An exact solution of delay-differential equations in association models

J.F. Rojas

Facultad de Ciencias Físico Matemáticas, Benemérita Universidad Autónoma de Puebla,
Río Verde y Av. San Claudio, C.U. Col. San Manuel, Puebla, 72570, Puebla, México,
e-mail: frojas@fcfm.buap.mx

I. Torres

Instituto Nacional de Astrofísica Óptica y Electrónica,
Luis Enrique Erro No. 1, Tonantzintla, Puebla, México.

In modeling automatic engines, like in physiological or biological systems or ecology dynamics, oftenly is necessary to include delay effects in the equations. This effect is related to reaction or transfer times and can be extended to the spatial case, for example, in cases such as the influence in local green biomass density due to dispersal of seeds. Spatial delay effects are present in liquid mixtures models such as the Cummings-Stell model (CSM) for associating molecules: in a series of publications they solve, for particular cases, an equation with spatial delay that must be satisfied by an auxiliary (Baxter's) function. In this paper, we present an analytical and general solution of the first order Delay-Differential Equation (or Differential-Difference Equation) DDE, for the auxiliary Baxter's function that appears in the CSM. A n-partition of the domain leaves a set of DDE's defined in the subintervals. We use recursive properties of these auxiliary functions and a matrix composed by differential and shift operators (MDSO) in order to obtain the solution of the original problem with an arbitrary value of n. The problem of solving spatial DDE's is common to other models of associative fluids, such as homogeneous and inhomogeneous mixtures of sticky shielded hard spheres, or models of chemical ion association and dipolar dumbbells and polymers. In all the cases the location of the potential, $L = m\sigma/n$, has different physical effects.

Keywords: Delay-differential equations; molecular association; biological.

En la modelación de máquinas automáticas, sistemas fisiológicos o biológicos, así como en dinámica de ecosistemas se hace necesario, muchas veces, incluir una corrección en las ecuaciones diferenciales correspondientes. Esta corrección consiste en la inclusión de un tiempo de "retraso" que está relacionado con tiempos de reacción o de transferencia, la cual puede hacerse para el caso espacial también. Por ejemplo, en el caso en el que la densidad de biomasa vegetal local se ve afectada por la dispersión de semilla en otro sitio. En otros modelos se ha incluido un "retraso" espacial como es el caso del modelo de moléculas reactivas de Cummings y Stell (CSM): en una serie de artículos ellos resuelven, para casos particulares, una ecuación con corri- miento (o "retraso") espacial que debe ser satisfecha por la función auxiliar de Baxter. En este trabajo presentamos una solución general y analítica para la ecuación diferencial con corrimiento (Delay Differential Equation) de la función auxiliar de Baxter que aparece en el CSM. Una partición de tamaño n del intervalo de interés lleva a la formulación de un sistema de ecuaciones diferenciales (DDE) definidas en los subintervalos. Usando propiedades recursivas y una matriz de operadores diferenciales y de "corrimiento" (MDSO) se obtiene una solución analítica del problema original para n arbitrario. El problema es común a otros modelos de fluidos reactivos tales como mezclas homogéneas e inhomogéneas de esferas duras con potencial interno de pegado. Lo mismo para asociación iónica, mancuernas dipolares y polímeros. En todos los casos el sitio del potencial de pegado, $L = m\sigma/n$, ocasiona diferentes efectos físicos.

Descriptores: Ecuaciones diferenciales con retardo; asociación molecular; biología.

PACS: 02.30.Ks; 61.20.Qg; 61.25.Em; 82.30.Nr

1. Introduction

In modeling automatic engines, phisiological or biological systems (such as human respiration [1], the dynamics of HIV [2], ecology dynamics [3] or another nonlinear systems [4]) it is often necessary, in order to obtain realistic models involving feedback, to include delay effects such as a reaction time. In 1994 Cooke and Turi published a discussion on stability of a set of delay equations to model patterns of ventilation in human respiration [1]:

$$\frac{d\tilde{x}}{dt} = p - (\tilde{x}(t) - x_I)\alpha W(\tilde{x}(t-\tau), \tilde{y}(t-\tau))$$

$$\frac{d\tilde{y}}{dt} = -\sigma + (y_I - \tilde{y}(t))\beta W(\tilde{x}(t-\tau), \tilde{y}(t-\tau)).$$

In these equations $\tilde{x}$ and $\tilde{y}$ denote arterial concentrations of CO_2 and O_2 respectively, W is the ventilation function (volume of gas moved by the respiratory system) and $\tau > 0$ is the transport delay. The quantities x_I and y_I are the inspirated concentrations of CO_2 and O_2 respectively, p is the CO_2 production rate and σ the O_2 consumption rate. α and β are positive constants referring to the diffusibility of CO_2 and O_2 respectively.

In nonlinear models of human inmunodeficiency virus (HIV) infection where an intracellular delay is included, more accurated representations of the biological data are obtained [2]. In ecosystems, the growth rate of species population will not respond immediately to changes in its own population, rather it will do so after a time lag. The effects

of overgrazing may depend not so much on the actual herbivore population, but on an average reaching back into the past over a time roughly equal to the characteristic regeneration time for the vegetation [3]. As an example a prototype model that considers a single species with growth rate r and a maximum sustainable population K of herbivores grazing over vegetation with recovery time τ, modifies the original logistic equation [5] as

$$\frac{dN(t)}{dt} = rN(t)\left[1 - \frac{N(t-\tau)}{K}\right].$$

This equation can be rewrote in a discrete form known as the *delayed logistic model*[i]

$$n_{t+1} = rn_t(1 - n_{t-1}), \tag{1}$$

so that the original behavior of the solutions of the discrete logistic model (nontrivial stable fixed points for $1 < r < 3$, and bifurcations for $r > 3$) changes to a stable fixed point for $r < 2$ and a stable *limit cycle* for $r > 2$ [6].

