Alternative approach to the semiclassical description of N-fermion systems

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An information-theory-based approach to the semiclassical treatment of the N-fermion problem is presented which improves upon the traditional ones in two respects: It is valid beyond the turning points and is able to describe shell effects. The method is illustrated by recourse to simple one-dimensional systems.

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I. INTRODUCTION

Semiclassical treatments were introduced already in the 1920s [1,2] but still enjoy wide popularity (see, for instance, [3–9]) as they are often able to provide useful insights concerning the intricacies of some physical phenomena. Of course, the concomitant literature is so extensive that no attempt can be made to list a comprehensive set of references (for an excellent recent review one could cite, for example, Ref. [10]). In particular, the idea of investigating the ground-state properties of an N-fermion system by recourse to the knowledge of the diagonal part of the one-body reduced density matrix has found extensive applications in atomic, nuclear, plasma, and solid-state physics [10–16].

Several derivations can be found in the literature of the so-called Wigner-Kirkwood expansion [17], of which the celebrated Thomas-Fermi (TF) approach constitutes the leading order [13–15,18]. A common trait characterizes these derivations: that of approximating the Wigner distribution by a Heaviside step function. From the Wigner transform, the diagonal one-body density, both in momentum and coordinate representations, is easily constructed. *This density has the range of its validity restricted to the interval bounded by the classical turning points*, a fact that certainly must be stressed and that receives adequate consideration if one attempts an *alternative* discussion of the Wigner-Kirkwood expansion on the basis of a semiclassical expansion of Schrödinger's equation (WKB) [19]. It is thus clearly appreciated that TF constitutes an approximate treatment of the N-fermion problem that retains terms up to order $\hbar$, while the Wigner-Kirkwood (WK) approach incorporates terms up to order $\hbar^2$, *while in both cases the level density is smoothed.*

Of course, one would like to deal with approximate one-body densities without worrying about their range of validity. A method that circumvents this difficulty is provided by the widely popular density-functional theory [11,12], which has enjoyed a considerable amount of success and attracted the attention of many authors. However, an essential feature of the N-body systems is the existence of shell effects, quantum fluctuations, and discontinuous behavior of the energy eigenvalues, which are averaged out both by the TF and WK treatments, on the one hand, and by density-functional techniques, on the other.

The purpose of the present effort is to approach the semiclassical treatment of the N-fermion problem from a different angle, so as to have one-body densities of unrestricted validity and also be in a position to describe "shell effects." Simple tools of information theory (IT) [20,21] will be used to this effect. Since this is an introductory work, attention will be restricted to the one-dimensional situation.

The manuscript is organized as follows. A brief summary of the main ingredients of the TF and WK approaches is given in Sec. II while some rudiments of IT are reviewed in Sec. III. Our present treatment is described in Sec. IV and some applications are presented in Sec. V. Finally, conclusions are drawn in Sec. VI.

II. THE THOMAS-FERMI AND WIGNER-KIRKWOOD APPROACHES

Following the ideas expounded in [19] and [22], the expectation value of a one-body operator F in a state of energy ϵ can be computed as

$$\langle F\rangle_\epsilon = \lim_{\lambda\to 0}\frac{1}{\lambda}[\epsilon(V+\lambda F)-\epsilon(V)]\ , \tag{1}$$

where $\epsilon(V+\lambda F)$ is the energy eigenvalue when the Hamiltonian $H=T+V$ is replaced by $H'=T+V+\lambda F$. If n is the number of zeros of the concomitant *exact* wave function, the energy eigenvalues ϵ_n are determined by the requirement

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

S being the function defined as

$$S=\oint(\chi+i\hbar\chi_1)dz\ , \tag{3}$$

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where χ is the solution of the associated Ricatti equation, of which χ_1 gives the contribution of order $\hbar$ [19]. The contour integration in the complex z plane encloses the segment of the real axis bounded by the turning points.

