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Mapping the Wigner distribution function of the Morse oscillator onto a semiclassical distribution function

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Abstract

The mapping of the Wigner distribution function (WDF) for a given bound state onto a semiclassical distribution function (SDF) satisfying the Liouville equation introduced previously by us is applied to the ground state of the Morse oscillator. The purpose of the present work is to obtain values of the potential parameters represented by the number of levels in the case of the Morse oscillator, for which the SDF becomes a faithful approximation of the corresponding WDF. We find that for a Morse oscillator with one level only, the agreement between the WDF and the mapped SDF is very poor but for a Morse oscillator of ten levels it becomes satisfactory. We also discuss the limit $\hbar \rightarrow 0$ for fixed potential parameters.

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1. Introduction

The Wigner description in phase space [1] provides a tool for comparing quantum and classical dynamics [2]. In a previous paper [3] we introduced a mapping relating the Wigner distribution function (WDF) corresponding to a given wavefunction, solution of the Schrödinger equation, to a semiclassical distribution function (SDF) satisfying the classical Liouville equation with the same potential. So far this mapping was applied to the ground state of the square well [3], the Pöschl–Teller potential [4] and to a modified harmonic oscillator potential [4].

Here this mapping is extended to the ground state of the unidimensional Morse oscillator. We vary the depth of the potential in order to study the effect of the level density on the mapping.

The Morse oscillator [5] plays an important role in many areas of physics, because it is a good approximation to diatomic molecular potentials [6]. Today the Morse potential is used in molecular spectroscopy, even for polyatomic molecules [7]. Some authors have used the Morse potential for studying the semiclassical limit of quantum mechanics [8].

The unidimensional Morse oscillator in phase space has already been studied by many authors. The classical motion [9] as well as the quantum representation [6] are well known for this potential.

In section 2 of this work we summarize the method developed in [3] for mapping a WDF onto the corresponding SDF. In section 3 we study the Morse oscillator and in section 4 we present our results and conclusions.

2. Description of the method

In this section we present a short derivation of the method used for the mapping [3]. We start with the quantum Liouville equation for the WDF ρ :

$$\frac{\partial \rho}{\partial t} + \frac{p}{m} \frac{\partial \rho}{\partial q} + \int K(q, p - p') \rho(q, p', t) dp' = 0 \quad (1)$$

where the kernel K is given by

$$K(q, p - p') = \frac{i}{\hbar} \int \frac{dv}{2\pi\hbar} \exp\left[\frac{i}{\hbar}(p - p')v\right] \left[V\left(q - \frac{v}{2}\right) - V\left(q + \frac{v}{2}\right) \right] \quad (2)$$

$V(q)$ being the potential. The corresponding classical Liouville equation may be written similarly as

$$\frac{\partial \rho_c}{\partial t} + \frac{p}{m} \frac{\partial \rho_c}{\partial q} + \int K_c(q, p - p') \rho_c(q, p', t) dp' = 0 \quad (3)$$

where

$$K_c(q, p - p') = -\frac{i}{\hbar} \int \frac{dv}{2\pi\hbar} \exp\left[\frac{i}{\hbar}(p - p')v\right] v \frac{\partial V}{\partial q} = -\frac{\partial V}{\partial q} \frac{\partial}{\partial p} \delta(p - p'). \quad (4)$$

We relate solutions ρ and ρ_c of equations (1) and (3) through the integral equation

$$\begin{aligned} \rho(q, p, t) = & \rho_c(q, p, t) - \int_{-\infty}^{\infty} dt' \int dq' dp' G_c(q, p; q', p', t - t') \\ & \times \int dp'' [K(q', p' - p'') - K_c(q', p' - p'')] \rho(q', p'', t') \end{aligned} \quad (5)$$

where G_c is the retarded Green's function corresponding to the classical Liouville equation (3). In fact (5) is the defining equation of ρ_c since the WDF ρ is already determined by fixing the wavefunction solution of the Schrödinger equation. Using the differential equation satisfied by G_c [3] one may easily verify that ρ_c satisfies (3) provided ρ obeys (1).

As K_c is the limit of K when \hbar goes to zero, from (5) we obtain that the limit of $\rho - \rho_c$ will also be zero.

In what follows we shall consider mostly the mapping of the time-independent WDF $\rho(q, p)$ corresponding to a bound state.

It can be shown [3] that for points (q, p) on closed classical orbits the expression given by (5) is equivalent to

$$\rho_c(q, p) = \frac{1}{T(q, p)} \int_{-T(q, p)}^0 dt \rho(Q(q, p, t), P(q, p, t)). \quad (6)$$

Here $(Q(q, p, t), P(q, p, t))$ describes the classical trajectory in phase space of a particle subject to the potential $V(q)$ which at time $t = 0$ occupies the point (q, p) and $T = T(q, p)$

is the period of the orbit. For open trajectories we have $T \rightarrow \infty$ and as for bound states the integral in (6) converges, we get $\rho_c = 0$. As will be discussed further, in the calculation of averages of physical quantities the quantity of interest is rather $T(q, p)\rho_c(q, p)$ which does not vanish for the open trajectories.

