Fisher information and semiclassical methods

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Using the Frieden and Soffer principle of extreme physical information we present a method for the construction of WKB wave functions that avoids the matching problem between the classically allowed and forbidden regions. When this formalism is applied in conjunction with the semiclassical methods for *N*-fermion systems, it provides one with Thomas-Fermi and Wigner-Kirkwood densities, valid beyond the turning points that also include shell effects. The method is illustrated with reference to both the sextic bistable and the Morse potential. [S1050-2947(99)01905-8]

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I. INTRODUCTION

Semiclassical methods, already introduced in the early days of quantum mechanics, still enjoy wide popularity [1–11] (see Ref. [1] for an excellent recent review), and are being applied to new subjects in quantum mechanics as, for instance, trapped Bose condensates [12], quantum dots [13,14], and quantum wires [15,16].

One of the most celebrated semiclassical methods is the Wentzel-Kramers-Brillouin (WKB) approximation, which clearly exhibits the similarity between the Schrödinger equation and its classical Hamilton-Jacobi counterpart. Although the Dunham formalism [17,18] yields a practical recipe for evaluating expectation values using the WKB expansion, the obtention of the WKB wave function becomes nevertheless cumbersome due to the connection problem at the classical turning points [19]. By recourse to the Shannon-Jaynes information theory (IT) ideas [20,21], it has recently been shown that this troublesome matching procedure can be nicely bypassed .

When applying semiclassical methods to many-fermion systems, one decomposes the level density into a smooth part and an oscillating one. Keeping only the smooth part of the level density and truncating the WKB expansion up to order $\hbar$, or up to order $\hbar^2$, the Thomas-Fermi (TF) and the Wigner-Kirkwood (WK) approaches are, respectively, obtained [22].

Within the strictures of these approaches (TF and WK) [1,23] the diagonal part of the one-body density matrix (i) has a validity range restricted to the interval between the classical turning points and (ii) lacks shell effects. This difficulty concerning the range of validity can be overcome by recourse to special approaches: one is the energy-density functional method [24–26]. Other treatments, based on the Shannon-Jaynes information theory ideas, are also able to include shell effects [27,28].

The purpose of the present work is to present a still different alternative in this respect: to tackle the semiclassical treatments either for single-particle orbitals (WKB) or for *N*-fermion systems (TF and WK), from a different angle, the Frieden and Soffer principle of extremal (Fisher) information (EPI) [29–31], it will be shown, provides WKB wave functions and TF or WK densities (i) with an unrestricted range of validity (ii) that incorporate shell effects. The paper is organized as follows. A brief review of the main ingredients of the semiclassical approaches is given in Sec. II. A summary of EPI is the subject of Sec. III. The present approach and some applications are described in Sec. IV and, finally, some conclusions are drawn in Sec. V.

II. THE SEMICLASSICAL APPROACHES

The method proposed in Refs. [17,18] and reviewed in Ref. [22] provides for a rapid determination of the WKB single-particle energy eigenvalues. Nevertheless, the above approximation, based on the $\hbar$ expansion of the quantized semiclassical action [22],

$$S(\epsilon_n, V, \hbar) = (n+\tfrac{1}{2})h, \tag{1}$$

does not allow for the derivation of an explicit semiclassical expansion of the wave functions.

A nice trick exists that permits one, nevertheless, to obtain semiclassical expansions *for the expectation value of a given operator* $F(x)$ *without recourse to the pertinent wave functions* [22]. For a given operator $F(x)$ one changes the Hamiltonian $H_0 = T + V$ in the Ricatti equation (associated with any Schrödinger equation [22]) in the fashion $H_1 = H_0 + \lambda F(x)$ (with $\lambda \ll 1$) so that, according to elementary perturbation theory, the expectation value of $F(x)$ in a state of energy ϵ can be computed as

$$\langle F \rangle_{\mathrm{WKB}} = \lim_{\lambda \to 0} \frac{1}{\lambda} \{ \epsilon[H_0 + \lambda F(x)] - \epsilon(H_0) \}, \tag{2}$$

where $\epsilon[H_0 + \lambda F(x)]$ and $\epsilon(H_0)$ are the eigenvalues of the Ricatti equation when the Hamiltonians are H_1 and H_0, respectively. As shown in [22], expanding the action S and the energy eigenvalues up to a given order in $\hbar$, one obtains an explicit expression for the expectation value of our one-body operator.

