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Free evolution of an incoherent mixture of states: a quantum mechanical approach to the Van Cittert - Zernike theorem

Free Evolution of an Incoherent Mixture of States: A quantum mechanical approach to the Van Cittert - Zernike Theorem

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Abstract. We study the time evolution of an incoherent mixture of quantum states and demonstrate, in very simple terms, a quantum mechanical equivalent of van Cittert - Zernike theorem, which can be easily explained to Quantum Physics students with a basic knowledge of the density matrix theory. Finally, we exemplify this result by applying it to the quantitative analysis of the coherence of a beam of particles in atomic collisions.

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1. Introduction

The Sun is a conspicuously incoherent source of light. However, when Sunlight reaches the surface of the Earth after an 8-minute journey, it exhibits spatial coherence over a length of tens of μm (Mashaal *et al* 2012). The explanation of this remarkable effect, where the light emitted from an incoherent source becomes approximately coherent at large distances, relies on a theorem (Born and Wolf 1999) demonstrated by Pieter H. van Cittert in 1934 (van Cittert 1934) and, in a different context by Frits Zernike in 1938 (Zernike 1938).

Based on a direct analogy between electromagnetic and de Broglie waves, this theorem from light optics is usually applied to the study of coherent properties of particle beams (Cronin *et al* 2009). This strategy of borrowing results from classical optics and applying them to the study of particle's coherence, might be sound for qualitative analysis, but should be validated by a Quantum Mechanical approach for quantitative applications. For instance, an atom optics version of the van Cittert-Zernike theorem was proposed by Taylor *et al* (1994) in terms of a second-quantization model. More recently, Inpens and Guéry-Odelin (2010) employed a classical phase-space approach based on the Truncated Wigner equation.

Anyway, the concept that a beam of particles can gain coherence with time is far from being easy to grasp. Here we present a very simple derivation of van Cittert-Zernike theorem for an incoherent mixture of quantum states. This demonstration aims to senior undergraduate students and relies on basic concepts of Quantum Mechanics, as the density matrix theory and the Born approximation in elastic collisions, as explained in standard textbooks (See, e.g. Ballentine 2000, Bransden and Joachain 2000, Galindo and Pascual 1990, Gasiorowicz 2003, Landau and Lifshitz 1977, Schiff 1968). We hope that this approach would provide Physics students with the understanding of a fascinating but rather counterintuitive concept.

In this article we study the time evolution of an incoherent mixture of an ensemble of particles of mass m, described by identical wave packets located at different positions upon a much larger region of dimension D. We evaluate the time evolution of the corresponding density operator ρ by solving the Liouville - von Neumann equation. Actually, we demonstrate that a coherence length ℓ can be defined, such that for distances shorter than ℓ the system behaves coherently (i.e. ρ can be approximated by the product of pure states). In particular, ℓ coincides with the coherence length of each individual wave packet for small times t, as expected; while for large values of t the standard expression $\ell \propto \hbar t/mD$, of van Cittert - Zernike theorem is recovered. But first, let us review some basic concepts of the time evolution of an individual wave packet.

2. Free time evolution of a wave packet

Let us consider the time evolution of a normalized wave packet Φ_t for a particle of mass m in the absence of a potential. For pedagogical reasons, let us assume that

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at time $t = 0$, the wave packet Φ_0 is separable in cartesian coordinates, namely, $\langle \mathbf{r}|\Phi_0\rangle = \langle x|\phi_0\rangle \langle y|\varphi_0\rangle \langle z|\psi_0\rangle$. Since this factorization is preserved for all times, we will only study the evolution of $\langle x|\phi_t\rangle$. However, it is important to point out that this assumption does not represent any loss of generality, since its removal is straightforward.