We observe here that one may verify directly that the time-independent Liouville equation is obeyed by applying the operator $p\partial/\partial q - (\partial V/\partial q)\partial/\partial p$ on the right-hand side of (6) and using the fact that $\rho(Q(q, p, -t), P(q, p, -t))$ satisfies the classical Liouville equation (3).

An important property of the stationary SDF is that it is constant along the classical trajectories [3].

Let $(Q(E, \nu, t), P(E, \nu, t))$ represent, for t in the interval $-T(E, \nu)/2 \leq t \leq T(E, \nu)/2$ (T may be infinity), the points of a trajectory in phase space corresponding to energy E and fixed value of ν . Here the discrete parameter ν ($\nu = 1, \dots, \nu_{\max}$) distinguishes between the different trajectories corresponding to the same value of E . By varying E and ν one covers the entire allowed phase space. Thus we may consider the transformation of points (E, ν, t) in the appropriate domains D_ν of the energy-time space onto the points (p, q) of the phase space

$$q = Q(E, \nu, t) \quad p = P(E, \nu, t). \tag{7}$$

Let us define the function

$$R_c(E, \nu) = \int_{-T(E, \nu)/2}^{T(E, \nu)/2} dt \rho(Q(E, \nu, t), P(E, \nu, t)). \tag{8}$$

According to (6) one has

$$\rho_c(q, p) = \frac{R_c(E(q, p), \nu)}{T(E(q, p), \nu)} \tag{9}$$

by choosing the value of ν appropriate to the trajectory containing the point (q, p) as follows from (7). We observe here that the relationship (8) between $\rho(q, p)$ and $R_c(E, \nu)$ is analogous to that between $R(q)$, the probability density in coordinate space and the WDF $\rho(q, p)$ [10]:

$$R(q) = \int \rho(q, p) dp. \tag{10}$$

The average of any Weyl function [10] $\mathcal{O}(q, p)$ corresponding to a certain operator O may be written as

$$\langle O \rangle = \int \mathcal{O}(q, p)\rho(q, p) dp dq = \sum_\nu \int_{D_\nu} o(E, \nu, \tau)r(E, \nu, \tau) dE d\tau \tag{11}$$

where we introduced the functions

$$o(E, \nu, \tau) = \mathcal{O}(Q(E, \nu, \tau), P(E, \nu, \tau)) \tag{12}$$

$$r(E, \nu, \tau) = \rho(Q(E, \nu, \tau), P(E, \nu, \tau)) \tag{13}$$

and we used the fact that the Jacobian J of the transformation (7) is unity [3].

In the special case in which the Weyl function \mathcal{O} is a constant of motion depending on (q, p) only through the energy $E(q, p)$, we obtain from (11), (13) and (8)

$$\langle O \rangle = \sum_\nu \int_{D_\nu} o(E, \nu)r(E, \nu, \tau) dE d\tau = \sum_\nu \int o(E, \nu)R_c(E, \nu) dE. \tag{14}$$

As ρ_c is an approximation of the Wigner function ρ , correct in the limit of $\hbar \rightarrow 0$, the average

$$\langle O \rangle_c = \int \mathcal{O}(q, p)\rho_c(q, p) dq dp \tag{15}$$

is also correct in the same limit. Expression (15) may also be written, by making use of the transformation (7), as

$$\langle O \rangle_c = \sum_{\nu} \int_{D_{\nu}} o(E, \nu, t) \frac{R_c(E, \nu)}{T(E, \nu)} dE dt = \sum_{\nu} \int \bar{o}(E, \nu) R_c(E, \nu) dE \quad (16)$$

where we used equations (9) and (12) and $\bar{o}(E, \nu)$ denotes the average

$$\bar{o}(E, \nu) = \int_{-T(E, \nu)/2}^{T(E, \nu)/2} o(E, \nu, t) \frac{dt}{T(E, \nu)}. \quad (17)$$

Thus the average $\langle O \rangle_c$ is obtained by replacing $o(E, \nu, t)$ in (11) by the average (17). In the case of open paths the limit $T(E, \nu) \rightarrow \infty$ is taken in equation (17). If, for fixed E , $o(E, \nu, t)$ depends weakly on t , the average $\langle O \rangle_c$ is expected to be a good approximation.

3. Wigner distribution function for the Morse potential

In 1929 Morse [5] suggested the potential $U_0(1 - e^{-ar})^2$ for studying diatomic molecules. The Schrödinger equation for this potential does not have an exact solution, but for the one-dimensional case the problem can be solved analytically [11, 12].

