Full Phase-Space Analysis of Particle Beam Transport in the Thermal Wave Model

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Abstract

Within the Thermal Wave Model framework a comparison among Wigner function, Husimi function, and the phase-space distribution given by a particle tracking code is made for a particle beam travelling through a linear lens with small aberrations. The results show that the quantum-like approach seems to be very promising.

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1 Introduction

A satisfactory description for the transverse dynamics of a charged particle beam is a fundamental requirement for the new generation of accelerating machines working at very high luminosity. To this aim, the recently proposed Thermal Wave Model (TWM) could represent an interesting framework for better describing the dynamics of charge particle beams.

According to this model, the beam transport is described in terms of a complex function, the beam wave function (BWF), whose squared modulus gives the transverse density profile. This function satisfies a Schrödinger-like equation in which Planck’s constant is replaced by the transverse emittance. In this equation, the potential term accounts for the total interaction between the beam and the surroundings. In particular, in a particle accelerator the potential has to take into account both the multipole-like contributions, depending only on the machine parameters, and the collective terms, which on the contrary depend on the particle distribution (self-interaction).

In transverse dynamics, TWM has been successfully applied to a number of linear and non-linear problems. In particular, it seems to be capable of reproducing the main results of Gaussian particle beam optics (dynamics for a quadrupole-like device), as well as of estimating the luminosity in final focusing stages of linear colliders in the presence of small sextupole- and octupole-like deviations. In addition, for the case of transverse dynamics in quadrupole-like devices with small sextupole and octupole deviations, TWM predictions have been recently compared with tracking code simulations showing a very satisfactory agreement.

More recently, in the framework of Nelson’s stochastic mechanics the Schrödinger-like equation of TWM has been derived.

This paper concerns with the transverse phase-space behaviour of a charged particle beam passing through a thin quadrupole with small sextupole and octupole deviations, in order to find the most suitable function to describe the phase-space distribution associated with the beam in the framework of TWM.

By using the BWF found in Ref., we compute the corresponding Wigner function (WF) which, according to the quantum mechanics formalism, should represent the most natural definition for the beam distribution function. Unfortunately, due to the uncertainty principle, the WF is not positive definite, hence for the above BWF we compute also the corresponding Husimi function (HF), the so-called Q-function, which is alternative to WF and is in fact positive definite. A comparison of both these predictions with the results of a particle tracking simulation is then performed in order to select the most appropriate definition of the beam phase-space function in TWM.

The paper is organized as follows. A brief presentation of BWF determination is given in section 2, whilst in section 3 we give the definition of both WF and HF. In section 4, the comparison of the theoretical predictions with the simulations results is presented. Finally, section 5 contains conclusions and remarks.
2 Beam Wave Function in presence of small sextupole and octupole aberrations

Let us consider a charged particle beam travelling along the $z$-axis with velocity $\beta c$ ($\beta \approx 1$), and having transverse emittance $\epsilon$.

We suppose that, at $z = 0$, the beam enters a focusing quadrupole-like lens of length $l$ with small sextupole and octupole deviations, then it propagates in vacuo. In this region, if we denote with $x$ the transverse coordinate (1-D case), the beam particles feel the following potential

$$U(x, z) = \begin{cases} \frac{1}{2!}k_1x^2 + \frac{1}{3!}k_2x^3 + \frac{1}{4!}k_3x^4 & 0 \leq z \leq l \\ 0 & z > l \end{cases} , \quad (1)$$

where $k_1$ is the quadrupole strength, $k_2$ is the sextupole strength and $k_3$ is the octupole strength, respectively. Note that $U(x, z)$ is a dimensionless energy potential, obtained dividing the potential energy associated with the transverse particle motion by the factor $m_0\gamma\beta c^2$, where $m_0$ and $\gamma$ are the particle rest mass and the relativistic factor $\sqrt{1 - \beta^2}^{-1/2}$, respectively.

As already stated, in the TWM, the transverse beam dynamics is ruled by the Schrödinger-like equation [1]

$$i\epsilon \frac{\partial \Psi}{\partial z} = -\frac{\epsilon^2}{2} \frac{\partial^2}{\partial x^2} \Psi + U(x, z)\Psi \quad . \quad (2)$$

The $z$-constancy of the integral $\int_{-\infty}^{+\infty} |\Psi(x, z)|^2 \, dz$, which is a consequence of the reality of $U(x, z)$ in (1), suggests to interpret $|\Psi(x, z)|^2$ as the transverse density profile of the beam. Hence, if $N$ is the total number of the beam particles, $\lambda(x, z) \equiv N |\Psi(x, z)|^2$ is the transverse number density.

