Ground-state wave functions and maximum entropy

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A modified version of the maximum-entropy principle is applied to distributions associated with special quantum states. In this way, it becomes feasible to make statistical inferences concerning the ground-state wave function and the associated potential from the sole knowledge of a few relevant mean values. The scheme is illustrated for the case of anharmonic and Morse potentials and yields excellent results.

I. INTRODUCTION

The use of just a small set of relevant mean values to describe a physical system is the essential feature of statistical mechanics. In recent developments based on information theory,[1-6] a statistical operator is constructed via the maximum-entropy principle, which provides the least biased description consistent with the available relevant information. The extended formalism is apt for dealing with quite a broad range of situations (including off-equilibrium statistical descriptions[6-11]).

The aim of this work is to apply some concomitant ideas to probability distributions associated with pure quantum states. In this way, statistical inference of a wave function (WF), based on diverse expectation values concerning the system, is made possible, provided the system is guaranteed to be in a pure state. In many physical problems, this constitutes a common occurrence. Quite often, expectation values of simple observables (for the ground state) are available, but there is no detailed knowledge of the pertinent effective Hamiltonian and WF.

Under such circumstances, the standard procedure is to make an intuitive choice concerning these objects, and then verify if the predictions are consistent with the available information. A great deal of "coupling constant fitting" is afterwards required.

We shall propose a scheme, however, that is both systematic and self-consistent, in the sense that it provides a "best" WF criterion that becomes exact in the case of complete information. Besides, the method provides very suitable functional forms for trial WF, so as to be in a position to approximate the ground-state WF (GSWF) in that case in which the Hamiltonian is known.

As we shall be dealing with statistical inference, one should keep in mind the fact that the concomitant approaches become the more powerful the less input information they require. Our goal shall thus be that of devising a technique that is able to yield predictions on the basis of a limited amount of information.

II. GENERAL SCHEME

Let us consider a quantum state $|\psi\rangle$ represented in a given complete orthonormal basis $\{|\varepsilon\rangle\}$ by the wave function

$$\psi(\varepsilon)=\langle\varepsilon|\psi\rangle\ , \tag{2.1}$$

which we assume to be positive definite, i.e., without nodes. The corresponding density or probability distribution $\rho(\varepsilon)$ in "ε space" is thus directly related to (2.1) by $\psi(\varepsilon)=[\rho(\varepsilon)]^{1/2}$. Examples are GSWF in the coordinate representation of a single particle in a given potential, many-body GSWF in boson systems, and also certain ground states in specific fermion model Hamiltonians.[12,13]

Let us suppose now that the available information concerning the system, assumed to be in its ground state, consists of the expectation values O_i of a set of linearly independent observables $\{\hat{O}_i, i=1,\ldots,n\}$,

$$O_i=\langle\psi|\hat{O}_i|\psi\rangle=\int\int\psi(\varepsilon)\langle\varepsilon|\hat{O}_i|\varepsilon'\rangle\psi(\varepsilon')d\varepsilon\,d\varepsilon'\ . \tag{2.2}$$

We assume now that the set is undercomplete, so that the constraints (2.2) do not suffice to determine $\psi(\varepsilon)$. Several wave functions will, in general, exist, which comply with the constraints (2.2). Let us define a quantal entropy[13] associated with the distribution $\rho(\varepsilon)$,

$$\begin{aligned}S&=-\int\rho(\varepsilon)\ln[\rho(\varepsilon)]d\varepsilon\\&=-\int 2\psi^2(\varepsilon)\ln[\psi(\varepsilon)]d\varepsilon\ .\end{aligned} \tag{2.3}$$

S measures the lack of information concerning the distribution in "ε space." It is thus explicitly "basis dependent," as opposed to the entropy $-\mathrm{Tr}[\hat{\rho}\ln(\hat{\rho})]$ of a proper statistical operator $\hat{\rho}$ (which vanishes for pure states). This is due to the fact that $\rho(\varepsilon)=\langle\varepsilon|\hat{\rho}|\varepsilon\rangle$, so that only the diagonal information in the chosen basis is taken into account in (2.3). An infinite irrelevant constant [independent of $\rho(\varepsilon)$] should be added to (2.3) in the continuous case.[4] Our S may be termed a "subjective" entropy.

