Quantum, classical and semiclassical momentum distributions. I. Theory and elementary examples

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Abstract. We discuss the basic properties of momentum distributions in quantum mechanics for elementary systems as well as their classical analogue. Semiclassical approximations can show a quantitative connection between the classical and quantum case. We believe, that such distributions provide a useful tool to improve the understanding of elementary quantum mechanics. Important differences between distributions in coordinate and momentum space are pointed out. Elementary examples (free and uniformly accelerating particle, harmonic oscillator and square well potential) are discussed.

1. Introduction

It is widely accepted that the Fourier transform of a time signal, i.e. its frequency spectrum, provides useful complementary information about the nature of the signal. In elementary quantum mechanics, however, one observes a preferential treatment of the wavefunction in coordinate (q) space (the 'coordinate representation'), whereas the corresponding Fourier transform to momentum (p) space (the 'momentum representation') is typically addressed only quite generally in the textbooks of quantum mechanics. Illustrating examples are, as a rule, omitted.

There are only two cases, where an explicite discussion of the momentum representation is presented: (a) The spreading of a Gaussian wave packet for the free particle, where it is shown that both representations are Gaussians, with width Δq and Δp, respectively, satisfying $\Delta p \Delta q = \hbar/2$. (b) The ubiquitous harmonic oscillator, which is, however, symmetric in coordinates and momenta, and therefore we observe the *same* behavior of the wavefunctions in coordinate and momentum space.

As a consequence, many students have the impression that the structural behavior of the wavefunctions in both representations are similar or even equivalent. This is, however, clearly *not* the case, as demonstrated below.

Such a preference of a one-sided picture centered on the coordinate distibutions is even more surprising in view of the unevitably discussed uncertainty relation

$$\Delta p \Delta q \geq \hbar/2 \tag{1.1}$$

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between the widths of both distributions which is, of course, a direct consequence of the Fourier transform.

It is the aim of the present paper to advocate the "thinking in p–space" [1] and to facilitate the use of the momentum representation in teaching elementary quantum mechanics by presenting a detailed discussion of some special cases allowing a closed form solution.

In addition to its conceptual importance, and to the momentum representation also has some advantages:

(1) In contrast to more abstract representations, the momentum representation yields the probability distribution of the momentum (or, equivalently, the velocity), which is a quantity clearly important also for a classical description of many quantum processes. One can find many approximate theoretical studies of quantum processes, using, e.g., an initial quantum momentum distribution combined with a classical treatment of the dynamics (see, e.g., [2] and references therein). Another example is the attachment of Rydberg electrons, where the cross sections can be approximately determined from the free electron one and the velocity distribution of the Rydberg electron [3]. Moreover, the outcome of some processes directly monitors the quantum momentum distribution of the initial quantum state, as for example the collision induced excitation of diatomic molecules under certain conditions [4, 5, 6].

(2) In scattering processes the distribution of momenta (or velocities) are directly measured experimentally in atomic or nuclear scattering experiments. In numerical simulations, the momentum space picture of the dynamics provides a more 'condensed' view of the scattering event (see, e.g., [7] for an example in one-dimensional scattering).

(3) There are cases, where a treatment in momentum space is much more convenient than in coordinate space. As an example we note the motion of a wave packet affected by a linear force. An elementary example is discussed in section 3.1 below (for a more elaborate analysis see [8]; see also the recent work on the chaotic quantum dynamics in dc and ac Stark systems [9, 10, 11] and references given there).

(4) Moreover, one of the most powerful techniques for solving the time dependent Schrödinger equation is the so-called split-operator method [12]. This method, which is routinely applied in numerous recent numerical studies of quantum dynamics, splits the Hamiltonian into a kinetic and potential energy part and switches (by means of a fast Fourier transform) periodically between coordinate representation (where potential operator is diagonal) and the momentum representation (where the kinetic energy is diagonal). This technique automatically provides a picture of the time dynamics in both, coordinate and momentum, space.

(5) As a last point, we mention the recent example of an analysis of chaotic billiard eigenfunctions in momentum space [13], showing the advantages of such

a representation in this case.

