A statistical approximation for solving some ordinary linear differential equations

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Abstract. We propose a physical analogy between finding the solution of some linear ordinary differential equations (ODEs) and doing the same for an N-particle problem in statistical mechanics. It makes use of the fact that finding the solution of an ODE is equivalent to obtaining the minimum of a functional. Then, we link these two notions, proposing this functional to be the interaction potential energy or thermodynamic potential of an equivalent particle problem. Therefore, solving this statistical mechanics problem amounts to solving the ODE. If only one solution exists, our method provides the unique solution of the ODE. If we treat an eigenvalue equation for which infinitely many solutions exist, we obtain the absolute minimum of the corresponding functional or fundamental mode. As a result, it is possible to establish a general relationship between statistical mechanics and ODEs which allows us not only to solve the related problems from a physical perspective, but also to obtain all relevant thermodynamical equilibrium variables of the equivalent particle system related to the differential equation.

Keywords: new applications of statistical mechanics

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1. Introduction

One way that physicists model physical phenomena is with ordinary differential equations. A great variety of analytical and numerical methods are available in the literature for solving such equations [1, 2].

Throughout this paper we wish to solve some problems that arise in vibration theory, by making an analogy with a system of particles (gas), a well known system treated in statistical mechanics. If this analogy is made, all the tools used in statistical mechanics are available for tackling such problems. From a more general perspective, we extend the same analogy and apply it to find the solutions of some ordinary linear differential equations (ODEs; see section 2).

The general method proposed here could be summed up in the following way. From a mathematical viewpoint, it is possible to obtain the solution of an ODE from the minimization of a functional. On the other hand, a thermodynamic potential or potential energy is represented by a functional. We connect these two notions, proposing a functional which leads to the solution of the selected ODE as the interaction potential energy or thermodynamic potential of an equivalent particle problem. Once the equivalent problem is so defined we ‘ignore’ the original one and treat this ‘new’ problem as that of a
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gas particle with the interaction potential energy given by the functional. Therefore, one is able to obtain the configuration of minimum potential energy—from the equilibrium distribution of this gas—when an order parameter analogous to temperature is slowing down to zero. It is the purpose of this paper to show that this minimum represents the solution of the ODE. For the situation where infinitely many solutions exist, as is the case in vibration theory, our method is capable of obtaining the fundamental mode or absolute minimum of the corresponding problem.

The principal aim of our work is to show (a) how the previously proposed correspondence is used to attain the solution of some ordinary linear differential equations, (b) the theoretical basis upon which it is sustained and (c) the way in which it can be treated within a stochastic framework.

The present work is organized as follows. In section 2, we show how the problem of solving a general kind of ODE can be transformed into a problem of minimization of a functional (a weak solution of the differential equation [3]). Section 3 presents the foundations of equilibrium statistical analysis viewed as a minimization of a thermodynamic potential. This provides the theoretical basis of our method. Section 4 describes the general aspects of the numerical scheme and algorithm implementation. Section 5 is devoted to finding the solution of an ODE employing a stochastic framework. This method allows us to solve the ODE by proposing an equivalent Langevin (stochastic) equation. At the end, in section 6, several numerical experiments which will support our theoretical hypothesis will be developed and solved. Finally, some conclusions will be outlined.

2. Mathematical problem

There are many possible approaches to finding the solutions of ODEs [1, 2]. Among them, we are interested in the one which transforms the problem of finding the solution of an ODE into that of the minimization of a functional. In view of this, we must recall some results from functional analysis.

2.1. Obtaining a minimum principle for the differential equation

The general form of the ODEs that will be treated in this paper can be written as [3]

\[ Au = \sum_{i=0}^{k} (-1)^{i} (p_i u^{(i)})^{(i)} = f \]  

(1)

where \( f \in L^2(a, b) \), \( p_i(x) \), \( i = 0, 1, \ldots, k \), are continuous functions with their derivatives up to the \( i \)th order inclusive in the closed interval \([a, b]\) and

\[ p_i(x) \geq 0 \text{ in } [a, b], \quad i = 0, 1, \ldots, k - 1 \]  

(2)

\[ p_k(x) \geq p \text{ in } [a, b], \quad p = \text{const.} \]  

(3)

\( L^2(G) \) is the Hilbert space of functions that are square integrable in the domain \( G \).
with the boundary conditions

\begin{align}
u(a) &= u'(a) = \cdots u^{k-1}(a) = 0 \\
u(b) &= u'(b) = \cdots u^{k-1}(b) = 0.
\end{align}

Operator $A$ denotes a differential operator with domain $M$ which is the linear set (dense in $L_2(a,b)$) of real valued functions $u$ which are continuous with their derivatives up to the $k$th order inclusive in $[a,b]$.