Our proposal for the wave function will be based on the maximum-entropy criterion. We shall choose that wave function which extremalizes (2.3) subject to the constraints (2.2). In this way the least biased and smoothest distribution in "ε space" is obtained. The solution can be attained by introducing n Lagrange multipliers λ_i and extremalizing the magnitude

$$S' = S - \sum_i \lambda_i O_i$$
$$= -\int\int \psi(\varepsilon)\left[2\ln[\psi(\varepsilon)]\delta(\varepsilon-\varepsilon') + \sum_i \lambda_i \langle \varepsilon|\hat{O}_i|\varepsilon'\rangle\right]\psi(\varepsilon')d\varepsilon\, d\varepsilon' \ . \quad (2.4)$$

The ensuing equation for $\psi(\varepsilon)$ resulting from $\delta S'=0$ is

$$0 = 2\psi\ln(\psi) + \psi + \sum_i \lambda_i \int g_i(\varepsilon,\varepsilon')\psi(\varepsilon')d\varepsilon' \ , \quad (2.5)$$

where

$$g_i(\varepsilon,\varepsilon') = \tfrac{1}{2}(\langle \varepsilon|\hat{O}_i|\varepsilon'\rangle + \langle \varepsilon'|\hat{O}_i|\varepsilon\rangle) \ . \quad (2.6)$$

If $\hat{O}_i$ is a Hermitic operator, (2.5) is a real equation.

The normalization of $\rho(\varepsilon)$ should be included as an additional constraint in (2.4), and can be represented by the operator $\hat{O}_0$, $\langle \varepsilon|\hat{O}_0|\varepsilon'\rangle = \delta(\varepsilon-\varepsilon')$, and the corresponding multiplier λ_0.

The second variation of (2.4) yields

$$\delta^2 S' = -2\int\int \delta\psi(\varepsilon)\left[\{2\ln[\psi(\varepsilon)]+3\}\delta(\varepsilon-\varepsilon') + \sum_i \lambda_i g_i(\varepsilon,\varepsilon')\right]\delta\psi(\varepsilon')d\varepsilon\, d\varepsilon' \ , \quad (2.7)$$

so that a maximum of S' is not guaranteed in every case.

Needless to say, the coordinate ε may represent a set of continuous or discrete labels (the integrals are to be replaced by sums in this case), or a mixture of both.

Notice that up to this point, we have considered the constraints (2.2) to be of a completely arbitrary character. Equation (2.5) is not easy to solve in the general case, and represents an integrodifferential equation for ψ if, for instance,

$$\langle \varepsilon|\hat{O}_i|\varepsilon'\rangle \propto \delta^{(k)}(\varepsilon-\varepsilon')$$

for some i (i.e., kth power of the momentum in ε space).

However, as pointed out in the last paragraphs of the preceding section, the method we are here proposing would not prove to be a useful one if it required a lot of input information. Contrariwise, we shall endeavor to show that things work out nicely with just a small amount of information of a very specific and simple character. Some special situations will be discussed later.

III. THE DIAGONAL CASE

In the rest of this work we shall concern ourselves just with diagonal observables in the basis $\{|\varepsilon\rangle\}$, i.e.,

$$\langle \varepsilon|\hat{O}_i|\varepsilon'\rangle = \delta(\varepsilon-\varepsilon')g_i(\varepsilon) \ . \quad (3.1)$$

This represents specific input information that is easily available. In this case, (2.5) yields the solution for ψ at once,

$$\psi(\varepsilon) = \exp\left[-\frac{1}{2}\left[\lambda_0' + \sum_{i=1}^{n}\lambda_i g_i(\varepsilon)\right]\right] \ , \quad (3.2)$$

where $\lambda_0' = \lambda_0 + 1$. The particular values of the Lagrange multipliers should be determined from the constraints (2.2).