In section 2 we derive the classical and semiclassical formulas for momentum space wavefunctions. We also discuss general properties of the momentum space representation. As instructive examples, we present a detailed discussion of very elementary special cases allowing a closed form solution in momentum space: Free and uniformly accelerating wave packets (section 3.1), the harmonic oscillator (section 3.2) and the square well (section 3.3). In a subsequent paper [14] we discuss more elaborated applications, namely the anharmonic Morse oscillator and the Coulomb potential as an example in three dimensions.

2. The momentum representation

Here we consider a one dimensional system with the Hamiltonian

$$H(p,q) = \frac{p^2}{2m} + V(q). \tag{2.1}$$

2.1. Quantum mechanics

The wavefunction $\phi(q)$ of system (2.1) in the coordinate representation of an eigenstate is given by a square-integrable solution of the Schrödinger equation

$$\phi_n''(q) + \frac{2m}{\hbar^2}\big(E_n - V(q)\big)\phi_n(q) = 0\,, \tag{2.2}$$

which specifies the energy eigenvalues E_n, $n = 0,\,1,\,\ldots$ $(E_n < E_{n+1})$. For convenience, we restrict ourselves to potentials with a discrete spectrum. Equation (2.2) can be directly obtained from (2.1) by inserting the coordinate representation of the momentum operator $p = -\mathrm{i}\hbar\mathrm{d}/\mathrm{d}q$.

The basic properties of the wavefunctions $\phi_n(q)$ in the coordinate representation are

- $\phi_n(q)$ can be chosen to be real.
- If the potential is symmetric, $V(-q) = V(q)$, the wavefunctions have even or odd parity for even or odd values of n, respectively:
  $\phi_{2\nu}(-q) = \phi_{2\nu}(q), \qquad \phi_{2\nu+1}(-q) = -\phi_{2\nu+1}(q); \qquad \nu = 0,\,1,\,\ldots\,.$
- $\phi_n(q)$ has n zeros.
- For potentials with a single minimum, the zeros are localized in the classically allowed region $V(q) < E_n$.

The momentum representation of the wavefunction

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}pq/\hbar}\phi(q)\,\mathrm{d}q\,, \tag{2.3}$$

is a projection on plane waves, i.e. the eigenstates of the momentum operator, and the Schrödinger equation (2.2) is transformed into an integral equation

$$\psi_n(p) + \frac{1}{E_n - \frac{p^2}{2m}} \int_{-\infty}^{+\infty} V(p-p')\psi_n(p')\,\mathrm{d}p' = 0\,, \tag{2.4}$$

with

$$V(p-p') = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}(p-p')q/\hbar} V(q)\,\mathrm{d}q\,. \tag{2.5}$$

It is important to note, that the transformation between the coordinate and the momentum representation is simply a Fourier transform. The basic properties of wavefunctions of the eigenstates $\psi_n(p)$ in the momentum representation follow directly from those of the coordinate representation:

- $\psi_n(-p) = \psi^*(p)$ because $\phi(q)$ is real. This implies that the momentum probability distributions are always symmetric: $\left|\psi_n(-p)\right|^2 = \left|\psi_n(p)\right|^2$.
- For coordinate wavefunctions with even or odd symmetry, e.g. $\phi(-q) = \pm\phi(q)$, we have in addition $\psi(-p) = \pm\psi(p)$. In combination with the general symmetry relation above, this implies that either $\psi(p)$ is purely real or purely imaginary.
- There is no general rule for the number of zeros of $\psi_n(p)$, which can vary between zero and infinity, as demonstrated by the examples below.

2.2. Classical mechanics

It is illustrative to compare the quantum distributions with the corresponding purely classical ones. The probability $w_E(q)\mathrm{d}q$ to find the particle with energy E in the interval $[q\,,\, q+\mathrm{d}q]$ is proportional to the time $\mathrm{d}t$, that the particle spends in this interval, i.e. $w_E(q)\mathrm{d}q = 2\mathrm{d}t/T$, where T is the period of oscillation and the factor 2 takes care of the fact that each value of q appears twice during one period with positive and negative momentum $p_\pm(q,E) = \pm\sqrt{2m(E-V(q))}$:

$$w_E(q) = \sum_{\nu=1,2} \frac{1}{T|\dot{q}|_\nu} = \frac{1}{T}\sqrt{\frac{2m}{E-V(q)}}\,. \tag{2.6}$$

