Finding all the stationary points of a potential-energy landscape via numerical polynomial-homotopy-continuation method

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The stationary points (SPs) of a potential-energy landscape play a crucial role in understanding many of the physical or chemical properties of a given system. However, unless they are found analytically, no efficient method is available to obtain *all* the SPs of a given potential. We present a method, called the numerical polynomial-homotopy-continuation method, which numerically finds all the SPs, and is *embarrassingly parallelizable*. The method requires the nonlinearity of the potential to be polynomial-like, which is the case for almost all of the potentials arising in physical and chemical systems. We also certify the numerically obtained SPs so that they are independent of the numerical tolerance used during the computation. It is then straightforward to separate out the local and global minima. As a first application, we take the XY model with power-law interaction, which is shown to have a polynomial-like nonlinearity, and we apply the method.

Introduction. A potential-energy landscape (PEL) is the hypersurface of some given potential $V(\vec{x})$, with $\vec{x} = (x_1, x_2, \ldots, x_N)$ being the variables (e.g., position coordinates, fields, etc.). Studying the stationary points (SPs) of the PEL, defined by the solutions of the system of N equations $\frac{\partial V(\vec{x})}{\partial x_i} = 0, i = 1, \ldots, N$, is crucial for learning many physical or chemical properties of the system described by $V(\vec{x})$. The SPs are classified according to the number of negative eigenvalues of the Hessian matrix, $\mathcal{H}$, evaluated at each SP. The SPs with no negative eigenvalue are called minima, and the SPs with at least one negative eigenvalue are called saddles. In statistical mechanics, for example, the stationary points of the PEL have been shown to be directly related to the nonanalyticity of thermodynamic quantities (i.e., phase transitions) in the respective models [1]. The global minimum of a spin-glass model is invaluable for studying its equilibrium properties. In theoretical chemistry, the study of properties of the PEL of supercooled liquids and glasses has been a very active area of research [2,3], specifically in the study of Kramer's reaction-rate theory for the thermally activated escape from metastable states and the computation of various physical quantities, such as the diffusion constant using the minima of the PEL [2]. In string theory, the SPs of the PEL of various supersymmetric potentials correspond to the so-called string vacua. Many current activities in string-phenomenology areas focus on developing different methods to find these string vacua [4–6].

If *all* SPs are found analytically for the given $V(\vec{x})$, then the problem is settled, obviously. But if the analytical solutions are intractable, then one has to rely on alternative methods. Though finding SPs is of the utmost importance in so many areas, the number of rigorous methods of finding SPs are few, compared to the number of methods for minimizing a potential.

One such method is the gradient-square-minimization method in which one minimizes $W = |\vec{\nabla} V(\vec{x})|^2$ using a traditional numerical-minimization method such as conjugate gradient, simulated annealing, etc. [7,8]. The minima of W,

with further restriction that $W = 0$, are the SPs of $V(\vec{x})$. However, minima of W also exist, where $W > 0$, and it has been shown that the number of these non-SPs grows as the system size increases [9,10], thus making the method inefficient.

The Newton-Raphson method (and its sophisticated variants) may also be used to solve the system of N nonlinear equations $\frac{\partial V(\vec{x})}{\partial x_i} = 0, i = 1, \ldots, N$. Here, an initial random guess is fed, and then refined to a given numerical precision, to obtain a solution of the system [9,11]. However, this method still suffers the major drawbacks of the gradient-square-minimization method: namely, the possible existence of large basins of attraction may lead us to repeatedly obtain the same SPs and, more importantly, no matter how many times we iterate the respective algorithms with different initial guesses, we are never sure if we have found all SPs.

If the system of stationary equations has polynomial-like nonlinearity, then the situation is enhanced. In the string-theory community, for such a system of equations, symbolic methods based on the Gröbner basis technique are used to solve the system [4–6], which ensure that all the SPs are obtained when the computation finishes. Roughly speaking, for a given system of multivariate polynomial equations (which is known to have only isolated solutions), the so-called Buchberger algorithm (BA) or its refined variants can compute a new system of equations, called a Gröbner basis, in which the first equation consists of only one of the variables, and the subsequent equations consist of increasing numbers of variables. The solutions of this alternative system remain the same as the original system, but the former is easier to solve. This method seems to resolve all of the above-mentioned problems. However, a few other problems occur. The BA is known to have suffered from the exponential space complexity, i.e., the memory (random access memory) required by the machine blows up exponentially with the number of variables, equations, and terms in each polynomial, etc. So, even for small-sized systems, one may not be able to compute a Gröbner basis. The BA is also inefficient for systems with irrational coefficients. Furthermore, the BA is highly sequential.