We thus regain the rather familiar expression for ρ, typical of the information theory approach to statistical mechanics. Hence, we can avail ourselves of all the general theorems on distributions usually employed in this field. In particular, the solution (3.2) can be proved to be unique if the mean values O_i's are compatible with all standard quantum-mechanical rules. One is always led to a maximum of S' [as is easily seen from (2.7)] for fixed values of the λ_i's, and of S for fixed O_i's.

The maximum entropy acquires the appearance

$$S = \sum_{i=1}^{n}\lambda_i O_i + \lambda_0' \ . \quad (3.3)$$

If the set $\{g_i(\varepsilon),\ i=0,\ldots,n\}$ [with $g_0(\varepsilon)=1$] forms a complete basis of functions in "ε space," $\psi(\varepsilon)$ is exactly determined. In this case we can expand $\psi^2(\varepsilon)$ in this basis,

$$\psi^2(\varepsilon) = \sum_{j=0}^{n} C_j g_j(\varepsilon) \ , \quad (3.4)$$

so that

$$O_i^* = \int \psi^2(\varepsilon)g_i^*(\varepsilon)d\varepsilon = \sum_{j=0}^{n} C_j D_{ij} \ , \quad (3.5)$$

where

$$D_{ij} = \int g_i^*(\varepsilon)g_j(\varepsilon)d\varepsilon \quad (3.6)$$

is the overlap kernel. Assuming all the O_i's are known, the C_j's are immediately obtained from (3.5),

$$C_j = \sum_{i=0}^{n} O_i^* D_{ji}^{-1} \ . \quad (3.7)$$

For an orthonormal set ($D_{ij}=\delta_{ij}$), $C_i = O_i^*$.

The expression (3.2) for $\psi(\varepsilon)$ represents in this situation the expansion of $\ln[\psi^2(\varepsilon)]$,

$$\lambda_i = -\sum_{j=0}^{n} D_{ij}^{-1}\int 2\ln[\psi(\varepsilon)]g_j^*(\varepsilon)d\varepsilon \ . \quad (3.8)$$

In this sense, our scheme can be viewed as an inversion method for the expansion (3.2) [and hence (3.4)] when not all O_i's are available. The maximum-entropy prescription yields $\lambda_i = 0$ if O_i is unknown.

The entropy (3.3) acquires its lowest value when all O_i's corresponding to a complete set are known. Otherwise, it provides obviously an upper bound to this minimum "exact" entropy.

Notice that since $\rho(\varepsilon)$ is not a statistical operator but rather a probability distribution in "ε space," a smaller set of observables than that needed in the statistical case is required to determine $\rho(\varepsilon)$ without recourse to the maximum entropy criterion. The set $\{\hat{O}_i,\ i=0,\ldots,n\}$

is not complete in the space of observables (they are diagonal), but their expectation values determine $\psi(\varepsilon)$ completely if the corresponding set of functions $g_i(\varepsilon)$ is complete. Moreover, a full quantum statistical operator may not even be normalizable for such a reduced set (for instance, $\hat{\rho}=\exp(-\lambda\hat{x}^2)$ has an infinite trace if $\hat{x}$ is the coordinate operator associated with a momentum $\hat{p}$).