Conditions (2) and (3) ensure that operator $A$ is positive definite in the linear set $M$ (see [3]). This condition asserts that the element $u^*$ which minimizes a functional $F(u)$ of the form

\[ F(u) = \sum_{i=0}^{k} \int_{0}^{L} p_i(u^{(i)})^2 \, dx - 2 \int_{0}^{L} fu \, dx \]

is the desired solution of (1) (see theorem 9.2 in [3]).

For the eigenvalue problem, $Au - \lambda u = 0$, $\lambda \in \mathbb{R}$, the functional to be minimized coincides with the corresponding eigenvalue $\lambda$ and it reduces to

\[ F(u) \equiv \lambda = \frac{\sum_{i=1}^{k} \int_{0}^{L} p_i(u^{(i)})^2 \, dx}{\int_{0}^{L} u^2 \, dx}. \]

In this case, infinitely many minima exist, each of them corresponding to the associated eigenvalues

\[ \lambda_1 \leq \lambda_2 \leq \cdots. \]

Equation (8) means that $\lambda_1$ is the minimum possible eigenvalue with corresponding eigenfunction $u_1$. Therefore $F(u_1)$ is the absolute minimum of $F(u)$.

From the above considerations, it can be said that differential operators of the form (1), or given by $Au - \lambda u = 0$, satisfying conditions (2)–(5), can be transformed into a functional so that minimizing this functional is equivalent to solving the corresponding ODE.

### 3. Statistical treatment

As a second step towards attaining the solution of ODEs, we must adapt the problem to be treated as a standard particle problem in statistical mechanics. To this end, we must think of an $n$-particle system in a one-dimensional box of size $L$, where a point in the $n$-dimensional configurational phase space can be denoted by $q = (q_1, q_2, \ldots, q_n)$, $q_j$ being the position of particle $j$. Now, a link between the representation of this system in configurational phase space $q$ with the description of possible candidate solutions of the ODE $u$ (see equation (1)) is proposed through an adequate discretization of the function $u$. 

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3.1. Discretization of $u$

Consider now any possible candidate solution of a particular kind of ODE, named $u$. This continuous function is an element of the linear set $M$, the domain of operator $A$. The proposed discretization of $u$ will be settled from the consideration of $n$ sites labelled with the discrete index $l$ of a one-dimensional lattice. Then, the function $u(x)$ is taken as the limit $n \to \infty$ from the field functions $u_l(x_l)$. So the link between our system of particles and that element $u(x)$ is naturally settled as $u_l(x_l) = q_l$. Each $u_l$ can take any value between $-\infty$ and $\infty$. A possible configuration of our $n$ particle system is then considered by specifying the value of $u_l$ at each site $l$ or simply the lattice vector $q \equiv \{u_l(x_l)\} = (u_1(x_1), u_2(x_2), \ldots, u_n(x_n))$. Through this connection, it is possible to apply the whole statistical framework to treat this equivalent new problem.

3.2. Equilibrium statistical analysis and the equivalent particle problem

The next step is to formulate the problem as in standard statistical mechanics. To do this, we will consider our particle system in the canonical ensemble. So far, we have made a connection between the domain of the functional $F(u)$ with the microstates of a thermal system, represented by $q$. With this in mind, our proposal may be put in this way. We propose $F(q)$ as the interaction potential energy of an equivalent particle problem (we will refer to this as the gas). Once it is so defined we ‘ignore’ the original problem and concentrate on this ‘new’ gas problem. With this idea in mind, entropy and thermodynamic variables are referred to this ‘new’ gas. As an example, for the spatial part of the string equation (Helmholtz equation), $F(q)$ is the Rayleigh quotient $[4,5]$ which is actually neither the Hamiltonian nor the interaction potential energy for the string problem. Nevertheless, it can be imagined as an interaction potential energy (the units must be adjusted) of our gas.

Finally, to calculate the equilibrium probability density for our equivalent particle problem, we consider only the potential energy, $F(q)$, of the Hamiltonian $(F(q) + \text{kinetic energy})$ of our ‘new’ gas in the same way as is done in the simulated annealing method $[6]$; then

$$\rho_q = \frac{\exp(-F(q)/\sigma)}{Z}. \quad (9)$$

Here, $Z$ represents the configurational partition function (this time $Z = \int e^{-F(q)/\sigma} \, dq$) and $\sigma$ can be considered a parameter equivalent to the temperature. Automatically, this probability density maximizes a ‘configurational’ entropy. A brief mathematical justification is given in the appendix, which assures us of the mathematical feasibility of the probability density proposed. This leads us to propose an equivalent state equation:

$$A = \langle F(q) \rangle - S\sigma \quad (10)$$

where $A$ can be thought as the corresponding ‘configurational’ Helmholtz potential of the gas. We point out that this analogy can be useful for gaining physical intuition into the minimization process. At high $\sigma$, the equilibrium state is reached by the maximization of $S$ (configurational dependent) and at low $\sigma$ the equilibrium state is governed by the minimization of $F(q)$ (potential energy).

