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LETTER TO THE EDITOR

How to calculate the Wigner function from phase space

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Abstract. We present a method for the direct computation of the Wigner function by solving a coupled system of linear partial differential equations in phase space. Our modified spectral method relies on Chebyshev polynomials. Since this approach allows us to include arbitrary high orders of partial derivatives, our procedure is applicable to arbitrary binding potentials. We apply our scheme to Wigner functions of the harmonic oscillator, the Morse oscillator, and an asymmetric double-well potential.

How do we calculate the Wigner function of a quantum system? Two approaches offer themselves. The first route utilizes the standard definition [1] of the Wigner function in terms of the density operator. The second approach [2–6] works directly from phase space and defines the Wigner function by a set of partial differential equations in phase space spanned by the position variable q and the momentum variable p . This approach is rarely used in the literature [2, 3, 5, 7] since in general the equations are of infinite order and so far no technique to solve these equations has been proposed.

In this letter we present the first approach that solves the phase-space equations for the Wigner function numerically for an arbitrary one-dimensional binding potential. The central ingredient of our work is a modified spectral method [8]. We illustrate our results for energy eigenstates of the harmonic oscillator, the Morse oscillator and an asymmetric double-well potential. Our procedure may provide new insight into the fascinating properties of quasiprobability distributions and may become a valuable tool for numerical computations of the Wigner function. Moreover our approach can be generalized to any similar system of partial differential equations and to any high-order differential equations.

The Wigner function

$$\Psi(q, p) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy e^{ipy/\hbar} \psi_E^* \left(q - \frac{y}{2} \right) \psi_E \left(q + \frac{y}{2} \right) \quad (1)$$

of an energy eigenfunction $\psi_E(q)$ of a one-dimensional potential $U \equiv U(q)$ arises in many branches of physics ranging from the foundations of quantum mechanics via atomic physics, nuclear physics, and quantum optics to plasma physics. For a detailed discussion of its properties we refer to [9, 10].

[4] has translated the Schrödinger energy eigenvalue problem

$$-\frac{\hbar^2}{2M} \frac{d^2}{dq^2} \psi_E(q) + U(q) \psi_E(q) = \tilde{E} \psi_E(q) \quad (2)$$

into the phase-space language arriving at a system of two real partial differential equations

$$L_1\Psi(q, p) \equiv \left[-\frac{p}{M} \frac{\partial}{\partial q} + \sum_{r=1,3,5,\dots}^{\infty} \frac{1}{r!} \left(\frac{i\hbar}{2} \right)^{r-1} \frac{d^r U}{dq^r} \frac{\partial^r}{\partial p^r} \right] \Psi(q, p) = 0 \quad (3)$$

and

$$L_2\Psi(q, p) \equiv \left[\frac{p^2}{2M} + U(q) - \tilde{E} - \frac{\hbar^2}{8M} \frac{\partial^2}{\partial q^2} + \sum_{r=2,4,6,\dots}^{\infty} \frac{1}{r!} \left(\frac{i\hbar}{2} \right)^r \frac{d^r U}{dq^r} \frac{\partial^r}{\partial p^r} \right] \Psi(q, p) = 0. \quad (4)$$

These two equations define the Wigner function directly from phase space. Here M and \hbar denote the mass of the particle in the potential and Planck's constant, respectively. In general, these equations are of infinite order in p . However, in the case of a polynomial potential $U(q)$ only a finite number of derivatives contribute. Since these equations are scaled with powers of \hbar one might expect that it is possible to neglect higher-order terms. However, our numerical results indicate that this is not necessarily the case.

To apply our spectral method it is convenient to map the properly chosen phase-space domain $[-q_1 \leq q \leq q_2] \times [-p_0 \leq p \leq p_0]$ onto the dimensionless square $\Omega \equiv [-1 \leq x \leq 1] \times [-1 \leq y \leq 1]$. This is the range for which the Chebyshev polynomials used in our spectral ansatz are defined. Apart from some slight changes in the prefactors, the structure of equations (3) and (4) remains unchanged by this mapping: we simply replace the position variable q by x and the momentum variable p by y .

