Stochastic simulation of quantum mechanics

1991 J. Phys. A: Math. Gen. 24 4081

(http://iopscience.iop.org/0305-4470/24/17/025)

J. Phys. A: Math. Gen. 24 (1991) 4081-4091. Printed in the UK

Stochastic simulation of quantum mechanics

S M Catterall, I T Drummond and R R Horgan

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Silver Street, Cambridge CB3 9EW, UK

Received 11 April 1991, in final form 23 May 1991

Abstract. Langevin methods have proved useful in simulating lattice field theories of many kinds. These methods are essentially a practical realization of the stochastic quantization approach to quantum mechanical systems. In this paper we wish to show that the Langevin method is effective in calculations of non-relativistic quantum mechanical systems. For a one-dimensional system a more conventional approach through the diagonalization of the Hamiltonian matrix using the method of Sturm sequencing is more efficient. However, in two and higher dimensions where the Hamiltonian is no longer tridiagonal the Langevin scheme is more efficient and accurate. It follows therefore that Langevin methods may actually have a great deal to offer in quantum mechanical problems in high dimensions especially in cases where the potential does not have spherical symmetry.

1. Introduction

In this paper we apply a second order Langevin [1-4] method with Fourier acceleration [5] to the computation of the energy levels of the anharmonic oscillator in one, two and three dimensions. We calculate the energies of the ground states and first excited states of these systems. In the one-dimensional case we compare the results with those of the more standard Sturm sequencing method for diagonalizing large matrices [6]. In higher dimensions the matrices become rapidly much larger and more complicated in structure. In these circumstances the diagonalization of the Hamiltonian becomes much less easy to bring about. The Langevin scheme is much less sensitive to the dimension of the system. It therefore becomes relatively more attractive for higher-dimensional problems, especially where the potential does not have spherical symmetry such as for the case of a particle in a crystalline environment. The Langevin scheme and the associated path-integral formalism [7] is of course closely related to probabilistic methods of analysing quantum mechanics [8].

We explain the underlying path-integral formalism together with the discrete version required for the purposes of numerical simulation in section 2. The Fourier accelerated Langevin method for evaluating the expectation values of relevant observables is described in section 3 and its extension by means of slave equations in section 4. An outline of the Sturm sequencing method as it applies to the present problem is described in section 5 and the numerical details of the simulation are given briefly in section 6. The results of the numerical simulations are presented in section 7. We consider the significance of the results in a concluding section.

0305-4470/91/174081+11$03.50

2. Theory

We wish to compute the ground state energy E_0 and the gap $\Delta E = E_1 - E_0$ between the ground state and the first excited state. We accomplish this by computing the partition function and the time correlation function of appropriate operators. The partition function Z for a quantum mechanical system at temperature T^{-1} is given by

$$Z = \sum_s e^{-E_s T}. \tag{1}$$

When $T \gg \Delta E^{-1}$ the partition function Z is dominated by the contribution from the ground state. For T sufficiently large we have

$$E_0 = -\frac{\partial}{\partial T} \log Z. \tag{2}$$

For the systems with which we shall be dealing a correlation function sensitive to the energy gap ΔE is

$$G_{ab}(t) = \langle x_a(t) x_b(0) \rangle_C = \langle x_a(t) x_b(0) \rangle - \langle x_a(t) \rangle \langle x_b(0) \rangle \tag{3}$$

where $x_a(t)$ is the ath component of the particle position operator at (Euclidean) time t and $\langle \ldots \rangle$ indicates the thermal average of the enclosed quantity. For T sufficiently large and $0 \ll t \ll T$ we have for our systems

$$G_{ab}(t) \propto \delta_{ab} e^{-\Delta E t}. \tag{4}$$

The imaginary-time Feynman path-integral formula for the partition function is [7]

$$Z = \int \mathcal{D}x(t) e^{-S} \tag{5}$$

where the paths $\{x(t)\}$ over which the integration is carried out are *periodic*, satisfying the boundary condition $x(T) = x(0)$, and S is the imaginary-time action for a particle of mass m moving in a potential $V(x)$. It is given by

$$S = \int_0^T dt \left(\tfrac{1}{2} m \dot{x}^2 + V(x)\right). \tag{6}$$

Expectation values relevant to the correlation function are given by the path integral with an appropriately modified integrand, for example

$$\langle x_a(t) x_b(0) \rangle = \frac{1}{Z} \int \mathcal{D}x(t) e^{-S} x_a(t) x_b(0). \tag{7}$$