The calculation of the time evolution of ϕ_t is trivial in momentum representation. It reads

$$\langle p|\phi_t\rangle = e^{-iE_p t/\hbar} \langle p|\phi_0\rangle \,, \tag{1}$$

with $E_p = p^2/2\,m$. The time evolution of the wave packet in coordinate space can be readily obtained,

$$\begin{aligned}\langle x|\phi_t\rangle &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \langle p|\phi_t\rangle \, \mathrm{d}p \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i(px-E_p t)/\hbar} \langle p|\phi_0\rangle \, \mathrm{d}p \,. \end{aligned} \tag{2}$$

It is important to note that, since the momentum distribution does not depend on time, namely $|\langle p|\phi_t\rangle|^2 = |\langle p|\phi_0\rangle|^2$, all the expectation values related to p are also time-independent,

$$\langle A(p)\rangle_t = \int_{-\infty}^{\infty} A(p)|\langle p|\phi_t\rangle|^2 \, \mathrm{d}p = \int_{-\infty}^{\infty} A(p)|\langle p|\phi_0\rangle|^2 \, \mathrm{d}p = \langle A(p)\rangle_{t=0} \,, \tag{3}$$

as expected for a free particle. In particular, so are $\langle p\rangle$ and $\Delta p = \sqrt{\langle p^2 - \langle p\rangle^2\rangle}$. On the contrary, $\Delta x = \sqrt{\langle x^2 - \langle x\rangle^2\rangle}$ varies in time as (Robinett *et al* 2005)

$$(\Delta x)^2 = (\Delta x)_0^2 + 2\,\mathrm{cov}(x, p, 0)\,t/m + (\Delta p)^2 t^2/m^2 \,, \tag{4}$$

where we have defined the generalized covariance of two operators A and B as

$$\mathrm{cov}(A, B, t) = \frac{1}{2}\langle [A - \langle A\rangle][B - \langle B\rangle] + [B - \langle B\rangle][A - \langle A\rangle]\rangle \,. \tag{5}$$

2.1. Gaussian Wave Packet

As a working example and for pedagogical reasons, from now on we will consider a gaussian wave packet of initial full width d (Kennard 1927, Darwin 1928, Lekner 2007, Cox and Lekner 2008), namely,

$$\langle x|\phi_0\rangle = \left(\frac{2}{\pi d^2}\right)^{1/4} e^{-x^2/d^2} \,, \tag{6}$$

and

$$\langle p|\phi_0\rangle = \left(\frac{d^2}{2\pi\hbar^2}\right)^{1/4} e^{-d^2 p^2/4\hbar^2} \,. \tag{7}$$

Replacing in eqs (1) and (2), we obtain

$$\langle x|\phi_t\rangle = \left(\frac{2d^2}{\pi\sigma^4}\right)^{1/4} e^{-x^2/\sigma^2} \tag{8}$$

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and

$$\langle p|\phi_t\rangle = \left(\frac{d^2}{2\pi\hbar^2}\right)^{1/4} e^{-iE_p t/\hbar} e^{-d^2 p^2/4\hbar^2}, \tag{9}$$

where we have defined

$$\sigma = d\sqrt{1 + i\frac{t}{\tau}}, \tag{10}$$

with $\tau = md^2/2\hbar$.

The expectation values of x and p are null, $\langle x\rangle = 0$ and $\langle p\rangle = 0$, and $\Delta x = |\sigma|^2/2d$ and $\Delta p = \hbar/d$, which are in accordance with the general result, eq. (4), i.e. $(\Delta x)^2 = (\Delta x)_0^2 + (\Delta p)^2 t^2/m^2$, for a null x-p covariance (Nicola 1972, Bradford 1976, Klein 1980). We see that the Gaussian wave function has its minimum value of $\Delta x \cdot \Delta p = \hbar/2$ at $t = 0$, and then increases (for both positive and negative times) as

$$\Delta x \, \Delta p = \frac{\hbar}{2}\sqrt{1 + \frac{t^2}{\tau^2}}. \tag{11}$$

Let us point out that these latter results can be generalized to a wave packet of arbitrary form, whenever the characteristic time τ is redefined as $\tau \equiv m(\Delta x)_0/\Delta p$, as can be seen easily seen in eq. (4).