IV. STATISTICAL INFERENCE OF GSWF AND POTENTIAL

Let us now apply the previous formalism to the case of the ground state of a single particle system under the action of a potential V. We assume that the available information deals with the expectation values of n linearly independent functions of the coordinate $x=(x_1,x_2,x_3)$,

$$g_i=\langle g_i(x)\rangle=\int \psi^2(x)g_i(x)dx \ . \tag{4.1}$$

The least biased wave function is thus

$$\psi(x)=\exp\left[-\frac{1}{2}\left[\lambda_0+\sum_{i=1}^{n}\lambda_i g_i(x)\right]\right] , \tag{4.2}$$

where the normalization constant λ_0 is given by

$$\lambda_0=\ln\left[\int \exp\left[-\sum_{i=1}^{n}\lambda_i g_i(x)\right]dx\right] , \tag{4.3}$$

$$\frac{\partial\lambda_0}{\partial\lambda_i}=-g_i \ . \tag{4.4}$$

With this choice of ψ, one is in a position to make statistical inferences concerning any quantity of interest. In addition to the standard trace predictions, represented here by inferred mean values of known functions of the coordinates, other types of inferences are feasible within the present, new context.

Of particular interest are the inferred values of the mean square momentum (we set herefrom $\hbar=1$)

$$\begin{aligned}\langle\hat{p}^2\rangle&=-\int\psi\nabla^2(\psi)dx\\&=-\tfrac{1}{2}\int\psi^2\nabla^2[\ln(\psi)]dx \ ,\end{aligned} \tag{4.5}$$

and of the associated potential and ground-state energy E (we assume a unit mass)

$$\begin{aligned}V(x)-E&=\frac{\nabla^2\psi}{2\psi}\\&=\frac{1}{4}\left[-\sum_i\lambda_i\nabla^2 g_i(x)+\frac{1}{2}\left[\sum_i\lambda_i\nabla g_i(x)\right]^2\right] ,\end{aligned} \tag{4.6}$$

as obtained from the stationary Schrödinger equation (∇^2 denotes the Laplacian while ∇ the gradient vector).

Thus, an approximate prediction of both the ground-state energy (measured from the bottom of the potential) and of the potential function is possible with just a few relevant mean values. Our inferred quantities will converge towards the exact values as additional constraints of the type (4.1) are included (i.e., new information is added). When the λ_i's become stable (up to a given accuracy) convergence is reached.

Usually, the available information is just that corresponding to the averages of moments $x_1^i x_2^j x_3^k$ (i.e., averages of multipole moments) or directly r^l in case of radially symmetric systems (r is the radius to the origin). For example, the GSWF in the Coulomb potential is of the form

$$\psi(r)=\exp[-\tfrac{1}{2}(\lambda_0+\lambda r)] \ .$$

Therefore, it is *exactly* reconstructed with the sole information of the mean radius $\bar{r}=3/\lambda$. The one-dimensional harmonic-oscillator GSWF is exactly derived with just the mean value of $\langle x_1^2\rangle$ ($\langle x_1^2\rangle$ and $\langle x_1\rangle$ in the case of a displaced potential). In these examples, the information saturates (i.e., the λ_i's become stable) with just one moment.

The corresponding entropies are

$$S=\lambda_0+\lambda\bar{r}=C_c+3\ln(\bar{r}) \ , \tag{4.7}$$

for the Coulomb potential [with $C_c=\ln(8\pi/27)+3$], and

$$S=C_h+\ln(\sigma) \ , \tag{4.8}$$

for the harmonic oscillator, where $\sigma=(\langle x_1^2\rangle-\langle x_1\rangle^2)^{1/2}$ and $C_h=[\ln(2\pi)+1]/2$. The entropy obviously increases with the dispersion.

The inferred WF (4.2) possesses an attractive and suitable functional form if the functions $g_i(x)$ are polynomials. In fact, it can be used as a trial WF for approximating the exact GS if the Hamiltonian $\hat{H}$ of the system is known. Moreover, in this case the available information can be used together with the minimization of $\langle\hat{H}\rangle$ to determine the best parameters λ_i.

