [-X,X] it is negligible (like gaussian functions) or has a periodic behaviour. In such situations, the kinetic operator, involving a second spatial derivative, can be evaluated more acurately by using a Fourier Transform than by using finite difference.

An interesting application of this method is the determination, by correlation and spectral techniques, of the energy levels and the corresponding eigenfunctions for the stationary states. (see [8]).

Also, the method can be adapted to non-Cartesian coordinates, like spherical coordinates (see [10]).

2.4 Chebyshev method

In this method the exponential operator is approximated by a polynomial expansion (see [6], [11]) :

$$exp(\frac{-iH\Delta t}{h}) \approx \sum_{n=0}^{N_b} a_n P_n(\frac{-iH\Delta t}{h}). \quad (24)$$

The Chebyshev scheme approaches this problem in analogy to the approximation of a scalar function. Consider a scalar function $F(x)$ in the interval $[-1, 1]$.

In this case it is known that the Chebyshev polynomial approximations are optimal, since the maximum error in the approximation is minimal compared to almost all possible polynomial approximations.

In the approximation of the evolution operator, the complex Chebyshev polynomials $\Phi_n(X)$ are used, replacing the scalar function by a function of an operator. In making this change, one has to examine the domain of the operator and adjust it to the range of definition of the Chebyshev polynomials. The range of definition of these polynomials is from $-i$ to i. This means that the Hamiltonian operator has to be renormalized by dividing it by $\Delta E_{grid} = E_{max} - E_{min}$, where $E_{min} = V_{min}$ and $E_{max} = V_{max} + K_{max}$ with $K_{max} = \sum_i \frac{\pi^2 h^2}{2\mu \Delta x_i^2}$ where Δx_i is the grid spacing on the i'th coordinate.

Also, for maximum efficiency, the range of eigenvalues is positioned from -1 to 1 by shifting the Hamiltonian to

$$H_{norm} = 2\frac{H - I(\Delta E_{grid}/2 + E_{min})}{\Delta E_{grid}}. \tag{25}$$

Denoting $\alpha = \Delta E_{grid} t/2h$, the evolution of the wavefunction ψ can be approximated as

$$\psi(t) = e^{-(i/h)(\Delta E_{grid}/2 + E_{min})t} \sum_0^{N_b} a_n(\alpha) \Phi_n(-iH_{norm})\psi(0). \tag{26}$$

The first term on the right-hand side is a phase shift compensating the shift in the energy scale. The expansion coefficients become:

$$a_n(\alpha) = 2J_n(\alpha) \tag{27}$$

with $a_0(\alpha) = J_0(\alpha)$. J_n are the Bessel functions.

The use of eq.26 requires the calculation of the operation of $\Phi_n(-iH_{norm})$ on $\psi(0)$. This is accompanied by the recursion relation of the Chebyshev polynomials

$$\phi_{n+1} = -2iH_{norm}\phi_n + \phi_{n-1} \tag{28}$$

with $\phi_n = \Phi_n(-iH_{norm})\psi(0)$.

The recurrence is started by $\phi_0 = \psi_0$ and $\phi_1 = -iH_{norm}\psi_0$.

The hamiltonian H is obtained by

$$H\psi_j \approx \frac{-\hbar^2}{2m}\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta x^2} + V_j\psi_j. \tag{29}$$

Its coefficients are considered as elements H_j of a vector and the operator H applied to ψ_j appear as a vector multiplication.

The number of expansion terms needed to converge the sum in 26 is determined by the size of the time-energy phase space volume: $\alpha = \Delta E_{grid} t/2\hbar$.

Examining the expansion coefficients as a function of n, one finds that when n becomes larger than α, the Bessel functions $J_n(\alpha)$ decay exponentially. This means that in a practical implementation, the maximum order N_b can be chosen such that the accuracy is dominated by the accuracy of the computer. Practical tests shown that N_b should be $15-20$ times greater than α.

The Chebyshev scheme does not conserve norm or energy which can be used to estimate error. It is however very accurate when ΔE_{grid} is relatively small. In such cases, long time steps can be used, sometimes a single time step completes the calculation.

Let us note that the MSD, split operator and Chebyshev methods allow straightforward extensions to several spatial dimensions. For more than two spatial dimensions, these methods should be used, since the Crank Nicholson scheme is not applicable.

