Indirect evidence for the Gouy phase for matter waves

I. G. da Paz *
Departamento de Matemática, Universidade Federal do Piauí, Campus Senador Helvídio Nunes de Barros, Picos, PI 64600-000, Brazil and
Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Caixa Postal 702, Belo Horizonte, MG 30123-970, Brazil, e-mail: irismar@fisica.ufmg.br,
Phone: +55-31-3499-5605, Fax: +55-31-3499-5688.

M. C. Nemes and S. Pádua
Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Caixa Postal 702, Belo Horizonte, MG 30123-970, Brazil

C. H. Monken
Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Caixa Postal 702, Belo Horizonte, MG 30123-970, Brazil and
Huygens Laboratory, P. O. Box 9504, 2300 RA Leiden, The Netherlands

J. G. Peixoto de Faria
Departamento de Física e Matemática, Centro Federal de Educação Tecnológica de Minas Gerais, Av. Amazonas 7675, Belo Horizonte, MG 30510-000, Brazil

* Corresponding author.
Abstract

We show that the well known geometric phase, the Gouy phase in optics can be defined for matter waves in vacuum as well. In particular we show that the underlying physics for the “matter waves” Gouy phase is the generalized Schrödinger-Robertson uncertainty principle, more specifically, the off diagonal elements of the covariance matrix. Recent experiments involving the diffraction of fullerene molecules and the uncertainty principle are shown to be quantitatively consistent with the existence of a Gouy phase for matter waves.

PACS numbers: 03.75.-b, 03.65.Vf, 03.75.Be

Keywords: Gouy Phase, Matter Waves
The extra phase shift experienced by a converging light wave passing through its focal point, also known as the Gouy phase shift, is a well-known phenomenon in optics. Since its observation reported by Gouy in 1890 [1, 2], this phase shift (sometimes referred to as a phase anomaly), its physical origin and its consequences have been objects of study, especially in the last decades [3–8]. Although it is often presented as a property of Gaussian light beams [9], the Gouy phase shift appears in any kind of wave that is submitted to some sort of transverse spatial confinement, be it by focusing or by diffraction through small apertures. As discussed in [7], when a wave is focused, the Gouy phase shift is associated to the propagation from $-\infty$ to $+\infty$ and is equal to $\pi/2$ for cylindrical waves (line focus), and $\pi$ for spherical waves (point focus). In the case of diffracted waves, the Gouy phase shift is associated to the propagation from the diffraction aperture to infinity, and amounts to $\pi/4$ ($\pi/2$) for one-dimensional (two-dimensional) apertures.

The Gouy phase shift has been observed in water waves [10], acoustic [11], surface plasmon-polariton [12], and phonon-polariton [13] pulses. In this work we show that it can also be observed in matter waves, despite the abstract nature of the latter, and is directly related to the generalized uncertainty principle. Some effects related to the Gouy phase shift in electromagnetic waves, such as pulse reshaping [14] and acceleration [15], anomalous spectral behavior [16], among others, rise interesting questions about their possible counterparts in matter waves.

We start our analysis by taking the simple route of a direct comparison between the Gaussian solutions of the paraxial wave equation and the two-dimensional Schrödinger equation. Later, we focus on the one-dimensional problem of diffraction of massive particles through a single slit. We take as an example a recent diffraction experiment with fullerene molecules [17, 18] and show that the Gouy phase shift can be inferred from the reported experimental data.

Consider a stationary electric field in vacuum

$$E(\vec{r}) = A(\vec{r}) \exp(ikz). \quad (1)$$

The paraxial approximation consists in assuming that the complex envelope function $A(\vec{r})$ varies slowly within one wavelength $\lambda_L = 2\pi/k$. Under this condition the equation for $A(\vec{r})$ can be immediately obtained and reads [19]

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + i4\pi \frac{1}{\lambda_L} \frac{\partial}{\partial z} \right) A(x, y, z) = 0. \quad (2)$$
Consider now the two-dimensional Schrödinger equation for a free particle of mass $m$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + 2i\frac{m}{\hbar} \frac{\partial}{\partial t}\right) \psi(x, y, t) = 0. \quad (3)$$