We fix the initial profile as a Gaussian density distribution of r.m.s. $\sigma_0$, which corresponds to the initial BWF

$$\Psi_0(x) \equiv \Psi(x, 0) = \frac{1}{[2\pi \sigma_0^2]^{1/4}} \exp \left( -\frac{x^2}{4\sigma_0^2} \right) \quad . \quad (3)$$

Provided that $\sigma_0k_2/(3k_1) \ll 1$ and $\sigma_0^2k_3/(12k_1) \ll 1$, the quantum mechanics formalism for time-dependent perturbation theory applied to (2) for the case of a thin lens ($\sqrt{k_1}l \ll 1$) allows us to give an approximate first-order normalized BWF in the configuration space. At the exit of the lens ($z = l$) it reads

$$\Psi(x, l) = \Psi_0(x) \exp \left( -\frac{iK_1x^2}{2\epsilon} \right) \left[ (1 - i3\omega) H_0 \left( \frac{x}{\sqrt{2}\sigma_0} \right) - i\frac{3\tau}{\sqrt{2}} H_1 \left( \frac{x}{\sqrt{2}\sigma_0} \right) \right. \right.$$

$$\left. - i3\omega H_2 \left( \frac{x}{\sqrt{2}\sigma_0} \right) - i\frac{\tau}{2\sqrt{2}} H_3 \left( \frac{x}{\sqrt{2}\sigma_0} \right) - i\frac{\omega}{4} H_4 \left( \frac{x}{\sqrt{2}\sigma_0} \right) \right] , \quad (4)$$

where $\tau \equiv \sigma_0^2K_2/6\epsilon$, and $\omega \equiv \sigma_0^3K_3/24\epsilon$, with $K_i \equiv k_i l$ ($i = 1, 2, 3$), the integrated aberration strengths. Remarkably, Eq. (4) shows that, due to the aberrations, the BWF after passing the kick stage is a superposition of only five modes, according to the simple selection rules due to (1). Thus, after a drift of length $L$ ($L \gg l$) in the free space we get
Ψ(x, L) = \exp \left[ -\frac{x^2}{4\sigma^2(L)} \right] \exp \left[ i \frac{x^2}{2\sqrt{2} \sigma(L)} + \frac{x}{2i} \right] \left[ (1 - i3\omega) H_0 \left( \frac{x}{\sqrt{2\sigma(L)}} \right) \right. \\
- \left. \frac{3\tau}{\sqrt{2}} H_1 \left( \frac{x}{\sqrt{2\sigma(L)}} \right) e^{i2\phi(L)} - i3\omega H_2 \left( \frac{x}{\sqrt{2\sigma(L)}} \right) e^{i4\phi(L)} \right. \\
- \left. \frac{\tau}{2\sqrt{2}} H_3 \left( \frac{x}{\sqrt{2\sigma(L)}} \right) e^{i6\phi(L)} - \frac{\omega}{4} H_4 \left( \frac{x}{\sqrt{2\sigma(L)}} \right) e^{i8\phi(L)} \right] , \quad (5)

where
\[ \sigma(L) = \left( \frac{\epsilon^2}{4\sigma_0^2} + K^2 \sigma_0^2 \right) (L-l)^2 - 2K_1 \sigma_0^2 (L-l) + \sigma_0^2 \]  \\
\frac{1}{R(L)} = \left. \frac{d\sigma}{\sigma \, dz} \right|_{z=L} , \\
\phi(L) = -\frac{1}{2} \left\{ \arctan \left[ \left( \frac{\epsilon}{2\sigma_0^2} + \frac{2K^2 \sigma_0^2}{\epsilon} \right) (L-l) - \frac{2K_1 \sigma_0^2}{\epsilon} \right] \right. \\
+ \left. \arctan \left[ \frac{2K_1 \sigma_0^2}{\epsilon} \right] \right\} . \quad (6)

Correspondingly, the Fourier transform of Ψ(x, z)
\[ \Phi(p, z) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, z) \exp(-ipx/\epsilon) \, dx \quad , \quad (7) \]
is the BWF in the momentum space.
Consequently, |Ψ(x, l)|² and |Ψ(x, L)|² give the transverse particle density profiles at z = l (after lens) and at z = L (after drift), respectively, whilst |Φ(p, l)|² and |Φ(p, L)|² give the momentum distributions of the particles, at z = l and at z = L, respectively.

In Ref. [3] the configuration-space and momentum-space distributions are reported for some significative values of parameters σ₀, ε, K₁, K₂, K₃, and L. They are compared with the corresponding results obtained from particle tracking simulations showing a very satisfactory agreement.

In the next section we extend this analysis, made separately both in configuration space and in momentum space, by introducing the appropriate distribution function in the context of TWM approach.

Since the approximate solution (4) and (5) for BWF is given for small sextupole and octupole deviations from a quadrupole potential (harmonic oscillator), the present analysis falls in the *semiclassical* description of the wave packet evolution (WKB theory) extensively treated in Ref. [7].

