Maximum-entropy principle with moment recursion relations as constraints

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We employ the maximum entropy ansatz to obtain reasonably accurate densities for a few quantum oscillators and discrete dynamical systems. An optimization scheme is suggested that does not require any *a priori* knowledge of values for moments. Instead, moment recursion relations are used as constraints. Pilot calculations, with trial densities conforming to correct asymptotic behavior as and when necessary, reveal the advantages readily.

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I. INTRODUCTION

The maximum entropy principle (MEP) [1] provides a recipe for constructing a probability density (PD) $p(x)$, $x \in [a,b]$ with the usual assumption that the power moments μ_n, $n=0,1,2,\ldots,N$, are available as input. The MEP prescription is to maximize the information entropy

$$S=-\int_a^b p(x)\ln p(x)dx \tag{1}$$

subject to these moment constraints. Introducing $(N+1)$ Lagrange parameters $\lambda_0,\lambda_1,\ldots,\lambda_N$ the constrained optimization problem yields the formal approximate solution [2]

$$\tilde{p}(x)=\exp\left(-\sum_n^N \lambda_{n=0}x^n\right)=\exp[-\tilde{g}(x)]. \tag{2}$$

The parameters λ_i are determined from the following set of nonlinear equations:

$$\int_a^b x^j \exp\left(-\sum_{n=0}^N \lambda_n x^n\right)dx=\mu_j, \quad j=0,1,2,\ldots,N. \tag{3}$$

The success of this scheme rests mainly on (i) the largeness of N and (ii) the ability to solve Eq. (3). The knowledge of the moments presupposes that the exact $p(x)$ is somehow known *beforehand*. In that case, the MEP methodology can at best have pedagogic interest only. For many physical problems one can, however, deduce with little effort a set of *recursion* relations involving the moments although the problems are *not* exactly solvable [3]. These recursion relations have the form

$$f_n=\sum_{p=K}^L c_p\mu_{n+p}=0. \tag{4}$$

The aim of this communication is to explore how the MEP formalism can be used in conjunction with Eq. (4) to eliminate the need for the *explicit* knowledge of any moment. In Sec. II we present the general technique and apply it to two cases drawn from two very different fields of study, namely the PD corresponding to the ground states of various anharmonic oscillators and the PD of a class of logistic maps in the chaotic regime.

II. FORMALISM

We construct a trial PD $\tilde{p}(x)$ by exploiting the symmetry of the problem and the knowledge of the boundary behavior. Departing from the common practice, the optimized values of the parameters embedded in the PD are here determined from the condition that $\Delta=\Sigma_n f_n^2$ is minimum, while $\tilde{S}$ corresponding to Eq. (1) is at its maximum. To tackle the optimization problem, we introduce here three alternative schemes: (a) minimization of Δ; (b) minimization of a penalized function of the form $-\tilde{S}+10^{\gamma}\Delta$, where γ is a parameter which is gradually increased to refine the results; and (c) minimization of $\Delta/\tilde{S}$. In all these schemes, the Lagrangian multipliers appearing in Eq. (2) acquire the status of *variational* parameters. One can then use the optimized PD to compute quantities of interest. This we illustrate below by treating the case of anharmonic oscillators first, and then logistic maps.

Consider a one-dimensional quantum system defined by $H=-\nabla^2+V(x)$ with a potential of the form

$$V(x)=\sum_m^M a_m x^{2m}, \quad x\in[-\infty,\infty]; m\in\mathbb{N}. \tag{5}$$

From the symmetry of the problem, it is obvious that the odd moments vanish. The even moments satisfy a recursion relation that can be deduced [3–5] by calculating the matrix elements of the commutator $[H,[H,x^{n+2}/(n+2)]]$ between two eigenstates of H. This recursion relation has the form

$$\begin{aligned} f_n=&4E_0(n+1)\mu_n-4\sum_m a_m(n+m+1)\mu_{n+2m}\\ &+(n+1)n(n-1)\mu_{n-2}\\ =&0, \end{aligned} \tag{6}$$

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TABLE I. Testing the accuracy of optimized densities for various oscillators. Exact results [11] are quoted in parentheses.