In our simulation we make use of a discrete approximation to the path integral. The time interval T is divided into N segments of length $\varepsilon = T/N$ and correspondingly the path $x(t)$ is approximated by a sequence of points $x_n = x(n\varepsilon)$. The periodicity of the path is enforced by requiring that $x_N = x_0$. The action in this approximation becomes

$$S = \sum_{p=0}^{N-1} \left(\frac{m}{2\varepsilon} (x_{p+1} - x_p)^2 + \varepsilon V(x_p) \right) \tag{8}$$

and the path integral for the partition function takes the form

$$Z = \left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \int \prod_{p=0}^{N-1} dx_p \, e^{-S} \tag{9}$$

The corresponding integral for the relevant term in the correlation function is

$$\langle (x_n)_a (x_0)_b \rangle = \frac{1}{Z}\left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \int \prod_{p=0}^{N-1} \mathrm{d}x_p \, \mathrm{e}^{-S} (x_n)_a (x_0)_b. \tag{10}$$

In applying (2) to the discrete version of the path integral it is inconvenient to vary T by varying N with fixed ε, even though in some ways this is the most natural approach. Instead we rescale $\varepsilon \to \lambda\varepsilon$ and then we find

$$E_0 = -\frac{1}{T}\frac{1}{Z}\left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \frac{\partial}{\partial\lambda}\left(\lambda^{-(D/2)(N-1)} \int \prod_p \mathrm{d}x_p \, \mathrm{e}^{-S_\lambda}\right)\Bigg|_{\lambda=1} \tag{11}$$

with

$$S_\lambda = \sum_{p=0}^{N-1}\left(\frac{m}{2\varepsilon\lambda}(x_{p+1}+x_p)^2 + \lambda\varepsilon V(x_p)\right). \tag{12}$$

This gives

$$E_0 = \frac{1}{Z}\left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \int \prod_p \mathrm{d}x_p \left[\frac{d}{2\varepsilon} + \frac{1}{N\varepsilon}\sum_p \left\{-\frac{m}{2\varepsilon}(x_{p+1}+x_p)^2 + \varepsilon V(x_p)\right\}\right] \mathrm{e}^{-S}. \tag{13}$$

The term in curly brackets above is the discrete version of H_p, the Euclidean energy density operator. That is

$$H_p = -\frac{m}{2\varepsilon}(x_{p+1}+x_p)^2 + V(x_p)\varepsilon. \tag{14}$$

Note that the expression for the ground state energy has a contribution, the first term in the integrand of (13), that is divergent in the limit $\varepsilon \to 0$. Its presence is due to the normalization factor in the definition of the path-integral [7]. The ground state energy is thus the difference between two terms both of which are large in the limit of small lattice spacing. This feature does not, in general, augur well for the numerical approach since the signal-to-noise ratio of such a difference of large numbers is likely to be much less than that of each of the two terms individually. Fortunately, in this case the problem is not serious. We can see why by examining the case of a free particle. We have

$$\frac{1}{Z_0}\left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \int \prod_p \mathrm{d}x \frac{1}{N\varepsilon}\sum_p \frac{m}{2\varepsilon}(x_{p+1}-x_p)^2 \, \mathrm{e}^{-S_0} = D\left[\frac{1}{2\varepsilon} - \frac{1}{2T}\right] \tag{15}$$