In Refs. 4, 1, 7, and 8 the parameter τ defines regions, in such way that the original domain must be partitioned and the local solutions joined over all the frontiers of the subintervals. In each one, the solution depends on the new form of the equation due to the solution in the previous interval. Same arguments can be applied to spatial delay models. As an example, consider the equation

$$\frac{dq(r)}{dr} = q(r - L) \tag{2}$$

whose solution, if $L = 0$, is obvious. The solution in the first interval $[0, L)$ depends on the values of $q(r)$ in $[-L, 0)$. This posibility of delay in differential equations models was an indirect result of the application of Baxter's technique in classical theory of liquids. In this work we focus our atention on a problem related with classical theory of liquids and we obtain an exact solution for a particular type of DDE.

2. The CSM of association: hard spheres with shielded sticky interaction

In 1984 Cummings and Stell [9] proposed a simplified hamiltonian model for a reactive system of two types of homogeneus fluids with the same density and diameter[ii]. In this model, two type of molecules A and B, can be associated by means of a selective square interaction that, in the appropriate limits, can be reduced to a sticky Baxter's potential [10] located inside the hard core at a distance $L = \sigma/n$ from the center of the particle (see Fig. 1 and Eqs. (8)). This model requires the explicit form of the auxiliary Baxter's function and this function must satisfy spatial Delay-Differential Equations (see Eqs. (8)) in this case related to interactions between different chemical species in the system.

The total and direct correlation functions are related by the Ornstein-Zernike (OZ) equation that, for this binary mixture, can be written as [11]

$$h_{ij}(r) = c_{ij}(r) + \sum_{k=A,B} \rho_{k,0} \int c_{ik}(s)h_{kj}(|\mathbf{r} - \mathbf{s}|)d\mathbf{s} \tag{3}$$

where the integral is evaluated in the whole space, $s = \|\mathbf{s}\|$, $i, j = A$ or B and $\rho_{k,0}$ is the numeric density of particles with species k. In the CSM both densities are considered equal.

The CSM [7] for chemical reactions represents the association of two species $A + B \rightleftharpoons AB$. The potential proposed in the CSM consists of a hard sphere repulsion between like species ($A - A$ or $B - B$) and a mound of width σ with a deep, narrow and attractive square well, with width w and centred on L. Here $L < \sigma/2$ and $L + w/2 \leqslant \sigma/2$ for AB interactions:

$$\phi_{AB}/k_B = \begin{cases} \epsilon_1 & \text{if} \quad 0 < r < L - w/2 \\ -\epsilon_2 & \text{if} \quad L - w/2 < r < L + w/2 \\ \epsilon_1 & \text{if} \quad L + w/2 < r < \sigma \\ 0 & \text{if} \quad r > \sigma \end{cases} \tag{4}$$

The geometric consideration of this model for AB interactions ensures steric saturation in the system (there is no formation of n-mers for $n \geqslant 3$) due to overlapping. In addition, this model has an analytical solution in the Percus-Yevick approximation (PYA), mapping the square well onto an infinitely deep and stretch well like the Baxter sticky potential [10]. The connection between the Baxter's original potential and this model, is obtained by comparing the second virial coefficients by considering the limit $\epsilon_1 \to \infty$, $\epsilon_2 \to \infty$, $w \to 0$. The limits $\epsilon_2 \to \infty$ and $w \to 0$ are taken to maintain tractable the problem in the PY approximation [10]. The limit $\epsilon_1 \to \infty$ (in the repulsive part: see Fig. 1) has a little effect on the results and simplifies the solution [12].

Briefly reviewing the formulation of the CS model, we need the factorized form of the Ornstein-Zernike (OZ) [13] Eqs. (3) with the PY closures

$$\left.\begin{array}{l} h_{AA}(r) = h_{BB}(r) = -1, \quad r < \sigma \\ c_{AA}(r) = c_{BB}(r) = 0, \qquad r > \sigma \end{array}\right\} \tag{5}$$

and, in the considered limits

$$\left.\begin{array}{l} h_{AB}(r) = -1 + \frac{\lambda L}{12}\delta(r - L), \quad r < \sigma \\ c_{AB}(r) = 0, \qquad\qquad\qquad r > \sigma. \end{array}\right\} \tag{6}$$

Given the conditions of the problem, the factorized OZ equations are written as [14,9,12,15]

$$rh_{11}(r) = -q'_{11}(r) + 2\pi\rho \int_0^\sigma dt(r - t)$$

$$\times [q_{11}(t)h_{11}(|r - t|) + q_{12}(t)h_{12}(|r - t|)]$$

$$rh_{12}(r) = -q'_{12}(r) + 2\pi\rho \int_0^\sigma dt(r - t)$$

$$\times [q_{11}(t)h_{12}(|r - t|) + q_{12}(t)h_{11}(|r - t|)]. \tag{7}$$

where we changed the index of h_{AA} and h_{AB} to h_{11} and h_{12} respectively. Same for all functions.