$^2$ In this sense, it is not possible to obtain the equation of motion for the string from $F(q)$. 

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Summarizing, since our problem of solving the ODE has been transformed into an equivalent thermal system problem, all the mathematical framework of statistical mechanics could be applied. For the sake of brevity, here we only outline how several typical thermodynamical equilibrium variables, such as entropy and specific heat, could be calculated for the gas using well-known relations from statistical mechanics [7]. For example, for the specific heat \( C(\sigma) \) we have,

\[
C(\sigma) = \frac{d\langle F(q) \rangle}{d\sigma} = \frac{[\langle F(q) \rangle^2 - \langle F(q) \rangle^2]}{\sigma^2}
\]

(11)

where \( \langle \rangle \) means the equilibrium or ensemble average and could be calculated for each \( \sigma \) via Monte Carlo sampling (see section 4).

Also the entropy could be obtained in the same form by applying the well known relation

\[
\frac{dS}{d\sigma} = \frac{C(\sigma)}{\sigma}
\]

(12)

which integrated, using equation (11), gives us

\[
S(\sigma) = S(\sigma_1) - \int_{\sigma_1}^{\sigma} \frac{[\langle F(q) \rangle^2 - \langle F(q) \rangle^2]}{\sigma^3} d\sigma'.
\]

(13)

4. Proposed algorithm

Having established this new equivalent problem, we apply the whole framework of equilibrium statistical analysis to obtain the extreme value of \( F(q) \). Our main tool for solving problems throughout this paper is based on the metropolis Monte Carlo algorithm [8]. Briefly, this algorithm ensures a way of sampling the canonical ensemble, proposing a transition probability \( P_{q'|q} \) which satisfies detailed balance. For our case, it takes the form

\[
P_{q'|q} = \frac{\rho_{q'}}{\rho_q} = \exp\left(-\frac{\Delta F(q',q)}{\sigma}\right).
\]

(14)

With this transition probability, we construct an algorithm that can sample our \( n \)-dimensional configurational phase space \( H_n \), whose limit as \( n \to \infty \) tends to the Hilbert space \( H_A \). Each equilibrium state, which can be reached by waiting sufficient time (Monte Carlo steps), is a function of parameter \( \sigma \) in which all possible configurations differ from each other in \( \pm \sigma \). Obviously, this also means that for a given \( \sigma > 0 \) there exist many equilibrium configurations and only for \( \sigma = 0 \) do they reduce to one.

The proposed algorithm takes the previous idea and uses it in the same way as in standard simulated annealing [9]. We have just revealed that equilibrium states are governed by parameter \( \sigma \). So, if one diminishes its value in a way as to go through successive equilibrium states, then, the most representative points of the ensemble will be sampled. In the limit as \( \sigma \to 0 \), each different configuration will differ from each other one by an infinitesimal quantity which means, from the notion of a variation of a functional, that we reach a minimum \( q^* = u^* \) (solution of the ODE). Thus, the algorithm is supposed to be capable of avoiding relative minima, providing the absolute minimum of the functional. For the eigenvalue problem, this just allows one to obtain the fundamental
mode and lowest eigenvalue. However, higher modes which correspond to relative minima could be obtained in principle if we impose restrictions on the functional, such as a symmetry or a number of nodes. These topics will be explored in future works.

Summarizing, we claim that the ODE solution is equivalent to the physical configuration of the gas when \( \sigma = 0 \) \((T = 0)\). All other intermediate ‘states’ of the gas represent neither a solution nor an approximation to the ODE’s solution.

### 4.1. Solution generation

Here, we address the problem of generating candidate solutions \( q' \) from an existing one \( q \) (the solution generation scheme).

To attempt this, we will first make a brief survey of the calculus of variations \([1]\). The variation of a functional \( F(u) = \int f(u, u^{(1)}, \ldots, u^{(s)}) \, dx \) which depends on the function \( u(x) \) and its derivatives of order \( \nu \), \( u^{(\nu)} \) is

\[
\delta F(u, u^{(1)}, \ldots, u^{(s)}) = \epsilon(u)\delta u
\]

where by definition

\[
\epsilon(u)\delta(u) = \int \sum_{\nu=0}^{s} (-1)^{\nu} \frac{d}{dx} \left[ \frac{\partial f(u, u^{(1)}, \ldots, u^{(s)})}{\partial u^{(\nu)}} \right] \delta u \, dx
\]

and \( \delta u \) is the variation of the function \( u(x) \) and is equal to \( \epsilon\eta(x), \epsilon \to 0; \) also \( \eta(x) \) is an arbitrary function satisfying sufficiently smooth conditions \([1]\).