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In this Rapid Communication, we present the numerical polynomial-homotopy-continuation (NPHC) method which solves all the above problems for systems of equations with polynomial-like nonlinearity. Numerical continuation methods have been around for some time [12] and the polynomial-homotopy-continuation method has also been an active area of research [13,14]. (See [15,16] for earlier accounts on the NPHC method for various areas in theoretical physics.) As with the Gröbner basis technique, the NPHC method extensively uses concepts from complex algebraic geometry, and hence we allow the variables to take values from the complex space, even if the physically important solutions are only the real ones. When a system of polynomial equations is known to have only isolated solutions, the NPHC guarantees that we obtain all complex solutions of the system, from which all the real solutions can subsequently be filtered out.

Numerical polynomial-homotopy-continuation method. Here we introduce the NPHC method to solve a system of multivariate polynomial equations. Specifically, we consider a system $P(\vec{x}) = 0$, which is known to have isolated solutions and where $P(\vec{x}) = (\frac{\partial V(\vec{x})}{\partial x_1}, \ldots, \frac{\partial V(\vec{x})}{\partial x_N})$. Now, the classical Bézout theorem asserts that for a system of N polynomial equations in N variables that is known to have only isolated solutions, the maximum number of solutions in $\mathbb{C}^N$ is $\prod_{i=1}^{N} d_i$, where d_i is the degree of the ith polynomial. This bound is called the classical Bézout bound (CBB).

Based on the CBB, a homotopy can be constructed as $H(\vec{x},t) = \gamma(1-t)Q(\vec{x}) + t\,P(\vec{x}) = 0$, where γ is a random complex number. The new system $Q(\vec{x}) = (q_1(\vec{x}), \ldots, q_N(\vec{x}))$, called the *start system*, is a system of polynomial equations with the following properties: (1) The solutions of $Q(\vec{x}) = H(\vec{x},0) = 0$ are known or can be easily obtained. The solutions of $Q(\vec{x}) = 0$ are called start solutions. (2) The number of solutions of $Q(\vec{x}) = H(\vec{x},0) = 0$ is equal to the CBB of $P(\vec{x}) = 0$. (3) The solution set of $H(\vec{x},t) = 0$ for $0 \leqslant t \leqslant 1$ consists of a finite number of smooth paths, each parametrized by $t \in [0,1)$. (4) Every isolated solution of $H(\vec{x},1) = P(\vec{x}) = 0$ can be reached by some path originating at a solution of $H(\vec{x},0) = Q(\vec{x}) = 0$. We can then track all the paths corresponding to each start solution from $t = 0$ to $t = 1$ and reach (or diverge from) $P(\vec{x}) = 0 = H(\vec{x},1)$. It is shown rigorously that for a generic value of complex γ, all paths are regular for $t \in [0,1)$, i.e., there is no singularity along the path [13]. By implementing an efficient-path-tracker algorithm, such as Euler's predictor and Newton's corrector method, all isolated solutions of $P(\vec{x}) = 0$ can be obtained. We do not delve into the discussion of the actual-path-tracker algorithms used in practice in this Rapid Communication, except to mention that in the path-tracker algorithms used in practice, almost all apparent difficulties have been resolved, such as tracking singular solutions, multiple roots, and solutions at infinity [13].

As a trivial illustration, let us take the univariate polynomial $P(x) = x^2 - 5 = 0$ from [13]. To find its solutions, we may, for example, choose $Q(x) = (x^2 - 1)$ as our start system as it satisfies the twin criteria of having the same number of solutions as the CBB of $P(x)$ and of being easily solved to obtain the start solutions $x = \pm 1$. The problem of getting all solutions of $P(x) = 0$ now reduces to simply tracking

the solutions of $H(x,t) = 0$ from $t = 0$ to $t = 1$ so that the paths beginning at $x = \pm 1$ lead us to the actual solutions $x = \pm\sqrt{5}$. Note that, in general, if there are more start solutions than actual solutions, then the remaining paths diverge as t approaches 1.

Several sophisticated computational packages exist, such as PHCPACK [17], BERTINI [18], and HOM4PS2 [19], which can be used to solve systems of univariate and, more importantly, multivariate polynomial equations, and the packages are available as freeware. For the sake of completeness, the solutions of the above-mentioned univariate equation are $x = \pm(2.236067977 + i\,10^{-10})$, i.e., $\pm\sqrt{5}$ up to the numerical precision.