$V(x)$	Optimization scheme	Form of $\tilde{p}(x)$	r	t	u	Number of recursion relations	E_0	R
x^4	A	MEP	3	0	1	5	1.060 365 5	1.0001
	A	MEP	4	0	1	6	1.060 362 2	0.999 996
	A	PPA	2	1	$\frac{1}{2}$	5	1.060 362 097	1.000 004
	A	PPA	2	2	$\frac{1}{4}$	5	1.060 362 094	1.000 003
	A	PPA	3	3	$\frac{1}{2}$	6	1.060 362 090 6	0.999 999 94
	B	PPA	2	1	$\frac{1}{2}$	4	1.060 362 095	0.999 9996
	B	PPA	2	4	$\frac{1}{8}$	6	1.060 362 090 5	1.000 000 03
	C	PPA	2	1	$\frac{1}{2}$	5	1.060 362 097	1.000 004
	C	PPA	2	4	$\frac{1}{8}$	6	1.060 362 090 5	1.000 000 06
							(1.060 362 090 48)	
x^2+x^4	A	PPA	2	1	$\frac{1}{2}$	5	1.392 351 641 7	1.000 001 5
	A	PPA	2	2	$\frac{1}{4}$	5	1.392 351 641 7	1.000 001 4
	A	PPA	3	3	$\frac{1}{2}$	6	1.392 351 641 53	1.000 000 02
							(1.392 351 641 53)	
$-x^2+x^4$	A	PPA	2	1	$\frac{1}{2}$	5	0.657 653 094	0.999 975 8
	A	PPA	2	2	$\frac{1}{4}$	5	0.657 653 007 5	0.999 998 3
	A	PPA	2	4	$\frac{1}{8}$	6	0.657 653 005 2	0.999 999 8
							(0.657 653 005 18)	
x^6	A	PPA	3	1	1	6	1.144 802 473	0.999 998 6
	A	PPA	4	2	1	6	1.144 802 455	0.999 999 5
							(1.444 802 453 79)	
x^2+x^6	A	PPA	3	1	1	6	1.435 624 643 8	0.999 999 92
	A	PPA	4	2	1	6	1.435 624 623 4	0.999 999 90
							(1.435 624 619 00)	
x^8	A	PPA	3	1	$\frac{1}{2}$	5	1.225 821 12	1.000 012
	A	PPA	3	2	$\frac{1}{4}$	6	1.225 820 189	1.000 004 75
							(1.225 820 113 80)	

where $n=0,2,4,...$, $\mu_n=\langle 0|x^n|0\rangle$, and E_0 is the energy of the ground state. Without any loss of generality, one can set $\mu_0=1$. The knowledge of the even moments from $n=2$ to $n=2M$ is then sufficient to generate all the higher even moments by recursive use of Eq. (6). Since the virial theorem relates E_0 to μ_4, the quartic oscillator ($M=2$) gives rise to a ''one-missing-moment problem'' [6]. A number of authors [4–6] have adopted different strategies to exploit Eq. (6) for the calculation of ground-state properties with varying degrees of accuracy. But, in the MEP context, these relations have never been employed. Note that the MEP ansatz $\tilde{p}(x)$ for the PD here has the form (2) with even powers of x only. This form, however, fails to satisfy the boundary behavior. For $V(x)=x^{2M}$, one can easily check that the true PD must decay as $\exp[-|x|^{M+1}/(M+1)]$ when $|x|\to\infty$. On the other hand, when $|x|\to 0$, $p(x)\sim\exp(-\alpha x^2)$, with $\alpha>0$. If we consider the specific case of $M=2$, it is not immediately obvious how a series $\tilde{g}(x)$, as in Eq. (2), of even powers of x can behave as $|x|^3/3$ for large x. Elsewhere [7], we have argued that in situations of this sort, it is expedient to modify the MEP ansatz so as to incorporate the correct boundary behavior. With this motivation, we replace the series $\tilde{g}(x)$ by a power-Padé approximant (PPA)

$$\tilde{g}(x)\approx\frac{[P_r(x)]^s}{[Q_t(x)]^u}\equiv[r,s/t,u]. \tag{7}$$

Here $P_r(x)$ is a polynomial in x^2 of degree r with the constant term zero, and $Q_t(x)$ is a polynomial in which the highest power of x^2 is t, while the constant term is taken as unity. On expansion, $\tilde{g}(x)$ in Eq. (7) generates the even series exponentiated in Eq. (2). A broad range of PD can be handled by choosing r, s, t, and u in such a way that the behavior of $p(x)$ for $|x|\to 0$ and $|x|\to\infty$ for a given potential problem is satisfied. Thus, for the ground state of the x^4 problem our simplest choice of $\tilde{p}(x)$ has the form $\tilde{p}(x)=C\exp[-(\lambda_1 x^2+\lambda_2 x^4)/(1+\lambda_3 x^2)^{1/2}]$, where C is fixed by the normalization condition.