Substituting the closure relations (5) and (6) in the set of OZ Eqs. (7), the following system of difference-differential equations (DDE) for the auxiliary Baxter's functions $q_{ij}(r)$ is obtained:

$$q'_{11}(r) + p[q_{12}(r+L) - q_{12}(r-L)]$$
$$= (a_{11} + Da_{12})r + b_{11} + Db_{12}$$

$$q'_{12}(r) + p[q_{11}(r+L) - q_{11}(r-L)] = (Da_{11} + a_{12})r$$

$$+ Db_{11} + b_{12} - \frac{\lambda L^2}{12}\delta(r-L), \qquad (8)$$

where $p = \pi\rho\lambda L^2/6$ and

$$a_{ij} = \delta_{ij} - 2\pi\rho\int_0^\sigma q_{ij}(t)dt \qquad b_{ij} = 2\pi\rho\int_0^\sigma tq_{ij}(t)dt$$

fulfilling the boundary conditions

$$q_{11}(\sigma) = q_{12}(\sigma) = 0$$

$$q_{12}(L^-) = q_{12}(L^+) + \frac{\lambda L^2}{12}. \qquad (9)$$

After integration, a step discontinuity appears at $r = L$ for the auxiliary function $q_{12}(r)$ due to delta in the term associated with the well.

The cases $L = \sigma/n$ for $n = 2, 3, 4$ for the Baxter's function have been solved in 9, 12 y 15 using the same formalism and, at [16], the results were applied for a pair of reactive fluids and a solvent. Lee and Rasaiah solved the $L = \sigma/4$ and $L = \sigma/5$ cases and proposed a solution for $L = \sigma/n$ in a system with chemical association and dipolar dumbbells [17].

The model of Lee and Rasaiah of association in electrolytes $A^+ + B^- \rightleftharpoons AB$ is studied in Ref. 18. In this case the authors add a selective coulombian interaction, $\pm e^2/r$, out of core, to the original CSM model (see in Fig. 1 the dashed lines at $r > \sigma$).

The sticky site inside the hard core incorporates geometrical conditions of steric saturation in the molecule. This idea is shown, using computational simulations in different ensembles, in Ref. 19. For different bounding length parameters the system allows dimers formation for small L, chains for slightly larger L values and vulcanization of species for bounding length values close to the diameter σ of particles. Huerta and Naumis studied the connectivity of a binary mixture using a selective superposition of hard sphere potential with an associating term [20]:

$$U_{ij}(r) = U_{ij}^{hd}(r) + (1 - \delta_{ij})U_{as}(r)$$

where

$$U_{ii}^{hd}(r) = \begin{cases} \infty, & r < 1 \\ 0, & r > 1 \end{cases}$$

$$U_{ij}^{hd}(r) = \begin{cases} \infty, & r < L - 0.5\,w \\ D, & L - 0.5\,w < r < 1 \\ 0, & r > 1 \end{cases}$$
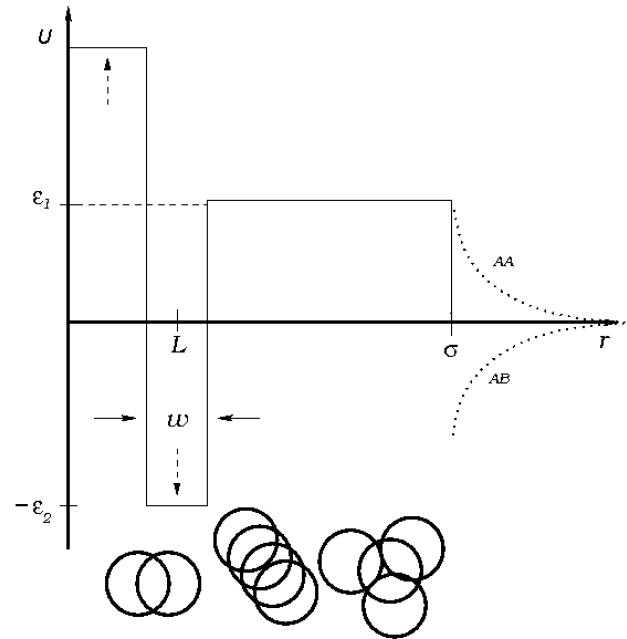

FIGURE 1. The image shows the basic form of the potential, including a coulombian part (dashed curves "AA" and "AB"). Below are shown structural effects for different L values (dimers for small values of L, strings for middle values, and clusters for high values of L, near of σ, in according to [20].

and

$$U_{as}(r) = \begin{cases} 0, & r < L - 0.5\,w \\ -\varepsilon_{as} - D, & L - 0.5w < r < l + 0.5\,w \\ 0, & r > L + 0.5\,w, \end{cases}$$

where L is the bounding distance, w the intracore square well width and i, j represents the species in the mixture. The final potential (see Fig. 1) is equivalent to the original Cummings-Stell in the adecuate limits for sticky approximation. This idea is implemented by Pizio and Blum [21] for a hard-sphere fluid with dimerization $A + A \rightleftharpoons A_2$.

Most of the models maintain L as a parameter (bounding distance) but, at the end, they take the case $L = \sigma/2$, although other possibilities have the analytical solution for arbitrary L. Kalyuzhnyi and Stell [22] present a recount of cases with different ranges of the location L. As we mentioned above, the sticky potential into the hard sphere shell produces a step discontinuity in the Baxter's auxiliary functions. This allows us to think in systems with more than one sticky site inside the shell or, even, a distribution of sticky wells.

The vertical dashed arrows shows the Baxter's sticky limit [9]. The molecular diameter is σ and the dashed curves (with labels "AA" and "AB") correspond to selective coulombian attractive and repulsive interaction for an electrolyte with A and B ions [18].

In the following sections, we develop the matrix of differential and shift operators MDSO, and its inverse, for the simplest case $n = 2$, followed by an inversion of the MDSO's for a very general case that corresponds to the set of n DDE's, to n subintervals of $[0,\sigma]$ and for a sticky location $L = m\sigma/n$.