where $S_0 = \Sigma_p \, (m/2\varepsilon)(x_{p+1}-x_p)^2$. Clearly the divergence arises from the integral of the kinetic term over the Wiener measure. This will also be true in (13). In the interacting case the potential generates important corrections but these remain finite in the limit $\varepsilon \to 0$. For large N a numerical evaluation of this integral will give a very good estimate of the divergent term since it is given by the average of the results from N identical gaussian integrals. The error consequently drops like $N^{-1/2}$ which for fixed ε corresponds to $T^{-1/2}$. This analysis extends to the full calculation of E_0 since the signal is the average of a *local* operator over the whole lattice and so the full error also drops like $N^{-1/2}$. This error is, of course, also reduced by the usual statistical factor equal to the square-root of the number of statistically independent evaluations, C, of the energy operator. The overall error is thus reduced by a factor $(NC)^{-1/2}$: NC is essentially the number of independent *lattice site* updates (in our case a typical value is of order 10^6). Since the errors are expected to be small the divergent term may be subtracted to give an accurate estimate for the ground state energy, E_0. In practice we

reduce the error yet further by measuring E_0 relative to the ground state energy, $E_0^{(0)}$, of a particle in a harmonic-oscillator potential. By performing a simulation of the harmonic-oscillator model in parallel with the original simulation using the same random numbers we can minimize the effect of statistical fluctuations on our estimate of the ground state energy.

$$E_0 - E_0^{(0)} = \frac{1}{Z}\left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \int \prod \mathrm{d}x_p \frac{1}{N\varepsilon} \sum H_p \, \mathrm{e}^{-S} - \frac{1}{Z^{(0)}}\left(\frac{m}{2\pi\varepsilon}\right)^{ND/2} \int \prod \mathrm{d}x_p \frac{1}{N\varepsilon} \sum H_p^{(0)} \, \mathrm{e}^{-S^{(0)}}. \tag{16}$$

The parameters of the harmonic-oscillator model are chosen so that $E_0^{(0)} \simeq E_0$. Because the estimates of the divergent pieces in both terms depend on the same random numbers the cancellation is more accurate than that the result of subtracting the divergence by hand.

The discrete version of the Green function which reveals the excitation ΔE is

$$G_{r,ab} = \langle (x_r)_a (x_0)_b \rangle_C = \langle (x_r)_a (x_0)_b \rangle - \langle (x_r)_a \rangle \langle (x_0)_b \rangle. \tag{17}$$

In fact considerable improvement in statistics can be obtained by replacing x_r in this correlator by the extended operator X_r where

$$X_r = \frac{1}{M} \sum_{m=r}^{M+r-1} x_m. \tag{18}$$

We then define $\mathcal{G}_{r,ab}$ so that

$$\mathcal{G}_{r,ab} = \langle (X_r)_a (X_0)_b \rangle_C = \langle (X_r)_a (X_0)_b \rangle + \langle (X_r)_a \rangle \langle (X_0)_b \rangle. \tag{19}$$

For $M \ll r \ll N$

$$\mathcal{G}_{r,ab} \propto \mathrm{e}^{-\Delta E t} \tag{20}$$

where $t = r\varepsilon$.

3. The Langevin method

The energies and correlation functions of the quantum system are evaluated as expectation values over the distribution function e^{-S}. We realize this distribution numerically by producing sample configurations from the Langevin updating scheme introduced by Parisi [1–4]. This amounts to integrating the stochastic differential equation [9]

$$\frac{\mathrm{d}}{\mathrm{d}\tau} x_r = U_r(x) + w_r(\tau) \tag{21}$$

where τ is the artificial Langevin time variable, $w(\tau)$ is a white noise process satisfying

$$\langle (w_r)_a(\tau)(w_s)_b(\tau') \rangle = 2\delta_{rs}\delta_{ab}\delta(\tau - \tau') \tag{22}$$

and

$$U_r(x) = -\frac{\partial}{\partial x_r} S. \tag{23}$$

The simplest discrete algorithm for carrying out this integration numerically is

$$\Delta x_r = U_r(x)\Delta\tau + (2\Delta\tau)^{1/2}\eta_r. \tag{24}$$

The components of the vectors η_r are independent Gaussian random numbers of zero mean and unit variance. The samples making up the numerical ensemble are obtained by first equilibrating the system and then selecting a configuration for measurement at appropriate intervals in τ. The above updating algorithm realizes the required distribution to within an error of $O(\Delta\tau)$.