V. APPLICATION

Let us consider first a one-dimensional quartic anharmonic oscillator. The corresponding Hamiltonian can be generally written as

$$\hat{H}=(\hat{P}^2+\alpha\hat{X}^2)/2+\beta\hat{X}^3+\gamma\hat{X}^4 \ , \tag{5.1}$$

with $[\hat{X},\hat{P}]=i$. This type of potential has been the subject of a great deal of work during the past years,[14-20] due to its relevance in the study of molecular vibrations and to its role in the modeling of nonlinear quantum field theories. Our aim is to approximately reconstruct the GSWF of (5.1) with the sole knowledge of a few expectation values $\{\langle x^l\rangle,\ l=1,\ldots,n\}$. The corresponding approximate WF is

$$\psi(x)=\exp\left[-\frac{1}{2}\left[\lambda_0+\sum_{l=1}^{n}\lambda_l x^l\right]\right] , \tag{5.2}$$

where the parameters λ_l can be obtained by means of a standard Newton-Raphson procedure.

If $n=2$, (5.2) is a Gaussian, and the inferred potential (4.6) is thus that of a harmonic oscillator. Our approach is, in this case, equivalent to a mean-field approximation (in the boson representation[18-20]). For $n>2$, we are thus in a position to go beyond mean-field treatments.

TABLE I. Mean-square momentum, energy, inferred energy, entropy, and the overlap with the exact WF, for the Hamiltonian (5.1) (quartic oscillator), with $\beta=0$. Case (a) corresponds to $\alpha=1$, $\gamma=1$, (b) to $\alpha=1$, $\gamma=10$, and (c) to $\alpha=-1.5\alpha_c$, $\gamma=1$ (bistable case). The quantity $m=n/2$ denotes the number of moments used in the approximate reconstruction [see (5.2)].

Case		$\langle \hat{P}^2 \rangle$	$\langle \hat{H} \rangle$	E_{inf}	S	Overlap
(a)	Exact	0.985 978	0.803 771		0.738 300	
	$m=1$	0.972 196	0.813 051	0.972 196	0.739 890	0.999 570
	$m=2$	0.986 032	0.803 798	0.816 305	0.738 304	0.999 999
	$m=4$	0.985 978	0.803 771	0.804 183	0.738 300	1
(b)	Exact	1.963 289	1.504 972		0.396 591	
	$m=1$	1.922 751	1.533 558	1.922 751	0.398 913	0.999 367
	$m=2$	1.963 494	1.505 075	1.540 536	0.396 597	0.999 998
	$m=4$	1.963 289	1.504 972	1.506 419	0.396 591	1
(c)	Exact	1.220 330	−1.761 382		1.254 676	
	$m=1$	0.173 477	0.963 904	0.173 477	1.601 647	0.899 541
	$m=2$	1.310 386	−1.716 354	−0.869 993	1.263 924	0.997 804
	$m=4$	1.225 705	−1.758 694	−1.396 386	1.254 953	0.999 932

First, we shall tackle the case $\beta=0$, $\alpha>0$, i.e., a symmetric potential with a sole minimum at the origin. Results for various quantities of interest are shown in Table I, for $n=2$, 4, and 8, $\alpha=1$ and $\gamma=1$ and 10 (only two of the three coupling constants are actually independent). The information has been obviously restricted to even moments. The exact WF and moments have been calculated according to the procedures followed in Refs. 18–20.

We see that excellent agreement between inferred and exact values is already achieved with $n=4$, and even with $n=2$ we attain a suitable description. The overlap $\langle \psi_{\text{ex}} | \psi_{\text{app}} \rangle$ between the exact and approximate WF is better than 0.999. Moreover, the accuracy of the results depends only slightly on the value of γ.

Notice that $\langle \hat{H} \rangle$ denotes the mean energy (assuming the Hamiltonian is known), while E_{inf} is the inferred GS energy as obtained from the constant term in (4.6) (assuming no knowledge of the potential and its couplings constants). The inferred potentials are shown in Fig. 1, together with the exact one.