3. The MDSO

In the first work of Cummings and Stell [9] a new pair of functions were used and defined as the sum

$$q_+(r) = q_{11}(r) + q_{12}(r)$$

and difference

$$q_-(r) = q_{11}(r) - q_{12}(r)$$

of the originals $q_{11}(r)$ and $q_{12}(r)$. The advantage of this trick is to obtain two uncoupled equations, one for $q_+(r)$ and another for $q_-(r)$ which can be solved in a separate way. With this definition and adding and substracting Eqs. (8),

$$q'_+(r) + p[q_+(r+L) - q_+(r-L)]$$
$$= a_+ r + b_+ - \frac{\lambda L^2}{12}\delta(r-L) \qquad (10)$$

and

$$q'_-(r) - p[q_-(r+L) - q_-(r-L)]$$
$$= a_- r + b_- + \frac{\lambda L^2}{12}\delta(r-L), \qquad (11)$$

with the obvious definitions[iii]

$$a_\pm = (1 \pm D)\left[1 - 2\pi\rho \int_0^\sigma dt q_\pm(t)\right]$$

and

$$b_\pm = (1 \pm D)2\pi\rho \int_0^\sigma dt t q_\pm(t).$$

The last term in (10) and (11) can be neglected since it is equal to zero in all subintervals except where $r = L = \sigma/n$. This condition is fixed in the boundary conditions (9). In the rest of subintervals, for the general case, must imply that [9,17]

$$q(m\sigma/n^-) = q(m\sigma/n^+), \quad \text{for} \quad m = 2, 3, \ldots, n-1. \quad (12)$$

We use, from here, $q(r) \equiv q_{11}(r) + q_{12}(r)$. The aim of this proposal is to find an analytical form of the function $q(r)$ assuming that: i) the solution must be obtained in subintervals [23], ii) this implies that $q(r)$ will be defined also in subintervals, and iii) the original functions $q_{ij}(r)$ can be recovered with the relations

$$q_{11}(r) = \frac{q_+(r) + q_-(r)}{2}$$

and

$$q_{12}(r) = \frac{q_+(r) - q_-(r)}{2}.$$

Identical procedure shows that it is sufficient to replace $\lambda \to -\lambda$, $p \to -p$, $\nu \to -\nu$ to obtain $q_-(r)$.

The cases shown in Refs. 9, 12, 15, and 17 are solved here by using MDSO. For convenience we show the case $L = \sigma/2$ of the CSM [9] in detail, and the cases $L = \sigma/3$ and $L = \sigma/4$ summarized.

3.1. The case $n = 2$

The first case yields to a system of two coupled differential equations associated with the two subintervals defined by $L = \sigma/2$,

$$\frac{dq_1(r)}{dr} + pq_2(r+\sigma/2) = ar + b, \quad \text{for} \quad 0 < r < \sigma/2 \quad (13)$$

and

$$\frac{dq_2(r)}{dr} - pq_1(r-\sigma/2) = ar + b,$$
$$\text{for} \quad \sigma/2 < r < \sigma. \qquad (14)$$

where, evidently, q_1 corresponds to the first half of the interval and q_2 to the second one. We define the differential operator $\mathcal{D}$ as

$$\mathcal{D}f(x) \equiv \frac{df(x)}{dx}$$

and the shift operator $\mathcal{E}^s$ by $\mathcal{E}^{\pm s}f(x) \equiv f(x \pm s)$. With this operators defined, the set of Eqs. (13) and (14) can be rewritten as

$$\mathcal{D}q_1(r) + p\mathcal{E}^{\sigma/2}q_2(r) = ar + b$$

and

$$\mathcal{D}q_2(r) - p\mathcal{E}^{-\sigma/2}q_1(r) = ar + b$$

or, in matricial form, as

$$\begin{pmatrix} \mathcal{D} & p\mathcal{E}^{\sigma/2} \\ -p\mathcal{E}^{-\sigma/2} & \mathcal{D} \end{pmatrix} \begin{pmatrix} q_1(r) \\ q_2(r) \end{pmatrix} = \begin{pmatrix} f_1(r) \\ f_2(r) \end{pmatrix}. \quad (15)$$

These equations can be reduced to a symbolic form

$$\mathcal{M}_2 \boldsymbol{q}(r) = \boldsymbol{f}(r) \qquad (16)$$

where $\mathcal{M}_2$ is the matrix of differential and shift operators, or MDSO, that appears in (15), applied to the vector $\boldsymbol{q}$ of functions $q_i(r)$. The right side is the vector $\boldsymbol{f}$ of functions $f_i(r)$ that, in this case, are linear functions of r. The index in $\mathcal{M}$, corresponds to the number of equations (or partitions in the interval of solution).

The main idea of this paper is to find a solution for the system represented in (16) as

$$\boldsymbol{q}(r) = \mathcal{M}_2^{-1} \boldsymbol{f}(r).$$

This implies the knowledge of an explicit analytical form of the inverse of $\mathcal{M}_2$, and how it operates on $\boldsymbol{f}(r)$. One way of

defining the inverse of the differential operator $\mathcal{D}$ is by using the equation

$$y'(x) \pm ay(x) = f(x) \tag{17}$$

or

$$(\mathcal{D} \pm a)y(x) = f(x)$$

whose solution leads us to define the inverse operator $(\mathcal{D} \pm a)^{-1}$ as

$$(\mathcal{D} \pm a)^{-1}f(x) \equiv Ce^{\mp ax} + e^{\mp ax}\int e^{\pm ax'}f(x')dx'. \tag{18}$$

In the previous expression, the case for $a = 0$ implies that the inverse MDSO is reduced to the trivial definition of inverse differential operator as an integral operator. The case where a is a complex number (or imaginary) implies harmonic solutions [7] and Fourier transform of the right hand side of differential equation.