We now briefly summarize our strategy to solve the coupled system of partial differential equations (3) and (4). In this letter we only present the basic ideas of our modified spectral method and refer to [11, 12] for more details. We note that in general the spectral method can also treat time-dependent as well as higher-dimensional problems.

To find a non-trivial solution of equations (3) and (4) we require the value of the solution at some point in the computational domain Ω to be non-zero. Since the basic equations are linear, we can select an arbitrary value, e.g. at the origin, and normalize the solution after the calculation. We approximate the solution of equations (3) and (4) by

$$\Psi_N(x, y) = \sum_{j=0}^{N_x} \sum_{k=0,2,\dots}^{N_y} a_{j,k} T_j(x) T_k(y) \quad (5)$$

where the Chebyshev polynomials $T_j(x)$ and $T_k(y)$ of order j and k , respectively, serve as one-dimensional shape functions and the $(N_x + 1)(N_y/2 + 1)$ coefficients $a_{j,k}$ are to be determined. [13] discusses the properties of Chebyshev polynomials in great detail. Note that due to the symmetry relation

$$\Psi(q, -p) = \Psi(q, p) \quad (6)$$

following from equations (3) and (4) only Chebyshev polynomials of even order in y are used. In our problem, no boundary conditions have to be satisfied by the shape functions.

We substitute our ansatz (5) into the dimensionless form of the differential equations (3) and (4) and recall that we can express derivatives and products of Chebyshev series arising from $\partial^r \Psi / \partial y^r$, $y^2 \Psi$ etc as Chebyshev series. Their coefficients are related to the original coefficients $a_{j,k}$ by recurrence relations [12, 13]. Note that for Chebyshev polynomials these relations remain simple even for high-order derivatives. It is this property that causes us to use Chebyshev polynomials rather than some other set of orthogonal polynomials. When

we treat all the terms appearing in the basic equations in this manner and also express the potential $U(x)$ as a Chebyshev series, we end up with the residuals

$$R_\ell \equiv L_\ell \Psi_N \equiv \sum_{j,k} a_{j,k}^{(\ell)} T_j(x) T_k(y) \quad \ell = 1, 2 \quad (7)$$

where R_1 corresponds to equation (3) and R_2 to equation (4). The coefficients $a_{j,k}^{(\ell)}$ are linear combinations of $a_{j,k}$ and are given explicitly in [11, 12]. We note that $a_{j,2k}^{(1)} = 0$ and $a_{j,2k+1}^{(2)} = 0$ due to the symmetry relation (6).

The residuals R_1 and R_2 will in general not be zero. Spectral methods determine the unknown coefficients $a_{j,k}$ by requiring that the integral of the weighted residual over the computational domain Ω vanishes. Moreover, weight and shape functions are chosen from the same set of orthonormal functions. Hence, when we multiply equation (7) by the product $T_\nu(x)T_\mu(y)$ and the Chebyshev weight $\chi(x, y) = \frac{1}{\sqrt{1-x^2}} \frac{1}{\sqrt{1-y^2}}$ and integrate over the domain Ω we arrive at the requirement

$$\begin{aligned} 0 &= \int_{-1}^1 \int_{-1}^1 R_\ell T_\nu(x) T_\mu(y) \chi(x, y) dx dy \\ &= \sum_{j,k} a_{j,k}^{(\ell)} \int_{-1}^1 \int_{-1}^1 T_j(x) T_k(y) T_\nu(x) T_\mu(y) \chi(x, y) dx dy \end{aligned} \quad (8)$$

with $\nu = 0, 1, \dots, N_x$ and $\mu = 0, 1, \dots, N_y$. Due to the orthogonality relation

$$\int_{-1}^1 \int_{-1}^1 T_j(x) T_k(y) T_\nu(x) T_\mu(y) \chi(x, y) dx dy = \text{constant } \delta_{j\nu} \delta_{k\mu} \quad (9)$$

for Chebyshev polynomials only the integrals with $j = \nu$ and $k = \mu$ give a non-vanishing contribution in equation (8). We conclude that in order to satisfy equation (8), the prefactors belonging to the product $T_\nu(x)T_\mu(y)$ must be zero. When we express the $a_{j,k}^{(\ell)}$ by the original coefficients $a_{j,k}$ this leads to the homogeneous linear system of equations

$$\Gamma_{j,k}^{\nu,\mu} a_{j,k} = 0 \quad j, \nu = 0, 1, \dots, N_x \quad k = 0, 2, \dots, N_y \quad \mu = 0, 1, \dots, N_y. \quad (10)$$

where the coefficients $\Gamma_{j,k}^{\nu,\mu}$ are derived explicitly in [12].