3 Artificial Boundary Conditions

When the natural domain of the problem being solved is infinite, we are obliged to use only a finite portion in the numerical calculations. This approximation leads to reflections which affect the propagated wave function and to errors in the calculation of the physical quantities. One solution is to increase the spatial grid, but in many cases it is necessary to use very large intervals, which is costly in computer time and memory requirements. In order to eliminate or at least to reduce reflections special procedures were conceived, thus allowing the use of smaller spatial grids. By these procedures special boundary conditions are imposed. We shall present two kinds of such procedures, namely **Transparent Boundary Conditions** (TBC) and **Absorbing Boundary Conditions** (ABC). They may be easily incorporated into the Crank-Nicholson scheme.

3.1 Transparent Boundary Conditions

The TBC algorithm is based on some suggestions contained in Hadley's papers ([12]), ([13]).

Let us consider the integral

$$\rho = \int_a^b |\psi|^2 dx \tag{1}$$

and calculate $\frac{\partial \rho}{\partial t}$ related to the energy conservation.

By simple manipulations, using TDSE eq.(1) we obtain:

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m}[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}]|_a^b = -F_b + F_a \tag{2}$$

where F_b represents the energy "flux" leaving the right boundary and F_a that entering through the left boundary. Since the treatment of the two boundaries

is essentially identical, we will focus on the right boundary. We next make the important assumption that near this boundary $\psi = \psi_0 \exp(ik_x x)$, where ψ_0 and k_x are complex constants, and k_x is (for the moment) unknown. With this assumption, F_b becomes

$$F_b = \frac{\hbar}{m} Real(k_x)|\psi(b)|^2. \tag{3}$$

Therefore, as long as the real part of k_x is positive, the contribution to the overall change in energy from this boundary will always be negative, i.e., radiative energy can only flow out of the problem region.

If we now consider the finite difference equivalent of (2) using a standard Crank-Nicholson scheme, it can be shown that the above energy balance relationship is preserved. Thus, assuming the same exponential dependence described above, we adjust the boundary value ψ^n_{M+1} (which without TBC is assumed to be 0) prior to the start of the $(n+1)$th propagation step so that

$$\frac{\psi^n_{M+1}}{\psi^n_M} = \frac{\psi^n_M}{\psi^n_{M-1}} = \exp(ik_x \Delta x). \tag{4}$$

This determines k_x and the boundary condition for the new propagation step is thus

$$\psi^{n+1}_{M+1} = \psi^{n+1}_M \exp(ik_x \Delta x). \tag{5}$$

However, prior to the application of (5), the real part of k_x must be restricted to be positive to ensure only radiation outflow.

In practice, this is done as follows. Let us note

$$\alpha = \exp(ik_x \Delta x) = \exp(i(k_1 + ik_2)\Delta x) = \exp(-k_2 \Delta x) \exp(ik_1 \Delta x).$$

We shall write:

$$\alpha = r + is = \rho \ \exp(i\theta) = \rho \ (\cos\theta + i \sin\theta).$$

Thus,

$$\rho = \exp(-k_2 \Delta x) = |\alpha|$$

and

$$\theta = \arctan(s/r) = k_1 \Delta x.$$

We want to keep $k_1 \geq 0$. As $k_1 < 0$ is equivalent to $\theta < 0$, we shall put in such a case $\theta = 0$.

Then we shall take $\alpha = \rho \ \exp(i\theta)$ with θ eventually set to 0 and the relation between ψ_{M+1} and ψ_M will be:

$$\psi^{n+1}_{M+1} = \alpha \ \psi^{n+1}_M. \tag{6}$$

An important feature of the above procedure is that k_x is allowed to change as the problem progresses, thus eliminating the need for a problem-dependent adjustable parameter.

3.2 Absorbing Boundary Conditions

In this approach it is supposed that TDSE admits plane wave solutions of the form

$$\psi = e^{-i(\omega t - kx)}; \tag{7}$$

ω is a function of wave number k through the **dispersion relation**. Equations having such solutions are called dispersive equations. The dispersion relation allows us to define the phase speed, $c(k) = \frac{\omega(k)}{k}$, of individual waves and the group velocity, $C(k) = \frac{\partial \omega}{\partial k}$, of wave packets. Energy, for instance, travels with group velocity.

A fundamental requirement of an absorbing boundary condition is that the interior solution that is generated is close to the unique solution that is produced if the boundary conditions were placed at a large distance (say, infinity) from the interior region. For interior schemes involving traveling waves, the absorbing boundary condition must have the ability to absorb waves incident on it rather than reflecting them back into the interior of the domain.