Continuing with the case $L = \sigma/2$, the inverse of $\mathcal{M}_2$ is

$$\mathcal{M}_2^{-1} = \frac{1}{\Delta_2}\begin{pmatrix} \mathcal{D} & -p\mathcal{E}^{-\sigma/2} \\ p\mathcal{E}^{\sigma/2} & \mathcal{D} \end{pmatrix} \equiv \frac{1}{\Delta_2}\check{\mathcal{M}}_2 \tag{19}$$

where the commutation properties of the operators $\mathcal{D}$ and $\mathcal{E}$ were used. Direct calculation gives the determinant-operator of $\mathcal{M}_2^{-1}$ as[iv]

$$\Delta_2 \equiv \mathcal{D}^2 + p^2 = (\mathcal{D} + ip)(\mathcal{D} - ip), \tag{20}$$

so that (19) and (20) define completely the inverse determinant-operator of $\mathcal{M}_2$ as the product of two inverse operators of the form of (18):

$$\frac{1}{\Delta_2} = \Delta_2^{-1} = \frac{1}{\mathcal{D} + ip}\frac{1}{\mathcal{D} - ip}. \tag{21}$$

This is the formal inverse determinant of the MDSO, however we still need to find the appropiate coefficients to satisfy the boundary conditions. So that, the direct application of the inverse MDSO, (19), on (13) and (14) gives

$$q_1(r) = A\cos pr + B\sin pr - \frac{a}{p}r + \frac{a}{p^2}(1 - \nu/2) - \frac{b}{p}$$

$$q_2(r) = C\cos pr + D\sin pr + \frac{a}{p}r + \frac{a}{p^2}(1 - \nu/2) + \frac{b}{p}$$

with $\nu \equiv p\sigma$. Now, considering (9) and the fact that (14) must be satisfied we obtain[5],

$$q_1(r) = A\cos pr + B\sin pr - \frac{a}{p}r + \frac{a}{p^2}(1 - \nu/2) - \frac{b}{p}$$

$$q_2(r) = A\sin p(r - \sigma/2) + B\cos p(r - \sigma/2)$$

$$+ \frac{a}{p}r + \frac{a}{p^2}(1 - \nu/2) + \frac{b}{p}, \tag{22}$$

which agree with the results in Ref. 9. The second equation has the same set of constants that the first one and the harmonic functions have been interchanged and their arguments shifted by $-\sigma/2$.

3.2. The case $n > 2$

In the case $L = \sigma/3$ there are three equations[vi] associated with three subintervals of length $\sigma/3$:

$$\frac{dq_1(r)}{dr} + pq_2(r + \sigma/3) = ar + b, \quad \text{for} \quad 0 < r < \sigma/3$$

$$\frac{dq_2(r)}{dr} + pq_3(r + \sigma/3) - pq_1(r - \sigma/3) = ar + b,$$

$$\text{for} \quad \sigma/3 < r < 2\sigma/3$$

$$\frac{dq_3(r)}{dr} - pq_2(r - \sigma/3) = ar + b,$$

$$\text{for} \quad 2\sigma/3 < r < \sigma \tag{23}$$

with the MDSO given as

$$\mathcal{M}_3 = \begin{pmatrix} \mathcal{D} & p\mathcal{E}^{\sigma/3} & 0 \\ -p\mathcal{E}^{-\sigma/3} & \mathcal{D} & p\mathcal{E}^{\sigma/3} \\ 0 & -p\mathcal{E}^{-\sigma/3} & \mathcal{D} \end{pmatrix}$$

and the inverse operator of $\mathcal{M}_3$

$$\mathcal{M}_3^{-1} = \frac{1}{\mathcal{D}(\mathcal{D}^2 + 2p^2)}$$

$$\times \begin{pmatrix} \mathcal{D}^2 + p^2 & -p\mathcal{D}\mathcal{E}^{\sigma/3} & p^2\mathcal{E}^{2\sigma/3} \\ p\mathcal{D}\mathcal{E}^{-\sigma/3} & \mathcal{D}^2 & -p\mathcal{D}\mathcal{E}^{\sigma/3} \\ p^2\mathcal{E}^{-2\sigma/3} & p\mathcal{D}\mathcal{E}^{-\sigma/3} & \mathcal{D}^2 + p^2 \end{pmatrix}$$

where

$$\frac{1}{\Delta_3} = \frac{1}{\mathcal{D}(\mathcal{D}^2 + 2p^2)}$$

$$= \frac{1}{(\mathcal{D} - 0)}\frac{1}{(\mathcal{D} + i\sqrt{2}p)}\frac{1}{(\mathcal{D} - i\sqrt{2}p)}$$

and[vii]

$$\check{\mathcal{M}}_3 = \begin{pmatrix} \mathcal{D}^2 + p^2 & -p\mathcal{D}\mathcal{E}^{\sigma/3} & p^2\mathcal{E}^{2\sigma/3} \\ p\mathcal{D}\mathcal{E}^{-\sigma/3} & \mathcal{D}^2 & -p\mathcal{D}\mathcal{E}^{\sigma/3} \\ p^2\mathcal{E}^{-2\sigma/3} & p\mathcal{D}\mathcal{E}^{-\sigma/3} & \mathcal{D}^2 + p^2 \end{pmatrix}. \tag{24}$$