Our solution generation scheme starts generating a Markov chain in which the next iterate is built from the previous one, making the change \( q' \to q + \delta q \). The proposal consists in taking \( \delta q \) in agreement with the master equation \([7]\). We consider \( R \) steps (fixed number of steps) for a given \( \sigma \). For the transition probability to have a value of \( 1/2 \), we set \( \Delta F(q', q) \approx \delta F \); then,

\[
P_{q'|q} = \frac{1}{2} = \exp \left( -\frac{\Delta F(q', q)}{\sigma} \right) \approx \exp \left( -\frac{\epsilon(q)\delta q}{\sigma} \right)
\]

where equation (15) has been used. Now, it is possible to calculate \( \delta q \equiv \{\delta u_i(x_i)\} = (\delta u_1(x_1), \ldots, \delta u_n(x_n)) \) by considering the integral in (15) as a sum over the \( n \) sites of the lattice. According to this, and considering every \( \delta u_i(x_i) \) identical and independent of \( x_i \), we can calculate an estimate of the jump \( \delta\overline{\pi} \) that satisfies (16)

\[
\delta u_i(x_i) = \delta\overline{\pi} = -\frac{\ln(1/2)}{\epsilon(u)} \frac{\sigma}{\epsilon(u)}
\]

Then, we obtain \( \delta q \equiv \{\delta\overline{\pi}\} = (\delta\overline{\pi}, \ldots, \delta\overline{\pi}) \). This form for calculating \( \delta q \) provides one possible way of setting an estimate for the jump for building the next iterate. Of course, other possibilities are feasible for implementation. However, this has the advantage of efficiently exploring configurational phase space in order to reach equilibrium states avoiding local minima (if there are any).

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4.2. Algorithm implementation

It is a relevant problem to determine the initial temperature $\sigma_0$ to start the algorithm. The one proposed by Kirkpatrick [9] for initial temperature guesses in the standard simulated annealing technique (SA) proves to be simple and very effective. Obviously, other means are possible, but we chose it for simplicity (see [10] and references therein). Briefly, it consists in conducting a pilot survey of the solution space in which all increases in the objective function (the functional $F(q)$) are accepted. The initial temperature is then calculated from (14), once the initial transition probability $P_{q'|q_0}$ has been given ($0.9–0.8$ is commonly selected), according to

$$\sigma_0 = -\frac{\Delta \tilde{f}}{\ln(P_{q'|q_0})} \quad (18)$$

where $\Delta \tilde{f}$ is an average increase in the objective function, $F(q)$. According to this formula, it is then possible to initiate the algorithm. To trigger it for the first time, a high $\sigma$ is chosen. Then, one computes $\Delta \tilde{f}$ for the first hundred of attempts and applies (18).

In the implementation of the algorithm, we decided to lower $\sigma$ half an order of magnitude between different equilibrium states. Then, we performed a maximum of $10^5$ runs to compute different equilibrium averages for a given $\sigma$ to ensure that we reached equilibrium.

Since it is impossible to reach absolute zero as a limiting value of the control parameter $\sigma$, a stopping criterion must be used as $\sigma \to 0$. This criteria could be condensed in the following way: the process of cooling of the system ends when, making a choice of a significant digit for the value of the functional being minimized, this digit averages to zero during the cooling procedure, while the other, more significant digits remain unchanged.

5. The Langevin approach

An alternative treatment of the problem is to present it within a stochastic framework. To this end, we propose to model the system with the Langevin equation. The use of the Langevin equation to stochastically sample an arbitrary field is not a new idea [11]. However, the authors do not know of the same approach having been attempted for finding solutions of ODEs. Briefly, the Langevin equation is a stochastic differential equation whose coefficients are random, with given stochastic properties [12]. It defines $u(x,t)$ as a stochastic process provided that an initial condition is added, $u(x,0)$. The method developed for solving ODEs consists in proposing a Langevin equation for the scalar field $u(x)$ in the simulation time $t$; this is

$$\frac{\partial u(x,t)}{\partial t} = -\frac{1}{\xi(T)} \frac{\delta F(u)}{\delta u} + \eta(x,t) \quad (19)$$

where $\xi$ is the friction coefficient which depends on $T$, the absolute temperature\(^3\), and $\eta(x,t)$ is a Gaussian thermal noise with zero mean and that satisfies

$$\langle \eta(x,t)\eta(x',t') \rangle = 2D(T)\delta(x-x')\delta(t-t'). \quad (20)$$

\(^3\) Here, we retain $T$ and not $\sigma$ as the control parameter since this time there is no need to make the change.