The system (10) is overdetermined: there are $(N_x + 1)(N_y/2 + 1)$ unknown coefficients $a_{j,k}$, but we have $(N_x + 1)(N_y + 1)$ equations from the integral relations (8) and one additional normalization equation (not included in equation (10)) to find a non-trivial solution. We apply a least-squares method to approximate the solution of equation (10). Thus the weighted residuals are not exactly zero, but are minimized in the Euclidean norm. Numerical experiments show that this approach yields solutions of high accuracy for our problem[†]. After solving the system (10), we compute the approximation for the Wigner function Ψ_N by substituting the coefficients $a_{j,k}$ into the ansatz (5).

We now illuminate different aspects of our method by applying it to three different examples. Throughout we use the dimensionless position variable $Q \equiv q/a_0$, where a_0 is a characteristic length and the dimensionless momentum $P \equiv (a_0/\hbar)p$. Note that it is important to find the balance in order to properly choose a phase-space domain $[-Q_1 \leq Q \leq Q_2] \times [-P_0 \leq P \leq P_0]$, which has to be large enough to resolve all properties of the Wigner function. However, when the domain is chosen too large we have to incorporate Chebyshev polynomials of higher order to obtain a certain error bound which enlarges the linear system of equations (10) and therefore the computational cost.

[†] For a proof of the convergence of our integration scheme see [11].

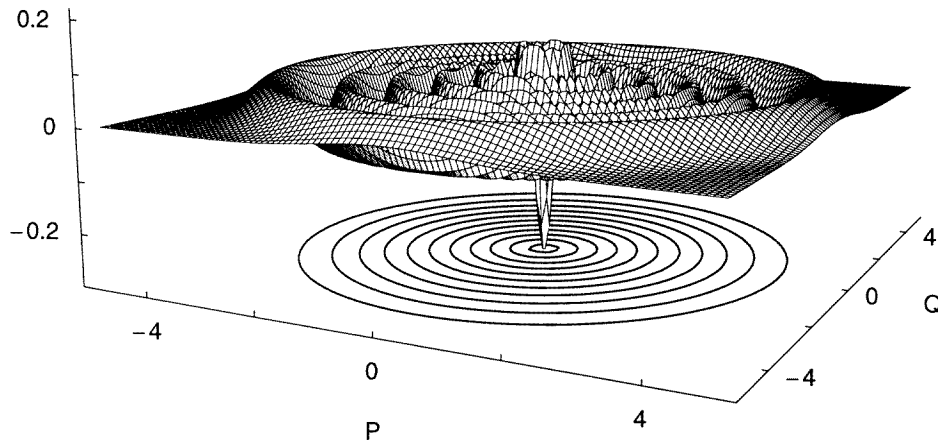


Figure 1. Wigner function (top) and zero phase-space contour lines (bottom) of the 11th energy eigenstate of the harmonic oscillator.

Table 1. The mean and maximal absolute errors for the Wigner function approximation equation (5) of the 11th energy eigenstate of the harmonic oscillator depending on the number $N = N_x = N_y$ of Chebyshev polynomials in our ansatz. For the definition of these errors see the footnote.

N	Mean absolute error	Maximal absolute error
50	$3.4 \times 10^{+1}$	$2.1 \times 10^{+4}$
60	4.8×10^{-2}	$3.0 \times 10^{+1}$
70	1.1×10^{-6}	6.6×10^{-4}
80	7.5×10^{-11}	1.4×10^{-8}
90	1.1×10^{-11}	7.8×10^{-9}
100	7.9×10^{-12}	5.9×10^{-9}

First we focus on a harmonic oscillator potential $U(Q) = Q^2/2$. Since U is a polynomial of second order, the equations for the Wigner function are also of second order. The Wigner function of an energy eigenstate is analytically known [14] for this potential. Therefore we are able to calculate exactly the errors of our approximation[†]. In figure 1 we show the Wigner function of the 11th energy eigenstate together with the contour lines of $\Psi(Q, P)$. Table 1 gives the mean and maximal absolute errors of our approximation of the Wigner function with $E = 11.5$. The data indicate that the errors rapidly decrease with increasing number $N_x = N_y$ of Chebyshev polynomials. For $N_x = N_y = 100$, we achieve an error of order 10^{-12} which is in the range of the machine precision.