Obviously $1/\Delta_3$ is a inverse product of operators in the form of (18). Applying these to the right hand side of (23) we obtain,

$$q_1(r) = A_1\cos\sqrt{2}pr + B_1\sin\sqrt{2}pr + \frac{a}{2}r^2$$

$$- \frac{a}{2p}(1 - 2\nu/3)r + br + F_1$$

$$q_2(r) = A_2\cos\sqrt{2}pr + B_2\sin\sqrt{2}pr + F_2$$

$$q_3(r) = A_3\cos\sqrt{2}pr + B_3\sin\sqrt{2}pr + \frac{a}{2}r^2$$

$$+ \frac{a}{2p}(1 - 2\nu/3)r + br + F_3$$

and, imposing bound conditions in the respective subintervals and the fact that (23) must be satisfied (as in (22) for $n = 2$), we obtain A_2, A_3, B_2 and B_3 in terms of A_1 and B_1

$$q_1(r) = A_1 \cos \sqrt{2}pr + B_1 \sin \sqrt{2}pr$$
$$+ \frac{a}{2}r^2 - \frac{a}{2p}(1 - 2\nu/3)r + br$$

$$q_2(r) = \sqrt{2}A_1 \sin \sqrt{2}p(r - \sigma/3)$$
$$+ \sqrt{2}B_1 \cos \sqrt{2}p(r - \sigma/3)$$

$$q_3(r) = -A_1 \cos \sqrt{2}p(r - 2\sigma/3) - B_1 \sin \sqrt{2}p(r - 2\sigma/3)$$
$$+ \frac{a}{2}r^2 + \frac{a}{2p}(1 - 2\nu/3)r + br. \tag{25}$$

The case $L = \sigma/4$ has a tridiagonal matrix $\mathcal{M}_4$, whose determinant $\Delta_4 = \mathcal{D}^4 + 3\mathcal{D}^2p^2 + p^4$ has roots

$$\pm i \frac{\sqrt{5} - 1}{2} p$$

and

$$\pm i \frac{\sqrt{5} + 1}{2} p$$

so that

$$\Delta_4 = \left[\mathcal{D} + i\frac{\sqrt{5} - 1}{2}p\right]\left[\mathcal{D} - i\frac{\sqrt{5} - 1}{2}p\right]$$
$$\times \left[\mathcal{D} + i\frac{\sqrt{5} + 1}{2}p\right]\left[\mathcal{D} - i\frac{\sqrt{5} + 1}{2}p\right].$$

Lee and Rasaiah, in Ref. 17, called these roots

$$x = \frac{\sqrt{5} - 1}{2}$$

and

$$y = \frac{\sqrt{5} + 1}{2},$$

and correspond to the α_k's defined below.

The case $n = 5$ or $L = \sigma/5$ has a determinant $\Delta_5 = \mathcal{D}^5 + 4\mathcal{D}^3p^2 + 3\mathcal{D}p^4$ whose roots are 0, $\pm ip$, $\pm i\sqrt{3}p$, and the solutions have the same structure as (22) and (25), and those in Refs. 9, 12, 15, and 16.

4. The general MDSO

4.1. The matrix

Computing the same construction for n divisions in the solution interval for a given $L = \sigma/n$, we obtain n functions q_i that represent a continuous solution. Each of them must fulfill

$$q_i'(r) + p[q_{i+1}(r + \sigma/n) - q_{i-1}(r - \sigma/n)] = ar + b,$$

$$\text{for} \quad \frac{i-1}{n}\sigma < r < \frac{i}{n}\sigma \tag{26}$$

where $i = 1, 2, 3 \ldots, n$ and $q_0 = q_{n+1} = 0$, in which

$$q_i(r) = \begin{cases} q(r), & \frac{i-1}{n}\sigma < r < \frac{i}{n}\sigma \\ 0, & \text{otherwise.} \end{cases} \tag{27}$$

The generalized MDSO for arbitrary n has a tridiagonal form

$$(\mathcal{M}_n)_{ij} = \begin{cases} \mathcal{D} & \text{for} & i = j \\ p\mathcal{E}^{\sigma/n} & \text{for} & i = j - 1 \\ -p\mathcal{E}^{-\sigma/n} & \text{for} & i = j + 1 \\ 0 & \text{oherwise} \end{cases} \tag{28}$$

or, in matrix form

$$\mathcal{M}_n = \begin{pmatrix} \mathcal{D} & p\mathcal{E}^s & 0 & 0 & \ldots & 0 \\ -p\mathcal{E}^{-s} & \mathcal{D} & p\mathcal{E}^s & 0 & \ldots & 0 \\ 0 & -p\mathcal{E}^{-s} & \mathcal{D} & p\mathcal{E}^s & \ldots & 0 \\ 0 & 0 & \ldots & \ldots & p\mathcal{E}^s & 0 \\ \ldots & \ldots & \ldots & -p\mathcal{E}^{-s} & \mathcal{D} & p\mathcal{E}^s \\ 0 & 0 & 0 & 0 & -p\mathcal{E}^{-s} & \mathcal{D} \end{pmatrix} \tag{29}$$

Due to symmetry of $\mathcal{M}_n$ the shift operators are mutually canceled in the inverse of Δ_n. This fact enables us to write all solutions $q_i(r)$ in terms of inverse differential operators of the form (18) and (21).