The idea is to construct an algebraic equation for k and ω and then to use the correspondence between the $x - t$ space and the $k - \omega$ space to construct a differential equation on the boundaries which is transparent for the plane waves.

By introducing the solution of form (7) into eq.(1) one obtains the relation

$$\hbar^2 k^2 = 2m(\hbar\omega - V). \tag{8}$$

This relation can be solved for k and yields

$$\hbar k = \pm\sqrt{2m(\hbar\omega - V)} \tag{9}$$

where the plus sign describes waves moving to the right boundary and the minus sign means waves moving to the left boundary. The left boundary has to be transparent for left-going waves and the right boundary must be transparent for right-going waves. Because we are involved with radial TDSE, we consider only the right boundary set to some finite $x = R$.

To transform (9) back into the $x-t$ space one needs an approximation for the square root which can be easily transformed into a differential equation at the boundary. Shibata ([14]) used a linear approximation of the square root function, while Kuska ([15]) used a rational function approximation.

The authors of ([16]) developed a more general approach to produce absorbing boundary conditions, which includes as special cases the previous methods. We shall present the main ideas of this procedure.

From eq.(8) results

$$\omega = \frac{1}{\hbar}(\frac{\hbar^2 k^2}{2m} + V). \tag{10}$$

Then we can calculate the group velocity:

$$C = \frac{\partial \omega}{\partial k} = \frac{\hbar}{m}k. \tag{11}$$

For a wave traveling to the right within the domain and impinging on the $x = R$ boundary, the group velocity from (11) must be positive, since the energy of the waves propagates at group velocity. This implies that the energy associated with k is leaving the interior domain. A negative group velocity would mean that energy is entering the interior domain and hence is a reflected wave.

Put in mathematical form, the symbol for the boundary condition has the following form at the $x = R$ boundary:

$$\frac{\hbar}{m}k = |\frac{\hbar}{m}k|. \tag{12}$$

Between the $x - t$ space and $k - \omega$ space the following correspondence exists:

$$k <=> -i\frac{\partial}{\partial x}, \quad \omega <=> i\frac{\partial}{\partial t}. \tag{13}$$

Thus from the condition (12) could be developed a differential boundary condition which is an exact absorbing boundary condition if satisfied on the boundary since all the group velocities on the boundary are positive (no spurious reflections off the boundary). But, this boundary condition cannot be realized in physical space by differential operators due to the absolute value function, and thus we must use an approximation to obtain an explicit rational differential form which can be applied on the boundary.

Since a single differential equation can absorb only waves of a certain group velocity, let us consider an approximation to (12) of the form

$$\frac{\hbar}{m}k = a \tag{14}$$

on the boundary, where a is positive and real. Using the correspondence between k and the partial derivative in x, we obtain the following differential operator relation from (14):

$$(i\frac{\partial}{\partial x} + \frac{ma}{\hbar})\psi = 0. \tag{15}$$

If this differential equation is satisfied on the boundary, then waves traveling to the right with group velocity a would be absorbed completely, leading to no reflections off the boundary from that component of the numerical solution for the wave.

But in general waves are composed of more than one component with different group velocities. Therefore, a generalization of the operator in (15) is

$$\Pi_{l=1}^{p} \, (i\frac{\partial}{\partial x} + \frac{ma_l}{\hbar}) \, \psi = 0. \tag{16}$$

where the group velocity values, a_l, are real.

If $a_k \neq a_l$, $k \neq l$, then the effect of the differential equation, when applied to the boundary, would be to completely absorb p different group velocities,

each being absorbed to the first order. If $a_k = a_l$, $k \neq l$, then the effect of this differential equation, when applied to the boundary, would be to completely absorb the component of the computed wave solution with group velocity a_l to the 2nd order. If all the group velocities a_l are the same, then (16) is essentially a series expansion of (8) to the pth order about the point $\frac{ma_l}{\hbar}$.