In order to obtain the Wigner distribution function [1]

$$\rho(q, p, t) = (2\pi\hbar)^{-1} \int_{-\infty}^{\infty} dv e^{\frac{i}{\hbar}pv} \psi\left(q - \frac{1}{2}v, t\right) \psi^*\left(q + \frac{1}{2}v, t\right) \quad (18)$$

where ψ is the solution of the Schrödinger equation, we need the eigenfunctions for the one-dimensional Morse potential

$$\mathcal{V}(x) = D(1 - e^{-ax})^2 \quad (19)$$

a and D being constant parameters. Starting with the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + D(1 - e^{-ax})^2 \right] \psi_n = \mathcal{E}_n \psi_n \quad (20)$$

we introduce the dimensionless parameter λ

$$\lambda = \frac{\sqrt{2mD}}{a\hbar} \quad (21)$$

and the dimensionless coordinate

$$q = ax \quad (22)$$

obtaining an eigenvalue equation depending only on one parameter

$$\left[-\frac{1}{\lambda^2} \frac{d^2}{dq^2} + (1 - e^{-q})^2 \right] \psi_n = \epsilon_n \psi_n \quad (23)$$

where

$$\epsilon_n = \frac{\mathcal{E}_n}{D}. \quad (24)$$

This equation is solved most conveniently using the variable

$$\xi = 2\lambda e^{-q} \quad -\infty < q < \infty. \quad (25)$$

The eigenfunctions and eigenvalues are [6]

$$\psi_n(\xi) = N(n, \lambda) e^{-\frac{\xi}{2}} \xi^{\lambda-n-\frac{1}{2}} L_n^{\lambda-n-\frac{1}{2}}(\xi) \quad (26)$$

$$\epsilon_n = \frac{2}{\lambda} \left(n + \frac{1}{2} \right) \left[1 - \frac{1}{2\lambda} \left(n + \frac{1}{2} \right) \right] \quad (27)$$

where the quantum number n takes the values

$$n = 0, 1, 2, \dots, \left[\lambda - \frac{1}{2} \right]. \tag{28}$$

Here $[\lambda - 1/2]$ denotes the largest integer smaller than $\lambda - 1/2$, L_n^s is the polynomial [6]

$$L_n^s = \sum_{j=0}^n \binom{n+2s}{n-j} \frac{(-\xi)^j}{j!} \tag{29}$$

and the normalization factor N is given by

$$N(\lambda, n) = \left[\frac{(2\lambda - 2n - 1)\Gamma(n+1)}{\Gamma(2\lambda - n)} \right]^{\frac{1}{2}} \tag{30}$$

where the normalization condition $\int \psi_n^* \psi_n dq = 1$ is assumed. The normalization constant with the usual normalization condition has been derived in [13].

From (27) one verifies that, for $\lambda \gg 1$ and $n \ll \lambda$, the energy spectrum of the Morse oscillator is written approximately as $\mathcal{E}_n \approx \hbar\omega_0(n + 1/2)$, which is the spectrum of a harmonic oscillator with frequency

$$\omega_0 = \frac{2D}{\hbar\lambda} = a\sqrt{\frac{2D}{m}} = \lambda\hbar\frac{a^2}{m}. \tag{31}$$

As the semiclassical distribution functions ρ_c for the harmonic oscillator coincide with the Wigner functions ρ we expect that if $\lambda \gg 1$ ρ_c does get close to ρ for the low lying levels. Thus it may be appropriate to use, instead of the variable q and its canonical conjugate momentum p , the variables which treat harmonic oscillators on the same footing, namely [6]

$$Q = \left[\frac{m\omega_0}{\hbar} \right]^{\frac{1}{2}} x = \left[\frac{2mD}{a^2\hbar^2\lambda} \right]^{\frac{1}{2}} q = \sqrt{\lambda}q \tag{32a}$$

$$P = \frac{1}{\sqrt{\lambda}}p. \tag{32b}$$

The coordinate Q and the momentum P have been used in figures 1–4. We define the dimensionless potential $V(Q)$

$$V(Q) = (\hbar\omega_0)^{-1}\mathcal{V}(x) = \frac{\lambda}{2} \left(1 - e^{-\frac{Q}{\sqrt{\lambda}}} \right)^2 \tag{32c}$$

and the corresponding dimensionless energy levels

$$E_n = (\hbar\omega_0)^{-1}\mathcal{E}_n = \left(n + \frac{1}{2} \right) - \frac{1}{2\lambda} \left(n + \frac{1}{2} \right)^2. \tag{32d}$$

We observe that the potential $V(Q)$ is independent of λ for $Q^2 \ll \lambda$.