Summing up, a procedure exists that easily allows one to find WKB eigenvalues. From these, the expectation values of a given operator can be obtained with recourse to Eq. (2), without explicitly using any wave function. Starting with these WKB expectation values as input information, the

method presented in Sec. III allows for the inference, using Frieden and Soffer's principle of extremal Fisher information, of associated wave functions.

The philosophy described above can be extended to the quantum many-body realm to obtain densities according to the TF and WK approaches. The main ingredient of such a formulation [22,27,28] is again the WKB expectation value (2) of relevant operators F, evaluated after a semiclassical expansion up to a given order in $\hbar$. The corresponding $\langle F\rangle_{\mathrm{TF}}$ and $\langle F\rangle_{\mathrm{WK}}$ expectation values (order $\hbar$ or $\hbar^2$, respectively) are obtained after integrating the appropriate $\langle F\rangle_{\mathrm{WKB}}$, from the bottom of the potential well ϵ_0 up to the Fermi energy ϵ_F, using a semiclassical smoothed level density $\tilde{g}(\epsilon)$,

$$\langle F\rangle = \int_{\epsilon_0}^{\epsilon_F} \langle F\rangle_{\mathrm{WKB}}\ \tilde{g}(\epsilon)\, d\epsilon, \tag{3}$$

where $\tilde{g}(\epsilon)$ is computed by expanding the quantal level density by recourse of the Euler-McLaurin method and then dropping the oscillating terms. The Fermi energy ϵ_F is simply obtained by requiring

$$\int_{\epsilon_0}^{\epsilon_F} \tilde{g}(\epsilon)\, d\epsilon = N, \tag{4}$$

where N is the correct number of particles.

Going up to order $\hbar^2$ in Eq. (3), the explicit expression for the expectation value of our one-body operator in the WK approach is readily obtained,

$$\langle F\rangle_{WK} = \frac{1}{h}\oint F\sqrt{\epsilon_F - V}\, dz + \frac{\hbar}{48\pi}\left(\oint \frac{FV''}{(\epsilon_F - V)^{3/2}}\, dz + \frac{3}{4}\oint \frac{FV'^2}{(\epsilon_F - V)^{5/2}}\, dz \right), \tag{5}$$

where the first term in the sum corresponds to the TF approach and the contour integration in the complex z plane encloses the segment of the real axis between the classical turning points. As stated above, the range of validity of the TF and WK densities is restricted to the interval between turning points.

Our goal here is the following: (i) start with some TF or WK expectation values computed according to Eq. (5) and (ii) with recourse not to the Shannon-Jaynes information theory but to a totally different approach, namely, Frieden and Soffer's principle of extremal Fisher information (EPI), obtain an appropriate semiclassical one-body density (i) valid everywhere and (ii) that includes shell effects.

III. THE FRIEDEN-SOFFER EPI PRINCIPLE

Using the principle of extremal physical (Fisher's) information (EPI), it has been shown [29–31] that the Lagrangian describing a given physical scenario is not an *ad hoc* construct. On the contrary, its integral ($\equiv$ action $\mathcal{A}$) represents some definite physical information. The dynamics of the concomitant physical process can be obtained by extremizing $\mathcal{A}$. On such a basis, the most important equations of physics (including quantum mechanics, relativity, and Maxwell's electromagnetism) can be derived [29–32].

In particular, assuming for a quantal system that the probability density is $\rho = \psi^*\psi$, Schrödinger's equation is obtained by extremizing the action [32]

$$\mathcal{A} = 4\int \nabla\psi\cdot\nabla\psi^* - \frac{2m}{\hbar^2}\langle \text{Kinetic energy}\rangle. \tag{6}$$

We shall restrict our attention here to the one-dimensional case, and we will consider the scenario discussed in [32]: a particle of mass m moving in a static real potential $V(x)$. In this case, what Frieden and Soffer call their ''demon's knowledge'' (reminiscent of Maxwell's demon) is just the expectation value of the kinetic energy. If E is the system's energy, extremization of the action $\mathcal{A}$ is made without changing the value of $\lambda[E - \langle V(x)\rangle]$, with λ the associated Lagrange multiplier, which Frieden and Soffer have shown to be equal to $2m/\hbar^2$ [32].