The period T can be obtained from

$$T = \oint \mathrm{d}t = 2m \int_{q_{\min}}^{q_{\max}} \frac{\mathrm{d}q}{\sqrt{2m(E-V(q))}}\,, \tag{2.7}$$

where $q_{\min}$ and $q_{\max}$ are the classical turning points ($p(q_{\min},E) = p(q_{\max},E) = 0$). The classical momentum distribution is obtained in a similar manner:

$$w_E(p) = \sum_{\nu=1,2} \frac{1}{T|\dot{p}|_\nu} = \sum_{\nu=1,2} \frac{1}{T\left|\frac{\mathrm{d}V}{\mathrm{d}q}\right|_\nu}\,, \tag{2.8}$$

where the derivative of V is taken at the roots q_ν of the equation $E = H(p, q_\nu)$ at a given value of p.

Alternatively, one can derive the probability distributions from the general formula

$$w_E(q) = N \int \mathrm{d}p' \, \mathrm{d}q' \, \delta(q - q') \, \delta(E - H(p', q')) = N \sum_\nu \left| \frac{\partial H}{\partial p} \right|_\nu^{-1} , \qquad (2.9)$$

where the sum is taken over all solutions of $H(p_\nu, q) = E$, i.e. the two values $p_\pm(q, E) = \pm\sqrt{2m(E - V(q))}$ for the Hamiltonian (2.1). The normalization factor is easily evaluated as

$$N^{-1} = \int \mathrm{d}p' \, \mathrm{d}q' \, \delta(E - H(p', q')) = \int \mathrm{d}q' \left| \frac{\partial H}{\partial p} \right|_\nu^{-1} = \int \mathrm{d}q' \, |\dot{q}'|_\nu^{-1} = \int \mathrm{d}t = T \, . \quad (2.10)$$

With $\partial H/\partial p = p/m$ we recover the distribution given in (2.6). In the same way we re-derive (2.8):

$$w_E(p) = N \int \mathrm{d}p' \, \mathrm{d}q' \, \delta(p - p') \, \delta(E - H(p', q')) = N \sum_\nu \left| \frac{\partial H}{\partial q} \right|_\nu^{-1} = N \sum_\nu \left| \frac{\mathrm{d}V}{\mathrm{d}q} \right|_\nu^{-1} , \qquad (2.11)$$

where the summation runs over all (in the present case two) solutions of $H(p, q_\nu) = E$. The momentum space probability distribution can also be obtained directly from the position space distribution by

$$w_E(p) = \int \delta(p - p(q, E)) w_E(q) \mathrm{d}q, \qquad (2.12)$$

which is the classical equivalent to the Fourier transformation (2.3) in quantum mechanics.

As an illustration, figure 1 shows the energy shell $H(p, q) = p^2/2m + V(q)$ and the contributing coordinate or momentum values, respectively, for the case of the Morse potential discussed below. The distributions appear as the projections of the energy shell onto the coordinate or momentum axis, weighted by the inverse derivative. Note that at the maximum allowed values of the coordinates of momenta, i.e. at the boundaries of the classically allowed region, the distributions diverge.

2.3. Semiclassics

In the semiclassical approximation the quantum wavefunction can be approximated by a superposition of classical contributions ν with amplitudes A_ν, where A_ν^2 is the classical probability, and phases are given by the classical action integral S_ν. Quite generally this approximation is expected to be valid if $\hbar$ is small compared to the classical action S; in many cases, however, one observes surprisingly good results, even for $S/\hbar$ of the order of unity. For the position space wavefunction this leads to the well-known WKB