Since each path can be tracked independently of all others, the NPHC is known as being *embarrassingly parallelizable*, a feature that makes it very efficient.

The multivariate case, $Q(\vec{x}) = (x_1^{d_1} - 1, \ldots, x_N^{d_N} - 1)$, is the simplest choice as a start system. For big systems, solving the start system itself may take significantly more time in general, although due to the simple form of the start system for the total-degree homotopy, obtaining the start solutions is straightforward. Once all the paths are tracked, we get all the complex solutions. To filter out the real solutions, we have to take more care. Here, by a 'solution' (complex or real) means a set of numerical values of the variables which satisfies each of the N equations with a given tolerance, $\triangle_{\text{sol}}$ ($\sim 10^{-10}$ in our setup). Since the variables are allowed to take complex values, all the solutions come with real and imaginary parts. We call a solution a real solution if the imaginary part of each of the variables is less than or equal to a given tolerance. [Note that $\triangle_{\mathbb{R}}$ ($\sim 10^{-7}$) is a robust tolerance for the equations we will be dealing with in the next section, below which the number of real solutions does not change.] All these solutions can be further refined with an arbitrary precision up to the machine precision.

The obvious question at this stage is whether the number of real solutions depends on $\triangle_{\mathbb{R}}$. To resolve this issue, we use a very recently developed algorithm, called alphaCertified, which is based on the so-called α-theory to certify the real nonsingular solutions of polynomial systems using both exact rational arithmetic and arbitrary precision-floating-point arithmetic [20]. This is a remarkable step because, using alphaCertified, we can prove that a solution classified as a real solution is actually a real solution independent of $\triangle_{\mathbb{R}}$, and hence these solutions are as good as the exact solutions.

A first application. As a first application, we choose the XY model a with long-range power-law (algebraically decaying) interaction, defined as $V(\vec{\theta}) = K \sum_{i=1}^{N} \sum_{j=1}^{\frac{(N-1)}{2}} \frac{1 - \cos(\theta_i - \theta_{i+j})}{j^\alpha}$, where N is odd for our purposes, the normalization constant $K = (2 \sum_{j=1}^{\frac{(N-1)}{2}} \frac{1}{j^\alpha})^{-1}$, and $\alpha \in [0,\infty)$ [21]. $\alpha = 0$ reproduces the mean-field XY model and $\alpha \to \infty$ reproduces the nearest-neighbor-coupling XY model for which all the SPs are analytically obtained [15,22,23]. We choose $\alpha = 0.75$, for which the coefficients take values from $\mathbb{R}$, unlike, for example, $\alpha = 1$, for which the coefficients are rational numbers. Hence, we are already in the domain of problems where the Gröbner basis technique is inefficient. We impose a periodic boundary condition, i.e., $\theta_{k+N} = \theta_k$. Spin-glass models with power-law

interaction have recently gained interest [24]. The chosen model is one of the simplest models of this kind with a continuous symmetry. The stationary equations are $\frac{\partial V(\vec{\theta})}{\partial \theta_k} = K \sum_{j=1}^{\frac{(N-1)}{2}} [\frac{\sin(\theta_k - \theta_{k+j}) + \sin(\theta_k - \theta_{k-j})}{j^\alpha}] = 0$, for $k = 1, \dots, N$. To eliminate the global-rotation symmetry $\theta_k \to \theta_k + \phi$, where $\phi \in \mathbb{R}$, we fix one of the angles, say $\theta_N = 0$, and remove the Nth equation out of the system, as done in [15,23]. Kastner [21] used a specific class of known solutions, called the stationary wave solutions, i.e., $\theta_m^{(n)} = \frac{2\pi mn}{N}$, where $m, n \in \{1, \dots, N\}$. Many more solutions for this model are possible, as discussed below.