In our case, we assume that the knowledge of the system is restricted to the expectation values of M commuting operators $\hat{O}_\kappa(\kappa = 1, \ldots, M)$, computed (i) with the WKB approach according to Eq. (2), or (ii) within the framework of the TF or WK approximations, with recourse to Eq. (5). The principle of extremal physical information leads to the problem of extremizing Fisher's information measure (FIM) [29,30]. It should be remarked that the EPI uses a rather special version of FIM, namely, one that is applicable in the case of translation families [33]. Such a FIM is to be extremized subject to the constraints posed by the M known expectation values plus normalization. The associated variational problem involves the quantity

$$Q = \frac{1}{8}\int dx\, \frac{1}{\rho}\left(\frac{\partial\rho}{\partial x}\right)^2 + \sum_{\kappa=1}^{M} \gamma_\kappa \int dx\, \rho\hat{O}_\kappa(x) - E\int dx\, \rho. \tag{7}$$

The first term above constitutes Fisher's information measure for translation families [33], the second one imposes the pertinent constraints through the corresponding Lagrange multipliers γ_κ, and the third term is the normalization condition, with Lagrange multiplier E, which can be regarded as a zeroth-order expectation value (that is, a term for index $\kappa = 0$ and $\hat{O}_0 = 1$). Assuming $\rho = |\psi(x)|^2$ and $\hbar^2/m = 1$, extremization of Q yields the Schrödinger-like equation

$$-\frac{1}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \left(\sum_{\kappa=1}^{M} \gamma_\kappa\hat{O}_\kappa(x)\right)\psi(x) = E\,\psi(x), \tag{8}$$

with the pseudopotential energy $V(x) = \Sigma_{\kappa=1}^{M}\gamma_\kappa\hat{O}_\kappa(x)$ imposed by the data constraints, while the Lagrange multiplier corresponding to normalization is simply the level energy E.

As shown in [34], the Lagrange multipliers that guarantee compliance with the constraints can be obtained by requiring

$$\frac{\partial E}{\partial\gamma_\kappa} = \langle\hat{O}_\kappa\rangle = d_\kappa. \tag{9}$$

Using Bayesian statistical inference, Silver [33] has proposed a powerful method to obtain the Lagrange multipliers

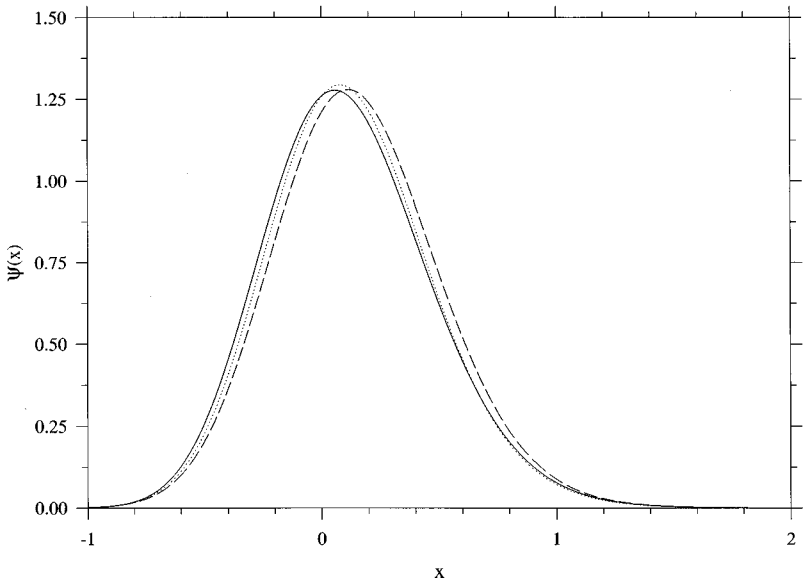

FIG. 1. The exact ground-state wave function (continuous line) is compared to the WKB0 (dotted line) and WKB2 (dashed line) inferred ones for the Morse potential (15).