In the special case in which we are interested, namely the ground state, $n = 0$, the wavefunction is given by

$$\psi_0(\xi) = \left[\frac{2\lambda - 1}{\Gamma(2\lambda)} \right]^{\frac{1}{2}} \xi^{\lambda - \frac{1}{2}} e^{-\xi}. \tag{33}$$

In order to calculate the Wigner function replace ψ by $\psi_n(2\lambda e^{-q})$ in (18), obtaining

$$\rho_n^{(\lambda)}(q, p) = (2\pi\hbar)^{-1} \int_{-\infty}^{\infty} dv \psi_n(2\lambda e^{[-q + \frac{v}{2}]}) \psi_n^*(2\lambda e^{[-q - \frac{v}{2}]}) e^{\frac{i}{\hbar}pv}. \tag{34}$$

Introducing the new integration variable

$$\tau = e^{\frac{v}{2}} \tag{35}$$

(34) becomes

$$\rho_n^{(\lambda)}(q, p) = (\pi\hbar)^{-1} \int_0^\infty \psi_n^* \left(\frac{\xi}{\tau} \right) \psi_n(\xi\tau) \tau^{2ip\hbar^{-1}} \frac{d\tau}{\tau} \quad (36)$$

where ξ is given by (25). Substituting ψ_n in (36) by expression (26) $\rho_n^{(\lambda)}$ becomes [6]

$$\rho_n^{(\lambda)}(q, p) = \left[\frac{\pi\hbar}{2} \right]^{-1} [N(\lambda, n)]^2 \xi^{2\lambda-2n-1} \sum_{r=0}^n \sum_{s=0}^n b(\lambda, n, r) b(\lambda, n, s) \xi^{r+s} K_{s-r+2ip\hbar^{-1}}(\xi) \quad (37)$$

where

$$b(\lambda, n, j) = \binom{2\lambda - n - 1}{n - j} \frac{(-1)^j}{j!} \quad (38)$$

and $K_\nu(\xi)$ is defined by [6]

$$K_\nu(\xi) = \frac{1}{2} \int_0^\infty e^{-\frac{\xi}{2}(\tau + \frac{1}{\tau})} \tau^\nu \frac{d\tau}{\tau} \quad (39)$$

ν being a complex variable. In the particular case in which $n = 0$ we get

$$\rho_0^{(\lambda)}(q, p) = \left(\frac{\pi\hbar}{2} \right)^{-1} \frac{2\lambda - 1}{\Gamma(2\lambda)} \xi^{2\lambda-1} K_{2ip\hbar^{-1}}(\xi). \quad (40)$$

The numerical method we used to calculate the function $K_\nu(\xi)$ will be given in the appendix.

The symmetries obeyed by the function K_ν are

$$K_{\nu^*}(\xi) = \frac{1}{2} \int_0^\infty e^{-\frac{\xi}{2}(\tau + \frac{1}{\tau})} (\tau^\nu)^* \frac{d\tau}{\tau} = (K_\nu(\xi))^* \quad (41)$$

$$K_{-\nu}(\xi) = \frac{1}{2} \int_0^\infty e^{-\frac{\xi}{2}(\tau + \frac{1}{\tau})} \tau^{-\nu} \frac{d\tau}{\tau} = K_\nu(\xi) \quad (42)$$

where the last step is obtained by making $\tau \rightarrow \tau^{-1}$. From equations (42) and (41) we get

$$K_{-a+ib} = K_{a+ib}^*. \quad (43)$$

Thus (37) may be written as

$$\rho_n^{(\lambda)}(q, p) = \left[\frac{\pi\hbar}{2} \right]^{-1} [N(\lambda, n)]^2 \xi^{2\lambda-2n-1} \sum_{r=0}^n \sum_{s=0}^n b(\lambda, n, r) b(\lambda, n, s) \xi^{r+s} \operatorname{Re}(K_{s-r+2ip\hbar^{-1}}(\xi)) \quad (44)$$

showing explicitly that $\rho_n^{(\lambda)}$ is real.

In order to calculate the semiclassical distribution function $\rho_c(q, p)$ given by (6) or (9), we need the solution of the classical equation of motion

$$m\ddot{x} = -D \frac{d}{dx} (1 - e^{-ax})^2 \quad (45)$$

which has already been obtained exactly [9]. Introducing the coordinate $q = ax$ and the variable θ given by