The semiclassical WKB approximation is obtained by assuming that χ (and, consequently, S and ϵ) admits a power expansion in $\hbar$

$$S = \sum_{m=0}^{\infty} (i\hbar)^{2m} S_m(\epsilon_n, V, \hbar) \quad , \tag{4}$$

and

$$\epsilon = \epsilon_0 + \hbar^2 \epsilon_1 + \hbar^4 \epsilon_2 + \cdots \quad . \tag{5}$$

One can recast (1) in the fashion

$$\langle F \rangle_\epsilon = -\frac{\delta S(F,\epsilon)}{\partial S/\partial \epsilon} \quad , \tag{6}$$

where

$$\delta S(F,\epsilon) = \lim_{\lambda \to 0} [S(\epsilon, V + \lambda F) - S(\epsilon, V)]/\lambda \, . \tag{7}$$

The expansions of S and ϵ_n can be truncated at the order $\hbar^2$, so that the expectation value of our one-body operator F acquires the appearance [19]

$$\langle F \rangle_\epsilon = \frac{\oint \frac{F}{\sqrt{\epsilon_0 - V}} dz}{\oint \frac{1}{\sqrt{\epsilon_0 - V}} dz} - \hbar^2 \left\{ \frac{\frac{1}{16} \oint \frac{V'' F}{(\epsilon_0 - V)^{5/2}} dz + \frac{5}{64} \oint \frac{V'^2 F}{(\epsilon_0 - V)^{7/2}} dz + \frac{1}{2} \frac{d}{d\epsilon_0} \left(\epsilon_1 \oint \frac{F}{(\epsilon_0 - V)^{1/2}} dz \right)}{\oint \frac{1}{(\epsilon_0 - V)^{1/2}} dz} \right\} + O(\hbar^4) + \cdots \, , \tag{8}$$

where ϵ_0 is the eigenenergy of order $\hbar$, determined by recourse to (2)

$$\oint \sqrt{\epsilon_0 - V} dz = (n + \tfrac{1}{2}) h \, , \tag{9}$$

while ϵ_1 is the corresponding correction of order $\hbar^2$

$$\epsilon_1 = -\frac{1}{24} \frac{\oint \frac{V''}{(\epsilon_0 - V)^{3/2}} dz}{\oint \frac{1}{(\epsilon_0 - V)^{1/2}} dz} \, . \tag{10}$$

All the contour integrations can be evaluated in the real axis by taking derivatives with respect to the energy

$$\frac{d}{d\epsilon_0} \oint (\epsilon_0 - V)^{-n/2} dz = -\frac{n}{2} \oint (\epsilon_0 - V)^{-(\frac{n+2}{2})} dz \tag{11}$$

and using

$$\oint dz = 2 \int_{x_-}^{x_+} dx \quad , \tag{12}$$

where $x\pm$ are the turning points.

In the case of one-dimensional N-fermion systems we can reach the TF and WK approaches by "smoothing" the level density and integrating (8) up to the Fermi energy. Following [19] we write down the quantal level density as a function of S [the number of states $N(\epsilon)$ equals the number of fermions N],

$$g(\epsilon) = \frac{dN}{d\epsilon} = \frac{1}{h} \frac{\partial S}{\partial \epsilon} \sum_{k=0}^{\infty} \delta \left(-\frac{1}{2} + \frac{1}{h} S(\epsilon, V, \hbar) - k \right) . \tag{13}$$

After averaging out the discontinuities of $g(\epsilon)$ by expanding (13) (using the method of Euler-McLaurin, for instance) and dropping the oscillating terms, the "smoothed" level density $\tilde{g}(\epsilon)$ is obtained

$$\tilde{g}(\epsilon) = \frac{1}{h} \frac{\partial S}{\partial \epsilon} \theta(\epsilon - \epsilon_m^0) \quad , \tag{14}$$

where ϵ_m^0 is defined by the condition $S(\epsilon_m^0) = 0$. Replacement of (4) into (14) leads to the proper semiclassical level density.

Of special importance for our purpose are the expectation values of one-body operators in the TF (order $\hbar$) or in the WK (order $\hbar^2$) approximation. They are computed by replacing sums over discrete levels by suitably weighted integrals up to the Fermi energy

$$\langle F \rangle = \int_{-\infty}^{\epsilon_F} \langle F \rangle_\epsilon \tilde{g}(\epsilon) d\epsilon \quad , \tag{15}$$

so that one finds

$$\begin{aligned} \langle F \rangle = & \frac{1}{h} \oint F \sqrt{\epsilon_F - V} dz \\ & + \frac{\hbar}{48\pi} \left(\oint \frac{F V''}{(\epsilon_F - V)^{3/2}} dz \right. \\ & \left. + \frac{3}{4} \oint \frac{F V'^2}{(\epsilon_F - V)^{5/2}} dz \right) . \end{aligned} \tag{16}$$

The Fermi energy ϵ_F is obtained by requiring that

$$\int_{-\infty}^{\epsilon_F} \tilde{g}(\epsilon) d\epsilon = N \, . \tag{17}$$

The integrals of (16) can be computed in the real axis, taking out derivatives with respect to the energy. When they are not analytical, to avoid losing accuracy, we compute them in the complex z plane.