γ_κ in the case of *mixed* states. As sketched in [34], the purpose of the present work is to present a method, valid for *pure* states, that, using only semiclassical expectation values as input information, allows one to obtain, with recourse to Eqs. (8) and (9), ''semiclassical wave functions or densities'' valid on the whole real axis, while properly including, at the same time, shell effects.

IV. PRESENT APPROACH AND APPLICATIONS

We advance now a self-consistent procedure for determining the Fisher Lagrange multipliers γ_κ. Our input information is restricted to a few expectation values, that of operators $\{\hat{O}_\kappa(x)\}$,

$$\langle \hat{O}_\kappa \rangle = d_\kappa; \quad \kappa = 1, \ldots, M. \tag{10}$$

Starting with arbitrary initial values for the γ's, we repeatedly solve Eq. (8). At each (N_{th}) iteration step, we obtain a semiclassical wave function $\psi_N(\gamma_1, \ldots, \gamma_M)$ and extremize the quantity

$$R(\gamma_1, \ldots, \gamma_M) = E - \sum_{\kappa=1}^{M} \gamma_\kappa \left(\frac{\int \rho_N(x) \hat{O}_\kappa(x)}{\int \rho_N(x)} - d_\kappa \right), \tag{11}$$

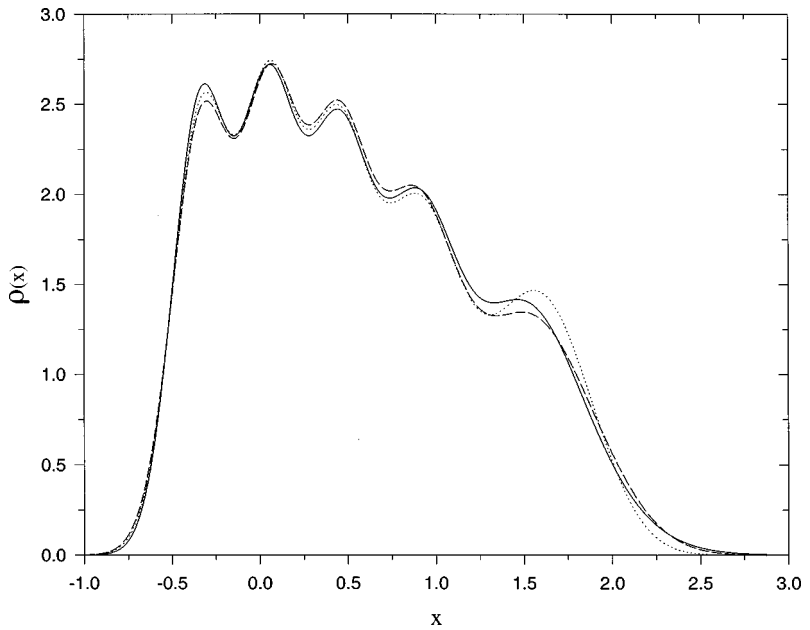

FIG. 2. Exact density (continuous line) and inferred WKB densities (WKB0 ≡ dotted line and WKB2 ≡ dashed line) for the Morse potential (15) with $N=5$ occupied states.