### 3 Phase-space distributions

According to Quantum Mechanics (QM), for a given BWF Ψ(x, z) we can introduce the density matrix ρ as
\[ \rho(x, y, z) \equiv \Psi(x, z)\Psi^*(y, z) \quad , \quad (8) \]
which, in the \langle bra | and | ket \rangle Dirac’s notation, is associated with the following \textit{density operator}

\[ \hat{\rho} = |\Psi \rangle \langle \Psi| \]  \hspace{1cm} (9)

Note that \( \hat{\rho} \) has the following two properties

i) probability conservation

\[ \text{Tr}(\hat{\rho}) = 1 \] ; \hspace{1cm} (10)

ii) hermiticity

\[ \hat{\rho}^\dagger = \hat{\rho} \] \hspace{1cm} (11)

On the basis of this density matrix definition, we can define the relevant phase-space distributions associated with the transverse beam motion within the framework of TWM.

### 3.1 Wigner function

One of the widely used phase-space representations given in QM is the one introduced by Weyl and Wigner. In this representation, by simply replacing Planck’s constant with \( \epsilon \), the phase-space beam dynamics can be described in terms of the following function, called Wigner function (WF)

\[ W(x, p, z) \equiv \frac{1}{2\pi \epsilon} \int_{-\infty}^{+\infty} \rho \left( x - \frac{y}{2}, x + \frac{y}{2}, z \right) \exp \left( \frac{i p y}{\epsilon} \right) dy , \]  \hspace{1cm} (12)

namely, by virtue of (8)

\[ W(x, p, z) = \frac{1}{2\pi \epsilon} \int_{-\infty}^{+\infty} \Psi^* \left( x + \frac{y}{2}, z \right) \Psi \left( x - \frac{y}{2}, z \right) \exp \left( \frac{i p y}{\epsilon} \right) dy . \]  \hspace{1cm} (13)

It is easy to prove from (13) that

\[ \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} W(x, p, z) \, dx \, dp = 1 \] , \hspace{1cm} (14)

\[ \lambda(x, z) = N \int_{-\infty}^{+\infty} W(x, p, z) \, dp \] , \hspace{1cm} (15)

and

\[ \eta(p, z) = N \int_{-\infty}^{+\infty} W(x, p, z) \, dx \] , \hspace{1cm} (16)

where \( \eta(p, z) \) represents the transverse momentum space number density (note that \( \eta(p, z) = N \, |\Phi(p, z)|^2 \)). Eqs. (15) and (16) show that \( N \) times \( W(x, p, z) \) is the phase-space distribution function associated with the transverse beam motion. Consequently, \( \lambda \) and \( \eta \) are its configuration-space and momentum-space projections, respectively.

The averaged-quantity description can be done by introducing the following second-order momenta of \( W \)

\[ \sigma^2_z(z) \equiv \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} x^2 W(x, p, z) \, dx \, dp \equiv \langle x^2 \rangle \] , \hspace{1cm} (17)

\[ \sigma_{xp}(z) \equiv \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} xp W(x, p, z) \, dx \, dp \equiv \frac{1}{2} \langle xp + px \rangle \] , \hspace{1cm} (18)
\[\sigma_p^2(z) \equiv \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p^2 \ W(x, p, z) \ dx \ dp \equiv \langle p^2 \rangle \ . \quad (19)\]

They are connected with the geometrical properties of the phase-space ensemble associated with the beam; here we have considered the case \(\langle p \rangle = \langle x \rangle = 0\).

According to QM and simply replacing \(\hbar\) with \(\epsilon\), we can easily say that \(W(x, p, z)\), defined by (13) when the BWF \(\Psi(x, z)\) is solution of (2) (with \(U\) arbitrary Hermitian potential), satisfies the following Von Neumann equation

\[
\left[ \frac{\partial}{\partial z} + \frac{p}{\partial x} + \frac{i}{\epsilon} \left( U \left( x + \frac{ie}{2} \frac{\partial}{\partial p} \right) - U \left( x - \frac{ie}{2} \frac{\partial}{\partial p} \right) \right) \right] W = 0 \ . \quad (20)
\]

Thus, in order to perform a phase-space analysis, one has two possibilities: either to solve (2) for \(\Psi(x, z)\) and then, by means of the Wigner transform (13), to obtain \(W(x, p, z)\), or to solve directly (20) for \(W(x, p, z)\).