In order to obtain better control over the systematic errors we use a higher-order Runge–Kutta type algorithm [3, 4] which realizes the distribution with an error $O(\Delta\tau^2)$. Such an algorithm involves an intermediate configuration $x^{(1)} = x + \Delta x^{(1)}$ specified by the equation

$$\Delta x_r^{(1)} = U_r(x)\Delta\tau/2 + (\Delta\tau)^{1/2}\eta_r^{(1)}. \tag{25}$$

The complete updating step is given by

$$\Delta x_r = U_r(x^{(1)})\Delta\tau + (\Delta\tau)^{1/2}(\eta_r^{(1)} + \eta_r^{(2)}) \tag{26}$$

when $\eta_r^{(1)}$ and $\eta_r^{(2)}$ are vectors with components that are independent Gaussian random numbers with zero mean and unit variance.

The above algorithm acts locally on the (one-dimensional) spacetime lattice. This has the result that the update acts more quickly on short wavelength modes than on long wavelength ones with a consequent retardation of both the full equilibration of the system and the statistical decorrelation of successive configurations. The remedy was given by Batrouni *et al* [5]. We update in Fourier transform space rather than configuration space and arrange for the longer-wavelength modes to receive an update enhanced relative that applied to the short wavelength modes. For the first-order update represented by (24) the modification of Fourier acceleration is simple. We define the Fourier transform variable $\bar{x}_k$ for $-N/2 < k \leq N/2$ to be

$$\bar{x}_k = \frac{1}{\sqrt{N}} \sum_{r=0}^{N-1} e^{-2\pi ikr/N} x_r. \tag{27}$$

Note that because the original variable x_r is real we have

$$\bar{x}_{-k} = \bar{x}_k^* \tag{28}$$

which implies that $\bar{x}_0$ and $\bar{x}_{N/2}$ are real. We can define similarly a Fourier transform version $\bar{\eta}_k$ of the random step η_r with the same reality properties as $\bar{x}_k$.

The first-order update becomes

$$\Delta\bar{x}_k = f(k)\bar{U}_k(x)\Delta\tau + (2f(k)\Delta\tau)^{1/2}\overline{\eta_k} \tag{29}$$

where

$$\bar{U}_k(x) = \frac{1}{\sqrt{N}} \sum_{r=0}^{N+1} e^{-2\pi ikr/N} U_r(x) \tag{30}$$

and where $f(k)$ is a function of the wavenumber k which is weighted towards small values of k. The particular choice of $f(k)$ made in this paper is based on intuition from the harmonic oscillator case. It is

$$f(k) = (L(N/2) + \mu^2)/(L(k) + \mu^2) \tag{31}$$

where

$$L(k) = \left(\frac{4}{\varepsilon^2}\right) \sin^2\left(\frac{\pi k}{N}\right). \tag{32}$$

The quantity $L(k)$ is the Fourier transform version of the Laplacian on the lattice. The value of the mass μ is chosen on the basis of computational experience but is related in size to the excitation energy of the system. The results are not idependent on the precise value of μ.

The steps in the update are as follows.

(i) Starting with the current value of $\bar{x}_k$ we invert the Fourier transform to obtain x_r.

(ii) From x_r we compute $U_r(x)$ and then use (30) to obtain $\bar{U}_k(x)$.

(iii) The updating formula in (29) is now used to obtain the new value of $\bar{x}_k$.

Clearly it is necessary at each stage to pass from the Fourier transform $\bar{x}_k$ to x_r and from $U_r(x)$ to its Fourier transform $\bar{U}_k(x)$. These steps are carried out by means of an effective fast Fourier transform algorithm.

The Fourier accelerated version of the second order algorithm is a natural generalization of the above, namely

$$\Delta\bar{x}_k^{(1)} = f(k)\bar{U}_k(x)\Delta\tau/2 + (f(k)\Delta\tau)^{1/2}\bar{\eta}_k^{(1)}. \tag{33}$$

The final step is given by

$$\Delta\bar{x}_k = f(k)\bar{U}_k(x^{(1)})\Delta\tau + (f(k)\Delta\tau)^{1/2}(\bar{\eta}_k^{(1)} + \bar{\eta}_k^{(2)}). \tag{34}$$

Of course we must invoke the fast Fourier transform algorithm in performing these steps in the simulation [10].