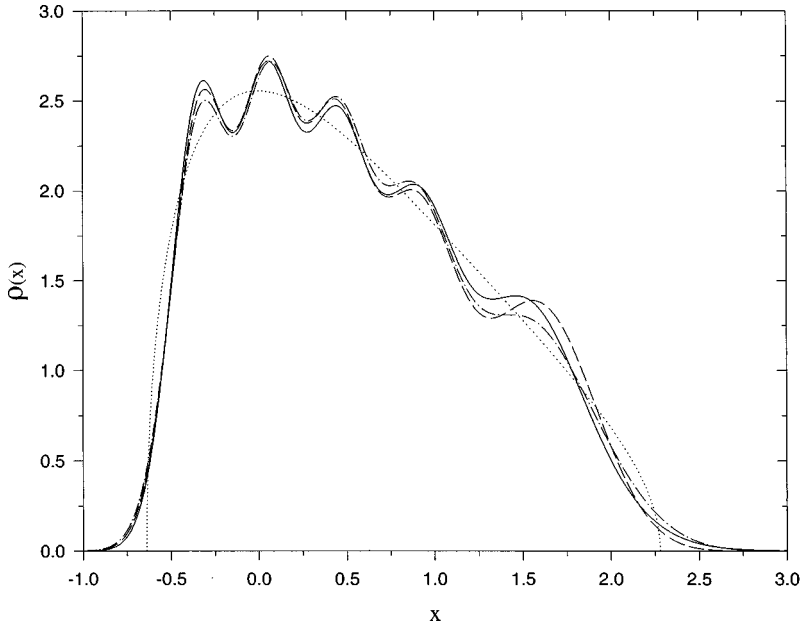

FIG. 3. The exact density (continuous line) is compared to the TF (dashed line) and WK (dot-dashed line) inferred ones for the same example of Fig. 2. The standard TF density (dotted line) is also shown for comparison purposes.

with $\rho_N(x)=|\psi_N(x)|^2$. Using the steepest-descent procedure one obtains the M optimal Lagrange multipliers that will, obviously, force the inferred potential to verify the virial theorem.

For technical reasons, it is convenient to use ''zero mean'' operators $[\hat{O}_\kappa(x)-d_\kappa]$ in Eq. (7). Consequently, the pseudopotential and the total energies are shifted according to

$$E^*=E-\sum_{\kappa=1}^{M}\gamma_\kappa d_\kappa, \tag{12}$$

$$V^*(x)=V(x)-\sum_{\kappa=1}^{M}\gamma_\kappa d_\kappa. \tag{13}$$

Notice that with the above choice $\langle V^*(x)\rangle=0$ and, as a consequence, the shifted total energy E^* corresponds only to the kinetic energy. Equation (9) gets transformed then into

$$\frac{\partial E^*}{\partial \gamma_\kappa}=0, \quad \kappa=1,\ldots,M, \tag{14}$$

that leads to the desired selfconsistent values of the γ's.

As a test for the semiclassical approximations just described, in the following subsection we will use as input information the expectation value of a few $\hat{x}^n$ (power of coordinate operators), computed according to Eq. (2) or Eq. (5) going up either to order $\hbar$ or to order $\hbar^2$.

A. Morse potential

As a typical example of an asymmetric potential, we shall use the Morse one, employed in modeling the interaction of diatomic molecules [35,36],

$$V(x)=A[1-\exp(-x)]^2, \tag{15}$$

where we take $A=40$ and assume foreknowledge of the global expectation values $\langle x^m\rangle (m=1,\ldots,4)$,

$$\langle x^m\rangle=\sum_{i=1}^{N}\langle x^m\rangle_{\epsilon_i}, \tag{16}$$

where N is the number of occupied states and each $\langle x^m\rangle_{\epsilon_i}$ is computed in the WKB approach with recourse to Eq. (2) for each ϵ_i energy level.

The solution of Eq. (8), subject to the constraints (16), yields a set of N orthogonal approximate WKB wave functions, valid beyond the turning points, and in good agreement with the exact ones. Assuming one particle per state and $N=5$ occupied levels, we compare in Fig. 1 the exact ground-state wave function with the WKB0 (order $\hbar$) and WKB2 (order $\hbar^2$) inferred ones using the previously described approach. Exact and inferred wave functions closely resemble each other. We depict in Fig. 2 the comparison between the exact density and the inferred WKB0 and WKB2 ones. In spite of the fact that usually the WKB approach fares rather poorly in the case of ground states [22], in *this* instance things are different. The input information obtained with recourse to Eq. (2) has been used and, contrary to what happens in the case of the method presented in Ref. [21], here we do not need any *ad hoc* variational treatment for the ground state. In the present scheme, the orthogonality of the inferred wave functions is guaranteed by construction.