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There is a certain arbitrariness in the selection of the diffusion and friction constants, $D(T)$ and $\xi(T)$, but the product $\xi(T)D(T)$ must satisfy the Einstein relation, i.e. $\xi(T)D(T) = k_B T$, to give the correct thermodynamical averages. It can be proved that the probability distribution $P(u,t)$ approaches the equilibrium distribution $P_{eq} \propto e^{-F(u)/k_B T}$ as $t \to \infty$ (see [13]). To obtain the minimum of $F(u)$ and consequently the solution of the ODE, we must solve (19) starting at a high temperature $T_0$ and then slowing it down gradually, which means passing through successive equilibria, until we reach a temperature near zero. Following the same reasoning as before, we will thus obtain the absolute minimum of the functional. Of course, the implementation of this cooling schedule is analogous to that of the previously developed procedure, so there is no need to go into detail again.

In the end, to make possible a numerical solution of the field equation (19), we work with the same discretization scheme as above. This time, the Langevin equation for the scalar lattice field $u_l(x_l)$ looks as follows:

$$\frac{\partial u_l(x_l,t)}{\partial t} = -\frac{1}{\xi(T)} \frac{\delta F(u_l)}{\delta u_l} + \eta(x_l,t) \quad l = 1 \cdots n. \tag{21}$$

6. Numerical experiments

In this section we present several ODEs which were solved by applying the previously developed methods. The cases under study are:

- Case 1. The Helmholtz equation.
- Case 2. The fourth-order beam equation.
- Case 3. The fourth-order beam deflection under a static load.

The proposed methods provide, for the eigenvalue problem (cases 1 and 2), the absolute minimum of the functional (lowest eigenvalue) and the corresponding eigenfunction (fundamental mode). For case 3, this situation no longer arises since there is only one minimum of the functional and this represents the unique solution of the ODE.

6.1. Case 1

For the case of the Helmholtz equation, $u''(x) + \lambda u(x) = 0$, the corresponding functional $F(u)$ reduces to

$$F(u) = \int_0^L (u'(x))^2 \, dx \over \int_0^L u(x)^2 \, dx. \tag{22}$$

This result is obtained from equation (7) after an easy manipulation. Fixed boundary conditions will be considered in this case; this means $u(0) = u(L) = 0$. The functional $F(u)$ is named the Rayleigh quotient $R(u)$, as mentioned before. Physically, it is derived from the principle of conservation of energy since, if the total energy of the system remains constant, one can be assured that $V_{\text{max}} = T_{\text{max}}$ (potential maximum energy equals kinetic maximum energy).
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Table 1. Rayleigh’s quotient for the configurations of figure 1 with $N_{\text{part}} = 16$. The control parameter $\sigma$ and the number of algorithm iterations are also shown.

| Config. | $R(u)$   | $\sigma$   | $N_{\text{iter}}$ |
|---------|----------|------------|-------------------|
| Initial | 0.396959 | $1 \times 10^{-4}$ | 0                 |
| Interm. 1 | 0.083343 | $1 \times 10^{-4}$ | $1 \times 10^{3}$ |
| Interm. 2 | 0.048746 | $1 \times 10^{-4}$ | $2 \times 10^{3}$ |
| Interm. 3 | 0.045338 | $1 \times 10^{-4}$ | $3 \times 10^{3}$ |
| Final 16 | 0.043871 | $1 \times 10^{-6}$ | $1 \times 10^{4}$ |

For a vibrating system, let $T_{\text{max}} = \omega^2 T^*_{\text{max}}$; that is, $T_{\text{max}}$ is the maximum kinetic energy of the system during a cycle of motion, with the square of the natural frequency, $\omega^2$, factored out. Thus, from the total constant energy requirement, one can write

$$\omega^2 = \frac{V_{\text{max}}}{T^*_{\text{max}}}$$

which is exactly (22) with $\omega^2 = \lambda$.

For the algorithm implementation and following the spirit of section 3, we define $F(q)$ as

$$F(q) \equiv F(\{u_l\}) = F(u_1, \ldots, u_n) = \sum_{l=1}^{n} (\nabla u_l)^2 \delta x_l / \sum_{l=1}^{n} u_l^2 \delta x_l$$

which is the discretized version of equation (22). Here, $\nabla u_l = (u_{l+1} - u_l)/\delta x_l$ and $\delta x_l = x_{l+1} - x_l$. This is the expression for the numerical evaluation of $F(u)$ that we will use for this case. We start with a random function $q_0$ and then apply the solution generation routine and the transition probability $P_{q'|q}$ of (14) together with the cooling schedule until the stopping criterion is reached. For this case, we have discretized the one-dimensional lattice to 16 sites, i.e. $n = 16$. However, to compute the functional values $F(u)$, we have employed a cubic spline interpolation scheme using Matlab® routines between $u$ values which smooths the representation of $u(x)$ for calculating $F(u)$.