4.2. The determinant inverse operator

From the tridiagonal matrix obtained, (29), the determinants for different values of n can be evaluated:

$$\Delta_0 \equiv 1$$

$$\Delta_1 = \mathcal{D}$$

$$\Delta_2 = \mathcal{D}^2 + p^2$$

$$\Delta_3 = \mathcal{D}^3 + 2\mathcal{D}p^2$$

$$\Delta_4 = \mathcal{D}^4 + 3\mathcal{D}^2p^2 + p^4$$

$$\Delta_5 = \mathcal{D}^5 + 4\mathcal{D}^3 p^2 + 3\mathcal{D}p^4$$

$$\Delta_6 = \mathcal{D}^6 + 5\mathcal{D}^4 p^2 + 6\mathcal{D}^2 p^4 + p^6$$

$$\dots$$

$$\Delta_{14} = \mathcal{D}^{14} + 13\mathcal{D}^{12} p^2 + 66\mathcal{D}^{10} p^4 + 165\mathcal{D}^8 p^6$$
$$+ 210\mathcal{D}^6 p^8 + 126\mathcal{D}^4 p^{10} + 28\mathcal{D}^2 p^{12} + p^{14}$$

$$\Delta_{15} = \mathcal{D}^{15} + 14\mathcal{D}^{13} p^2 + 78\mathcal{D}^{11} p^4 + 220\mathcal{D}^9 p^6$$
$$+ 330\mathcal{D}^7 p^8 + 252\mathcal{D}^5 p^{10} + 84\mathcal{D}^3 p^{12} + 8\mathcal{D}p^{14}$$

$$\dots$$

It is easy to prove that the recurrence relation between MDSO determinants of different order is, for $n \geqslant 2$,

$$\Delta_n = \mathcal{D}\Delta_{n-1} + p^2 \Delta_{n-2} \qquad (30)$$

where $\Delta_1 \equiv \mathcal{D}$ and $\Delta_0 \equiv 1$. The index of Δ_n corresponds to the MDSO order. From this recurrence relation we obtain the general expression for Δ_n

$$\Delta_n = \mathcal{D}^n + \sum_{j=1}^m \frac{\mathcal{D}^{n-2j} p^{2j}}{j!} \prod_{k=j}^{2j-1} (n-k)$$
$$= \sum_{j=0}^m \frac{\mathcal{D}^{n-2j} p^{2j}}{j!} \frac{(n-j)!}{(n-2j)!}$$

which, finally, can be reduced to

$$\Delta_n = \sum_{j=0}^m \binom{n-j}{j} \mathcal{D}^{n-2j} p^{2j} \qquad (31)$$

where additionally, in terms of the imaginary roots of (31),

$$\Delta_n = \prod_{k=1}^n (\mathcal{D} - x_k). \qquad (32)$$

In these expressions $m = \lfloor n/2 \rfloor$ is the integer part of $n/2$. In (32) we have written Δ_n in factorized polynomial form. Here x_k are all the n roots of Δ_n which are all pure imaginary and proportional to p. When n is even there are exactly $m = n/2$ pairs of complex conjugated roots[viii] $\pm i\alpha_k p$ and, if n is odd, there is an additional null root of Δ_n, which requires an additional integration to obtain the q_i functions.

We can write Δ_n, with m as defined above, as

$$\Delta_n = \begin{cases} \prod_{k=1}^m \mathcal{D}_k^2 & \text{for} \quad n \quad \text{even} \\ \mathcal{D}_0 \prod_{k=1}^m \mathcal{D}_k^2 & \text{for} \quad n \quad \text{odd} \end{cases} \qquad (33)$$

where we define $\mathcal{D}_k^2 \equiv (\mathcal{D} - x_k)(\mathcal{D} - \tilde{x}_k)$ and $x_k \equiv is_k \equiv i\alpha_k p$. Also, $\tilde{x}_k$ is the complex conjugate of x_k, α_k is a real number, and $\mathcal{D}_0$ is the operator associated with the root $x_0 = 0$ for n odd.

Direct application of individual inverse $\mathcal{D}_k^2$ on a linear function gives

$$\mathcal{D}_k^{-2}(cr + d) = A_k \cos s_k r$$
$$+ B_k \sin s_k r + \frac{1}{s_k^2}(cr + d). \qquad (34)$$

Same as before, s_k is defined by mean of $x_k \equiv is_k \equiv i\alpha_k p$ and $D_k^{-2} \equiv (D_k^2)^{-1}$. In the general case, an even partition n of the interval $[0, \sigma]$ results in

$$\mathcal{D}_1^{-2}\mathcal{D}_2^{-2}\dots\mathcal{D}_m^{-2}(cr + d) = \sum_{k=1}^m [A_k \cos s_k r + B_k \sin s_k r]$$
$$+ \frac{1}{\prod_{k=1}^m s_k^2}(cr + d). \qquad (35)$$

In both cases (34) and (35) is obvious that in the homogeneus case the solution is an oscilatory one, as shown in Ref. 7.

It is easy to see that if we define the vectorial funcion $\boldsymbol{v}(r)$, using the definition in (19) or (24), as the application of $\check{\mathcal{M}}_n$ to the vector $\boldsymbol{f}(r)$,

$$\boldsymbol{v}(r) = \check{\mathcal{M}}_n \boldsymbol{f}(r),$$

we obtain a linear function $\boldsymbol{v}(r)^{ix}$. The general solution of the system of equations become

$$\boldsymbol{q}(r) = \frac{1}{\Delta_n} \boldsymbol{v}(r)$$

where

$$\boldsymbol{q}(r) \equiv \begin{pmatrix} q_1(r) \\ q_2(r) \\ \dots \\ q_n(r) \end{pmatrix},$$

and $q_i(r)$ is as defined in (27). The constants A_i and B_i that appear in (35) can be established from bound conditions at the frontiers of the subintervals given by (9) and (12) and the recurrence established in the original set of equations.