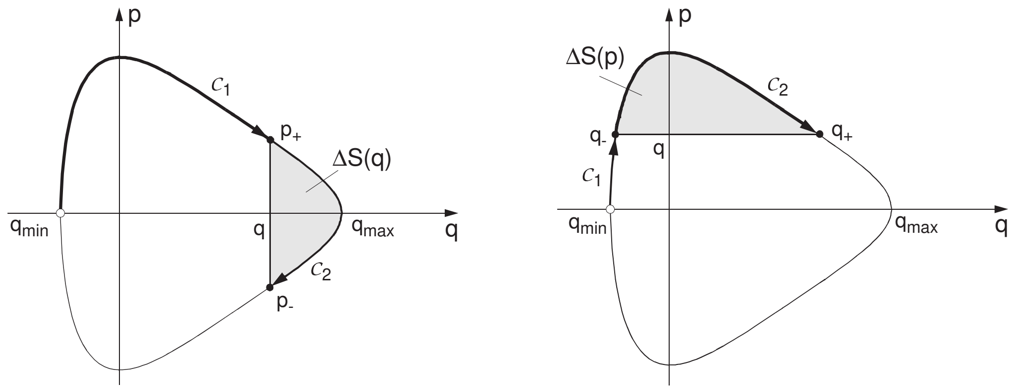

Figure 1. *Classical energy shell $H(p,q) = E$ and momenta $p_\pm$ contributing to the position space density $w_E(q)$ (left) and coordinates $q_\pm$ contributing to the momentum distribution $w_E(p)$ (right). The areas $\Delta S(q)$ or $\Delta S(p)$ determine semiclassically the interference oscillations in the distributions in position or momentum space, respectively.*

wavefunction. In the present case of the Hamiltonian (2.1) with a single minimum potential, the two equal amplitudes are (compare (2.6) and (2.9))

$$A_1(q) = A_2(q) = \left| \frac{1}{T} \sqrt{\frac{2m}{E - V(q)}} \right|^{-1/2} = \sqrt{\frac{w_E(q)}{2}}. \tag{2.13}$$

We choose the left turning point q_{min} as a phase reference point. There are two paths $\mathcal{C}_\nu$ leading from q_{min} to the coordinate point q: A direct path $\mathcal{C}_1$ connecting $(p = 0, q_{min})$ and (p_+, q) and a path $\mathcal{C}_2$ which connects $(p = 0, q_{min})$ with (p_-, q) after a reflection at the right turning point $q_{\rm max}$, which is a prolongation of $\mathcal{C}_1$ (see figure 1). Consequently we have two actions

$$S_1(q) = \int_{\mathcal{C}_1} p(q', E)\, \mathrm{d}q' = \int_{q_{min}}^{q} p(q', E)\, \mathrm{d}q' \quad \text{and} \quad S_2(q) = \int_{\mathcal{C}_2} p(q', E)\, \mathrm{d}q' = S - S_1, \tag{2.14}$$

where

$$S = \oint p(q', E)\, \mathrm{d}q' \tag{2.15}$$

is the action for a full period.

For the semiclassical wavefunction in position space we use the ansatz

$$\phi_E(q) \approx A_+(q)\, \mathrm{e}^{\mathrm{i}S_1(q)/\hbar} + A_-(q)\, \mathrm{e}^{\mathrm{i}\left[S_2(q)/\hbar - \pi/2\right]}, \tag{2.16}$$

where the additional phase $-\pi/2$ results from a phase change by reflection at the classical turning point q_{max}. Inserting (2.13) we obtain

$$\phi_E(q) = \sqrt{2w_E(q)}\, \exp\left\{ \mathrm{i}\left(\frac{\Delta S(q)}{2\hbar} - \frac{\pi}{4} \right) \right\} \cos\left(\frac{\Delta S(q)}{2\hbar} + \frac{\pi}{4} \right) \tag{2.17}$$

with

$$\Delta S(q) = S_2(q) - S_1(q) = S - 2S_1(q). \tag{2.18}$$

The absolute value is

$$|\phi_E(q)|^2 = 2w_E(q)\cos^2\left[\frac{\Delta S(q)}{2\hbar} + \frac{\pi}{4}\right]. \tag{2.19}$$

This is, of course, only valid in the classically allowed region. The classically forbidden region can be treated semiclassically by complex valued classical trajectories, which will not be considered here, as well as the taming of the singularities at the turning points.