Although for the potential given by (11) the exact solution of the Schrödinger-like equation (2) is unknown, time-dependent perturbation theory can be applied to give, at any order of the perturbative expansion, the approximate solution [8]: for example, (4) is the first-order approximate solution of (2) for the potential (11). Also for the Von Neumann equation, (20), the exact solution is not available in the case of potential (11), with the exception of the case with \(k_2 = k_3 = 0\) (pure quadrupole/harmonic oscillator). Nevertheless, it has been shown [9] that, for a more general Hamiltonian which includes our case as a special case, a perturbative Dyson-like expansion for the Wigner function can be constructed which converges to the solution of the corresponding quantum Liouville equation. In general this approach, providing \(W(x, p, z)\) directly from the phase-space dynamics, should yield a smaller error.

For a thin lens the Wigner transform, (13), of the approximate BWF, as given by (4) and (5), coincides with the approximate first-order solution of quantum Liouville equation [3]: the two approaches are therefore equivalent. As TWM has been mainly developed in the configuration space [1], and the approximate BWF for the typical potential used in particle accelerators has already been calculated (see, for example, [1]-[3]), in this paper we have chosen to proceed with this latter approach.

For what concerns the calculation of the higher-order solutions, solving directly (20) for \(W(x, p, z)\) should, in principle, be preferable to the procedure in which we first solve for BWF and then use (13), because less approximations are required, and therefore smaller errors are involved. Unfortunately it is very difficult to treat the Von Neumann equation, (20), numerically, especially if the classical potential contains powers in \(x\) higher than the quadratic one. In fact, in this case operators \(U \left[ x \pm i(\epsilon/2) \frac{\partial}{\partial p} \right] \) make (20) a partial differential equation of order higher than the second in the \(p\)-derivative, which is rather difficult to handle numerically. In order to treat BWF and Wigner transform numerically, instead, one can profit of the very powerful methods developed for the Schrödinger equation, as it has been done, for instance, in Ref. [10].

Although \(W\) is the distribution function of the system in the framework of TWM, due to well-known quantum mechanical properties, it is not positive definite. However, in QM it results to be positive for some special harmonic oscillator wave functions, called coherent states [11, 12, 13], which give purely Gaussian density profiles.

Coherent states for charged particle beams have been recently introduced in TWM in order to describe the coherent structures of charged particle distributions produced in an accelerating machine [15]. The fact that \(W\) can assume negative values for some
particular cases, reflects the quantum-like properties of both the wave function and the density operator.

Remarkably, in the case of a pure quadrupole-like lens \( U = k_1 x^2 / 2 \) an interesting quantity, which estimates the r.m.s. area of the ensemble, can be expressed in terms of these momenta, namely

\[
\pi \left[ \langle x^2 \rangle \langle p^2 \rangle - \frac{1}{4} \langle xp + px \rangle^2 \right]^{1/2} = \pi \left[ \sigma^2_x(z) \sigma^2_p(z) - \sigma^2_{xp}(z) \right]^{1/2} .
\]  

(21)

Since in this case the ground-like state is

\[
\Psi_0(x, z) = \frac{1}{\sqrt{2\pi \sigma_0^2(z)}} \exp \left( -\frac{x^2}{4\sigma_0^2(z)} \right) \exp \left( -\frac{i}{2} \sqrt{k_1} z \right) ,
\]

(22)

the formula (13) produces the following bi-Gaussian Wigner distribution

\[
W_0(x, p) = \frac{1}{\pi \epsilon} \exp \left( -\frac{x^2}{2\sigma_0^2} - \frac{2\sigma_0^2}{\epsilon^2} p^2 \right) .
\]

(23)

In addition, for the following non-coherent Gaussian-like state associated with the charged-particle beam [15]

\[
\Psi(x, z) = \frac{1}{\sqrt{2\pi \sigma^2(z)}} \exp \left[ -\frac{x^2}{4\sigma^2(z)} + i\frac{x^2}{2\epsilon R(z)} + i\phi(z) \right] ,
\]

(24)

where

\[
\frac{d^2 \sigma}{dz^2} + k_1 \sigma - \frac{\epsilon^2}{4\sigma^3} = 0 , \quad \frac{1}{R} = \frac{1}{\sigma} \frac{d\sigma}{dz} , \quad \frac{d\phi}{dz} = -\frac{\epsilon}{4\sigma^2} ,
\]

(25)

definition (13) of \( W \) easily gives

\[
W(x, p, z) = \frac{1}{\pi \epsilon} \exp \left[ -\frac{x^2}{2\sigma^2(z)} - \frac{2\sigma^2(z)}{\epsilon^2} \left( \frac{x}{R(z) - p} \right)^2 \right] .
\]

(26)

Note that in this simple case of pure quadrupole the exact analytical solution (23) and (26) can be easily obtained directly by integrating (20).