$$\theta = \omega_0 t \quad (46)$$

where ω_0 is given by (31), (45) becomes

$$2 \frac{d^2 q}{d\theta^2} = -\frac{d}{dq} (1 - e^{-q})^2. \quad (47)$$

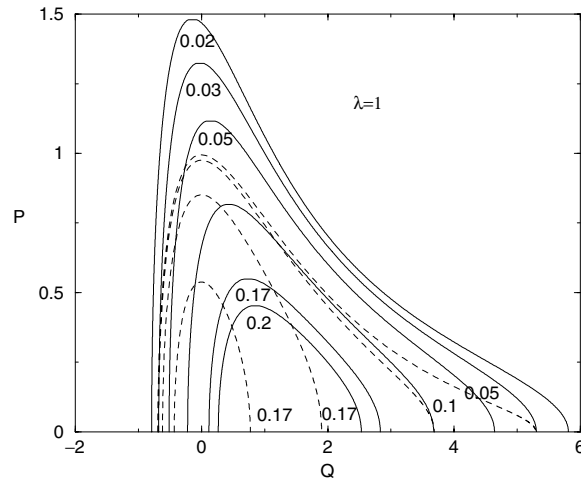


Figure 1. Solid curves are curves with a constant value of the Wigner distribution function ρ and dashed curves have constant value of the semiclassical distribution function ρ_c for the ground state of the Morse oscillator with $\lambda = 1$. Except for $\rho = 0.2$, for each solid curve with a given ρ one has one or two corresponding dashed curves with ρ_c such that $\rho_c = \rho$.

The solution of (47) for $\epsilon = E/D < 1$, where E is the energy associated with the trajectory, is

$$q(E, t) = \ln \left\{ \frac{1}{1 - \epsilon} [1 + \sqrt{\epsilon} \sin(\sqrt{1 - \epsilon}(\omega_0 t - \theta_0))] \right\}. \quad (48)$$

The canonical momentum associated with q is

$$p = \frac{m\dot{q}}{a^2} \quad (49)$$

which using equations (48) and (31) gives

$$p(E, t) = \hbar\lambda \frac{\sqrt{\epsilon}\sqrt{1 - \epsilon} \cos[\sqrt{1 - \epsilon}(\omega_0 t - \theta_0)]}{1 + \sqrt{\epsilon} \sin[\sqrt{1 - \epsilon}(\omega_0 t - \theta_0)]}. \quad (50)$$

The period associated with the orbit is

$$T(E) = \frac{2\pi}{\omega_0\sqrt{1 - \epsilon}}. \quad (51)$$

Analysing (48) one obtains that for $E \ll D$ the trajectories are close to those of a harmonic oscillator of frequency ω_0 .

4. Results

In this section we present the results of our calculations. We calculated the WDF ρ and the corresponding SDF ρ_c for the ground state of the Morse oscillator choosing for the parameter λ the values 1, 2, 4 and 10 corresponding to oscillators with 1, 2, 4 and 10 levels respectively. In the figures we used the dimensionless coordinates Q and the conjugate momenta P (in units of \hbar) defined by (32a) and (32b).

Let us first consider the results for the WDF. Figures 1, 2, 3 and 4 reproduce our calculations of the WDF for $\lambda = 1, 2, 4$ and 10 respectively through curves of constant density $\rho(Q, P)$ (solid curves). The value of ρ varies from $\rho \approx 0.3$ to $\rho = 0$ in the region

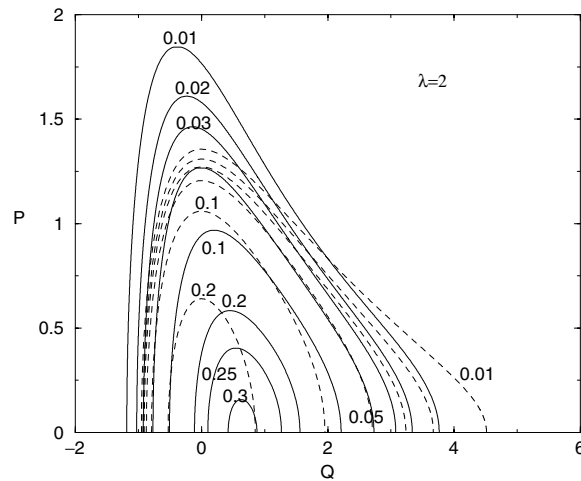


Figure 2. Same as figure 1 for $\lambda = 2$. Except for $\rho = 0.3$ and $\rho = 0.25$, for each full curve one has a corresponding dashed curve with ρ_c such that $\rho_c = \rho$.

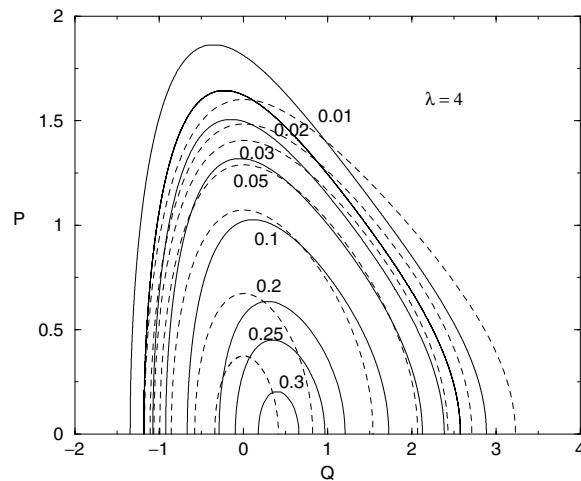


Figure 3. Same as figure 1 for $\lambda = 4$. Except for $\rho = 0.3$, for each full curve one has a corresponding dashed curve with ρ_c such that $\rho_c = \rho$.