For the algorithm to perform the iterations over different configurations, new configurations are settled from old ones with a jump estimation $\delta q$ that is calculated from equation (17):

$$\delta \hat{u} = -\frac{\ln(1/2)\sigma ||u||^2}{2G(u)}$$

where $G(u) = \int (u'' + \lambda u) \, dx$ represents Galerkin’s error function and $||u||^2 = \int u^2 \, dx$. Here, $\epsilon(u) = 2G(u)/||u||^2$ as can be seen by comparing equations (25) and (17). Obviously, $u''(x) + \lambda u(x) = 0$ is only satisfied by the solution of the ODE $u^*$.

The initial random function $q_0$ can be observed in figure 1 as initial config. In the same figure, intermediate candidate solutions which correspond to different equilibrium situations for different temperatures are shown. The final configuration was chosen following the stopping criterion. Numerical values of the configurations considered are presented in table 1, where the number of algorithm iterations is also shown for time estimation calculations.

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Figure 1. Initial, intermediate and final configurations for the Helmholtz equation with fixed ends, showing the convergence of the algorithm to the minimum of the functional, $N_{\text{part}} = 16$.

Table 2. Rayleigh’s quotient for the final configuration of figure 2 with $N_{\text{part}} = 64$. Here, the difference between the exact solution and the solution provided by the algorithm (final configuration) differs only within 0.01%.

| Config  | $R(u)$     | $\sigma$ | $N_{\text{iter}}$ |
|---------|------------|----------|-------------------|
| Final   | 0.0438650  | $1 \times 10^{-9}$ | $5 \times 10^4$   |
| Exact   | 0.0438649  | —        | —                 |

The selection of $n = 16$ or hereafter $N_{\text{part}} = 16$ was not arbitrary. The few particles at the beginning of the run make the algorithm run faster at large values of the prescribed $F(u)$ (we can call it the ‘energy’ of the system). As this ‘energy’ goes down, the algorithm starts to slow down its convergence rate due to the finite number of particles. At this stage, we increment the number of particles as many times as is necessary to get further significant reductions. This process has been named ‘stable resizing’ due to the ‘resizing’ of the number of particles considered. Figure 2 shows the results for $N_{\text{part}} = 64$. The exact solution (fundamental mode) appears as a full line and the function that results from the minimization process is shown as a cross line. The numerical values of the Rayleigh quotient are presented in table 2. It can be noted that the difference between the exact and obtained $R(u)$ is below 0.01%, which demonstrates the convergence of the method to the exact solution.
6.2. Langevin approach to the Helmholtz equation

For the case of the Helmholtz equation $u''(x) + \lambda u(x) = 0$, we have already shown that the corresponding functional is $F(u) = \int_0^L (u'(x))^2 \, dx / \int_0^L u(x)^2 \, dx$ which, in its discretized version, results in the same expression as (24). With that form of $F(\{u_l\})$ and applying an Euler updating scheme [13], it can be substituted in (21) to give

$$u_l(t + \delta t) = u_l(t) - \delta t \left( -2 \frac{(u_{l+1} - 2u_l + u_{l-1})/\delta x_l + \lambda u_l \delta x_l}{\|u_l\|^2} \right) + \sqrt{\delta t} \sqrt{2D(T)} \eta_l(t)$$

where

$$\|u_l\|^2 = \sum_{l=1}^{n} u_l^2 \delta x_l.$$

Fixed boundary conditions are also considered in this case. Numerical values of the configurations obtained are presented in table 3 where the number of algorithm iterations is also shown for the time estimation calculations.

A stable resizing routine could also be applied in this case. The results for $N_{\text{part}} = 64$ are shown in table 4.

6.3. Case 2

For the fourth-order beam equation, $u^{(IV)}(x) - \lambda u(x) = 0$, the corresponding functional is

$$F(u) = \frac{\int_0^L (u''(x))^2 \, dx}{\int_0^L u(x)^2 \, dx}. \quad (26)$$

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Figure 3. Initial, intermediate and final configurations for the Helmholtz equation with fixed ends for the simulations obtained with the Langevin approach. The convergence of the algorithm to the minimum of the functional with $N_{\text{part}} = 16$ is also illustrated.

Table 3. Rayleigh’s quotient for the configurations of figure 3 with $N_{\text{part}} = 16$ for simulations with the Langevin approach. The temperature $T$ and number of algorithm iterations are also shown.

| Config. | $R(u)$  | $T$     | $N_{\text{iter}}$ |
|---------|---------|---------|-------------------|
| Initial | 0.273213| —       | 0                 |
| Interm. 1 | 0.115614 | $1 \times 10^{-2}$ | $1 \times 10^4$ |
| Interm. 2 | 0.053995 | $1 \times 10^{-3}$ | $1 \times 10^4$ |
| Interm. 3 | 0.044929 | $1 \times 10^{-4}$ | $1 \times 10^4$ |
| Interm. 4 | 0.044005 | $1 \times 10^{-5}$ | $1 \times 10^4$ |
| Interm. 5 | 0.043875 | $1 \times 10^{-6}$ | $1 \times 10^4$ |
| Final 16 | 0.043866 | $1 \times 10^{-7}$ | $1 \times 10^4$ |

Clamped boundary conditions are considered for this case, i.e. $u(0) = u(L) = \partial u(x)/\partial x|_{x=0} = \partial u(x)/\partial x|_{x=L} = 0$.