III. A BRIEF SUMMARY OF ELEMENTARY IT CONCEPTS

Information theory [23] provides one with a powerful *inference* methodology in order to describe general properties on the basis of scarce information. Indeed, it purports to yield the "least-biased" description that can be devised on the basis of some specific data, in any possible situation [20,21]. The essential aspects of IT relevant for our present purposes can be summarized as follows. Let A_α ($\alpha = 1, ..., N$) be a set of random variables that characterize some system of interest. These variables adopt the values $A_\alpha(i)$ with probabilities $p(i)$. Assume that our knowledge concerning the system is limited to the set of expectation values

$$\langle A_\alpha \rangle = \sum_i p(i) A_\alpha(i), \qquad \alpha = 1, ..., N \ . \tag{18}$$

The question is the following: What can we assert with respect to the (unknown) probability distribution $p(i)$?

Of course, many such distributions are compatible with the amount of information provided by (18). It claims that the "best" (or least-biased) one is that which maximizes Shannon's entropy [23] (or, more appropriately perhaps, Shannon's ignorance function [20])

$$S = -\sum_i p(i) \ln p(i). \tag{19}$$

The concomitant extremalization problem can be solved in analytical fashion and yields the recipe for constructing the "one and only" probability distribution:

$$p(i) = \exp\left(-\lambda_0 - \sum_{\alpha=1}^{N} \lambda_\alpha A_\alpha(i)\right) \ , \tag{20}$$

where the λ's are Lagrange multipliers that guarantee compliance with the set of "constraints" (18). In particular, λ_0 ensures that the probability distribution (20) is a properly normalized one. The concrete values that these multipliers adopt is obtained by solving the coupled set of equations

$$\frac{\partial \lambda_0}{\partial \lambda_\alpha} = -\langle A_\alpha \rangle \ , \tag{21}$$

where

$$\lambda_0 = \ln \sum_i \exp\left(-\sum_\alpha \lambda_\alpha A_\alpha(i)\right). \tag{22}$$

It can be proved that $p(i)$ always exists and is uniquely determined by (21) and (22), provided the input information (18) is not self-contradictory [20]. A standard well-known numerical algorithm is available that yields the λ's in (20) [24].

If, in addition to (18), some additional piece of information is available, such as, for example, that $p(i)$ is of the form $g_1(i)g_2(i)$, with g_1 known and g_2 unknown, one can incorporate this knowledge by maximizing [instead of (19)] the so-called *relative* entropy [21]

$$S' = -\sum_i p(i) \ln\{p(i)/g_1(i)\} \ , \tag{23}$$

which produces no essential change in (20), (21), and (22), except for the fact that on the left hand side of (20) one should place the unknown function $g_2(i)$.

IV. THE PRESENT APPROACH

The main idea of the present approach is that of *inferring* with the IT methodology an appropriate one-body density valid *beyond* the interval bounded by the turning points. The input information refers here to either TF or WK expectation values.

As stated in Sec. II, these input values are of the form

$$\begin{aligned} \langle F \rangle_{\rm TF} &= \int_{\epsilon_0}^{\epsilon_F} \langle F \rangle_{\epsilon_\hbar} \ \tilde{g}(\epsilon)\, d\epsilon, \\ \langle F \rangle_{\rm WK} &= \int_{\epsilon_0}^{\epsilon_F} \langle F \rangle_{\epsilon_{\hbar^2}} \ \tilde{g}(\epsilon)\, d\epsilon, \end{aligned} \tag{24}$$

where ϵ_0 refers to the bottom of the appropriate potential well $V(x)$ and $\langle F \rangle_{\epsilon_\hbar}$, $\langle F \rangle_{\epsilon_{\hbar^2}}$ is the expectation value of the one-body operator computed using (8) up to order $\hbar$ or $\hbar^2$. One is thus led to [19]

$$\langle F \rangle_{\rm TF} = \frac{1}{\pi\hbar} \int_{x^-}^{x^+} F \sqrt{\epsilon_F - V(x)}\, dx \tag{25}$$

and (x^+, x^- refer, of course, to the turning points)

$$\langle F \rangle_{\rm WK} = \langle F \rangle_{\rm TF} + \frac{\hbar}{24\pi} \left(\int_{x^-}^{x^+} \frac{F V''}{(\epsilon_F - V)^{3/2}} dx + \frac{3}{4} \int_{x^-}^{x^+} \frac{F V'^2}{(\epsilon_F - V)^{5/2}} dx \right) . \tag{26}$$