The present method was also tested within the framework of the Thomas-Fermi and Wigner-Kirkwood approaches. For this purpose we have assumed, as input information, the expectation values $\langle x^m\rangle (m=1,\ldots,4)$ computed with recourse to Eq. (5). The solution of Eq. (8), with the constraints posed by the TF or WK input expectation values, yields again a set of orthogonal wave functions that allows for the inference of TF or WK densities, valid everywhere, and including shell effects. The quality of the approach is exhibited in Fig. 3,

TABLE I. Morse potential. Inferred Thomas-Fermi (ITF) and Wigner-Kirkwood (IWK) single-particle energies, obtained from the TF and WK global information corresponding to $N=5$ particles, are compared to the quantal ones.

	Quantal	ITF	IWK
ϵ_1	4.347	4.450	3.986
ϵ_2	12.29	12.93	12.07
ϵ_3	19.24	20.32	19.35
ϵ_4	25.18	26.22	25.55
ϵ_5	30.12	30.74	30.28

where the exact density is compared to both the TF and WK inferred ones.

Using only global input-information values, computed either in the TF or the WK approaches, the present method provides single-particle energies of rather good quality, as illustrated in Table I, where the quantal results are compared to the inferred ones for the potential (15) assuming a number of particles $N=5$.

B. Sextic bistable potential

As an example of a bistable potential, we take $V(x)$ to be of the form

$$V(x)=x^6+x^4-30x^2. \tag{17}$$

The possible exact solutions for this sextic potential have been recently discussed in Refs. [37,38]. We have assumed that our input information reduces to that of $\langle x^2\rangle$ and $\langle x^4\rangle$, obtained with recourse to Eq. (5) in both the TF and WK approaches. We shall take $N=10$ particles, accommodating, for sake of simplicity, one particle per level.

As before, the self-consistent solution of Eq. (8), subject to the constraints posed by the TF or WK input expectation values, yields a set of N orthogonal wave functions that allows one to infer TF or WK densities for the potential (17). We depict in Fig. 4 the comparison between the exact ground-state wave function and the inferred Thomas-Fermi one. The inclusion of the $\hbar^2$ correction in the input information (5) does not considerably improve upon this result. Figure 5 displays, for $N=10$, the TF density, our inferred ρ (ITF), and the exact quantal one. In our ITF density shell effects are clearly appreciable and quite well reproduced (as compared to the quantal ones) by using as the only input information $\langle x^2\rangle$ and $\langle x^4\rangle$, in turn obtained with the first term of Eq. (5). The inferred potential exhibits also a rather good quality (see Fig. 6). The same applies for the inferred eigenenergies displayed in Fig. 6 for the first three eigenvalues, which correspond to the first six occupied states due to degeneracy effects.

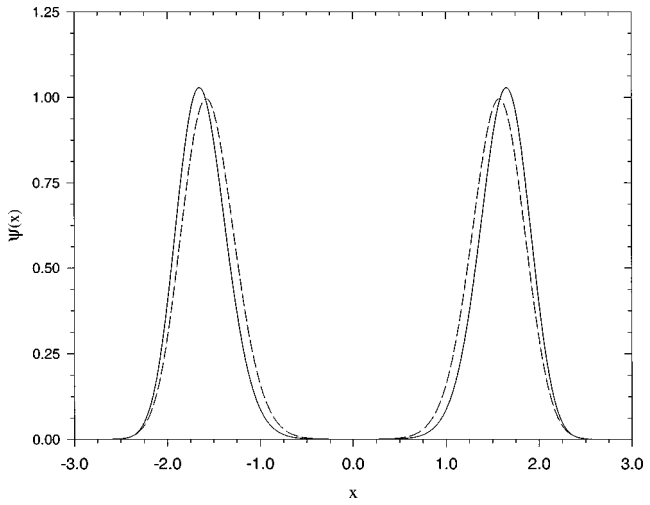

FIG. 4. The exact ground-state wave function (continuous line) is compared to the inferred TF one (dashed line) for the bistable potential (17). See Sec. IV B for additional details.