Finally, the Gaussian wave functions in space (8) and momentum (9) representations can be related by this simple equation, $\langle x|\phi_t\rangle = \sqrt{2\hbar/\sigma^2}\,\langle p|\phi_t\rangle$ with $p = 2\hbar x/\sigma^2$; which, for $t \gg \tau$, reads

$$\langle x|\phi_t\rangle \approx \left(\frac{m}{it}\right)^{1/2} e^{imx^2/2\hbar t}\,\langle p|\phi_0\rangle \qquad \text{with} \qquad p = \frac{mx}{t}. \tag{12}$$

It can be easily shown, by means of a stationary phase approximation of (2), that this asymptotic limit is valid for any functional form of ϕ_0 (Dollard 1971), and not only for Gaussian wave functions. We will return to this general result in section 4.

2.2. Coherence Length

When a compressed wave packet is colliding with a structured target, the result would strongly depend on the distance between the source of the projectiles and the target region. The reason is that if this distance is too short, then the wave packet might not *illuminate* the full target coherently, but only a portion of it. But as time goes by, the width of the wave packet will increase, until it reaches a critical distance, where all the target will be illuminated coherently.

To be more specific, let us consider that the wave interacts with two similar delta potentials separated by a given distance x_o, namely $V_+(x) \propto \delta(x - x_o/2)$ and $V_-(x) \propto \delta(x + x_o/2)$. In a first Born approximation (See, e.g. Bransden and Joachain 2000, Galindo and Pascual 1990, Gasiorowicz 2003, Landau and Lifshitz 1977, Schiff 1968), the cross section, proportional to the squared modulus of the transition matrix element $\langle p|V_+ + V_-|\phi_t\rangle$, would present an interference term given by

$$I(p) = 2\,\mathrm{Re}\,\langle p|V_-|\phi_t\rangle\langle\phi_t|V_+|p\rangle \propto \exp\left(-\frac{x_o^2}{2\ell^2}\right)\,\cos(p\,x_o/\hbar) \tag{13}$$

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with

$$\ell = 2\Delta x = d\sqrt{1 + \frac{t^2}{\tau^2}} \tag{14}$$

This term would be sizable for targets of the order of $x_o = \ell$ or smaller. Thus, we might define ℓ as the "coherence" length of the wave function at a given time t. This definition, which relies on the conditions necessary for the appearance of an interference structure, is standard in optical studies (Svelto 2010), but still might differ from other diverse and even contradictory definitions. For instance, Cohen-Tannoudji and Guéry-Odelin (2011) define the coherence length as the width of the global spatial coherence,

$$G(x_o) = \int_{-\infty}^{\infty} \langle x - x_o/2|\phi_t\rangle\langle\phi|x + x_o/2\rangle\mathrm{d}x , \tag{15}$$

corresponding to the overlapping between two wave packets separated by a distance x_o. For a gaussian wave packet (eqs. (8) and (9)) we obtain, $G(x_o) = e^{-x_o^2/2d^2}$. Thus, in the approach by Cohen-Tannoudji and Guéry-Odelin (2011), the coherence length is time-independent and equal to d.

Here, on the contrary, we retain the definition (14). Note that the more sharply peaked the wave packet is at $t = 0$ (i.e. for smaller values of d), the faster its coherence length spreads (for $t > 0$) since

$$\ell \approx \frac{2\hbar t}{md} \qquad \text{for} \qquad t \gg \tau . \tag{16}$$

As a side comment, let us point out that in Optics this limit is named in honor of Joseph von Fraunhofer, although he was not actually involved in the development of the theory. Putting some numbers, let us consider an electron impulsively removed from the ground state of a Hydrogen atom. For a corresponding initial width of $d = 1$ Å, the time necessary to achieve condition (16) is in the range of tens of attoseconds (i.e. $\tau = 40$ as), whereas the coherence length increases at a constant rate, $\ell/t \approx 23$ km/s.

Finally, let us assume that the wave has a group velocity $\mathbf{v}$, such that it travels a distance $\mathbf{z} = \mathbf{v}t$ in a given time t. Even thought we are considering a one dimensional problem, $\mathbf{v}$ might not be necessarily parallel to the direction $\hat{\mathbf{x}}$. We will come back to this point in the following section. Now, replacing $\mathbf{z} = \mathbf{v}t$ in the previous equation, we obtain,

$$\ell \approx \frac{\lambda}{\pi d} z \qquad \text{for} \qquad \ell \gg d , \tag{17}$$

with $\lambda = h/mv$ the particle's wavelength.