The concomitant TF and WK one-body densities are given in terms of the Heaviside function by

$$\rho_{\rm TF} = \frac{1}{\pi\hbar} \sqrt{\epsilon_F - V}\, \Theta(\epsilon_F - V) \tag{27}$$

and

$$\rho_{\rm WK} = \rho_{\rm TF} + \frac{\hbar}{24\pi} \left(\frac{V''}{(\epsilon_F - V)^{3/2}} + \frac{3}{4} \frac{V'^2}{(\epsilon_F - V)^{5/2}} \right) \theta(\epsilon_F - V) \ . \tag{28}$$

It is our purpose, that of inferring from a set of M expectation values of the form (25) [or of the form (26)] an *extended* semiclassical density valid beyond the turning points, that incorporates shell effects. This latter point can be adequately reflected in IT terms by noticing that it will lead to a one-body density ρ for the N-fermion system that exhibits N "ripples." In line with the discussion of Sec. III we advance the following ansatz:

$$\rho(x) = [P_{N-1}(x)]^2 \exp\left(-\lambda_0 - \sum_{\alpha=1}^{M} \lambda_\alpha F_\alpha(x)\right) , \quad (29)$$

where P_n is an arbitrary nth degree polynomial (squared so as to guarantee the positivity of ρ) that plays the role of the function g_1 in Sec. III. We assume that a set of semiclassical expectation values $\langle F_\alpha \rangle$ $(\alpha = 1, ..., M)$ is available.

A serious difficulty must be faced, however, since we do not know the coefficients of $P_{N-1}(x)$, so that a straightforward application of the IT approach (and of the concomitant numerical procedure given in [24]) is thereby precluded. Consequently, we proceed now to put forward a self-consistent algorithm that yields both the λ's and the coefficients of P_{N-1}.

We start by expressing ρ in the form

$$\rho(x) = (P_{N-1})^2 \mathcal{F}(\lambda_1, ..., \lambda_M) \ , \quad (30)$$

where $\mathcal{F}$ is, of course, of the exponential IT appearance. The idea is now to devise an iterative process that yields the λ's at each step, in the usual fashion [24] supplemented with additional manipulations involving $P_{N-1}(x)$. At order zero one sets $P^{(0)}_{N-1} = 1$ and obtains, via the algorithm of [24], the concomitant λ's of that order $(\lambda^{(0)}_1, ..., \lambda^{(0)}_M)$. Thus $\rho^{(0)}$ is of the form $(P^{(0)}_{N-1})^2 \mathcal{F}^{(0)}$. We now proceed to construct the N first orthogonal polynomials $\{Q^{(1)}_n(x)\ (n = 0, ..., N-1)\}$ with respect to the weighting function $\mathcal{F}^{(0)}$ by recourse to the Gramm-Schmidt procedure. $P^{(1)}_{N-1}$ is then constructed according to

$$[P^{(1)}_{N-1}(x)]^2 = \sum_{n=0}^{N-1} [Q^{(1)}_n(x)]^2 \ . \quad (31)$$

The new density $\rho^{(1)} = (P^{(1)}_{N-1})^2 \mathcal{F}^{(1)}$ is obtained by upgrading $\mathcal{F}$ with the usual IT procedure. We see that, proceeding in a similar fashion, a double-step iterative algorithm emerges in which information concerning the coefficients of P_{N-1} is fed into the IT machinery so as to influence the value of the Lagrange multipliers. These, in turn, affect, at order k, a fine tuning of the polynomial coefficients via the Gramm-Schmidt process according to

$$[P^{(k+1)}_{N-1}(x)]^2 = \sum_{n=0}^{N-1} [Q^{(k+1)}_n(x)]^2 \ . \quad (32)$$

As will be shown below, this scheme works nicely and produces quite reasonable results.

V. RESULTS

A. The harmonic oscillator

This constitutes the obvious test to be performed. We obtain the gratifying result that our "inferred Thomas-Fermi" (ITF) approach yields the *exact* quantal values, i.e., our one-body density coincides with the exact one. Some concomitant figures are listed in Table I for $N = 5$ (M = 1 and $F = x^2$).

TABLE I. Harmonic oscillator. Relative errors of the expectation values of x^6, x^8, and x^{10} for $N = 5$ particles. The predictions of the Thomas-Fermi (TF) and the inferred Thomas-Fermi (ITF) approaches are compared to the quantal ones.