of phase space corresponding approximately to the region of classical particles bound by the potential. On the remaining part of phase space ρ is much smaller in magnitude and there occur close spaced domains (not represented in the figures), such that ρ alternates in sign in the adjoining domains. Also the magnitude of ρ decreases rapidly as the domain gets farther away from the origin.

We found that in the case $\lambda = 1$ the minimum value of ρ is (in units of \hbar^{-1}) of the order of -10^{-2} . This minimum approaches zero as λ increases, thus for $\lambda = 4$ the minimum of ρ is reduced to about -10^{-4} .

The maximum of ρ moves from the point $(Q, P) = (1.2, 0)$ to $(Q, P) = (0.3, 0)$ as λ increases from 1 to 10 and its value increases slightly as λ increases. Thus the WDF curve for $\rho = 0.3$, which is present for $\lambda \geq 2$, does not occur for $\lambda = 1$.

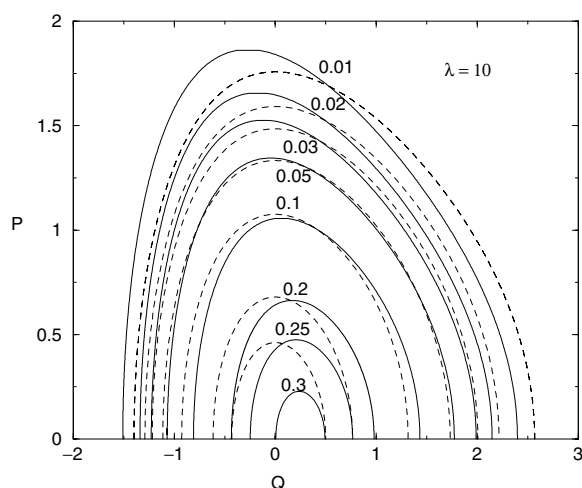


Figure 4. Same as figure 1 for $\lambda = 10$. Except for $\rho = 0.3$, for each full curve one has a corresponding dashed curve with ρ_c such that $\rho_c = \rho$.

Another feature of the WDF is that the curves of constant density ρ become more symmetric with respect to an axis parallel to the P -axis as λ increases, becoming close to the form of an ellipse. This tallies with the fact that for $Q \ll \sqrt{\lambda}$, $V(Q)$ is the potential of a harmonic oscillator.

Also in figures 1–4 we present SDF curves for fixed ρ_c (dashed curves) together with WDF curves with $\rho = \rho_c$ for comparison. It will be seen that as λ increases the SDF improves, which means also that the WDF curves of constant ρ become closer to classical trajectories. For the Morse oscillator with $\lambda = 1$, our semiclassical approximation is anomalous considering that ρ_c increases from $\rho_c = 0.145$ to $\rho_c = 0.179$ as the classical energy E varies from $E = 0$ to $E = 0.26\hbar\omega_0$ but decreases as E increases further. For $\lambda \geq 2$, ρ_c decreases as the energy E increases until reaching the value $\rho_c = 0$. As a consequence, for $\lambda = 1$ one has two closed curves with the same ρ_c for $0.145 < \rho_c < 0.179$ whereas for $\lambda \geq 2$, for each ρ_c one has only one such curve. Also for the WDF there is only one closed curve for each ρ from the maximum value of ρ up to the curve $\rho = 0$.

In figure 1 we compare the WDF curves of constant ρ with the SDF curves for which $\rho = \rho_c$ in the case $\lambda = 1$. One notices that the discrepancies between both curves are very large.

Making the same comparison for $\lambda = 2, 4$ and 10 in figures 2, 3, 4 we observe that for $\rho \gtrsim 0.05$ both curves are quite similar but displaced from each other. This displacement becomes less pronounced as ρ gets closer to 0.05 so that the best agreement between ρ and ρ_c is reached for $\rho \approx 0.05$. Also as λ increases the displacement between both curves decreases, as can be seen by comparing the oscillators $\lambda = 4$ and $\lambda = 10$. For $\rho < 0.05$ the curves of fixed ρ_c compared with the curves of fixed ρ contain a certain amount of distortion which becomes less pronounced as λ increases.