The second application of our method is the Morse oscillator potential [14]

$$U(Q) = \frac{1}{2}\lambda(1 - e^{-Q/\sqrt{\lambda}})^2 \quad (11)$$

where the parameter λ gives a measure for the number of bound states. To obtain satisfactory results for this potential we have to include higher-order terms of equations (3) and (4). To obtain a reference solution of high accuracy we use the known analytic expression for the

[†] In order to compare our approximation with the exact solution we evaluate our spectral solution on an equidistant grid consisting of 100×100 points. At each grid point we calculate the absolute difference between the approximate and the exact solution. The mean value of these differences we call mean absolute value and their maximum we call maximal absolute error.

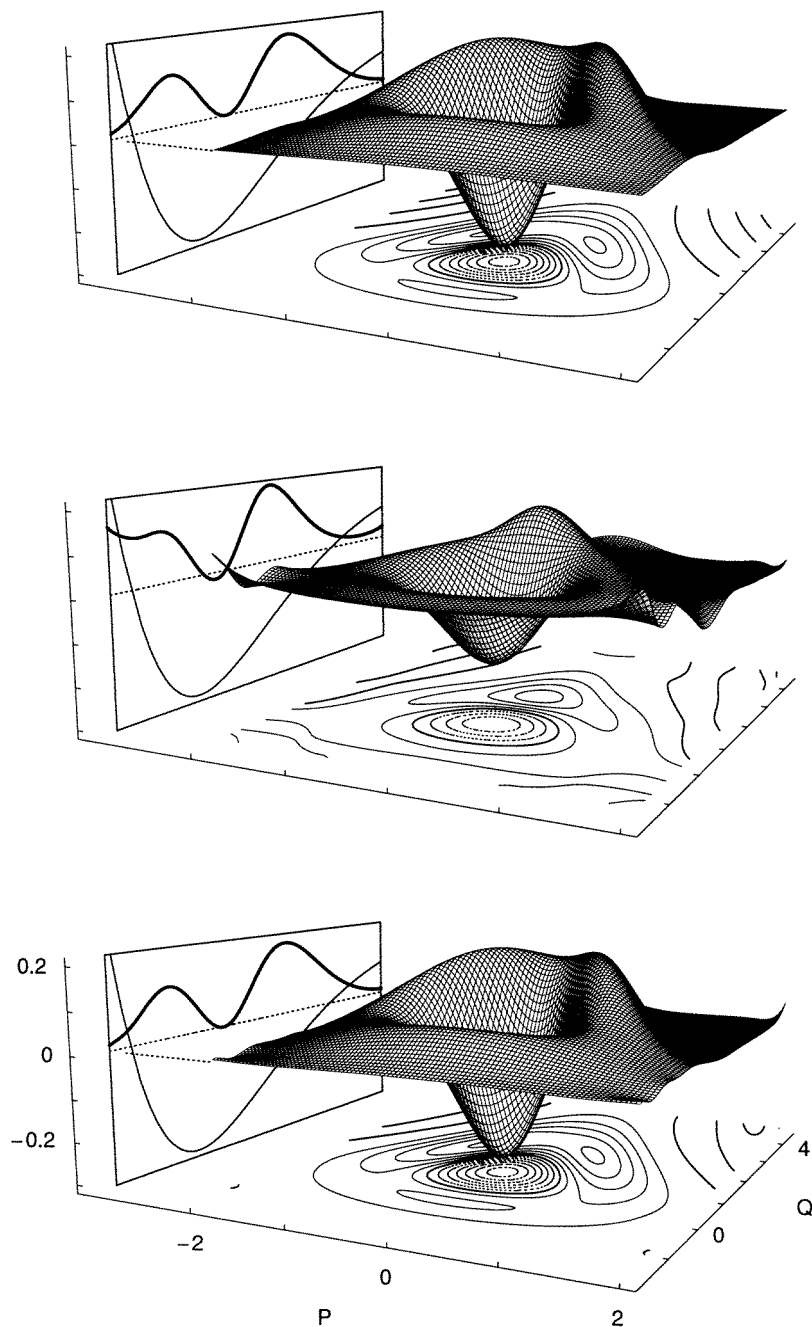


Figure 2. Exact Wigner Function (top) and approximations (middle and bottom) of the first excited energy eigenstate of the Morse oscillator potential. The potential with the energy level of the energy eigenstate and the