In (2.16) we have only summed over two classical paths from $q_{\min}$ to q. It is clear, however, that there is an infinite number of such paths, which are simply the paths $\mathcal{C}_1$ and $\mathcal{C}_2$ plus a number of full cycles. All these contributions interfere destructively, unless the WKB quantisation formula

$$S = \oint p(q, E_n)\,\mathrm{d}q = 2\pi\hbar(n + 1/2)\,, \tag{2.20}$$

is satisfied. Using (2.18) we finally obtain

$$|\phi_E(q)|^2 = 2w_E(q)\cos^2\left[S_+(q)\hbar - \pi/4\right]. \tag{2.21}$$

The action difference determines the interference oscillations of the wavefunctions and the phase varies between 0 and $(n+1/2)\pi$ and the position wavefunction has n zeros, all in the region between the classical turning points, in agreement with the exact quantum result.

The semiclassical momentum space wave functions can be obtained in the same way. However, the two amplitudes are different and the absolute value of the probability distribution is

$$|\psi_E(p)|^2 \approx A_+^2(p) + A_-^2(p) + 2A_+(p)A_-(p)\cos\left[\Delta S(p)/\hbar + \pi/2\right] \tag{2.22}$$

with amplitudes (2.8)

$$A_\nu(p) = \left|T\frac{\mathrm{d}V}{\mathrm{d}q}\right|_\nu^{-1/2} \tag{2.23}$$

where the derivative in the amplitude is taken at the two points $q_\pm$ ($q_- < q_+$) on the energy shell $H(p,q) = E$. $\Delta S(p)$ is the difference between the actions along the two paths $\mathcal{C}_1$, $\mathcal{C}_2$ from $p = 0$ to $q_\pm$, as illustrated in figure 1. Defining $q_\pm(p,E)$ ($q_-(p,E) < q_+(p,E)$) as the two branches of the coordinate q as a function of the momentum and the two action integrals

$$S_\pm(p) = \int_0^p q_{\nu_\pm}(p', E)\,\mathrm{d}p' \tag{2.24}$$

the phase difference can be expressed as

$$\Delta S(p) = S_+(p) - S_-(p) - S/2\,. \tag{2.25}$$

Using again the WKB quantisation formula (2.20), the semiclassical momentum space wave functions are finally given as

$$|\psi_n(p)|^2 \approx A_+^2(p) + A_-^2(p) + 2(-1)^n A_+(p)A_-(p)\cos\left[(S_+(p) - S_-(p))/\hbar\right] \tag{2.26}$$

(note that one of the paths again needs a phase correction because of an additional reflection at the turning point). Averaging over the oscillations, one recovers the classical momentum distribution (2.8)

$$w_E(p) = A_+^2(p) + A_-^2(p). \tag{2.27}$$

From (2.26) we see that at $p = 0$ the interference is always constructive for even values of n and destructive for odd ones. This is due to the fact that in such a situation the action difference is exactly equal to $n\hbar$.

3. Elementary examples

3.1. Free and uniformly accelerating wave packets

As an introductory application, we will consider some well-known examples of free wave packets and wave packets affected by a constant force. Let us start with a Gaussian packet in coordinate space, i.e. a plane wave $\exp(\mathrm{i}p_0 q/\hbar)$ with momentum p_0 and a Gaussian modulation of the amplitude centered at q_0. The wave function in coordinate space is

$$\phi(q) = \left(\frac{s}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{s(q-q_0)^2}{2\hbar} + \frac{\mathrm{i}}{\hbar}p_0\left(q - \frac{q_0}{2}\right)\right\} \tag{3.1}$$

with mean value $\overline{q} = q_0$ and width $\Delta q = \sqrt{\hbar/2s}$ (the phase term $\mathrm{i}p_0 q_0/2$ has been added for convenience). The Fourier transform (2.3) gives the momentum wave function

$$\psi(p) = \left(\frac{1}{\pi\hbar s}\right)^{1/4} \exp\left\{-\frac{(p-p_0)^2}{2s\hbar} - \frac{\mathrm{i}}{\hbar}\left(p - \frac{p_0}{2}\right)q_0\right\} \tag{3.2}$$

with $\overline{p} = p_0$ and width $\Delta p = \sqrt{\hbar s/2}$. The symmetric structure of this minimum uncertainty wave packet ($\Delta p \Delta q = \hbar/2$) is modified, when the wave packet evolves in time t. This is most easily carried out in momentum space, where the Hamiltonian $H = p^2/2m$ is diagonal:

$$\psi(p,t) = \exp\left\{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}t\right\}\psi(p)\,. \tag{3.3}$$

Apparently, this time dependent phase term does not change the momentum distribution $|\psi(p)|^2$, contrary to the coordinate distribution, whose width increases in time (this can be easily worked out by carrying out the Fourier transform of (3.3)).