We remark here that for the Morse oscillator the largest value of ρ_c is smaller than the largest value of ρ . Thus for each λ there is a range of values of ρ such that no classical trajectories exist for which ρ_c is equal to ρ . The maxima of ρ_c are 0.227 , 0.271 and 0.299 respectively for $\lambda = 2, 4$ and 10 whereas the maxima of ρ are of the order of 0.3 for these values of λ . From the above values of ρ_c one verifies that the value of the maximum of ρ_c increases as λ increases, getting for $\lambda = 10$ close to the maximum of ρ .

The maximum of ρ_c for $\lambda \geq 2$ occurs at the origin of phase space, which is a point of stable equilibrium. As mentioned already, the position of the maximum of ρ gets closer to the origin of phase space as λ increases.

These results are in agreement with the assumption that as the number of levels of the Morse oscillator increases the WDF tends to coincide with the corresponding SDF and that $\lambda \sim 10$ is a satisfactory value of the potential parameter.

If the parameters a and D of the potential (cf (19)) are fixed and \hbar is made to decrease then λ according to the definition (21) will increase. In the limit $\hbar \rightarrow 0$ we have $\lambda \rightarrow \infty$ and the WDF and the SDF will coincide. If instead of the variables Q and P (32) we use the original variables x and the corresponding canonical momentum, the WDF and SDF will be delta functions describing a particle located at rest at the origin of phase space, a classical limit consistent with our previous results [3, 4].

Appendix. Numerical evaluation of the Wigner function

Here we discuss the numerical calculation of the quantity K_ν defined in (39) of section 3,

$$K_\nu(\xi) = \frac{1}{2} \int_0^\infty e^{-\frac{\xi}{2}(\tau + \frac{1}{\tau})} \tau^\nu \frac{d\tau}{\tau}. \quad (\text{A1})$$

Here ν is complex,

$$\nu = N + 2ik \quad (\text{A2})$$

where N is an integer and k is the dimensionless momentum p/\hbar and according to (25) and (22)

$$\xi = 2\lambda e^{-q} \quad q = ax. \quad (\text{A3})$$

Making the transformation

$$\tau = e^u \quad (\text{A4})$$

and considering that only the real part of K_ν enters into expression (44) for the Wigner function we get from (A1), substituting also ν according to (A2),

$$\text{Re}[K_\nu(\xi)] = \frac{1}{2} \int_{-\infty}^\infty e^{-\xi \cosh u} e^{uN} \cos(2ku) du. \quad (\text{A5})$$

Let us take initially $N = 0$, which is the only value needed for the ground state of the Morse oscillator. Consider also $k \neq 0$ as the case $k = 0$ is calculated separately. For convenience we introduce the new variable of integration

$$z = 2ku \quad (\text{A6})$$

and use the fact that the integrand is an even function of u , obtaining from (A5)

$$\text{Re}[K_\nu(\xi)] = \frac{1}{2k} \int_0^\infty dz e^{-\xi \cosh(\frac{z}{2k})} \cos z. \quad (\text{A7})$$

The integral in (A7) is of the form

$$I = \int_0^\infty f(z) \cos z dz \quad (\text{A8})$$

where $f(z)$ is a positive decreasing function of z . In order to avoid numerical cancellations arising from the change of sign of $\cos(z)$, we replace this integral by an integral in the interval $[0, \pi/2]$ of a series of functions.

We decompose I as follows:

$$I = I_1 + I_2 \tag{A9}$$

where

$$I_1 = \int_0^{\frac{\pi}{2}} f(z) \cos z \, dz \tag{A10}$$

and

$$I_2 = \int_{\frac{\pi}{2}}^{\infty} f(z) \cos z \, dz = - \int_0^{\infty} f\left(y + \frac{\pi}{2}\right) \sin y \, dy \tag{A11}$$

where we made the substitution $z = y + \frac{\pi}{2}$ in I_2 . The interval of integration of the integral I_2 is divided into the set of intervals $[2\pi s, 2\pi(s + 1)]$, $s = 0, 1, \dots$, so that I_2 is written as

$$I_2 = - \sum_{s=0}^{\infty} \int_{2\pi s}^{2\pi(s+1)} f\left(y + \frac{\pi}{2}\right) \sin y \, dy. \tag{A12}$$

Making now the substitution

$$z = y - 2\pi s \tag{A13}$$

for the integral in the interval $[2\pi s, 2\pi(s + 1)]$, one obtains for (A12)

$$I_2 = - \sum_{s=0}^{\infty} \int_0^{2\pi} f\left(z + \left(2s + \frac{1}{2}\right)\pi\right) \sin z \, dz. \tag{A14}$$

However $\sin z$ changes sign in the interval $[0, 2\pi]$ which leads to cancellation errors if f is slowly varying in the interval. In order to eliminate the oscillation of sign of the integrand we decompose again the integral in the intervals $[0, \pi]$ and $[\pi, 2\pi]$ obtaining

$$I_2 = - \sum_{s=0}^{\infty} \left\{ \int_0^{\pi} \left[f\left(z + \left(2s + \frac{1}{2}\right)\pi\right) - f\left(z + \left(2s + \frac{3}{2}\right)\pi\right) \right] \sin z \, dz \right\}. \tag{A15}$$