The entropy (2.3) is also quoted, for exact and approximate WF. The relative entropy[21] $S(\rho_{\text{ex}}/\rho_{\text{app}})=S_{\text{app}}-S_{\text{ex}}$ measures the information which the approximate WF lacks with respect to the exact one. From the obtained values, we conclude that only a small amount of information is stored in higher moments. Nevertheless, quanti-

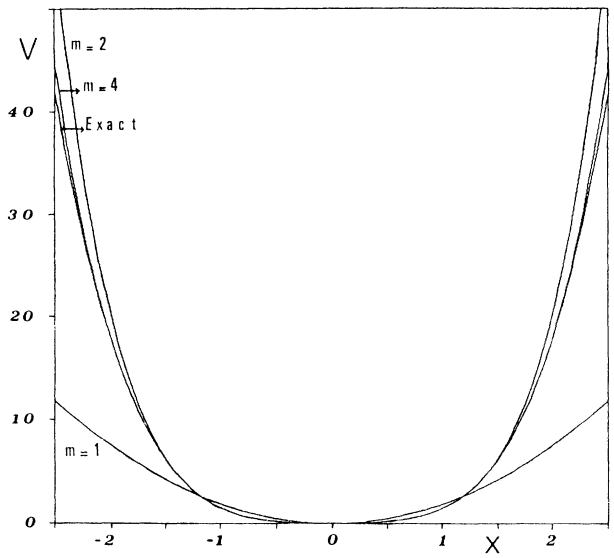

FIG. 1. Exact and inferred potentials for quartic oscillator (5.1), with $\alpha=\gamma=1$, $\beta=0$. The same notation of Table I is utilized. [In all figures, if x is measured in units of L (arbitrary), V is measured in units of $\hbar^2/mL^2$.]

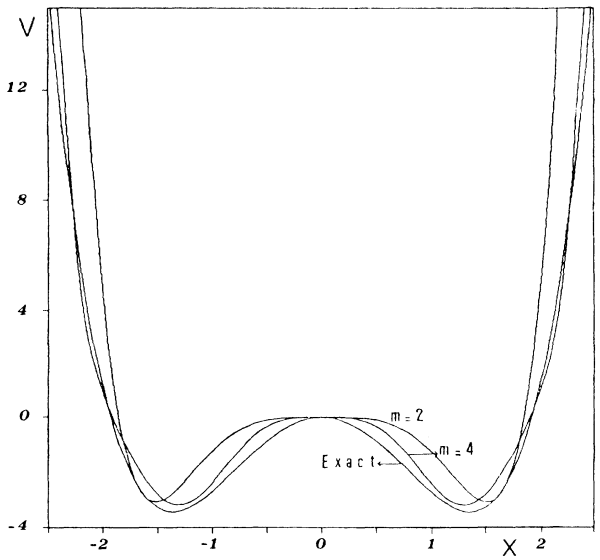

FIG. 2. Exact and inferred potentials for the bistable case ($\alpha=-1.5\alpha_c$, $\gamma=1$, $\beta=0$).

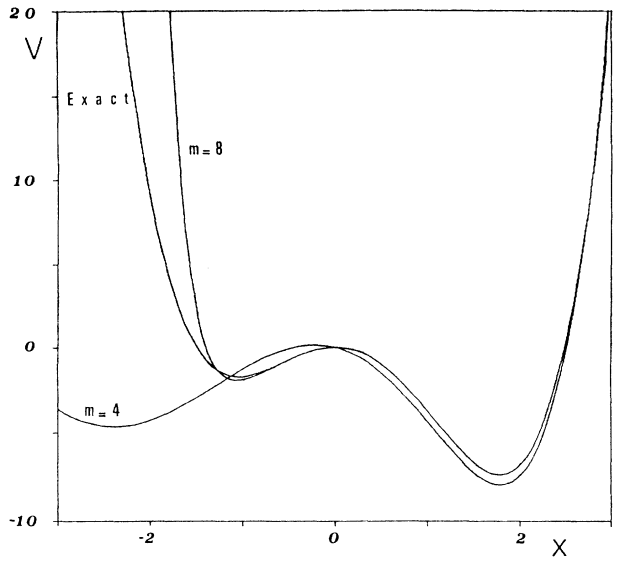

FIG. 3. Exact and inferred potentials for the case $\alpha=-1.5\alpha_c$, $\gamma=1$, $\beta=-1$.