Here, $\psi(x, y, t)$ stands for the wave function of the particle in time $t$. Assuming that the longitudinal momentum component $p_z$ is well-defined \[20\], i.e., $\Delta p_z \ll p_z$, we can consider particle’s movement in the $z$ direction is classical and its velocity in this direction remains constant. In this case one can interpret the time variation as the variation in this direction according to the relation $t = z/v_z$. Now using the fact that $\lambda_P = h/p_z$ and substituting in Eq. (3) we get

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + i4\pi \frac{1}{\lambda_P} \frac{\partial}{\partial z}\right) \psi(x, y, t = z/v_z) = 0. \quad (4)$$

The condition of constant velocity in the propagation direction has been used in the analysis of recent diffraction experiments with fullerene molecules \[17, 18\]. A theoretical model using this assumption was also shown to qualitatively reproduce the data well \[20\].

We show the particle’s counterpart using the initial gaussian state

$$\psi(x, y, 0) = \left(\frac{1}{b\sqrt{\pi}}\right) \exp\left[-\frac{(x^2 + y^2)}{b^2}\right], \quad (5)$$

we get for an arbitrary time $t$ \[21\]

$$\psi(x, y, t) = \left[\frac{1}{B(t)\sqrt{\pi}}\right] \exp\left(\frac{x^2 + y^2}{B^2(t)}\right) \times \exp\left\{i \left[\frac{m}{2\hbar} (x^2 + y^2) + \mu(t)\right]\right\}, \quad (6)$$

where $\mu(t)$ is the analogous to the Gouy phase. The comparison with the solution of the wave equation in the paraxial approximation with the same condition at $z = 0$ yields

$$B(t) = b \left[1 + \left(\frac{t}{\tau_b}\right)^2\right]^{\frac{1}{2}}, \quad (7)$$

$$R(t) = t \left[1 + \left(\frac{\tau_b}{t}\right)^2\right], \quad (8)$$

$$\mu(t) = -\arctan\left(\frac{t}{\tau_b}\right), \quad (9)$$

and

$$\tau_b = \frac{mb^2}{\hbar}. \quad (10)$$
Notice that the parameter $\tau_b$ is related to the initial condition only and is responsible for two regimes of the growing width $B(t)$, in close analogy to Rayleigh range which separates the width $w(z)$ in two qualitatively different regimes, as is well known [19].

Next we show that $\mu(t)$ is directly related to the Schrödinger-Robertson generalized uncertainty principle. For quadratic evolutions (as the free evolution in the present case) the determinant of the covariance matrix saturates to its minimum value,

$$\det \begin{pmatrix} \sigma_{xx} & \sigma_{xp} \\ \sigma_{xp} & \sigma_{pp} \end{pmatrix} = \frac{\hbar^2}{4} \quad (11)$$

where $\sigma_{xx} = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = \frac{B(t)^2}{2}$, $\sigma_{pp} = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2 = \frac{\hbar^2}{2\delta p}$, and $\sigma_{xp} = \frac{1}{2} \langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle - \langle \hat{x} \rangle \langle \hat{p} \rangle = \frac{\hbar t}{2\tau_b}$.

Since the covariance $\sigma_{xp}$ is non-null if the gaussian state exhibits squeezing [22], if one measures $\sigma_{xp}$, from the above relation it is possible to infer the Gouy phase for a matter wave which can be described by an evolving coherent wave packet.

Now an important question is in order: What does experiment say?

In Ref. [17] an experimental investigation of the uncertainty principle in the diffraction of fullerene molecules is presented. In that experiment, a collimated molecular beam crosses a variable aperture slit and its width is measured as a function of the slit width (see Fig. 3 in Ref. [17]).