3. Time evolution of an incoherent mixture of wave packets

Let us now consider the free evolution of an incoherent mixture of an ensemble of particles described by wave packets $\langle x|\phi_t\rangle$, as defined in (2), which are identical except for their initial positions b, which are distributed along the x axis according to a

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normalized distribution $f(b)$. Initially (i.e. at $t = 0$), the corresponding density operator $\rho(t)$ reads,

$$\langle x|\rho(0)|x'\rangle = \int \mathrm{d}b\, f(b) \langle x - b|\phi_0\rangle\langle\phi_0|x' - b\rangle \,, \tag{18}$$

in space representation, and $\langle p|\rho(0)|p'\rangle = \langle p|\phi_0\rangle\langle\phi_0|p'\rangle \tilde{f}(p - p')$ in momentum representation, with $\tilde{f}(q) = \int \mathrm{d}b\, e^{-iq\cdot b} f(b)$.

As in the previous sections, and for the sake of simplicity, we are considering a one-dimensional case. This does not mean any loss of generality, since the generalization to the three dimensional case is straightforward. The density operator $\rho(t)$ evolves in time according to the the Liouville - von Neumann equation with a free Hamiltonian H_o,

$$\frac{\partial\rho}{\partial t} = \frac{i}{\hbar}[\rho, H_o] \,. \tag{19}$$

This equation is trivially solved in momentum representation, namely

$$\langle p|\rho(t)|p'\rangle = \langle p|\rho(0)|p'\rangle \, e^{-i\left(E_p - E_{p'}\right)t/\hbar} \,, \tag{20}$$

with $E_p = p^2/2m$; from which the time dependent expression for the space dependent matrix element can be easily obtained,

$$\langle x|\rho(t)|x'\rangle = \frac{1}{2\pi\hbar} \int \mathrm{d}p\, \mathrm{d}p' \, \langle p|\rho(t)|p'\rangle \, e^{i(px-p'x')/\hbar} \,. \tag{21}$$

3.1. Gaussian wave packet and impact parameter distribution

In what follows, we will consider that both the wave packets ϕ and the distribution $f(b)$ are of a gaussian shape, namely,

$$\langle x|\phi_0\rangle = \left(\frac{2}{\pi d^2}\right)^{1/4} e^{-x^2/d^2} \,, \tag{22}$$

and

$$f(b) = \left(\frac{2}{\pi D^2}\right)^{1/2} e^{-2b^2/D^2} \,. \tag{23}$$

Thus, in momentum representation,

$$\langle p|\rho(t)|p'\rangle = \langle p|\phi_t\rangle \langle\phi_t|p'\rangle \, e^{-D^2(p-p')^2/8\hbar^2} \,, \tag{24}$$

with $\langle p|\phi_t\rangle$ given by (9), namely,

$$\langle p|\phi_t\rangle = \left(\frac{d^2}{2\pi\hbar^2}\right)^{1/4} e^{-iE_p t/\hbar} \, e^{-d^2 p^2/4\hbar^2} \,. \tag{25}$$

Similarly, in space representation,

$$\langle x|\rho(t)|x'\rangle = \langle x|\phi_t\rangle \langle\phi_t|x'\rangle \, e^{-(x-x')^2/2\,\Sigma^2} \,, \tag{26}$$

where

$$\Sigma = \frac{d}{D} \sqrt{D^2 + d^2 + d^2 t^2/\tau^2} \,, \tag{27}$$

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with $\tau = md^2/2\hbar$, and

$$\langle x|\phi_t\rangle = \left(\frac{2\,\mathrm{Re}(\sigma^2)}{\pi\sigma^4}\right)^{1/4} e^{-x^2/\sigma^2}\,, \tag{28}$$

with

$$\sigma = \sqrt{\frac{D^2 + d^2 + d^2 t^2/\tau^2}{1 - it/\tau}}\,. \tag{29}$$

Let us note that in both space and momentum representations, the density matrix (26) is composed of a gaussian pure state, incoherently modulated by a gaussian distribution of standard deviation Σ. We will come back to this result in the following section. But first, let us notice that, as expected,