To treat equation (26) numerically, this time $F(q)$ results as

$$F(q) \equiv F(u_i) = \sum_{l=1}^{n} (u_{l+1} - 2u_l + u_{l-1})^2/(\delta x_l)^3/\sum_{l=1}^{n} u_l^2 \delta x_l.$$  \hspace{1cm} (27)

As before, the jump estimation can be calculated from equation (17), resulting in the same expression, (25). The only change is in $G(u)$ which results as

$$G(u) = \int (u^{(IV)} - \lambda u) \, dx.$$  \hspace{1cm} (28)
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Figure 4. Initial, final and intermediate configurations as the algorithm runs towards the solution of the beam equation for clamped ends. $N_{\text{part}} = 16$.

Table 4. Rayleigh’s quotient for the final configuration of the simulations with Langevin approach with $N_{\text{part}} = 64$; the exact value of Rayleigh’s quotient is shown for comparison.

| Config. | $R(u)$  | $T$       | $N_{\text{iter}}$ |
|---------|---------|-----------|-------------------|
| Final   | 0.043 8661 | $1 \times 10^{-8}$ | $1 \times 10^4$  |
| Exact   | 0.043 8649  | —         | —                 |

We start the algorithm with a sinusoidal function, $q_0$, which is not the solution of the differential equation in this case (see figure 4). This was done to illustrate that the algorithm converges to the solution of the ODE independently of the initial condition that has been employed. In figure 4 we also show the convergence of the algorithm to the solution of the beam equation as $\sigma$ goes down. The number of particles is $N_{\text{part}} = 16$ for the first steps of the process, as was explained before. Numerical values are shown in table 5.

To improve the precision of the algorithm and accelerate its convergence, the number of particles was increased to five times ($N_{\text{part}} = 128$) its initial value. The final results can be observed in figure 5 where the Rayleigh quotient $R(u)$ is also shown. It is noticeable that we have better accuracy of the attained solution due to the ‘stable resizing’.

6.4. Case 3

For the fourth-order beam deflection under a static load the equation is $u^{(IV)}(x) = g(x)$. We have selected a concentrated load of the form $g(x) = \delta(x - x_0)$, $\delta(x)$ being the Dirac
delta function. This time, the functional is

\[ F(u) = \int_0^L (u''(x))^2 \, dx - 2 \int_0^L u(x)g(x) \, dx. \tag{29} \]

Simply supported boundary conditions are selected this time: \( u(0) = u(L) = \frac{\partial^2 u(x)}{\partial x^2} |_{x=0} = \frac{\partial^2 u(x)}{\partial x^2} |_{x=L} = 0 \). In this case, the functional simply represents twice the potential energy in a beam subjected to the transverse force \( g(x) \). Applying equation (16), one is able to obtain the estimated jump which results as

\[ \delta u_a = -\frac{\ln(1/2)\sigma + 2\delta u(x_a)}{2G(u)} \tag{30} \]

where \( G(u) = \int u^{(IV)} \, dx \). This equation states that the estimated jump could be obtained once \( \delta u(x_a) \) is provided. Since we have no knowledge of this quantity, it is reasonable to
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Figure 6. Initial, final and intermediate configurations in the convergence to the solution of a beam under a static load; $N_{\text{part}} = 16$.

Table 6. Functional value, $I(u)$, for the case of the elastic beam equation under a static force of delta type with simply supported boundary conditions.

| Config. | $I(u)$         | $\sigma$              | $N_{\text{iter}}$ |
|---------|----------------|-----------------------|--------------------|
| Initial | 1.7231         | $1 \times 10^{-4}$    | 0                  |
| Interm. 1 | 0.1172       | $1 \times 10^{-4}$    | $1 \times 10^{3}$ |
| Interm. 2 | 0.001995   | $1 \times 10^{-4}$    | $5 \times 10^{3}$ |
| Interm. 3 | −0.0038      | $1 \times 10^{-4}$    | $1 \times 10^{4}$ |
| Interm. 4 | −0.00808     | $1 \times 10^{-6}$    | $2 \times 10^{4}$ |
| Interm. 5 | −0.01103     | $1 \times 10^{-7}$    | $1 \times 10^{5}$ |
| Final   | −0.011334     | $1 \times 10^{-8}$    | $1 \times 10^{5}$ |

propose it to be of the order of $\delta \bar{u}$. With this assumption, equation (30) results as

\[ \delta \bar{u} = \frac{\ln(1/2)\sigma}{2(G(u) - 1)}. \]  

(31)

The algorithm was initialized with an initial configuration of the form of a sine function with random noise. This configuration, together with intermediate and final configurations, is shown in figure 6. $N_{\text{part}} = 16$ was chosen again since it provides good initial results. Numerical values for the different configurations are shown in table 6 for $x_a = 0.5L$, where $I(u) \equiv F(u)$.