4. Slave equations

An attractive feature of the Langevin method is that it can be extended by means of slave equations [2, 4] to yield directly an estimator for the connected part of any correlation function. In the present case we are interested in the correlation function $\mathcal{G}_{r,ab}$ the asymptotic behaviour of which yields the value of the energy gap ΔE. The slave equation for this estimator can be derived by first modifying the action by the addition of a term $\boldsymbol{J}\cdot\boldsymbol{X}_0$ (see (18)). That is

$$S \to S_J = S + \boldsymbol{J}\cdot\boldsymbol{X}_0. \tag{35}$$

We exploit the fact [1, 2, 4] that

$$\langle (x_r)_a (X_0)_b \rangle_C = \frac{\partial}{\partial J_b} \langle (x_r)_a \rangle \Big|_{J=0} \tag{36}$$

where $\langle \ldots \rangle_C$ means the connected part of the corresponding correlator and it is being assumed that the averages are evaluated with the modified action S_J. It follows that the quantity $g_{r,ab} = \partial (x_r)_a / \partial J_b$ is an estimator for the above connected correlation function.

For non-zero $\boldsymbol{J}$ the langevin equation for x_r is modified by replacing S by S_J. We have

$$\frac{\mathrm{d}}{\mathrm{d}\tau} x_r = U_r^J(x) + w_k(\tau) \tag{37}$$

where

$$U_r^J(x) = -\frac{\partial}{\partial x_r} S_J. \tag{38}$$

That is

$$U_r^J(x) = U_r(x) + J_r \tag{39}$$

where $J_r = s_r J$ and $s_r = 1/M$ for $0 \leqslant r < M$ and is zero otherwise. The equation of motion for $g_{r,ab}$ can be obtained by differentiating (37) with respect to J_b. We find

$$\frac{\mathrm{d}}{\mathrm{d}\tau} g_{r,ab} = \sum_{n=0}^{N-1} \sum_c \frac{\partial}{\partial(x_n)_c} (U_r)_a g_{n,cb} + s_r \delta_{ab}. \tag{40}$$

This is the continuous time version of the slave equation for $\mathscr{G}_{r,ab}$. Note that the white noise term is not present. Its influence is felt, however, through its effect on $x(\tau)$.

The discrete time version is obtained by applying the same approach to the discrete updating algorithms for x_r. The relevant case for us is the second-order algorithm. In the unaccelerated form we find for the intermediate step

$$\Delta g_{r,ab}^{(1)} = \left(\sum_{n=0}^{N-1} \sum_c \frac{\partial}{\partial(x_n)_c} (U_r)_a g_{n,cb} + s_r \delta_{ab} \right) \Delta\tau/2. \tag{41}$$

For the final step we have

$$\Delta g_{r,ab} = \left(\sum_{n=0}^{N-1} \sum_c \frac{\partial}{\partial(x_n)_c} (U_r^{(1)})_a g_{n,cb}^{(1)} + s_r \delta_{ab} \right) \Delta\tau \tag{42}$$

where the superscript (1) indicates that the quantity has been evaluated at the intermediate point. The Fourier accelerated version is obtained by taking the Fourier transform of these equations and modifying the time step so that it depends on the wavenumber as discussed in the last section. We have for the intermediate step

$$\Delta \bar{g}_{k,ab}^{(1)} = \left(\sum_{-N/2 < q \leqslant N/2} \sum_c \mathcal{M}_{kq,ac} \bar{g}_{qcb} + h_{k,ab} \right) f(k) \Delta\tau/2 \tag{43}$$

where

$$\mathcal{M}_{kq,ac} = \frac{1}{N} \sum_{r=0}^{N-1} \sum_{s=0}^{N-1} \mathrm{e}^{+2\pi i k r} \mathrm{e}^{2\pi i q s} \frac{\partial}{\partial(x_s)_c} (U_r) \tag{44}$$

and

$$h_{k,ab} = \sum_{r=0}^{N+1} s_r \, \mathrm{e}^{-2\pi i k r} \delta_{ab}. \tag{45}$$

The final step is

$$\Delta \bar{g}_{k,ab} = \left(\sum_{+N/2 < q \leqslant N/2} \mathcal{M}_{kq,qc}^{(1)} \bar{g}_{q,cb}^{(1)} + h_{k,ab} \right) f(k) \Delta\tau. \tag{46}$$

Here the superscript (1) has the same significance as before indicating a quantity evaluated at the intermediate point.