In the case $p = 1$ we deal just with eq.(15), which we write for point $x = x_j$ and moment $t = t_n$:

$$i\frac{\partial \psi_j^n}{\partial x} + \frac{ma}{\hbar}\psi_j^n = 0. \tag{17}$$

The following approximations are used ([14]) :

$$\psi_j^n \approx \frac{1}{4}(\psi_{j+1}^{n+1} + \psi_j^{n+1} + \psi_{j+1}^n + \psi_j^n), \tag{18}$$

$$\frac{\partial \psi_j^n}{\partial x} \approx \frac{1}{2\Delta x}(\psi_{j+1}^{n+1} - \psi_j^{n+1} + \psi_{j+1}^n - \psi_j^n). \tag{19}$$

By introducing these approximations in (14) we obtain for $j = M - 1$:

$$\alpha\psi_{M-1}^{n+1} + \beta\psi_M^{n+1} = -\alpha\psi_{M-1}^n - \beta\psi_M^n \tag{20}$$

with $\alpha = -\frac{i}{2\Delta x} + \frac{ma}{4\hbar}$ and $\beta = \frac{i}{2\Delta x} + \frac{ma}{4\hbar}$.

Eq.(20) replaces the last equation in linear system (8) derived from the Crank - Nicholson scheme.

For $p > 1$, boundary differential equations of higher orders are obtained.

4 Applications

We used the above methods to compute proton decay rates for the ground state of spherical ^{109}I ($Q_p = 0.829$ MeV).

The initial wavefunction, i.e. the metastable state, was provided by solving the radial stationary Schrodinger equation in a modified potential (usually taking a constant value starting from some distance R_{mod} beyond the top of the barrier) with boundary conditions appropriate to bound states $[Q_p < V(R_{mod})]$.

The success of the time - dependent approach to the decay of low - lying metastable states by quantum tunneling depends crucially on the preparation of this initial wave packet. In particular, it has to be as pure as possible to avoid the background produced by high energy components.

The most convenient numerical method to solve TDSE appeared to be Crank - Nicholson. The tridiagonal system solution at each time step is by far compensated by the step-size Δt required (much greater than for MSD2). For instance, for a mesh size of $1/4$ a time step of $1/8$ is sufficient for CN, while for MSD2 a time step of order $1/1000$ is necessary to ensure stability. The units are 'fm' and '10^{-22} sec'.

Moreover, artificial boundary conditions (TBC and ABC) can be easily incorporated into CN, thus reducing the computational domain by a factor of 5.

The TBC procedure proved to be more conveninent, since it adjusts itself the value of parameter k involved, while ABC requires additional input parameters (the coefficients a_i). Actually we have taken all a_i equal for p = 3, depending on the parameter k_0 whose optimal value has to be found by tests.

The following physical quantities are calculated:

a)- the norm of the wavefunction

b)- the value of the energy during the propagation in time

c)- the quantity ρ = Norm - Norm(int), where Norm is the norm on the whole interval and Norm(int) is the norm calculated between 0 and R_b, where R_b was chosen to be the last turning point. ρ represents the **Tunneling Probability**.

d)- the **decay rate** given by the relation:

$$\lambda(t) = \frac{1}{1-\rho(t)} \frac{d\rho(t)}{dt}.$$

Let us note that the CN method, conserving the norm and energy, is best suited for such calculations, while the others methods exhibit restrictive conditions to be applied.

Some examples of decay rates calculation are presented in Figs.1 - 4. They correspond to the ground state of ^{109}I with $l = 2$, $j = 5/2$ and a nuclear potential of Woods - Saxon form . The eigenfunction corresponding to the energy $E =$ 0.829 MeV was taken as initial wavefunction. It has been produced by setting the potential from $R_{mod} = 50$ fm to the constant value $V(R_{mod})$ and imposing bound state conditions at both ends of the spatial grid $[0, 128]$.

Fig.1 shows the **decay rate** obtained with CN, using TBC with a multiplication factor of the grid equal to 5. $\Delta x = 1/4$, $\Delta t = 1/16$. It is seen how the **decay rate** converges to an asymptotic value.

In Fig.2 the result obtained with the same parameters, but without TBC is given. One can see how the reflexions perturbed the evolution of the solution.

In Fig.3 the calculation with MSD2 is presented. A step $\Delta t = 1/1024$ and a factor of 20 have been necessary, to obtain accurate values.

In Fig.4 is shown an application of ABC procedure. We used the formula with $p = 3$. For the involved parameters we have taken the values: $k_0 = 10$ and $a_1 = a_2 = a_3 = \frac{\hbar k_0}{m} = 2.14$. One sees that Absorbing Boundary Conditions are slightly less performant than Transparent Boundary Conditions in reducing the reflections on the numerical boundaries.