As our second example, we consider the logistic map

$$x_{n+1}=\beta x_n(1-x_n^j)=\phi(x_n), \tag{8}$$

which serves as a rudimentary laboratory for the study of some aspects of chaos. The case $j=1$ has been extensively studied [8] over decades. The asymmetric map corresponding to $j=2$ has also attracted some attention [9]. Such maps turn chaotic at some critical value of β, say, β_c. To confine x in the range [0, 1], we choose $\beta \leqslant \beta_{\max}$, where $\ln \beta_{\max} = (j+1)\ln(j+1)/j - \ln j$. For these maps we can define $p(x)$ such that

$$\mu_t=\int_0^1 y^t p(y)dy, \quad t=0,1,2,\ldots. \tag{9}$$

The density function satisfies the Frobenius-Perron integral equation

$$p(y)=\int_0^1 p(x)\,\delta(y-\phi(x))dx, \tag{10}$$

which, in general, cannot be solved analytically. Only for the case $j=1$, the analytical form of $p(x)$ corresponding to $\beta=\beta_{\max}=4$ is known. For $j=2$ onwards, $p(x)$ can only be obtained numerically [10]. Here we construct this PD within the framework of the MEP, using the procedure described earlier. To this end, we first obtain a set of recursion relations involving the moments of the PD by raising both sides of Eq. (8) to their kth powers and taking the averages of each term over a sufficiently large number of iterations. In the chaotic regime, $\langle x_n^{k+1}\rangle = \langle x_n^k\rangle = \mu_k$. So, we get

$$f_k=\mu_k-\beta^k\sum_{r=0}^{k}(-1)^{k-r}\mu_{(j+1)(k-r)+r}=0. \tag{11}$$

For reasons of symmetry, we use the following form of PD for the quadratic map ($j=1$):

$$\tilde{p}(x)=\exp\left(-\sum_i \lambda_i(x-1/2)^i\right)+\exp\left(-\sum_i \lambda_i(1/2-x)^i\right). \tag{12}$$

For other values of j, we employ the MEP form (2). The Lyapunov exponent Λ corresponding to a given value of the control parameter β and order of the map j can now be computed from the formula $\Lambda=\int \tilde{p}(x)\ln|d\phi/dx|dx$ (see, e.g, [10]).

III. RESULTS AND DISCUSSION

Let us first take up the case of anharmonic oscillators. In Table I we display a few results for the potential form (5) with $M \leqslant 4$. The trial PD $\tilde{p}(x)$ has the power-Padé form given by Eqs. (2) and (7) with $s=1$ and r, t, u so chosen that $\tilde{p}(x)$ satisfies the boundary behavior for the specific potential problem. The total number of adjustable parameters in $\tilde{p}(x)$ is $r+t$. These are determined via the optimization schemes A, B, and C. The number of recursion relations (6) taken into consideration are indicated in Table I. For the purpose of comparison, we also exhibit some results corresponding to the traditional MEP form of $\tilde{p}(x)$. The values of the global properties like the ground-state energy E_0 and the virial ratio $R=2\langle T\rangle/\langle dV/d\ln x\rangle=1$, where T is the kinetic energy, provide a test of the accuracy of the optimized $\tilde{p}(x)$. From the quoted near-exact results [11], we happily note that our strategy works satisfactorily. The three optimization schemes outlined in Sec. II yield almost identical results as is evident from our data for the x^4 problem. This is because, by virtue of the choice of the MEP form (or its variant) of $\tilde{p}(x)$, $\overline{S}$ after optimization is *nearly at its maximum value* in all the cases. However, our numerical experience is that scheme A possesses a better convergence profile. Therefore, we stick to scheme A for the other problems. Our results reveal that as few as three parameters in the trial PD yield highly accurate values of E_0 and R. Further, the PPA form of $\tilde{p}(x)$ gives much better results than the traditional MEP form. This is expected, because the latter ignores information regarding the boundary behavior of the PD. Canosa *et al.* [2] employed the MEP in this context. Our present work has successfully modified the method to achieve higher accuracy.