Finally we construct the estimator for $\mathscr{G}_{r,ab}$. It is

$$\sum_{s=r}^{M+r-1} g_{s,ab}/M. \tag{47}$$

5. Diagonalization of the Hamiltonian

In order to have a basis for comparing the Langevin method with more conventional methods for potential problems we considered an evaluation of the energy levels as

the eigenvalues of an appropriate Hamiltonian matrix. For the present problem the natural form for such a matrix is obtained by creating a grid of sufficient extent and density in the position space of the particle. For the one-dimensional system we have

$$H_{xx'} = -\frac{1}{2m}\nabla_+\nabla_- + V(x)\delta_{xx'} \tag{48}$$

where the points x lie on the grid at a separation a and $\nabla_\pm$ are the forward and backward difference operators on the spatial grid. We have

$$\nabla_+\nabla_- = \frac{1}{a}\begin{pmatrix} -2 & 1 & 0 & \cdots & \\ 1 & -2 & 1 & \cdots & \\ 0 & 1 & -2 & \cdots & \\ & & & \ddots & \\ & & & & 1 \\ & & & 1 & -2 \end{pmatrix} \tag{49}$$

Because this matrix is tridiagonal it is possible to compute its eigenvalues very efficiently by an algorithm based on a Sturm sequence method [6] for solving for the zeros of the characteristic polynomial. In practice we were able to obtain a 1% level of accuracy by using a grid of 1000 points with a separation $a = 0.1$. Some of the results are quoted in table 1.

Table 1. Results for the 1D anharmonic oscillator. The potential is $V(x) = ax^2 + bx^4$. The theoretical results are from a Sturm sequencing evaluation of the eigenvalues.

a	b	E_0	ΔE	E_0^{th}	ΔE^{th}
0.0	1.0	0.666 ± 0.003	1.720 ± 0.002	0.668	1.726
0.0	2.0	0.8364 ± 0.004	2.162 ± 0.005	0.842	2.174
0.0	11.0	1.438 ± 0.002	3.805 ± 0.08	1.486	3.837
0.5	1.0	0.8029 ± 0.0002	1.928 ± 0.002	0.804	1.934
0.5	10.0	1.460 ± 0.002	3.781 ± 0.1	1.372	3.617
−0.5	1.0	0.511 ± 0.002	1.502 ± 0.002	0.515	1.506
−1.0	1.0	0.334 ± 0.002	1.271 ± 0.003	0.338	1.275
−2.0	1.0	-0.136 ± 0.002	0.784 ± 0.03	−0.130	0.791
+2.5	1.0	-0.469 ± 0.002	0.547 ± 0.03	−0.460	0.558
−3.0	1.0	-0.909 ± 0.002	no convergence	−0.895	0.352

For higher dimensions D the attainment of comparable accuracy requires the use of a matrix of size $1000^D \times 1000^D$. Not only does this rapidly become formidably large but it does not have the simple tridiagonal shape of the one-dimensional problem thus precluding the straightforward application of the Sturm sequencing method for finding the eigenvalues. We were not able to obtain conveniently, acceptable results for these higher-dimensional problems using the Sturm sequencing method.

6. Numerical simulation

In applying the above algorithm we used a lattice length $N = 256$, a lattice spacing $\varepsilon = 0.1$, a Langevin time step in the range $\Delta\tau = 0.001$ to 0.004 and an interval between

measurements of 10 iterations. since correlations between results appeared to persist for about 10 measurements, the Langevin correlation time for measurements was roughly $\tau_{cor} = 0.4$. The precise value is sensitive to the value of the acceleration mass parameter which was chosen to be $\mu^2 = 4.0$ so as to be comparable with the first excitation energies of the systems that we investigated. The lattice was equilibrated for 1000 iterations before measurements were begun.