We can conclude that the best results are obtained with Crank - Nicholson method coupled with Transparent Boundary Conditions and very narrow initial wave packets.

The lessons learned from this study will be subsequently applied to the more interesting case of bi - dimensional tunneling for long - lived metastable states.

5 Figures Caption

Fig. 1 - Ground - state decay rate of ^{109}I calculated by integrating TDSE on a grid of total length 5×128 fm using Transparent Boundary Conditions implemented in Crank - Nicholson numerical scheme.

Fig. 2 - Same as in Fig. 1 but without implementing TBC

Fig. 3 - Ground state decay rate of ^{109}I calculated by integrating TDSE using MSD2 numerical scheme. To reach similar accuracy as in Fig. 1, a 4 times larger grid and about 100 times smaller time step was necessary.

Fig. 4 - Same as in Fig. 1, but using Absorbing Boundary Conditions of order $p = 3$.

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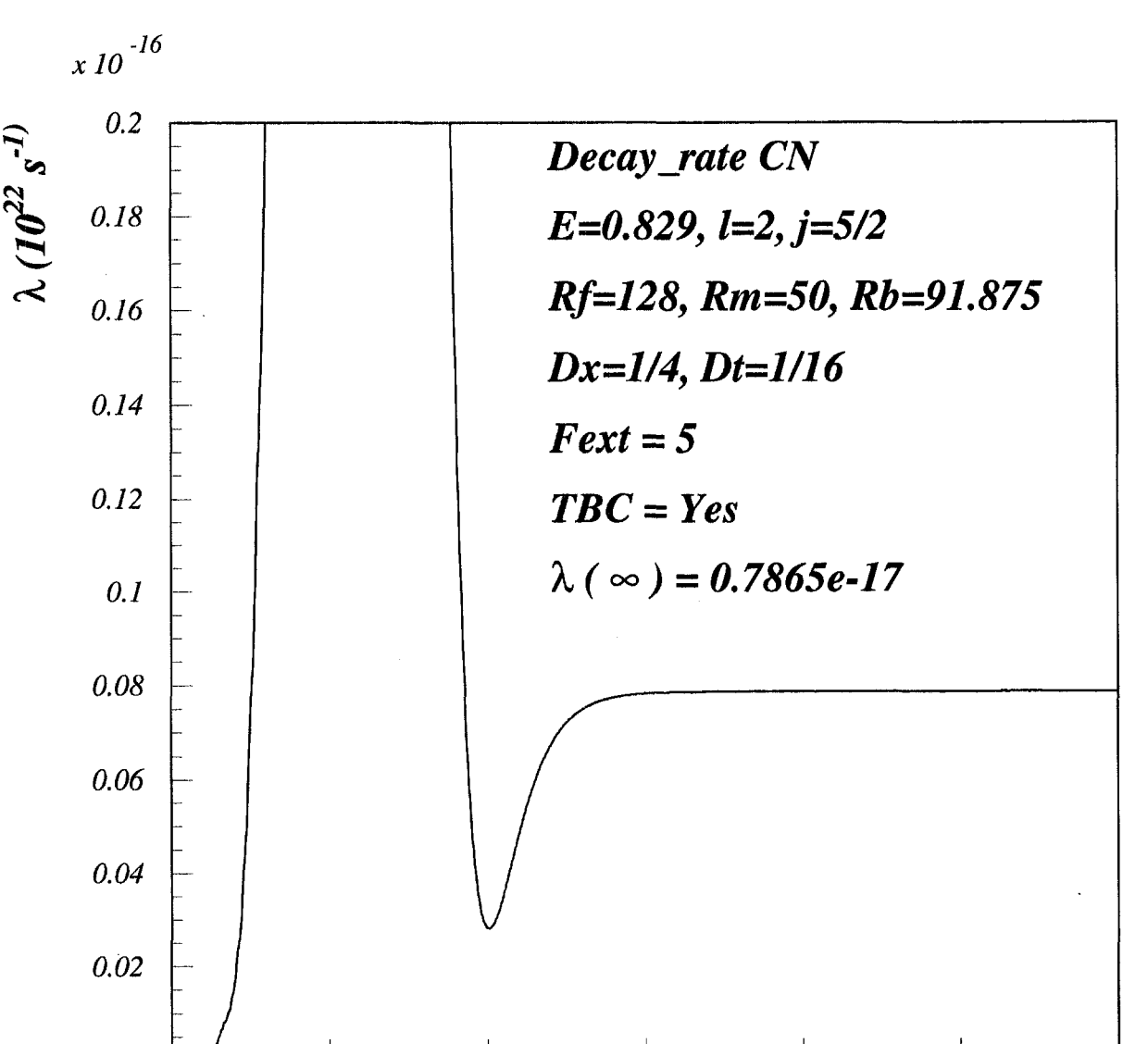
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0.12
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0.08