Also in the case of an homogeneous field

$$V(q) = Fq \quad \text{with} \quad (F > 0) \tag{3.4}$$

the analysis is simplified in the momentum representation. We will confine ourselves to the construction of a solution of the time independent Schrödinger equation for an energy E. The experienced reader will immediately write down the Fourier transform (2.5) for the linear potential (3.4)

$$V(p-p') = \frac{F}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}(p-p')q/\hbar} q \,\mathrm{d}q = \mathrm{i}\hbar F\,\delta'(p-p') \tag{3.5}$$

and use this to bring the integral equation (2.4) to the simple form

$$\frac{\psi'(p)}{\psi(p)} = \frac{\mathrm{i}}{\hbar F}\left(\frac{p^2}{2m} - E\right). \tag{3.6}$$

One can, however, arrive at the same result by writing the coordinate operator $\hat{q}$ in the Schrödinger equation in the momentum representation

$$\hat{H} = \frac{\hat{p}^2}{2m} + F\hat{q} \quad \longrightarrow \quad \frac{p^2}{2m} - \mathrm{i}\hbar F\,\frac{\mathrm{d}}{\mathrm{d}p}. \tag{3.7}$$

Integration of (3.6) yields

$$\psi(p) = \exp\left\{\frac{\mathrm{i}}{\hbar F}\left(\frac{p^3}{6m} - Ep\right)\right\}. \tag{3.8}$$

The Fourier transform to coordinate space is an Airy function. Let us furthermore note, that the wave function in momentum space (3.8) fully agrees with its semiclassical analog: The classical action (2.24) is

$$\begin{aligned} S(p) &= -\int_0^p q(p', E)\,\mathrm{d}p' \\ &= -F^{-1}\int_0^p (E - p'^2/2m)\mathrm{d}p' = F^{-1}\left(\frac{p^3}{6m} - Ep\right) \end{aligned} \tag{3.9}$$

(there is only a contribution from a single classical trajectory) and the classical amplitude is proportional to $|\mathrm{d}V/\mathrm{d}q|^{-1/2}$, i.e. constant. Therefore the semiclassical momentum wave function exactly agrees with the quantum one, which is, of course, *not* the case in the coordiante representation, where the primitive semiclassical approximation considered here breaks down in the vicinity of the classical turning point.

3.2. Harmonic oscillator

For the harmonic oscillator in natural units (length measured in units of $\sqrt{\hbar/m\omega}$) the Hamiltonian is

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 \tag{3.10}$$

with the energy eigenvalues $E_n = n + 1/2$. The eigenfunctions are

$$\phi_n(q) = \left[\sqrt{\pi}2^n n!\right]^{-1/2} \mathrm{e}^{-q^2/2} H_n(q) \tag{3.11}$$

in position space (H_n is the Hermite polynomial of order n) and

$$\psi_n(p) = \mathrm{i}^n \left[\sqrt{\pi}2^n n!\right]^{-1/2} \mathrm{e}^{-p^2/2} H_n(p) \tag{3.12}$$

in momentum space; i.e., they are identical up to the phase factor i^n. This is a consequence of the symmetry of the harmonic oscillator Hamiltonian in q and p.