As f is assumed to be monotonically decreasing each integrand in (A15) is now always positive. As the domain of integration of the integral I_1 is the interval $[0, \pi/2]$ we make the translation $v = z - \frac{\pi}{2}$, obtaining

$$I_2 = - \sum_{s=0}^{\infty} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} [f(v + (2s + 1)\pi) - f(v + (2s + 2)\pi)] \cos v \, dv. \tag{A16}$$

Making $v \rightarrow -v$ for the contribution from the interval $[-\frac{\pi}{2}, 0]$ in (A16) and adding the contribution from I_1 one obtains finally

$$\int_0^{\infty} f(x) \cos x \, dx = \int_0^{\frac{\pi}{2}} dx \cos x \left\{ f(x) - \sum_{s=0}^{\infty} [f((2s + 1)\pi - x) + f((2s + 1)\pi + x) - f((2s + 2)\pi - x) - f((2s + 2)\pi + x)] \right\}. \tag{A17}$$

For $f(x)$ monotonic each term of the series contributes with the same sign, however errors may arise from the subtraction of the sum of the series from $f(x)$.

In the general case in which $N \geq 0$ in (A5), the function $f(z)$ in (A8) becomes

$$f_N(z) = \frac{1}{2k} e^{-\xi \cosh \frac{z}{2k}} \cosh\left(\frac{Nz}{2k}\right) \quad z \geq 0 \quad N = 0, 1, \dots \tag{A18}$$

The function $f_N(z)$ has M ($M \leq N$) extremes at the real positive points $z_1^{(N)}, z_2^{(N)}, \dots, z_M^{(N)}$, labelled in order of increasing magnitude. This function decreases monotonically for $z > z_M^{(N)}$ and it may still be useful to apply the decomposition (A17) in order to eliminate errors due to cancellations of contributions of opposite sign from the integrand $f_N(z) \cos z$. In the general case only the sign of the first s_N terms of the series in (A17) may oscillate, where s_N is given roughly by the smallest integer satisfying $(2s_N + 1)\pi > z_M^{(N)}$. For $s > s_N$ the sign of the terms of the series in (A17) is always positive.

In fact, one may determine the extremes of $f_N(z)$ by expressing $f_N(z)$ in terms of $\cosh(z/2k)$ and applying the condition $\partial f_N(z)/\partial z = 0$. By making this substitution one obtains for (A18) the expression

$$f_N(z) = \frac{1}{2k} e^{-\xi y} \sum_{j=0}^{[N/2]} A_j (-1)^j y^{N-2j} \quad y = \cosh\left(\frac{z}{2k}\right) \quad (\text{A19})$$

where $[N/2]$ denotes the largest integer contained in $N/2$ and

$$A_j = \sum_{i=j}^{[N/2]} \binom{N}{2i} \binom{i}{j}. \quad (\text{A20})$$

Thus we get the extrema of $f_N(z)$ as the roots of a polynomial of degree N . For $N = 1$ the maximum occurs at

$$z_1^{(1)} = 2k \cosh^{-1}\left(\frac{1}{\xi}\right). \quad (\text{A21})$$

For $N = 2$ the maximum will be at

$$z_1^{(2)} = 2k \cosh^{-1}\left(\frac{2}{\xi} + \sqrt{\frac{4}{\xi^2} + 2}\right). \quad (\text{A22})$$

References

- [1] Wigner E 1932 *Phys. Rev.* **40** 749
- [2] Lee H W and Scully M O 1982 *J. Chem. Phys.* **77** 4604
- [3] Bund G W 1995 *J. Phys. A: Math. Gen.* **28** 3709
- [4] Bund G W and Tijero M C 2000 *Phys. Rev. A* **61** 052114
- [5] Morse P M 1929 *Phys. Rev.* **34** 57
- [6] Dahl J P and Springborg M 1988 *J. Chem. Phys.* **88** 4535
- [7] Frank A *et al* 1996 *Ann. Phys., NY* **252** 211
- [8] Dahl J P 1985 *Semi-classical Descriptions of Atomic and Nucleon Collisions* ed J Bang and J de Boer (Amsterdam: Elsevier)
- [9] De Marcus W C 1978 *Am. J. Phys.* **46** 733
- [10] Groot S R and Suttrop L G 1972 *Foundations of Electrodynamics* (Amsterdam: North-Holland)
- [11] Nieto M M and Simmons L M Jr 1979 *Phys. Rev. A* **19** 438
- [12] ter Haar D 1975 *Problems in Quantum Mechanics* 3rd edn (London: Pion)
- [13] Matsumoto A 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2863