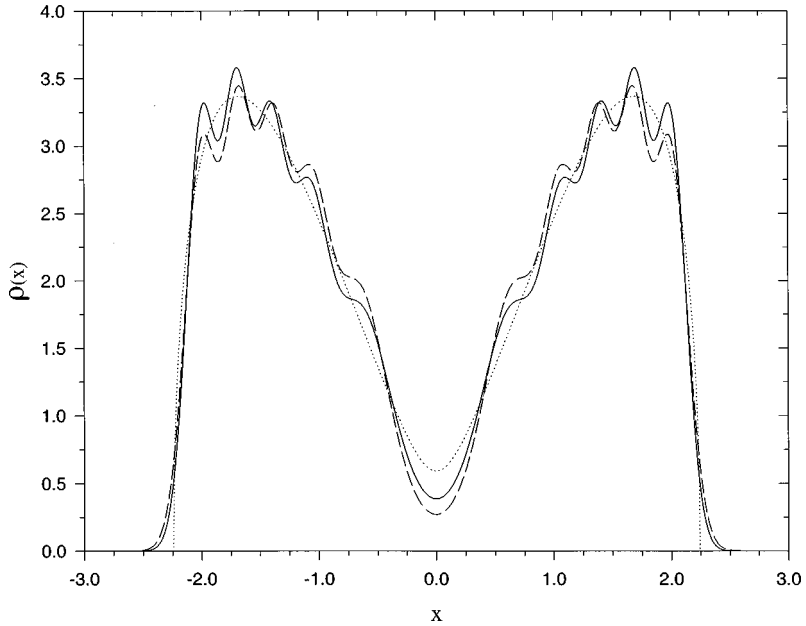

FIG. 5. Comparison between the exact density (continuous line) and the inferred TF one (dashed line) for the bistable potential (17) with $N=10$ particles. The standard TF density (dotted line) is also shown.

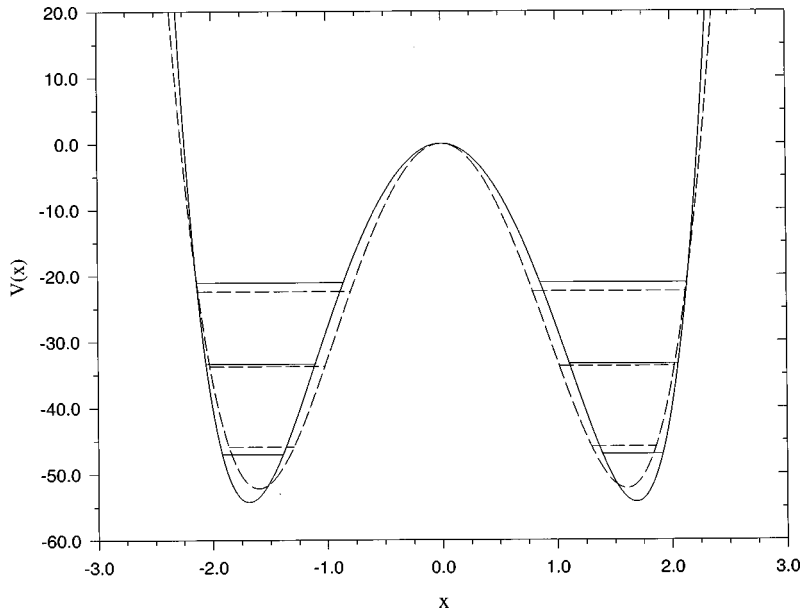

FIG. 6. The inferred bistable potential using TF information (dashed line) is compared to the exact one (continuous line). In addition, the inferred and exact eigenenergies for the first three degenerate levels are also shown.

V. CONCLUSIONS

Based on Frieden and Soffer's principle of extremal physical information (EPI) we have presented a method that allows one to obtain WKB wave functions, valid everywhere, without the need of any matching procedure. For this purpose we extremize Fisher's information for translation families subject to the constraints posed by the expectation values of a few commuting operators obtained in the WKB approach, and then follow the recipes of [22]. In the extremization process the Lagrange multipliers are self-consistently obtained.

The algorithm presented here has also been applied to the TF or WK approaches and yields one-body densities valid everywhere and including shell effects. With a very modest informational input (only a few TF or WK expectation values that are easily evaluated) our method is also able to infer approximate single-particle wave functions and eigenenergies of rather good quality.

The test presented in this effort for one-dimensional potentials is of a rather satisfactory character and should encourage application of the method to more realistic problems.

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