The above system of equations is not a system of polynomial equations. But we can transform it into one [15,16] by first using the trigonometric identities $\sin(\theta_k - \theta_{k+j}) = \sin\theta_k \cos\theta_{k+j} - \sin\theta_{k+j}\cos\theta_k$, etc.; abbreviating each $\sin\theta_k = s_k$ and $\cos\theta_k = c_k$, in all the $N-1$ equations; and, finally, adding $N-1$ additional constraint equations as $s_k^2 + c_k^2 - 1 = 0$, for $k = 1, \dots, N-1$. We get a system of $2(N-1)$ polynomial equations consisting of $2(N-1)$ algebraic variables c_ks and s_ks:

$$K \sum_{j=1}^{\frac{(N-1)}{2}} \frac{(s_k c_{k+j} - s_{k+j} c_k + s_k c_{k-j} - s_{k-j} c_k)}{j^\alpha} = 0,$$
$$s_k^2 + c_k^2 - 1 = 0, \tag{1}$$

for $k = 1, \dots, N-1$. The removal of the global-rotation symmetry ensures that the system will have only isolated solutions. We can now use the NPHC to (i) solve Eq. (1) for all the s_ks and c_ks, (ii) filter the real solutions out using the above-mentioned tolerances, and (iii) get the original θ variables back by $\theta_k = \tan^{-1}(\frac{s_k}{c_k}) \in (-\pi, \pi]$, for all $k = 1, \dots, N-1$. The results are as follows.

First, the number of SPs for $N = 3, 5, 7, 9, 11, 13$ are $6, 20, 168, 972, 4774, 24\,830$, respectively. Figure 1(a) shows the number of SPs as a function of N. The SPs for different models with similar sizes have been studied using the gradient-square-minimization and Newton-Raphson's methods, though the final number of SPs is always open to debate [9,10], whereas, using the NPHC method, we can find all the SPs with confidence. In the gradient-square-minimization method, it is difficult to obtain the SPs with higher indices [9]. In the NPHC, however, all the SPs are treated equally, irrespective of their indices. Figure 1(b) shows the index $I/(N-1)$ versus number of SPs for a given N. Apparently, the number of minima grows linearly in this model, which is contrary to current understanding [9,10]. However, the number of SPs indeed grows exponentially with increasing system size, as expected [9,10]. We also observe that the global minimum is always the configuration with all $\theta_i = 0, i = 1, \dots, N-1$, and that at the global minimum, the energy density V/N is zero. In Fig. 2, we plot V/N versus I for $N = 7, 9, 11, 13$. The apparent nonlinear relation between these two quantities in the plots shows a different behavior to the linear relationship observed for the Lennard-Jones models [9,10]. Note that to solve the systems presented here, we have mainly used a regular desktop computer, except in the largest systems (i.e., $N = 13$), for which we have used a cluster with a parallel version of the NPHC method. In the systems for $N \leqslant 9$, the
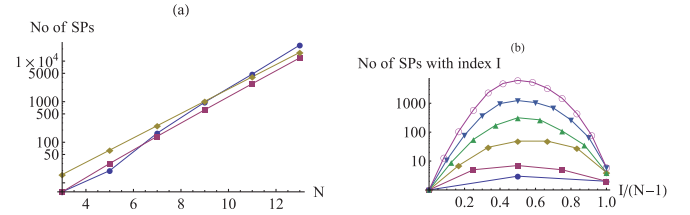

FIG. 1. (Color online) (a) Plot for N vs number of SPs. Circles, squares, and diamonds represent data points for the algebraic-decaying XY model, the one-dimensional nearest-neighbor XY model for periodic conditions [15,23], and antiperiodic conditions [22], respectively. The lines are drawn as a guide. (b) The plot for index I vs number of SPs with index I. From top to bottom, $N = 13, 11, 9, 7, 5, 3$. The normalization on I is $N - 1$ since we have taken $\theta_N = 0$.

desktop machine was able to track all the paths in less than an hour, for $N = 11$ all the paths were tracked in around 5 hours, and for $N = 13$ all the paths were tracked in around 30 processor hours.