As discussed in Ref. [20], given the way the fullerene molecules are produced, it is reasonable to assume that the outgoing beam after the diffraction slit has a random transverse momentum. Here, we suppose that the transverse momentum follows a gaussian distribution with zero mean and width $\delta k_x$, that is related to the experimental angular divergence of the beam, as explained in Ref. [23]. So, the state of fullerene molecules which leave the slit with width $b$ is given by (in transverse direction)

$$\rho(x, x', 0) = \frac{1}{b\sqrt{\pi}} \int \exp \left( -\frac{x^2 + x'^2}{2b^2} \right) \exp \left[ ik_x (x - x') \right] g(k_x) dk_x \quad (12)$$

where

$$g(k_x) = \frac{1}{\sqrt{\pi \delta k_x}} \exp \left( -\frac{k_x^2}{\delta k_x^2} \right) \quad (13)$$

is a gaussian probability distribution function for the transverse momentum with width $\delta k_x/\sqrt{2}$.

At $t = \frac{(z-L)}{v_z}$, where $v_z$ is the most probable velocity in $z$ direction, the calculation of the time evolution is straightforward and the elements of the covariance matrix are now given
\[ \sigma_{xx} = \frac{B(t)^2}{2} \left[ 1 + \left( \frac{\tau_b B(t) \delta k_x}{R(t)} \right)^2 \right] = \frac{\bar{B}(t)^2}{2}, \]  
\[ \sigma_{pp} = \frac{\hbar^2}{2} \frac{(1 + b^2 \delta k_x^2)}{b^2}, \]  
\[ \sigma_{xp} = \frac{\hbar}{2} \left( \frac{t}{\tau_0} \right) \left( 1 + b^2 \delta k_x^2 \right). \]

In Eq. (14), we define \( \bar{B}(t) \) as the counterpart of the width \( B(t) \) for the partially coherent gaussian state given in Eq. (12). The effective detected intensity is a convolution of the detector resolution function \( D(x) \) and the real intensity \( I(x,t) \) (where \( I(x,t) = \rho(x,x,t) \)) [17, 20].

For pure states, the Gouy phase \( \mu(t) \) and the width \( B(t) \) are related by the expression [7]

\[ \mu(t) = -\frac{\hbar}{2m} \int^t dt \frac{B(t)^2}{B(t)^2}. \]  

We conjecture that this relation holds for partially coherent states. So, for the state given in Eq. (12), the Gouy phase is

\[ \mu(t) = -\frac{1}{2\sqrt{1 + b^2 \delta k_x^2}} \arctan \left( \frac{2\sigma_{xp}}{\hbar \sqrt{1 + b^2 \delta k_x^2}} \right). \]  

Note that, again \( \mu(t) \) is related to \( \sigma_{xp} \) and is affected by the partial coherence of the initial wave packet.

Furthermore, as discussed before from the saturation of the determinant of the covariance matrix we get for \( \sigma_{xp} \),

\[ \sigma_{xp} = \frac{\hbar}{2} \sqrt{1 + b^2 \delta k_x^2} \left[ \left( \frac{W_{FWHM}}{2\sqrt{\ln 2}b} \right)^2 - 1 \right]^{\frac{1}{2}}, \]  

where \( W_{FWHM} \) is the full width at half maximum of the diffraction pattern at the screen. The experimental results for \( W_{FWHM} \) as reported in Ref. [17] is shown in Fig. 1 and compared with our theoretical calculation Eq. (14) (where \( W_{FWHM} = 2\sqrt{2 \ln 2} 2\sigma_{xx} \)). We use \( b \to b/3 \) due to van der Waals forces for the smallest slit width [17, 20, 24] and \( D = 12 \mu m \) for the spatial resolution of the detector [17]. The curve for \( \sigma_{xp} \) is shown in Fig. 2.

Now we show that this experiment is consistent with the existence of a phase. In Fig. 3 we show the phase, taken from Eq. (18). As expected the phase variation is \( \pi/4 \).
FIG. 1: Width of a beam of fullerene C\textsubscript{70} molecules as a function of the slit width. The solid curve corresponds to our calculation and the points are the results obtained in the experiment reported in Ref. [17]. We used $\delta k_x = 9.0 \times 10^6$ m$^{-1}$ and $t = 6.65$ ms.

The parameter which measures the partial coherence in transverse direction of the beam is given by $\delta k_x$. By fitting the data in Fig. 1 we obtained $\delta k_x = 9.0 \times 10^6$ m$^{-1}$. It corresponds to an angular aperture of 2.4 $\mu$rad. This is completely compatible with the experimental value quoted in Ref. [23] ($2 \leq \theta \leq 10$ $\mu$rad).