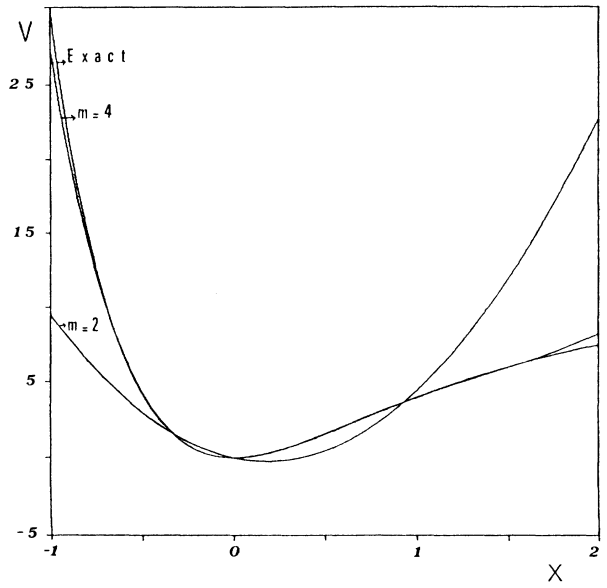

FIG. 4. Exact and inferred potentials for the Morse case, with $A=10$.

ties depending on the derivatives of the WF, such as $V(x)-E$, are quite sensible to the value of the Lagrange parameters, which are shown in Table III. Exact values refer to the coefficients of the expansion of $\ln\psi^2_{\rm ex}(x)$ [see (3.8)], and can be obtained from (4.6).

As a second and more challenging example, we shall consider the case of a bistable potential, with $\alpha=-1.5\alpha_c$, and $\gamma=1$. $\alpha_c=(243/2)^{1/3}\gamma^{2/3}$ denotes the critical value such that for $|\alpha|>|\alpha_c|$, the mean-field approach possesses a symmetry-breaking degenerate solution[20] (at zero temperature), centered at one of the wells. The Gaussian approximation is in this case unfit to provide an accurate picture of the GSWF. The corresponding results are also shown in Table I. Notice that already with $n=4$, a bistable inferred potential is obtained (Fig. 2), together with an excellent value of the overlap. However, in this case the corresponding λ's converge slowly towards the exact values.

The situation where the two minima of the potential possess unequal depth is depicted in Table II, case (a), for $\beta=-1$, with γ and α assuming the same values as in the bistable potential. In this case, information about odd moments must be obviously included. The inferred GSWF, which is centered at the deepest well, predicts a second shallow well already for $n\geq 4$, although we need to go up to $n=8$ to obtain a more accurate picture of the potential. We exhibit the corresponding results in Fig. 3.

Finally, we shall consider the case of a Morse potential, which has also attracted a great deal of attention over the past years,[22,23] as it provides one with a quite realistic description of molecular vibrations. The corresponding Hamiltonian is

$$\hat{H}=\tfrac{1}{2}\hat{P}^2+A\,[1-\exp(-\hat{X})]^2\ . \tag{5.3}$$

TABLE II. Same quantities quoted in Table I, for asymmetric potentials. Case (a) corresponds to Hamiltonian (5.1) with $\alpha=-1.5\alpha_c$, $\beta=-1$, $\gamma=1$ (the third column denotes the inferred GS energy measured from the bottom of the potential well), while (b) and (c) to the Morse potential (5.3), with $A=1$ (b) and $A=10$ (c).