$$\mathrm{Tr}(\rho) = \int_{-\infty}^{\infty} \langle x|\rho|x\rangle\,\mathrm{d}x = \int_{-\infty}^{\infty} |\langle x|\phi_t\rangle|^2\,\mathrm{d}x = 1\,, \tag{30}$$

while

$$\mathrm{Tr}(\rho^2) = \left(1 + \frac{D^2}{d^2}\right)^{-1/2}\,, \tag{31}$$

so that the total coherence of the beam remains constant in time. Let us point out that a simple calculation in momentum space can show that $\mathrm{Tr}(\rho^2)$ is independent of time, independently of the functional forms employed for ϕ_0 and $f(b)$.

3.2. Emerging coherence from an incoherent mixture of wave packets

It is clear that for $D \to 0$, the width Σ of the modulating gaussian reaches infinity, and the system becomes completely coherent, consisting of a single gaussian wave centered at $x = 0$. The corresponding density matrix element reads

$$\langle x|\rho(t)|x'\rangle = \langle x|\phi_t\rangle\,\langle\phi_t|x'\rangle \tag{32}$$

with a wave function given by (8), i.e.

$$\langle x|\phi_t\rangle = \left(\frac{2d^2}{\pi\sigma^4}\right)^{1/4} e^{-x^2/\sigma^2}\,, \tag{33}$$

where

$$\sigma = d\sqrt{1 + i\frac{t}{\tau}}\,. \tag{34}$$

Without going all the way to this purely coherent case, we see that for any finite value of Σ it would be possible to define a characteristic distance for which, if $|x' - x|$ is smaller than it, the modulating gaussian would be approximately constant and the system would mimic a completely coherent state. The emergence of this spatial coherence out of an incoherent system is the essence of the van Cittert – Zernike theorem.

Now, we find the same dependence on x_o for the interference term (13) than the one obtained in the previous section, i.e.

$$I(p) = 2\,\mathrm{Re}\,\langle p|V_-\,\rho\,V_+|p\rangle \propto \exp\left(-\frac{x_o^2}{2\ell^2}\right)\,\cos(p\,x_o/\hbar)\,, \tag{35}$$

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but with a different coherence length,

$$\ell = \sqrt{d^2 + \frac{4\hbar^2 t^2}{m^2(d^2 + D^2)}} \ . \tag{36}$$

Note that for $D = 0$, we recover the same result obtained in the previous section for a purely coherent system.

As a marginal note, let us point out that, when dealing with the concept of spatial coherence, the corresponding coherence length ℓ might be defined as the distance between two points in space for which the right term in (35) is a given fraction ξ of its maximum value. Thus, in general, we might define

$$\ell = \sqrt{|2\ln\xi|}\sqrt{d^2 + \frac{4\hbar^2 t^2}{m^2(d^2 + D^2)}} \ . \tag{37}$$

A standard definition is that of the full-width at half-maximum (FWHM), for which $\xi = 1/2$. In our case, we have arbitrarily chosen $\xi = e^{-1/2}$, so that (36) is obtained.

3.3. Small and large t limits

For very small values of t (a limit that in Optics is usually named after Augustin-Jean Fresnel), we obtain $\ell \approx d$. This means that the coherence length is limited to that of an individual wave packet. On the contrary, for $t \gg \tau\sqrt{1 + D^2/d^2}$, it grows linearly with time as

$$\ell \approx \frac{2\hbar t}{m\sqrt{d^2 + D^2}} \ . \tag{38}$$

Let us also point out that in general situations, $d \ll D$. This is the case, for instance, in particle accelerators, where the projectile's wave packets are much smaller than the macroscopic size of the collimators. In these cases, for $t \gg mDd/2\hbar$, we can approximate (36) by,

$$\ell \approx \frac{2\hbar t}{mD} \ . \tag{39}$$

Finally, replacing $t = z/v$, we write equations (36) and (39) as,

$$\ell = \sqrt{d^2 + \left(\frac{\lambda z}{\pi\sqrt{d^2 + D^2}}\right)^2} \ , \tag{40}$$

and

$$\ell \approx \frac{\lambda}{\pi D} \ z \ , \tag{41}$$

respectively, with $\lambda = h/mv$ the particle's wavelength. As we already mentioned in a previous section, the velocity $\mathbf{v}$ is not necessarily parallel to x. For instance, in the standard geometry of the collision experiments, the beam of particles is moving in a direction perpendicular to that of the impact parameter $\mathbf{b}$, a situation that is usually referred to as of "transversal" coherence.