corresponding position probability distribution is shown projected on the left-hand wall. Below the three-dimensional representation of the Wigner function we show its contour lines. The heavier contour lines denote the zero level, the light contours denote positive values in steps of 0.04, and the broken contours the negative values, respectively. For both approximations we have chosen $N_x = N_y = 50$ with maximum order of the derivatives $r = 4$ (middle) and $r = 7$ (bottom).

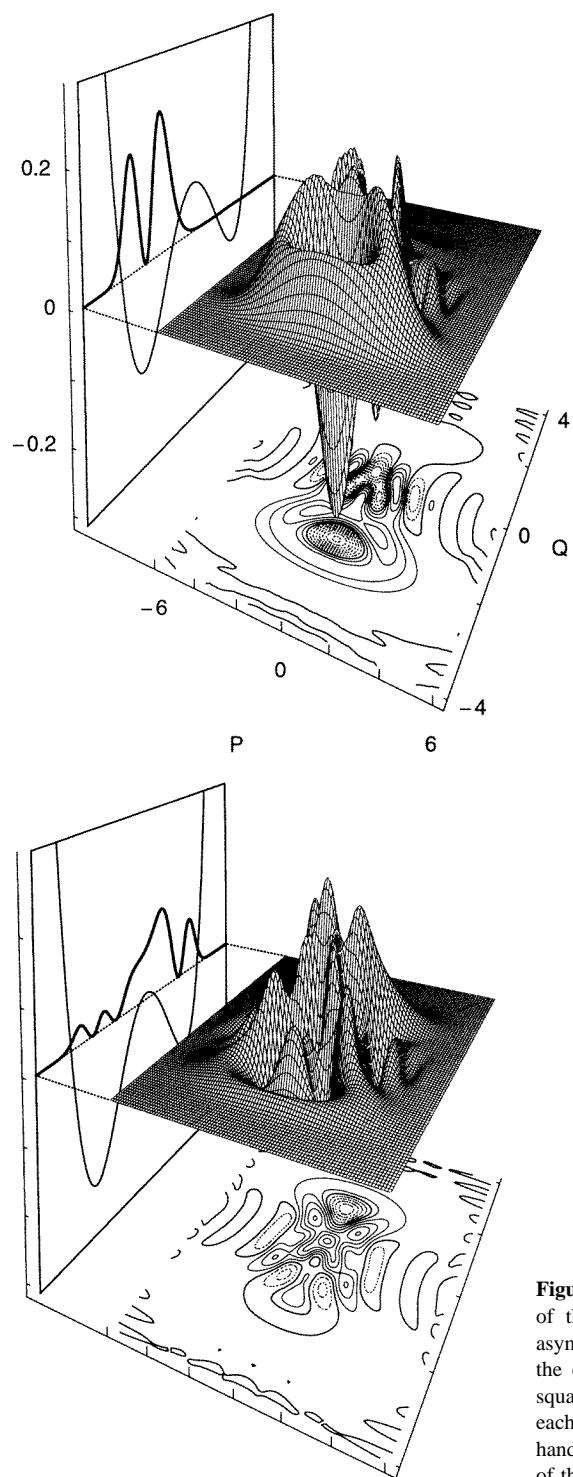


Figure 3. Approximations for the Wigner functions of the second and third energy eigenstates of the asymmetric double-well potential. The potential with the energy levels of the energy eigenstates and the square of the approximated position wavefunction of each particular state are shown projected on the left-hand wall for each energy eigenstate. The meaning of the contour lines is the same as in figure 2.

wavefunctions of the energy eigenstates and numerically perform the Fourier transform (1) defining the Wigner function.