Note also that the argument of the exponential in (26) is a quadratic form in the variables \( x \) and \( p \), which can be written as

\[
F(x, p, z) \equiv -\frac{2}{\epsilon} \left[ \gamma(z)x^2 + 2\alpha(z)xp + \beta(z)p^2 \right] ,
\]

(27)

where

\[
\alpha(z) = -\frac{\sigma^2(z)}{\epsilon R(z)} , \quad \beta(z) = \frac{\sigma^2(z)}{\epsilon} , \quad \gamma(z) = \frac{\epsilon}{4\sigma^2(z)} + \frac{\sigma^2(z)}{\epsilon R^2(z)} .
\]

(28)

These quantities are usually called Twiss parameters [16]. By substituting (26) into (17)-(19), we obtain \( \alpha(z) = -(1/2)d\beta(z)/dz \), \( \gamma(z) = \sigma^2_p(z)/\epsilon \) and

\[
\sigma_x(z) = \sigma(z) , \quad \sigma^2_p(z) = \frac{\epsilon^2}{4\sigma^2(z)} + \frac{\sigma^2(z)}{R^2(z)} = \frac{\epsilon^2}{4\sigma^2(z)} (1 + 4\alpha^2(z)) .
\]

(29)
Consequently, we immediately get the following quantum-like version of the Lapo\sittle{\textaccentserial{s}}ottle
definition of emittance \cite{16}
\[\langle x^2 \rangle \langle p^2 \rangle - \frac{1}{4} (xp + px)^2 = \frac{\epsilon^2}{4} = \text{const.}, \tag{30}\]
from which uncertainty relation of TWM can be easily derived
\[\sigma^2(x) \sigma_p^2(z) \geq \frac{\epsilon^2}{4}. \tag{31}\]
Furthermore, the equation
\[\gamma(z)x^2 + 2\alpha(z)xp + \beta(z)p^2 = \frac{\epsilon}{2}, \tag{32}\]
represents, for each \(z\), an ellipse in the phase-space of area \(\pi \epsilon/2\) associated with the particle beam motion.
Consequently, the operator
\[\hat{J}(x, p, z) \equiv \gamma(z)x^2 + 2\alpha(z)xp + \frac{\beta(z)p^2}{2} + \gamma(z)p^2 \tag{33}\]
is the quantum-like version of one of the well-known Courant-Snyder invariant \cite{17}. In fact, it easy to prove that
\[i\epsilon \frac{\partial \hat{J}}{\partial z} + [\hat{J}, \hat{H}] = 0, \tag{34}\]
where \(\hat{H}\) is the Hamiltonian operator for the case of a quadrupole.

### 3.2 Husimi function

The phase-space description of a quantum system can be done in terms of another function which has been introduced by Husimi \cite{8}, the so-called \textit{Q-function} or \textit{Husimi function} (HF). In order to give an analogous definition of HF for charged particle beams in the context of TWM, we still replace Planck’s constant with \(\epsilon\), obtaining
\[Q(x_0, p_0, z) \equiv \frac{1}{2\pi \epsilon} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Theta^*(u, z; x_0, p_0) \rho(u, v, z) \Theta(v, z; x_0, p_0) \, du \, dv, \tag{35}\]
where \(\Theta(x, z; x_0, p_0)\) is a coherent state associated with the charged particle beam defined as \cite{15}
\[\Theta(u, z; x_0, p_0) = \frac{1}{[2\pi \sigma_0^2]^{1/4}} \exp \left[ -\frac{(u - x_0(z))^2}{4\sigma_0^2} + i \frac{p_0(z)}{\epsilon} u - i\delta_0(z) \right], \tag{36}\]
with
\[x_0(z) \equiv \langle u \rangle = \int_{-\infty}^{\infty} u \, |\Theta|^2 \, du, \tag{37}\]
\[p_0(z) \equiv \langle \hat{p} \rangle = \int_{-\infty}^{\infty} \Theta^* \left( -i\epsilon \frac{\partial}{\partial x} \right) \Theta \, dx, \tag{38}\]
and
\[ \frac{d\delta_0}{dz} = \frac{p_0^2}{2\epsilon} - \sqrt{\frac{k_1}{4\sigma_0^2}} + \frac{\sqrt{k_1}}{2} \].  
(39)

Note that here \( x_0 \) and \( p_0 \) play the role of classical phase-space variables.

By substituting (8) and (36) in (35) we obtain
\[
Q(x, p, z) = \frac{1}{2\pi \epsilon \sqrt{2\pi \sigma_0^2}} \exp \left( -\frac{x^2}{2\sigma_0^2} \right) \int_{-\infty}^{\infty} dv \int_{-\infty}^{\infty} du 
\times \exp \left[ -\frac{u^2 + v^2}{4\sigma_0^2} + \frac{x(u + v)}{2\sigma_0^2} + i\epsilon(p(u - v)) \right] \Psi^*(u, z)\Psi(v, z) ,  
\]
(40)

where for simplicity we have replaced the classical variables \( x_0 \) and \( p_0 \) with \( x \) and \( p \), respectively.