5. Comments

A general solution of the set of DDE's for the original CSM has been discussed here. It requires the roots of the polinomial expresion for the inverse determinant Δ_n^{-1} which are black imaginary numbers of the form $is_k p$ with s_k a real number. One of the advantages of this method in the CSM is that it allows us to choose the site of the sticky potential, not only at $L = \sigma/n$ for a few values of n: the solution is valid for any n. Furthermore, it allows to change the sticky potential site to positions close (or further) to the center of the particle. For example in the case $n = 3$ the step of discontinuity $\lambda L^2/12$ can be defined at $L = \sigma/3$ or at $L = 2\sigma/3$.

The symmetry of the MDSO comes from the symmetry in the original set of differential equations. This fact is a particular characteristic of the model that enables us to set the well at $r = m\sigma/n(m < n)$, to obtain different molecular structures [20] by locating the step $\lambda L^2/12$ in the site of sticky. This term will represents a step discontinuity in the solution

at the position $L = m\sigma/n$. With this in mind one can think, also, the posibility of two or more sticky square wells inside the spheric shell adding step discontinuities at the sites of wells: it only requires to modify the border conditions in the adequate sites (see Eqs. (9)). This fact is applied by O. Pizio, based in a solution restricted to $\sigma/3 \leqslant L \leqslant \sigma/2$ values [24], to solve the restricted primitive model of electrolytes [25].

The CSM has a set of symmetrical DDEs with "positive" and "negative" delays respect to r. With this property the shifting in the inverse determinant of the MDSO is carried off and only the inverse (integral) part of Δ_n^{-1} is applied on the right hand side of the equations (26). It is possible that using some auxiliary function, this technique could be applied to another set of DDEs that does not have "positive" and "negative" delay together, such as the time delay models.

Acknowledgements

$i.$ Originally represents a population whose individuals need a certain time to reach sexual madurity and was proposed by Maynard Smith [5].

$ii.$ It will be detailed in next section.

$iii.$ From [15] $D = 1$, so that $a_- = b_- = 0$. This does not imply changes in the results. We asume this fact in the rest of paper.

$iv.$ The application of inverse shifting operators is the identity: $\mathcal{E}^s\mathcal{E}^{-s}f(x) = \mathcal{E}^s f(x + s) = f(x + s - s) = f(x)$.

$v.$ This fact allows us to establish the same set of constants for the harmonic part of the solution.

$vi.$ The first and last equations always have one term less, due to the condition of PYA, $q(r) = 0$ out of $[0,\sigma]$.

$vii.$ With this we are defining $\mathcal{M}_n^{-1} = \frac{1}{\Delta_n}\check{\mathcal{M}}_n$.

$viii.$ This was proved for $n = 1, 2, \ldots, 26$.

$ix.$ The harmonic part comes from the inverse determinant.

1. K.L. Cooke and J. Turi, *J. Math. Biol.* (1994) 535.

2. T. Dumrongpokaphan, Y. Lenbury, R. Ouncharoen, and Y. Xu, *Mathematical Modelling of Natural Phenomena* **2** (2007) 75.

3. R.M. May, *Stability and Complexity in Model Ecosystems (Princeton Landmarks In Biology)*. (Princeton University Press, 2001).

4. T. Erneux, *Applied Delay Differential Equations* (Springer-Verlag, 2009).

5. G.W. Flake, *The Computational Beauty of Nature (Computer Explorations of Fractals, Chaos, Complex Systems and Adaptation)* (The MIT Press, 2001).

6. N. Boccara, *Modeling Complex Systems* (Springer-Verlag, 2004).

7. G.M. Munguía-Gámez and M.G. García-Alvarado, *Memorias de la XVII Semana Regional de Nivel Superior Investigación y Docencia en Matemáticas. Mosaicos Matemáticos.* (August 2007).

8. R. Bellman and K.L. Cooke. *Proc. N.A.S.* **45** (1959) 1026.

9. P.T. Cummings and G. Stell, *Mol. Phys.* **51** (1984) 253.

10. R.J. Baxter, *J.Chem.Phys.* **49** (1968) 2770.

11. L.S. Ornstein and F. Zernike, *Proc. K. Ned. Akad. Wet* **17** (1914) 793.

12. P.T. Cummings and G. Stell, *Mol. Phys.* **55** (1985) 33.

13. L. Blum, J.F. Rojas, and J.N. Herrera. *Rev. Mex. Fis.* **39** (1993)799.

14. P.T. Cummings, *Kinam* **16** (1984) 121.

15. P.T. Cummings and G. Stell, *Mol. Phys.* **60** (1987) 1315.

16. S.H. Lee, P.T. Cummings, and G. Stell. *Mol. Phys.* **62** (1987) 65.

17. S.H. Lee and J.C. Rasaiah, *J. Chem. Phys.* **86** (1987) 983.

18. S.H. Lee and J.C. Rasaiah, *J. Chem. Phys.* **83** (1985) 317.

19. A. Huerta, *Mol. Phys.* **96** (1999) 795.

20. A. Huerta and G.G. Naumis, *Phys. Lett. A* (2002) 660.

21. O. Pizio and L. Blum, *Phys. Rev. E* **52** (1995) 572.

22. Y.V. Kalyuzhnyi and G. Stell, *Mol. Phys.* **78** (1993) 1247.

23. R. Bellman and K.L. Cooke. *Differential-Difference Equations* (Academic, Press, 1963).

24. Y. Zhou and G. Stell, *J. Chem. Phys.* **98** (1993) 5777.

25. O. Pizio, *J. Chem. Phys.* **100** (1994).