We investigate for $\lambda = 4$ the first excited state. Figure 2 shows the exact Wigner function (top) and two approximations (middle and bottom). In both approximations we chose $N_x = N_y = 50$, but the order r of the derivatives in equations (3) and (4) included in the calculations differ. Therefore the two figures visualize the truncation error. In the middle we have $r = 4$ which does not represent a satisfactory approximation for the Wigner function. Indeed the mean truncation error is larger by a factor of 10^3 than the error of the approximation on the bottom where $r = 7$. The latter is a very good approximation with a mean absolute error of 10^{-4} . We can confirm this result by investigating the probability distribution in position, that is the marginal distribution of the Wigner function with respect to P . In figure 2 we have projected this distribution onto the left wall. When we compare the numerical integrals of the approximated Wigner functions with the exact curve we observe a large deviation for $r = 4$ and a good agreement for $r = 7$. Hence any scaling argument of \hbar in the original equations as a justification to neglect higher-order terms leads in this case to incorrect results.

Our last example addresses the potential[†]

$$U(Q) = \frac{1}{2}Q^4 + \frac{1}{4}Q^3 - \frac{7}{2}Q^2 \quad (12)$$

which describes an asymmetric double well as illustrated on the left wall of figure 3. In the foreground of this figure we present approximations for the corresponding Wigner functions obtained by our method. Here we show the Wigner functions of the second and the third excited energy eigenstate. By integrating the Wigner function over P we have again computed the marginal distribution which is the square of the eigenfunctions ψ_E . Our results are in good agreement with our numerical calculations of the eigenfunctions obtained by applying the spectral method to equation (2). Since for this potential the Wigner function is not known analytically, this comparison brings out most clearly the validity and qualitative correctness of our solution.

To summarize, we have presented a novel approach for the direct computation of the Wigner function from phase space. The numerical examples illustrate that our approximations are of high accuracy for various potentials where a reference solution is known. Moreover, in the asymmetric double-well potential where no such reference solution exists a barrier is present for the lowly excited states. Here we face a situation where usual semiclassical approaches [16] fail. In contrast our method generates a good approximation for the Wigner function. Last but not least, our method is a valuable tool to solve any differential equations of arbitrary high order or any similar system.

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References

- [1] Wigner E 1932 *Phys. Rev.* **40** 749–59
- [2] Uhlhorn U 1956 *Ark. Fys.* **11** 87–100

[†] This potential has been [15] frequently studied as a test case for numerical solutions of the Schrödinger equation. Since we can easily apply our method to the time-independent Schrödinger equation (2) we are able to reproduce the eigenfunctions ψ_E numerically calculated in [15].

- [3] Fairlie D B 1964 *Proc. Camb. Phil. Soc.* **60** 581–6
- [4] Kundt W 1967 *Z. Nat.forsch.* a **22** 1333–6
- [5] Dahl J P 1983 *Energy Storage and Redistribution in Molecules* ed J Hinze (New York: Plenum) pp 557–71
- [6] Wang L and O'Connell R F 1988 *Found. Phys.* **18** 1023–33
- [7] Carruthers P and Zachariasen F 1983 *Rev. Mod. Phys.* **55** 245–85
- [8] Gottlieb D and Orszag S A 1977 *Numerical Analysis of Spectral Methods: Theory and Applications* (Philadelphia, PA: SIAM-CBMS)
- [9] Hillery M, O'Connell R F, Scully M O and Wigner E P 1984 *Phys. Rep.* **106** 121–67
- [10] Lee H-W 1995 *Phys. Rep.* **259** 147–211
- [11] Hug M, Menke C and Schleich W P 1998 *Phys. Rev. A* **57** Part I
- [12] Hug M, Menke C and Schleich W P 1998 *Phys. Rev. A* **57** Part II
- [13] Fox L and Parker I B 1968 *Chebyshev Polynomials in Numerical Analysis (Oxford Mathematical Handbooks)* (London: Oxford University Press)
- [14] Dahl J P and Springborg M 1988 *J. Chem. Phys.* **88** 4535–47
- [15] Feit M D, Fleck J A Jr and Steiger A 1982 *J. Comput. Phys.* **47** 412–33 and references therein
- [16] For a good presentation and resolution of this problem see Berry M V *Phil. Trans. R. Soc. A* **287** 237–71