However, the integration over \( p \) and over \( x \), does not give configuration-space and momentum-space distributions, respectively. But this function removes the pathology of negativity exhibited by \( W \), and thus gives a more accurate description in the phase-space region where \( W \) is negative.

Some properties of \( Q \) are in order.

i) It is easy to prove the following normalization relation
\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Q(x, p, z) \, dx \, dp = 1 .  
\]
(41)

ii) Definition (40) can be cast in the following more convenient form
\[
Q(x, p, z) = \frac{1}{8\pi \epsilon \sqrt{2\pi \sigma_0^2}} \left| \int_{-\infty}^{\infty} dy \exp \left( -\frac{y^2}{16\sigma_0^2} - i\frac{py}{2\epsilon} \right) \right|^2 .  
\]
(42)

Note that (42) clearly shows that \( Q \) is positive definite.

iii) Definition (33) of Husimi function, or equivalently (12), does not give in general a phase-space distribution coinciding with WF. But, in the case of a Gaussian BWF they must coincide, because in this case both \( Q \) and \( W \) reduce to the classical distribution. In particular, we observe that since in (33) or in (12) the constant \( \sigma_0 \) is involved, the present definitions of \( Q \) are suitable only to describe the phase-space distribution of eigenstates: this way \( Q \) does not explicitly depend on \( z \). The natural generalization of \( Q \) for \( z \)-dependent BWF will be introduced later. Now we point out that, in connection with the Gaussian BWF given by (22), Eq. (12) gives a bi-Gaussian \( Q \)-function that does not coincide with (23) because of a scaling disagreement. This problem can be easily removed, by introducing the following new definition for \( Q \)
\[
Q(x, p, z) = \frac{1 + \lambda^2}{8\pi \epsilon \lambda^2 \sqrt{2\pi \sigma_0^2}} \left| \int_{-\infty}^{\infty} dy \exp \left( -\frac{y^2}{16\sigma_0^2 \lambda^2} - i\frac{\sqrt{1 + \lambda^2}py}{2\epsilon \lambda} \right) \right|^2 ,  
\]
(43)
for any real number \( \lambda \). This is equivalent to introduce the following substitutions in the definition (35)

\[
x \rightarrow \sqrt{1 + \lambda^2} x \quad , \quad p \rightarrow \frac{\sqrt{1 + \lambda^2}}{\lambda} p \quad , \quad Q \rightarrow \frac{1 + \lambda^2}{\lambda} Q .
\]

(44)

Under these substitutions, the normalization condition (41) is preserved. In order to symmetrize (44), we choose \( \lambda = 1 \). Consequently,

\[
x \rightarrow \sqrt{2} x \quad , \quad p \rightarrow \sqrt{2} p \quad , \quad Q \rightarrow 2 Q ,
\]

(45)

and (13) becomes

\[
Q(x, p) = \frac{1}{4\pi\epsilon\sqrt{2\pi\sigma_0^2}} \int_{-\infty}^{\infty} dy \exp \left( -\frac{y^2}{16\sigma_0^2} - \frac{i}{\sqrt{2}\epsilon} py - \frac{i}{\sqrt{2}\epsilon} \right) \Psi \left( \sqrt{2}x + \frac{y}{2}, z \right)^2 .
\]

(46)

Thus, by using (22) in (46) we obtain

\[
Q(x, p) = \frac{1}{\pi\epsilon} \exp \left( -\frac{x^2}{2\sigma_0^2} - \frac{2\sigma_0^2}{\epsilon^2} p^2 \right) ,
\]

(47)

which now coincides with the corresponding Wigner function (23).

iv) For the non-coherent Gaussian-like BWF (24), Eq. (46) is no longer valid, because it does not coincide with (26). In particular, at any \( z \), the phase-space ellipses associated with \( W \) do not coincide with the contours of (46) for BWF given by (24). This problem can be overcome by generalizing definition (10) with the following

\[
Q(x, p, z) = \frac{1}{4\pi\epsilon\sqrt{2\pi\sigma_0^2(z)}} \int_{-\infty}^{\infty} dy \exp \left( -\frac{y^2}{16\sigma_0^2(z)} - \frac{iy^2}{8\epsilon R(z)} - \frac{i}{\sqrt{2}\epsilon} py - \frac{i}{\sqrt{2}\epsilon}u - \frac{i}{\sqrt{2}\epsilon}p \right) \Psi \left( \sqrt{2}x + \frac{y}{2}, z \right)^2 .
\]

(48)

By substituting (24) in (48) we easily obtain

\[
Q(x, p, z) = \frac{1}{\pi\epsilon} \exp \left[ -\frac{x^2}{2\sigma_0^2(z)} - \frac{2\sigma_0^2(z)}{\epsilon^2} \left( \frac{x}{R(z)} - p \right)^2 \right] ,
\]

(49)

which now coincides with the corresponding WF given by (26).