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Finally, let us point out that by comparing equations (14) and (36), we see that the coherence length grows at a much faster rate for a coherent state than in an incoherent superposition. In particular, for large values of t, the corresponding ratio becomes proportional to $\sqrt{1 + D^2/d^2}$. This characteristic of the coherence length evolution is already evident when comparing the generalized widths σ in equations (8) and (26).

4. Non-gaussian wave functions and position distribution

In the previous sections, we have assumed Gaussian shapes for the initial position distribution $f(b)$ and the wave packets ϕ. The reason for this choice was purely pedagogical, since all the calculations can be performed analytically. In this respect let us point out that this analysis in terms of Gaussian functions is simple enough as to be included in a problem to be solved by the student. However, it is important to point out that most of the results obtained with Gaussian functions are also valid for general non-gaussian $f(b)$ and ϕ functions. Take equation (39), for instance; one of the main results associated to the van Cittert - Zernike theorem. By replacing the general asymptotic form (12) of the wave function in the interference term (13), a simple demonstration leads to $\ell \propto t/d$ for pure states. Similarly, replacing (12) in (35), and performing a straightforward change of the integration variable, it can be shown that for an incoherent mixture of wave functions,

$$\ell \propto \frac{t}{D} , \tag{42}$$

for large values of t. Perhaps, this latter demonstration is too cumbersome to be of any pedagogical value. However, it can be numerically tested for different functional forms of $f(b)$ and ϕ, providing a complementary avenue for exploration and/or exercises.

5. Conclusions

We have shown in section 3 that it is possible to develop a generalization of van Cittert - Zernike theorem for massive particles, as a direct application of the density matrix concept. In particular, we see that this analysis does not imply any difficulty greater than those encountered in the study of the coherence length of a pure state, as shown in section 2. Furthermore, similar results are obtained in both cases, but with the difference that for large values of t the characteristic distance for the incoherent mixture is the size D of the source, instead of the initial width d of each of its individual waves. The reason for this result is that coherence emerges as result of the superposition of each of the individual components of the mixture. In spite of its simplicity, this difference is trascendental, and goes to the very heart of the van Cittert - Zernike theorem. It makes the coherence length of the Sunlight to be of the order of tens of μm, instead of larger than the Earth itself, as it would be for each of its individual photons. The same occurs in a particle accelerator, where the coherence length at the target region is of atomic dimensions and can be varied by changing its relative position along the beam's line.

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Recently, this peculiarity of the van Cittert - Zernike theorem has made it possible to develop a new set of atomic and molecular collision experiments where the cross sections are shown to depend on the degree of coherence of the projectiles beam. The coherence properties of particle beams have been extensively studied for decades, most notably in connection with neutrino interference and oscillations (Nussinov 1976, Kayser 1981), but represents a rather new issue in the area of atomic collisions (Egodapitiya *et al* 2011). It has been usually assumed that under very general and common conditions, the outcome of a scattering experiment does not depend on the properties of the projectiles beam (Taylor 1972). However, recent evidence in ionization (Egodapitiya *et al* 2011) and electron capture (Sharma *et al* 2012) experiments points to a breakdown of these conditions and a dependence of the collision outcome on the incident beams coherence properties. Finally let us point out that in the present article we have focussed our attention on the dependence of the spatial degree of coherence with the distance to the source, but not on its intensity distribution. This element of van Cittert - Zernike theorem is relevant in Optics, but not in its application to atomic collision experiments, where the projectile's beam is assumed to be homogeneously distributed over the transversal plane.

Acknowledgments

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