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0.02
0
0
50
100
150
200
250
300
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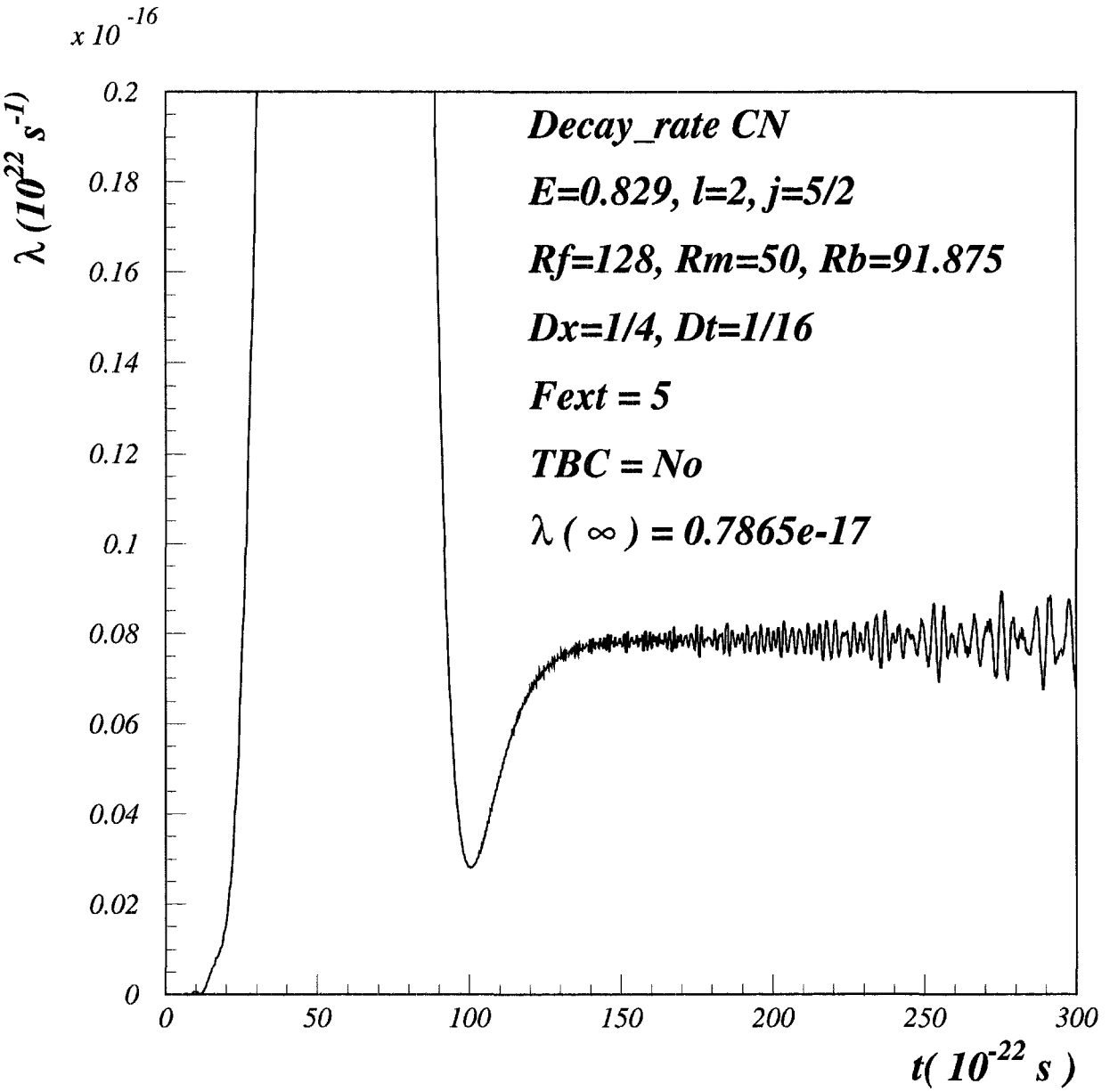
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Dx=1/4, Dt=1/16
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250
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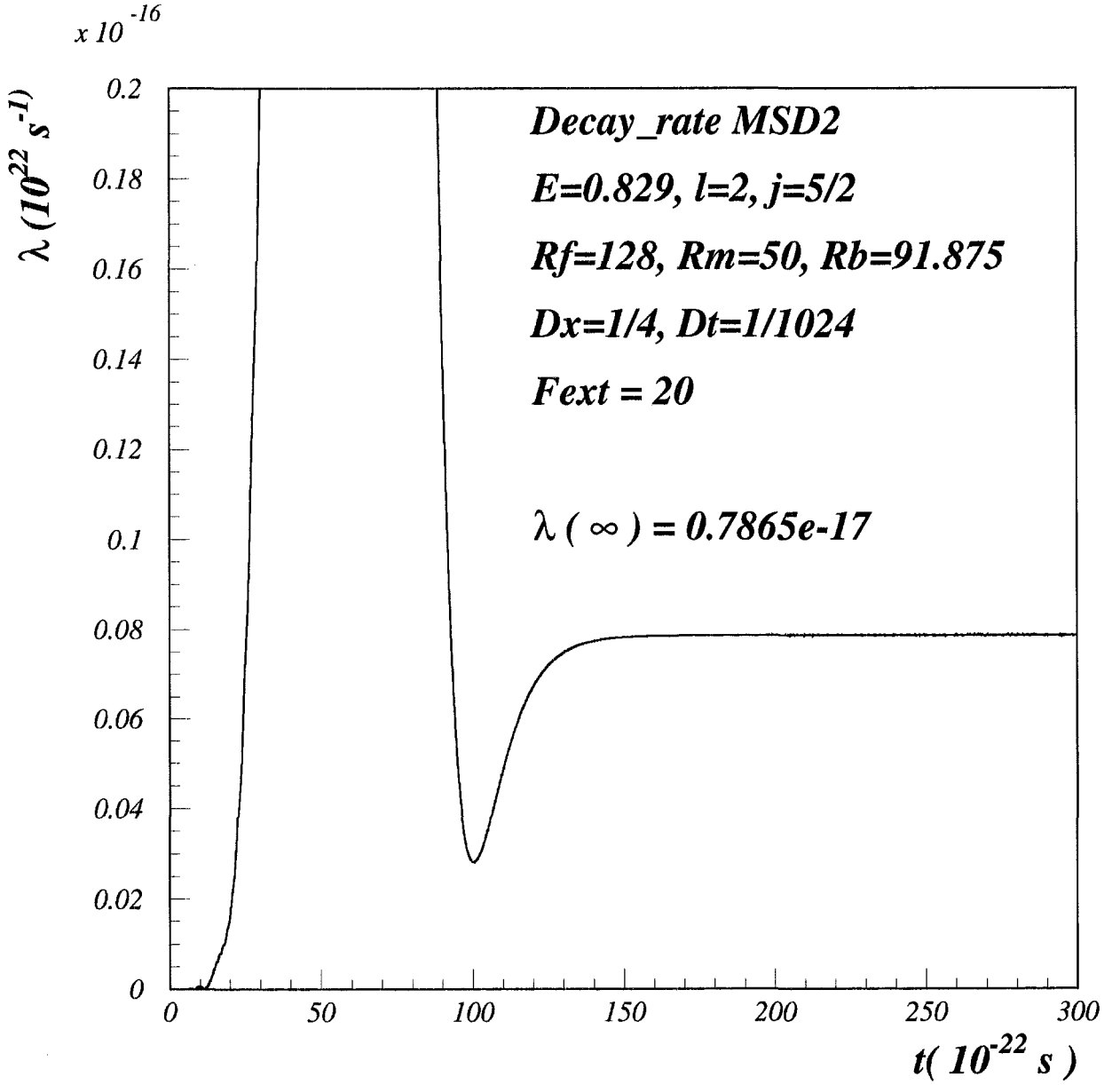
t(10^-22 s)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0.02
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Rf=128, Rm=50, Rb=91.875