If a better precision is to be reached, more particles must be included. Nevertheless, with $N_{\text{part}} = 16$ the difference between the exact and final solution is below 3%.

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7. Conclusions

A statistical approximation for the solution of some linear ODEs was presented; in particular we solved some problems related to vibration theory. The method developed establishes a way to attain the solution of an ODE proposed for solving physical problems from statistical mechanics. The idea consists in thinking of the domain of any functional (representing the ODE) as microstates of an equivalent particle system (gas) in contact with a heat bath at ‘temperature’ $\sigma$ (canonical ensemble), that interacts through a potential energy represented by the functional. Then, obtaining the minimum of the potential energy of this gas when $\sigma \to 0$ is the same as getting the solution of the ODE. If only one solution exists, our method provides the unique solution of the ODE. If we treat an eigenvalue equation for which infinitely many solutions exist, we obtain the absolute minimum of the corresponding functional or fundamental mode, as well as the fundamental eigenvalue.

Three examples have been provided to show the convergence of the method to the solution of the ODEs; the first two represent a typical eigenvalue problem, for the Helmholtz equation and for the fourth-order beam equation, with infinitely many possible solutions. In these cases the method has been shown to converge to the fundamental mode. For the third case, the beam equation under a static load, the method converges to its unique solution. Additionally, a resizing of the corresponding one-dimensional lattice called ‘stable resizing’, which increases the discretization, was used to provide further reductions of the functional, accelerating its convergence and improving its precision.

With the same outcome, but from a different perspective, a general approach to the problem within a stochastic framework was presented, with similar success. We proposed using an equivalent Langevin equation for the scalar field $u$ as a way of finding the minimum of the functional, the solution of the ODE. Numerical experiments have been run which showed that the method also converges to the exact solution for the Helmholtz equation. Of course, the other two cases, analysed with the first method developed, can be treated within the same scheme. However, for the sake of brevity, we postpone this to future work.

Summarizing, the present article does not pretend to claim a place as providing an alternative to other numerical, probably faster and more precise methods. Its virtue consists in showing that it is possible to establish a link between the problem of finding the solution of some linear ODEs and that of finding the solution for an equivalent interacting particle system or gas which can be treated within the framework of statistical mechanics. In this sense, we showed that some typical thermodynamical equilibrium variables, such as the entropy and specific heat of this gas, could be, in principle, calculated and this could help us to gain an intuitive idea of the process of convergence towards the minimum of the functional, the solution of the ODE. This may provide a different perspective and new insights in solving ODEs.

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Appendix

When modelling a thermal system in equilibrium, the supportive mathematical structure is simple and not exclusive to physical systems. In this mathematical structure, the entropy $S$ is defined over a convex subset $\Sigma$ of $\mathbb{R}^{m+1}$, where a point of $\mathbb{R}^{m+1}$ is denoted by $(X_0, X_1 \ldots X_m)$, so there can be defined a $C^1$ function, $S : \Sigma \rightarrow \mathbb{R}$, such that [14]:

- $S$ is concave.
- $\partial S/\partial E > 0$, with $E = X_0$.
- $S$ is positively homogeneous of degree 1.

For a probabilistic model there is also a measure needed; then, the requirement is fulfilled if:

- there is a class $\mathcal{A}$ defined by $\mathcal{A} = \{\rho : \Omega \rightarrow (0, \infty)\}$ (in physical systems, a point of $\Omega$ is called a microstate).
- $\rho$ is $\pi$-measurable ($\pi$ is the reference measure).
- $\int_{\Omega} \rho d\pi = 1$ ($\rho$ is the density of the microstate measure $\rho d\pi$).
- $E(X, \rho) = \langle X \rangle = \int_{\Omega} X \rho d\pi$ ($X$ is called an observable).

There is a well known theorem [14] which ensures that

$$\varrho = \frac{\exp (-\beta \cdot X)}{Z}$$  \hspace{1cm} (A.1)

maximizes $S(\rho) = -\int_{\Omega} \rho \ln(\rho) d\pi$ for all possible $\rho \in \mathcal{A}$. Here, $\beta \in \mathbb{R}^{m+1}$ and

$$Z = \int_{\Omega} e^{-\beta \cdot X} d\pi.$$  \hspace{1cm} (A.2)

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