Expectation value	TF(%)	ITF(%)
$\langle x^6 \rangle$	7,41	0.0
$\langle x^8 \rangle$	16,83	0.0
$\langle x^{10} \rangle$	29,50	0.0

B. Anharmonic potentials

We shall concentrate our efforts on Hamiltonians of the type

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\alpha}{2}x^2 + \gamma x^4 \ , \quad (33)$$

which continues to draw the attention of many authors due to its relevance in several disciplines [25–34]. We shall compare the results obtained with our approach with those yielded by the TF one. In those cases in which second-order corrections improve significantly over the TF figures, we shall also discuss inferences obtained with WK inputs. We shall take $M = 2$ and consider as input the pair $\langle x^2 \rangle, \langle x^4 \rangle$ as provided by a semiclassical approach. We "predict" with our inference technique the expectation values of x^{2n} with $n = 3, 4$, and 5 in order to illustrate the power of our method.

For the case $\alpha = 1$ and $\gamma = 10$ Table II compares the values of $\langle x^6 \rangle$, $\langle x^8 \rangle$, and $\langle x^{10} \rangle$, for N running between 2 and 10, as obtained in five different fashions: (1) quantal

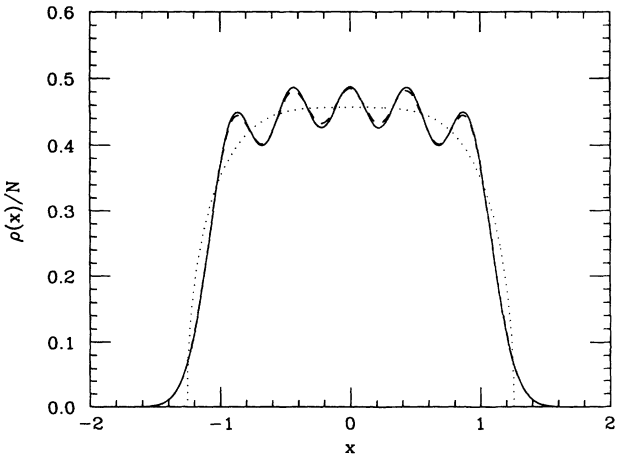

FIG. 1. Densities $\rho(x)/N$ for the quartic anharmonic oscillator ($\alpha = 1$ and $\gamma = 10$). The number of particles N is 5. The solid line represents the quantal (exact) result. The dotted line exhibits the TF prediction and the dashed line the results of the inferred Thomas-Fermi prescription.

(exact), (2) TF, (3) WK, (4) inferred (from) TF (ITF), and (5) inferred (from) WK (IWK). It is seen that ITF improves upon TF and IWK upon WK. The effect of terms of the order $\hbar^2$ is readily appreciated (already at the semiclassical level).

Our inference technique works well for other anharmonic oscillators and in all the cases analyzed the ITF and the IWK approaches improve the TF and WK results, respectively. For instance, in the case $\alpha = 1$ and $\gamma = 1$ our ITF prediction for $\langle x^6 \rangle$ approaches the quantal value with a precision between 13% and 0.5% when the number of particles N runs between 2 and 10. The TF method gives errors between 20% and 1% for the same results.

We have also applied our method to a double-well bistable potential ($\gamma = 1, \alpha = -1.5\alpha_c$) where α_c is a critical value discussed in Refs. [33, 34]. In this case our ITF prediction for $\langle x^{10} \rangle$ approaches the quantal result with a precision between 16% and 2% for N running

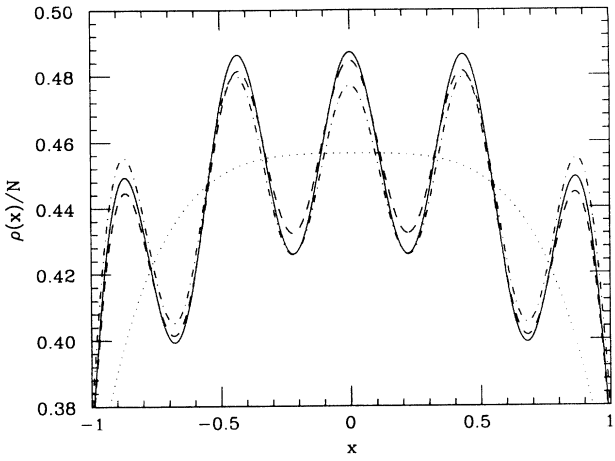

FIG. 2. "Ripples" of the densities $\rho(x)/N$ for the quartic anharmonic oscillator ($\alpha = 1$ and $\gamma = 10$). Additional details are the same as in Fig 1.