Case		$\langle\hat{P}^2\rangle$	$\langle\hat{H}\rangle$	$E_{\rm inf}$	S	Overlap
(a)	Exact	2.038 384	−5.222 045	2.149 228	0.380 544	
	$m=2$	1.971 266	−5.189 709	1.971 267	0.386 453	0.998 622
	$m=4$	2.038 781	−5.221 846	2.139 804	0.380 555	0.999 977
	$m=8$	2.038 384	−5.222 045	2.149 490	0.380 544	1
(b)	Exact	0.457 107	0.582 107		1.206 731	
	$m=2$	0.346 084	0.772 470	0.217 030	1.256 329	0.987 721
	$m=4$	0.446 454	0.584 565	0.546 476	1.207 711	0.999 788
(c)	Exact	1.986 068	2.111 068		0.403 670	
	$m=2$	1.863 853	2.190 178	1.631 635	0.414 468	0.997 321
	$m=4$	1.985 223	2.111 170	2.109 014	0.403 681	0.999 997

TABLE III. Exact and approximate Lagrange multipliers for a symmetric [case (a)] and an asymmetric [case (b)] potential. (a) corresponds to the quartic oscillator (5.1), with $\alpha=\gamma=1$, $\beta=0$, whereas (b) to the Morse potential (5.3), with $A=10$.

		Case (a)		
	λ_2	λ_4	λ_6	λ_8
Exact	1.607 541	0.264 032	−0.020 149	0.001 025
$m=1$	1.944 392	0.0	0.0	0.0
$m=2$	1.632 609	0.220 010	0.0	0.0
$m=4$	1.608 366	0.261 001	−0.016 422	0.003 019
		Case (b)		
	λ_1	λ_2	λ_3	λ_4
Exact	−1.000 000	4.472 136	−1.490 712	0.372 678
$m=2$	−1.362 991	3.727 707	0.0	0.0
$m=4$	−1.008 181	4.528 170	−1.487 683	0.256 839

In this case, the exact GSWF possesses an analytic expression,

$$\psi_{ex}(x) \propto \exp\{-[C\exp(-x)+(C-\tfrac{1}{2})x]\} , \qquad (5.4)$$

where $C=(2A)^{1/2}$. The exact multipliers $\lambda_l=2(-1)^l C/l!$ $(l>1)$ decrease thus rapidly with l. Results corresponding to a finite number of moments (see Tables II and III) are in excellent agreement with the exact figures, as are the inferred potentials (for $n>2$) in the region close to the bottom of the potential well (see Fig. 4).

VI. DISCUSSION AND CONCLUSIONS

We have presented a general method of statistical inference based on information theory, that allows for the "reconstruction" of a node free quantal WF and the corresponding effective potential, from an incomplete set of expectation values.

The formalism is very easy to apply in the case of expectation values concerning diagonal observables (in the "unbiased" basis), and is specially suitable for the reconstruction of single particle effective GSWF. The numerical results shown in Sec. V indicate that excellent agreement with the exact WF can be attained with just a few relevant mean values of diagonal observables.

The proposed scheme yields the least biased, most flat distribution, consistent with the available information. Whether this choice of WF is appropriate or not, can be self-consistently ascertained from the stability of the physical quantities of interest. If by adding new available data our former predictions do not change beyond our desired precision, no new relevant information is obtained. The information is concentrated only on the former expectation values and hence, predictions with acceptable accuracy can be made.

Important physical quantities become stable with a rather small amount of information (for instance, S, $\langle \hat{H} \rangle$ and the overlap, as numerical results depict), suggesting that they depend rather weakly on the detailed values of the Lagrange parameters. On the other hand, quantities involving derivatives of the inferred WF are more sensible and their inference requires, correspondingly, a larger informational input.

One might perhaps argue that the (subjective) maximum-entropy criterion is in philosophical agreement with the Copenhagen interpretation of a quantal WF, in the sense that $|\psi|^2$ describes the observer's knowledge of the particle position (or state), although it is not our intention here to delve into philosophical subjects.

Summing up, we have shown that a modified version of the maximum-entropy principle, involving only diagonal elements of the density operator, allows for a quite successful inference approach regarding ground-state properties. The method should be also of some value in those situations in which the ground-state wave function is too complicated to be dealt with, and one must make do with just some of its most salient features.

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