In summary we have shown that a geometrical phase for matter waves can be defined and shown to be compatible with existing experimental data. We have also given interpretation as to the physical content of this phase for matter waves: it is intimately related to the
FIG. 3: Gouy phase as a function of the slit width. The solid curve corresponds to our calculation and the points were obtained from the experimental results reported in Ref. [17]. The parameters are the same as in Fig. 1.

uncertainty principle, more specifically to the off diagonal element of the covariance matrix, $\sigma_{xp}$. We have also shown that the existence of this phase is compatible with experimental data involving the diffraction of fullerene molecules. We hope our results encourage experimentalists to implement a direct measure of this phase, since nowadays the fabrication of lenses capable of focusing matter beams are available [25]. Of course the experiment with fullerene molecules is not the best candidate for exhibiting the phase due to its incoherence in transverse direction. In this aspect experiment with neutrons should be “cleaner”, unfortunately not available yet.

We would like to thank K. M. Fonseca Romero for a careful reading of the manuscript. This work was partially supported by CNPq.

[1] G. Gouy, C. R. Acad. Sci. Paris 110 (1890) 1251.
[2] G. Gouy, Ann. Chim. Phys. Ser. 6, 24 (1891) 145.
[3] R. W. Boyd, J. Opt. Soc. Am. 70 (1980) 877.
[4] R. Simon, N. Mukunda, Phys. Rev. Lett. 70 (1993) 880.
[5] P. Hariharan, P. A. Robinson, J. Mod. Opt. 43 (1996) 219.
[6] Simin Feng, Herbert G. Winful, Robert W. Hellwarth, Opt. Lett. 23 (1998) 385.
[7] Simin Feng, Herbert G. Winful, Opt. Lett. 26 (2001) 485.
[8] Jun Yang, Herbert G. Winful, Opt. Lett. 31 (2006) 104.

[9] A. E. Siegman, Lasers, Sausalito (CA), University Science Books, 1986.

[10] Dominique Chauvat, Olivier Emile, Marc Brunel, Albert Le Floch, Am. J. Phys. 71 (2003) 1196.

[11] N. C. R. Holme, B. C. Daly, M. T. Myaing, T. B. Norris, Appl. Phys. Lett. 83 (2003) 392.

[12] Wenqi Zhu, Amit Agrawal, Ajay Nahata, Opt. Express 15 (2007) 9995.

[13] T. Feurer, Nikolay S. Stoyanov, David W. Ward, Keith A. Nelson, Phys. Rev. Lett. 88 (2002) 257402.

[14] Z. L. Horváth, Zs. Bor, Phys. Rev. E 60 (1999) 2337.

[15] Z. L. Horváth, J. Vinkó, Zs. Bor, D. von der Linde, Appl. Phys. B 63 (1996) 481.

[16] G. Gbur, T. D. Visser, E. Wolf, Phys. Rev. Lett. 88 (2002) 013901.

[17] O. Nairz, M. Arndt, A. Zeilinger, Phys. Rev. A 65 (2002) 032109.

[18] O. Nairz, M. Arndt, A. Zeilinger, Am. J. Phys. 71 (2003) 319.

[19] B. E. A. Saleh, M. C. Teich, Fundamentals of Photonics, p. 86, New York, John Wiley et Sons, 1991.

[20] A. Viale, M. Vicari, N. Zanghi, Phys. Rev. A 68 (2003) 063610.

[21] I. G. da Paz, Master thesis. Departamento de Física, Universidade Federal de Minas Gerais (2006).

[22] L. A. M. Souza, M. C. Nemes, M. F. Santos, J. G. Peixoto de Faria, Opt. Comm. 281 (2008) 4694.

[23] O. Nairz, M. Arndt, A. Zeilinger, J. Modern Opt. 47 (2000) 2811.

[24] R. E. Grisenti, W. Schöllkopf, J. P. Toennies, Phys. Rev. Lett. 83 (1999) 1755.

[25] I. G. da Paz, M.C. Nemes, J.G. Peixoto de Faria, J. Phys.: Conference Series 84 (2007) 012016.