Dx=1/4, Dt=1/1024
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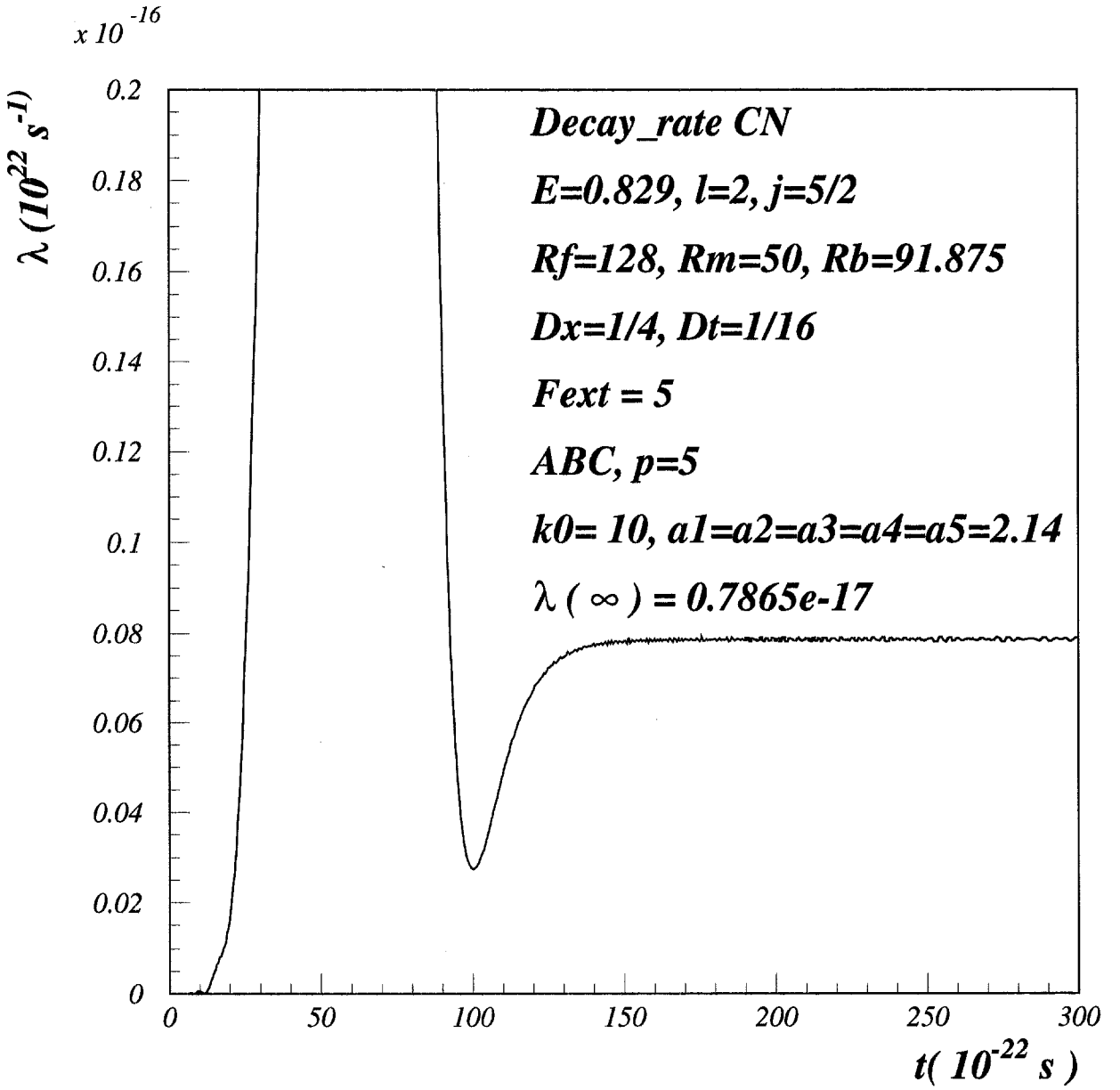
150
200
250
300
t(10^-22 s)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λ (10^22 s^-1)
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0.16
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0.12
0.1
0.08
0.06
0.04
0.02
0
0
50
100
150
200
250
300
t(10^-22 s)
Decay_rate CN
E=0.829, l=2, j=5/2
Rf=128, Rm=50, Rb=91.875
Dx=1/4, Dt=1/16
Fext = 5
ABC, p=5
k0= 10, a1=a2=a3=a4=a5=2.14
λ (∞) = 0.7865e-17