(v) Note that the generalized definition (18) suggests to start from (35) where the coherent states \( \Theta(u, z; x_0, p_0) \) are replaced by the following non-coherent Gaussian-like states

\[
\Theta_0(u, z; x_0, p_0) = \frac{1}{\sqrt{2\pi\sigma_0^2(z)}} \exp \left[ -\frac{(u - x_0(z))^2}{4\sigma_0^2(z)} + \frac{i}{\epsilon} p_0(z)u - i\delta_0(z) + \frac{(u - x_0(z))^2}{2\epsilon R(z)} \right] .
\]

(50)

This way if we start from (35) with (50), it is very easy to prove that it is equivalent to (18) for any \( \Psi \). Consequently, the generalized definition of (35) with (50) produce the same results of Wigner function definition (13) for any Gaussian-like states.
vi) Note that (50) are the non-coherent fundamental modes of the following set of solutions of (2) in the case of $U = (1/2)K_1x^2$

$$\Theta_n(x, z; x_0, p_0) = \frac{\Theta_0(x, z; x_0, p_0)}{\sqrt{2^n n!}} H_n \left( \frac{x - x_0(z)}{\sqrt{2\sigma(z)}} \right) \exp \left( i2n\phi(z) \right). \quad (51)$$

These modes are analogous to squeezed and correlated Fock’s states used in quantum optics \cite{18}. In the next section we check if the equivalence between (35) with (50) and (13) is still valid for non-Gaussian BWF. In particular, we make a comparison between definition (13) and (35) with (50) for the case of BWF given by (4) and (5), and in addition we compare them with the corresponding results of a multi-particle tracking simulation.

4 Numerical analysis

A numerical study has been pursued in order to compare the description of the phase-space as given by TWM, both by means of WF and by means of HF, with the one resulting from standard particle tracking.

A Gaussian flat (1-D) particle beam has been used as starting beam, with emittance $\epsilon = 120 \times 10^{-6}$ m rad, and $\sigma_0 = 0.05$ m. From Eq. (29) it follows that, if $\alpha(0) = 0$ at the start, $\sigma_{p0} \equiv \sigma_0 = 1.2 \times 10^{-3}$ rad. (Note that the definition of emittance given in (30) differs from the definition used in classical accelerator physics by a factor $1/2$.)

A simple device made of a quadrupole magnet plus a drift space has been considered as beam transport line: in addition sextupole and/or octupole aberrations have been included in the quadrupole.

The Wigner function (13) and the $Q$-function (48) have been computed by numerical integration for different combinations of aberration strengths, and have been compared with the results of the tracking of $7 \times 10^5$ particles.

Isodensity contours at 1, 2 and 3 $\sigma$ have been used to describe the particle distribution in phase-space, both before and after the passage through the simple device specified above. It is worth noting that with this choice only 2% of the particles are found beyond the contour at 2 $\sigma$, and only 0.01% of them are beyond the contour at 3 $\sigma$.

In Figure 1. the starting distribution is shown together with the distribution emerging from the linear transport line. As already shown, in the linear case both WF and HF can be computed analytically (Eqs. (26) and (49)) yielding exactly the same result of the conventional accelerator physics. Therefore, the output from tracking and the TWM predictions are in full agreement, and thus their superposition is not shown here.

In the cases shown in Figure 2. non-linear perturbations have been added to the quadrupole lens: a sextupole perturbation in the first column, an octupole perturbation in the second column, and perturbations of both kinds in the third column. The results from the numerical computation of WF and HF are shown also superposed to the tracking results for a first set of perturbation values, corresponding to the distortions $D = 0.125$ in the case of $K_2 = 0.06$ m$^{-2}$ and $D = 0.042$ in the case of $K_3 = 1.2$ m$^{-3}$. It should be noted that these values of distortion, chosen with the aim of enhancing the effects desired,

1 The phase-space distortion can be defined as the ratio between the deflection $\Delta p(x) \equiv p(x) - p(x_0)$, at $x = \sigma_0$, and $\sigma_{p0}$, namely $D \equiv \Delta p(\sigma_0)/\sigma_{p0}$. It is easy to prove that $D = 6\sigma = \sigma_0^3K_2/\epsilon$ for pure sextupole, and $D = 8\omega = \sigma_0^3K_3/3\epsilon$ for pure octupole.
are huge compared with what could be considered acceptable in any realistic single pass device.

A quite good agreement with tracking can be observed for the contours at 1 and 2 $\sigma$ for both WF and HF. The contours at 3 $\sigma$ show some discrepancies, more pronounced in the case of the Wigner function, which, as discussed in Section 3.1, in the periphery of the distribution produces regions with negative phase-space density which yield an unrealistic distortion of the phase-space. By the use of the $Q$-function, instead, this effect is largely smoothed out, as shown in the last two rows of Figure 2.