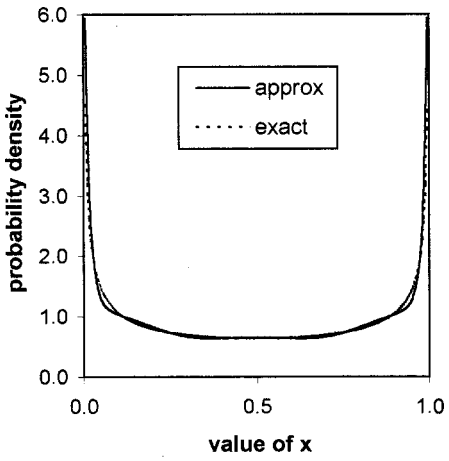

FIG. 1. Plot of exact and approximate probability densities for the quadratic ($j=1$) map.

We now turn our attention to the generalized logistic map (8). The optimized densities are obtained by taking a trial PD

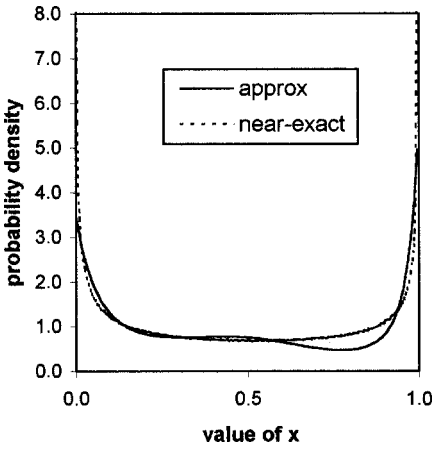

FIG. 2. Plot of near-exact and approximate probability densities for the cubic ($j=2$) map.

of the form (2) [and the symmetrized form (12) for $j=1$]. Here, we have fixed the number of parameters in the trial PD to 6. Figures 1 and 2 show plots of the optimized PD for cases $j=1$ and $j=2$. Exact $p(x)$ are also displayed for comparison. As regards the efficacy of our scheme, the figures speak for themselves. Let us note that an application of MEP to the $j=1$ case was made earlier [12], assuming explicit knowledge of moments. But, a lack of symmetrization and the use of just two parameters in $\tilde{p}(x)$ yielded far less accurate results. Here, we have also computed Λ from the optimized PD, and have plotted Λ vs j in Fig. 3. The nature of the variation is similar to what is found from *accurate* computations. In fact, the error is around 0.5%. Workability of the present endeavor is thus justified further.

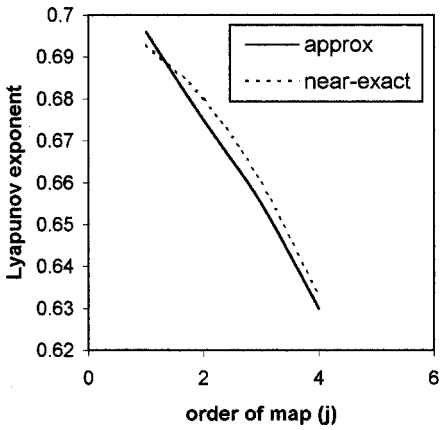

FIG. 3. Variation of the Lyapunov exponent with order j (see text).

IV. CONCLUDING REMARKS

Requiring the knowledge of exact or near-exact values for individual moments has been a serious practical limitation of the MEP. In this work we have suggested an alternative route where the chosen density is optimized by insisting on minimization of a certain function constructed from a set of moment relations satisfied by exact densities. We have also demonstrated how profitable it can be, in certain situations, to employ a variant of the MEP ansatz for the trial density that takes due care of the asymptotic behavior or the symmetry of the problem. The performance of a power-Padé form for $\tilde{g}(x)$ in dealing with oscillators, and a symmetrized form for the same in connection with the logistic map, supports our contention that such modifications may prove rewarding.

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