Although it is quite difficult to claim any result in the thermodynamic limit using such small-sized systems, we note that the minimum value of $|\text{Det}\mathcal{H}|^{1/N}$ is always either at the SPs, where all $\theta_i \in \{0, \pi\}$ for all $i = 1, \dots, N-1$, or at the SPs, where $\theta_{i+1} - \theta_i = \frac{2\pi k}{N} \mod 2\pi$ for all $i = 1, \dots, N$, with k being an integer. Using a recently spelled out condition for a class of spinglass models to have phase transition, that $|\text{Det}\,\mathcal{H}|^{1/N}$ evaluated at a class of stationary points tend to go to zero at the critical energy in the $N \to \infty$ limit, the phase transition in our model would occur at this specific class of solutions [25,26]. For $N = 7, 9, 11, 13$, the corresponding plots are drawn in Fig. 3, where the plot has started to fill by densely populated points around the critical-energy density $V/N \sim 0.5$. Hence, we have reproduced the results that Kastner worked out from another approach [21], just by studying these small-sized systems. These particular SPs are usually neither minima nor maxima. It should be stressed that this is a remarkable result since we extracted the information about the energy density at the phase transition without having to evaluate any complicated multidimensional path integration. All we needed for our approach was to find the SPs and to
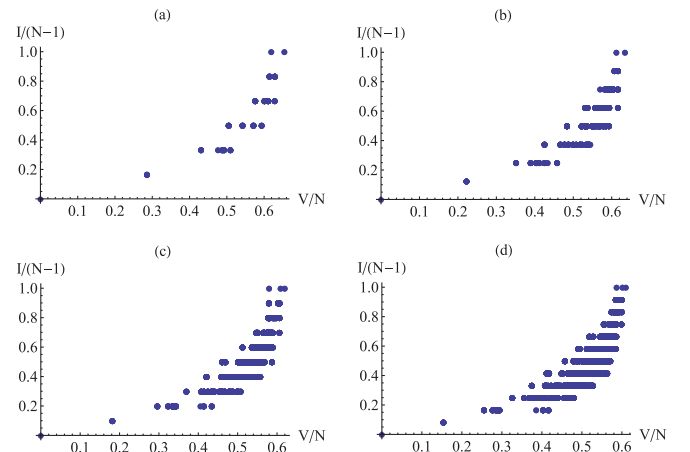

FIG. 2. (Color online) Plot for V/N vs index density. Starting from the upper left corner, $N = 7, 9, 11, 13$, respectively.
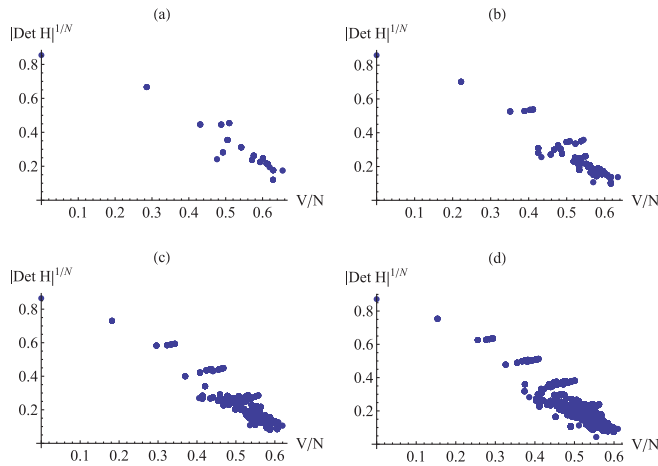
FIG. 3. (Color online) Plot for V/N vs $|\text{Det } \mathcal{H}|^{1/N}$. Starting from the upper left corner, $N = 7,9,11,13$, respectively. Though these small-sized systems can in no way be considered as representatives of the model in the thermodynamic limit, we still see the expected singularity of $|\text{Det } \mathcal{H}|^{1/N}$ at $V/N \to 0.5$.

filter out those SPs which satisfied the criteria of the above condition. Moreover, this specific class of SPs would not have been found using any other numerical minimization methods (because they would have found only the minima) or any other numerical methods (since they may not have hit these SPs at all).

It would be interesting to get all the SPs for $\alpha \in (1,2]$, find out the relevant SPs for the phase transition, and extrapolate the analysis in the thermodynamic limit, as suggested in [21]. A recent conjecture that the critical-energy density of a class of spin-glass models can be computed using only the Ising-like SPs (see [27] for the definition of these SPs and the conjecture) will need to be verified, and this will also be another important application of the NPHC method.

Conclusion. In this Rapid Communication, we have described and applied a method, called the numerical polynomial-homotopy-continuation method, that finds all SPs of a given potential, provided that the potential has polynomial-like nonlinearity. As shown in this Rapid Communication, even if the given potential is not apparently in polynomial form, its stationary equations could be transformed into a polynomial form by adding suitable constraint equations. So, the method is very widely applicable. Because the method can find all SPs, and because it is completely parallelizable, the method is quite promising for further application in many areas of theoretical physics and chemistry, for example, finding all the SPs and hence all the minima of the Lennard-Jones potential and its numerous variants, obtaining the string vacua of the models for which the symbolic algebraic geometry methods fail due to their algorithmic complexities, and studying phase transitions in various spin-glass models with the above-mentioned criterion on the Hessian determinant. We anticipate that this work will encourage research in related areas.

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