The computer we used was an AMT DAP 610 which because of its highly parallel architecture allowed us to update 16 independent lattices simultaneously. The statistical errors quoted are based on the following numbers.

Dimensions	number of iterations	CPU time (s)
1	10 000	3300
2	7 000	6130
3	6 000	9940

In order to assess the significance of times for the above runs we note that the DAP 610 runs at approximately 40 M flops.

7. Numerical results

The particular form of the anharmonic potential we used was in one dimension,

$$V(x) = ax^2 + bx^4 \tag{50}$$

and in two and higher dimensions,

$$V(x) = ax^2 + b(x^2)^2 + c\sum_i x_i^4. \tag{51}$$

The results of the simulation for a one-dimensional oscillator are shown in table 1 where they are compared with the results of Sturm sequencing. The two sets of figures agree to within 1% for most choices of the parameters in the potential except perhaps for some of the larger values of these parameters. The discrepancy is very probably due to the size of the lattice spacing.

The two-dimensional oscillator results are shown in table 2. Here the theoretical results are inferred from the analytical results of Hioe *et al* [11]. Again the correspondence between simulation and theory is quite acceptable although there is again an understandable tendancy to show discrepancies for the larger values of the parameters. In three dimensions we were unable to find theoretical results with which to compare those of our simulation. The results, however, show acceptable scaling properties in the coupling b or c when the other two couplings are zero. In each case we expect the result to behave as $b^{1/3}$ or $c^{1/3}$. The results of this scaling prediction are shown in the theory column of table 3 and are quite reasonably consistent with those of our simulation.

It should be remarked that the Green functions $\mathcal{G}_{r,at}(t)$, from which the values of ΔE were extracted, in all cases fitted a simple exponential form very well for $t > 2$, and the numerical errors on these functions were too small to be discernible in graphical plots of $\mathcal{G}$.

Table 2. Results for the 2D anharmonic oscillator. The potential is $V(x) = ax^2 + b(x^2)^2 + c\Sigma_i x_i^4$. The theoretical results are based on those of Hioe *et al.* *means that appropriate scaling has been applied to compute the results and †means that scaling and interpolation has been used.

0.0	1.0	1.0	1.765 ± 0.002	2.279 ± 0.004	1.780†	2.311†
0.0	1.0	5.0	2.415 ± 0.004	3.20 ± 0.01	2.478†	3.340†
0.5	0.0	1.0	1.595 ± 0.002	1.927 ± 0.003	1.6075	1.9342
0.5	0.0	1.0	1.326 ± 0.002	1.719 ± 0.004	1.3370*	1.7264*
−0.05	0.0	1.0	1.023 ± 0.0008	1.510 ± 0.003		
−1.0	0.0	1.0	0.668 ± 0.0008	1.280 ± 0.003		
−2.0	0.0	1.0	−0.273 ± 0.002	1.926 ± 0.002		
0.0	1.0	0.0	1.467 ± 0.002	1.926 ± 0.002	1.478*	1.9217*
0.0	5.0	0.0	2.486 ± 0.003	3.442 ± 0.005	2.5274*	3.2860*
−0.5	1.0	0.0	1.196 ± 0.001	1.730 ± 0.002		
+1.0	1.0	0.0	0.891 ± 0.001	1.531 ± 0.003		

Table 3. Results for the 3D anharmonic oscillator. The potential is $V(x) = ax^2 + b(x^2)^2 + c\Sigma_i x_i^4$. The theoretical results are based on a scaling law.

a	b	c	E_0	ΔE	E_0^{th}	ΔE^{th}
0.5	0.0	1.0	2.391 ± 0.005	1.925 ± 0.003		
0.5	0.0	5.0	3.593 ± 0.007	3.041 ± 0.02		
0.0	0.0	1.0	1.985 ± 0.005	1.716 ± 0.004		
0.0	0.0	2.0	2.497 ± 0.003	2.178 ± 0.003	2.500	2.162
0.0	0.0	4.0	3.136 ± 0.002	2.725 ± 0.006	3.151	2.724
0.0	0.0	10.0	4.172 ± 0.007	3.702 ± 0.05	4.276	3.697
0.0	1.0	0.0	2.370 ± 0.003	2.086 ± 0.002		
0.0	5.0	0.0	4.028 ± 0.005	3.6 ± ?*	4.05	3.56
−0.5	1.0	0.0	2.006 ± 0.002	1.915 ± 0.002		
−1.0	1.0	0.0	1.596 ± 0.002	1.738 ± 0.003		