In the plots displayed in the different columns of Figure 3, the same kinds of perturbations are included as in Figure 2, but with twice the strength, therefore yielding twice the distortion.

These large values of distortion approach the limits of applicability of perturbation theory which, for the starting parameters and the quadrupole strength selected, are given by $D \ll 3\sigma_0^2 K_1/\epsilon = 2.25$ for the sextupole perturbation and $D \ll 4\sigma_0^2 K_1/\epsilon = 3.00$ for the octupole perturbation.

Indeed larger discrepancies between TWM and tracking can be observed now, in particular where the sextupole perturbation is present ($D = 0.25$). Nevertheless in these cases (columns 1 and 3 of Figure 3) HF still describes fairly well the phase-space distribution for particles with amplitudes up to $1 - 1.5 \sigma$, whilst the WF distortion due to its negativity starts to show up already at amplitudes of the order of $1\sigma$.

In spite of the discrepancies observed at large amplitudes due to the particularly strong perturbations used in this study, these results can be considered very satisfactory: the TWM phase-space description of beam dynamics in the presence of a non-linear lens, and in particular the one given by the HF, will be in more than reasonable agreement with the one given by classical accelerator physics for all realistic values of perturbation.

5 Remarks and conclusions

In this paper we have studied the phase-space distribution associated with the transverse motion of a charged particle beam travelling through a quadrupole-like device with sextupole and octupole deviations. In particular, a quantum-like phase-space analysis within the Thermal Wave Model has been developed and its predictions have been compared with the results of particle tracking simulations.

To this end, we have first introduced the density matrix for the beam wave function (8). Then, following the usual definitions, we have constructed the Wigner transform (Eq. (13)), and the Husimi transform (Eq. (35)) with $\Theta$ given by (50). These functions represent the best candidates for describing the full phase-space evolution of the beam. Our aim was to compare the results of tracking simulations with the predictions of TWM, given in terms of $W$ and $Q$, in order to enquire if the equivalence between (83) with (50) and (13) is valid also for non-Gaussian BWF, and thus to determine the appropriate function to describe the phase-space dynamics.

The Wigner transform of the BWF, which represents the natural quantum analogous of the classical phase-space distribution associated with the beam, has been numerically computed for the present problem. Its $x$ and $p$-projections reproduce the configuration and momentum space distribution well [3], up to the first order of the perturbation theory. According to the results presented in section 4, this function reveals to be in good agree-
ment with the tracking results for small values of the integrated multipole-like strengths, for which conditions $\sigma_0 K_2/(3K_1) \ll 1$ and $\sigma_0^2 K_3/(12K_1) \ll 1$ are fully satisfied. For larger values of these parameters a little discrepancy appears. The reason is that in the last case the first-order perturbative expansion is not reliable enough. Nevertheless, we stress the fact that, beyond the contours at 2 $\sigma$ and 3 $\sigma$, only the 2% and 0.01% of the beam particles are present, respectively. Summarizing, the comparison between the tracking results and the TWM predictions shows that:

i) for small aberrations (conditions $\sigma_0 K_2/(3K_1) \ll 1$ and $\sigma_0^2 K_3/(12K_1) \ll 1$ well satisfied), both $Q$ and $W$ are in good agreement with the tracking results;

ii) for larger aberrations, WF and HF exhibit the same order of discrepancy with respect to the tracking contours, but the distortions in the Wigner contours are much more evident due to the negativity of this function which is responsible for a change in the contour concavity.

In conclusion, up to the first order in the perturbation theory, and for thin lens approximation, it results that Wigner function can be adopted as appropriate phase-space distribution in TWM. In fact it gives the correct $x$- and $p$-projections, which are in good agreement with the tracking configuration and momentum distribution, respectively. Finally, although Husimi function does not give the right $x$ and $p$-projections, according to our analysis it provides a better description as far as the only phase-space dynamics is concerned.
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Figure Captions

Figure 1. Phase-space distribution at the starting point (left) and after a quadrupole lens plus drift space (right). Starting from the center of the distributions the isodensity contours correspond to 1, 2 and 3 $\sigma$, respectively.

Figure 2. Comparison of TWM phase-space description with tracking (dotted lines) results. Parameter set No. 1. Starting from the center of the distributions the isodensity contours correspond to 1, 2 and 3 $\sigma$, respectively.

Figure 3. Comparison of TWM phase-space description with tracking (dotted lines) results. Parameter set No. 2. Starting from the center of the distributions the isodensity contours correspond to 1, 2 and 3 $\sigma$, respectively.
Fig. 3