The same is true, of course, for the classical and semiclassical wavefunctions in coordinate and momentum space, which are well-known: From (2.23) we immediately find (with $p_E = \sqrt{2E}$)

$$A_+(p) = A_-(p) = |2\pi q|^{-1} = \frac{1}{2\pi\sqrt{p_E^2 - p^2}} = \frac{1}{2}w(p) \tag{3.13}$$

and

$$S_\pm(p) = \pm\left\{\frac{p}{2}\sqrt{p_E^2 - p^2} + \frac{p_E^2}{2}\arcsin\frac{p}{p_E}\right\}. \tag{3.14}$$

(2.26) finally yields the momentum distributions

$$|\Psi_n(p)|^2 = w(p)\left(1 + (-1)^n \cos 2S_+\right) = 2w(p)\begin{cases}\cos S_+ & n \text{ even} \\ \sin S_- & n \text{ odd,}\end{cases} \tag{3.15}$$

where the semiclassically quantised energy (2.20) $E_n = n + 1/2$ exactly coincide with the quantum one.

3.3. Square-well potential

For the square-well potential

$$V(q) = \begin{cases} 0 & |q| < a \\ \infty & |q| \geq a \end{cases}, \tag{3.16}$$

the momentum distributions are obtained immediately by working out the elementary Fourier integrals (2.3) for the position wavefunctions $\phi_n(q) = \cos(k_n q)/\sqrt{2a}$ (n even) or

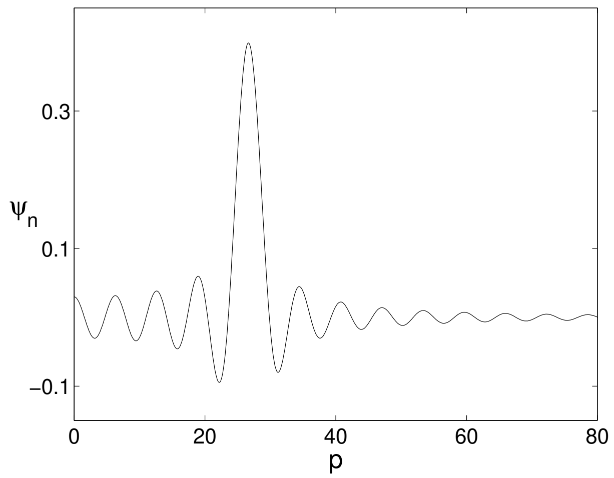

Figure 2. *Momentum wave function for the square well with $a = 1$ and $n = 16$.*

$\phi_n(q) = \sin(k_n q)/\sqrt{2a}$ (n odd) for $|q| < a$ and $k_n = (n+1)\pi/(2a)$, $n = 0, 1, \ldots$. The result is (compare also [1])

$$\psi_n(p) = g\sqrt{\frac{a}{4\pi\hbar}}\left(\frac{\sin[\,(n+1)\pi/2 - ap/\hbar\,]}{(n+1)\pi/2 - ap/\hbar} + (-1)^n \frac{\sin[\,(n+1)\pi/2 + ap/\hbar\,]}{(n+1)\pi/2 + ap/\hbar}\right) \tag{3.17}$$

with $g = 1$ or $g = -\mathrm{i}$ for n even or odd, respectively. As an example, figure 2 shows the momentum wavefunction for $n = 16$ for $p \geq 0$. We observe a spike at the position of the classical momentum

$$p = \pm p_{\rm cl} = \pm\sqrt{2mE_n} = \pm\hbar k_n = \pm\hbar\pi(n+1)/(2a)\,, \tag{3.18}$$

i.e. at $p \approx \pm 26.7$ for the case shown in figure 2. Furthermore, we clearly observe an infinite number of zeros in the momentum distribution, whereas there are $n = 16$ zeros in the position wavefunction. However, 8 of these momentum zeros are inside the classically allowed region $-p_{cl} < p < +p_{cl}$. In the limit $\hbar \to 0$ the momentum distribution approaches δ-functions at $\pm p_{cl}$, i.e. the classical distribution.

4. Summary

In the present article we have presented some (known) results for quantum momentum distributions for simple systems as well as their classical and semiclassical counterparts. Here we confined ourselves to very elementary, however instructive examples. In a subsequent paper [14] we will illustrate the properties of the quantum momentum distributions by a detailed discussion two important examples, an anharmonic one–dimensional potential (the Morse oscillator) and the three–dimensional Coulomb potential, where the distributions can be evaluated in closed form.

27 October 1999

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