8. Conclusion

We have applied a second-order Fourier accelerated Langevin method to the evaluation of the energies of the ground states and first excited states of various versions of the anharmonic oscillator. We found it easy to achieve accuracies of 1%. For the case of the one-dimensional oscillator the Langevin method was not as efficient as one based on Sturm sequencing. However, this latter method becomes rapidly less and less possible as the dimension of the oscillator increases. Already in two dimensions it involves matrices of formidably high dimension and complexity of structure to achieve comparable accuracy. The Langevin method therefore can be expected to be useful for problems in several dimensions such as those involving a number of particles. The method is particularly well suited to cases where the potential is not spherically symmetric, such as the potentials that occur in typical crystalline environments.

There are of course circumstances where the method for calculating the energy gap ΔE can be expected to encounter difficulties. In general these are situations where ΔE to the first excited state is anomalously small. Such a situation can arise in one dimension

where a, the coefficient of the quadratic term in the potential, is large and negative which results in a double well that allows only weak penetration of the barrier between the wells. The resulting energy gap between the symmetric ground state and the antisymmetric excited state is exponentially small in the barrier penetration factor. In the Langevin formalism this problem shows up in the existence of 'kink'-type instanton solutions which are stationary points of the action. It turns out that in the neighbourhood of such solutions there are configurations which give rise to negative eigenvalues for the matrix $\mathcal{M}$ in (44). This can result in an uncontrollable instability of the slave equations with a consequent breakdown of the method. General considerations show that the problem is worst when there is one kink and one antikink on the lattice which occurs for barriers of intermediate height. For very high barriers the probability of finding a kink is very small (there is virtually no tunnelling during the lifetime of the simulation). For relatively low barriers there are many kink-antikink pairs on the lattice and the tunnelling is well simulated. In higher dimensions this situation does not arise so easily in the anharmonic oscillator potentials we have considered since barriers of the kind encountered in one dimension are not so readily constructed. For example, in two dimensions the Mexican hat potential has a stationary point on the peak but the lifetime in the simulation of any configurations with lattice fields on or near the peak is very short: there are no stabilizing topological constraints preventing the decay of such configurations to more likely ones which lie mainly around the brim. Hence in more than one dimension where our method is most applicable the instabilities associated with instanton configurations are much less likely to occur. It should finally be emphasized that these instabilities affect the measurement of ΔE only, and in all circumstances and in all dimensions studied the evaluation of the ground state energy suffered no such instability.

References

[1] Parisi G and Wu Yongshi 1981 *Sci. Sin.* **24** 483
[2] Parisi G 1981 *Nucl. Phys.* B **180** [FS 2] 378
[3] Drummond I T, Duane S and Horgan R R 1983 *Nucl. Phys.* B **220** [FS8] 119
[4] Drummond I T, Duane S and Horgan R R 1987 *Nucl. Phys.* B **280** [FS18] 25
[5] Batrouni G, Katz G R, Kronfeld A S, Lepage G P, Svetitsky B and Wilson K G 1985 *Phys. Rev.* D **32** 2736
[6] Wilkinson J H 1965 *The Algebraic Eigenvalue Problem* (Oxford: Oxford University Press)
[7] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
[8] Simon B, Truman A and Davies I M (eds) 1989 *Proc. 9th IAMP Congress, Swansea 1988* (Bristol: Hilger) pp 234–63
[9] Sobczyk K 1991 *Stochastic Differential Equations* (Dordrecht: Kluwer Academic)
[10] Press W H, Flannery P, Teukolsky S A and Vetterling W T 1986 *Numerical Recipes* (Cambridge: Cambridge University Press)
[11] Hioe F T, MacMillen D and Montroll E W 1978 *Phys. Rep.* **43** 305