TABLE II. Anharmonic quartic oscillator ($\gamma = 10$). The expectation values of x^6, x^8, and x^{10} are evaluated according to different prescriptions. The number of particles N runs from 2 to 10. ITF and IWK denote, respectively, the inferred Thomas-Fermi and the inferred Wigner-Kirkwood prescription.

N	Expectation value	Quantal	TF	WK	ITF	IWK
2	$\langle x^6 \rangle$	0.1375	0.1120	0.1425	0.1212	0.1421
	$\langle x^8 \rangle$	0.1112	0.0677	0.1173	0.0860	0.1164
	$\langle x^{10} \rangle$	0.1065	0.0436	0.1094	0.0701	0.1125
3	$\langle x^6 \rangle$	0.4211	0.3827	0.4287	0.3984	0.4281
	$\langle x^8 \rangle$	0.3914	0.3042	0.4027	0.3489	0.4010
	$\langle x^{10} \rangle$	0.4185	0.2580	0.4300	0.3460	0.4309
4	$\langle x^6 \rangle$	0.9650	0.9135	0.9750	0.9365	0.9738
	$\langle x^8 \rangle$	1.0237	0.8816	1.0416	0.9629	1.0374
	$\langle x^{10} \rangle$	1.2219	0.9076	1.2470	1.1041	1.2416
5	$\langle x^6 \rangle$	1.8569	1.7923	1.8695	1.8225	1.8673
	$\langle x^8 \rangle$	2.2173	2.0102	2.2432	2.1351	2.2348
	$\langle x^{10} \rangle$	2.9347	2.4047	2.9791	2.7580	2.9613
6	$\langle x^6 \rangle$	3.1850	3.1074	3.2000	3.1442	3.1966
	$\langle x^8 \rangle$	4.2211	3.9394	4.2560	4.1134	4.2414
	$\langle x^{10} \rangle$	6.1396	5.3270	6.2093	5.8862	6.1710
7	$\langle x^6 \rangle$	5.0374	4.9467	5.0549	4.9897	5.0498
	$\langle x^8 \rangle$	7.3204	6.9552	7.3654	7.1825	7.3420
	$\langle x^{10} \rangle$	11.597	10.431	11.699	11.245	11.629
8	$\langle x^6 \rangle$	7.5023	7.3985	7.5223	7.4471	7.5150
	$\langle x^8 \rangle$	11.835	11.378	11.891	11.661	11.856
	$\langle x^{10} \rangle$	20.259	18.663	20.399	19.780	20.282
9	$\langle x^6 \rangle$	10.668	10.551	10.690	10.605	10.680
	$\langle x^8 \rangle$	18.117	17.560	18.185	17.902	18.134
	$\langle x^{10} \rangle$	33.274	31.171	33.460	32.638	33.276
10	$\langle x^6 \rangle$	14.622	14.492	14.647	14.550	14.634
	$\langle x^8 \rangle$	26.549	25.885	26.631	26.286	26.558
	$\langle x^{10} \rangle$	52.005	49.313	52.244	51.171	51.968

from 2 to 10. The corresponding TF prediction gives errors between 24% and 4%.

Figure 1 depicts our one-body densities for $N = 5, \alpha = 1$, and $\gamma = 10$ and compares them to both the exact quantal one and the TF results. Notice that no WK density exists (it yields actually a distribution). Shell effects are clearly appreciated. Figure 2 is an amplification of the pertinent ripples so as to be in a position to distinguish between ITF and IWK. It is seen that both densities are reasonably good ones.

VI. CONCLUSIONS

We have presented in this work a semiclassical approach, based upon information theory, that uses as input expectation values evaluated in orthodox semiclassical fashion. Our approach improves upon the traditional one in two respects: (1) the resulting one-body density is valid everywhere, whereas the original one is restricted to the interval bounded by the turning points; and (2) shell effects are well described, which is not possible otherwise, a fact that constitutes one of the main drawbacks of both the semiclassical approximations and the density functional theories.

From the practical point of view our method requires a very modest informational input, consisting in just a few semiclassical expectation values that are easily evaluated. The concomitant numerical effort should pose no undue troubles, as only two standard programs are required: one for the Gramm-Schmidt orthogonalization and the other for the determination of the IT Lagrange multipliers [24].

As the present one-dimensional results are of a rather satisfactory character, they should encourage one to tackle in a similar fashion more realistic problems.

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