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**“Quantum-mechanical phase vortices in the two-dimensional infinite square well”**

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**0. Referee’s worksheet.** I found this paper to be at several points so unclear, and at many points so computationally dense (a circumstance which, curiously, the authors do not explicitly acknowledge, and to which they do not draw the reader’s attention), that I could not simply read it through, from beginning to end, and be confident that I understood the authors’ intentions. I had therefore no option but to write out my own account of what I take to be the essential upshot of their work, and my own attempt to reproduce their calculations. Whence the following material, which I include because it exposes points to which I will, on occasion, want to make reference.

Working initially in 3D, the free-particle Schrödinger equation reads

$$-(\hbar^2/2m)\nabla^2\psi(\mathbf{x}, t) = i\hbar\partial_t\psi(\mathbf{x}, t)$$

The probability current is constructed

$$\mathbf{J}(\mathbf{x}, t) = -i(\hbar/2m)\{\psi^*\nabla\psi - \psi\nabla\psi^*\}$$

and enters into the continuity equation  $\partial_t P(\mathbf{x}, t) + \nabla\cdot\mathbf{J}(\mathbf{x}, t) = 0$ , where

$$P(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2$$

describes probability density. Familiar stuff, presented only to set the notational conventions from which I will soon depart.

Let the complex  $\psi$ -field be written in polar form:

$$\begin{aligned}\psi(\mathbf{x}, t) &= R(\mathbf{x}, t) \cdot e^{(i/\hbar)S(\mathbf{x}, t)} \\ &= R(\mathbf{x}, t) \cdot e^{i\phi(\mathbf{x}, t)} \quad : \quad \text{phase } \phi(\mathbf{x}, t) = S(\mathbf{x}, t)/\hbar\end{aligned}$$

One then has

$$P(\mathbf{x}, t) = [R(\mathbf{x}, t)]^2 \tag{1}$$

$$\mathbf{J}(\mathbf{x}, t) = P(\mathbf{x}, t) \cdot \frac{\nabla S(\mathbf{x}, t)}{m} \tag{2}$$

It becomes dimensionally/physically natural at this point to introduce the “velocity field”

$$\begin{aligned}\mathbf{V}(\mathbf{x}, t) &= \frac{\mathbf{J}(\mathbf{x}, t)}{P(\mathbf{x}, t)} \\ &= \frac{1}{m}\nabla S(\mathbf{x}, t) = (\hbar/m)\nabla\phi(\mathbf{x}, t)\end{aligned} \tag{3}$$

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which is an object central to the “hydrodynamical interpretation of quantum mechanics” and central also to the present discussion, for the reason that  $\mathbf{V}(\mathbf{x}, t)$  becomes singular at points where  $P(\mathbf{x}, t)$  vanishes (unless  $\mathbf{V}(\mathbf{x}, t)$  happens also to vanish there).

An aside: separating  $t$  from the  $\mathbf{x}$ -variables sends  $S(\mathbf{x}, t) \mapsto W(\mathbf{x}) - Et$  and we obtain

$$\begin{aligned}\psi(\mathbf{x}, t) &= R(\mathbf{x}) e^{(i/\hbar)W(\mathbf{x})} \cdot e^{-(i/\hbar)Et} \\ P(\mathbf{x}) &= [R(\mathbf{x})]^2 \\ \mathbf{J}(\mathbf{x}) &= P(\mathbf{x}) \cdot \frac{\nabla W(\mathbf{x})}{m} \\ \mathbf{V}(\mathbf{x}) &= \frac{1}{m} \nabla W(\mathbf{x})\end{aligned}$$

The continuity equation  $\partial_t P(\mathbf{x}, t) + \nabla \cdot \mathbf{J}(\mathbf{x}, t) = 0$  simplifies:  $\nabla \cdot \mathbf{J}(\mathbf{x}, t) = 0$ .

When confronted with a velocity field it becomes natural—whatever the physical context—to consider the associated “vorticity field”

$$\mathbf{\Omega}(\mathbf{x}, t) = \nabla \times \mathbf{V}(\mathbf{x}, t) \tag{4}$$

and with every bounded surface  $\mathcal{S}$  to associate a “circulation”

$$\Gamma = \oint_{\partial\mathcal{S}} \mathbf{V} \cdot d\mathbf{s} = \iint_{\mathcal{S}} \mathbf{\Omega} \cdot d\boldsymbol{\sigma} \tag{5}$$

Bringing (3) to (4), we find that the quantum velocity field is irrotational

$$\mathbf{\Omega} = \nabla \times \frac{1}{m} \nabla S = \mathbf{0}$$

except at points where the velocity field becomes singular (points where the probability density vanishes), and that the circulation is sure to vanish except when the curve  $\partial\mathcal{S}$  encircles such a singularity.

The intent of the MPF paper is to draw attention to these points (a useful undertaking, since the points in question—though they are entirely elementary—are known to strike deep in some important physical contexts, yet are developed in none of the standard introductory quantum texts) and to the fact that the quantum mechanics of particle that moves freely within a square box is rich enough to illustrate them. I follow them down that road:

We note first that the pullback from 3D to 2D, though it causes  $\mathbf{J}$  and  $\mathbf{V}$  to lose a component, and  $\mathbf{\Omega}$  to acquire the character of a pseudo-*scalar* field, is otherwise inconsequential, except that it opens up a world of graphic possibilities.

Adopt units in which the free particle Schrödinger equation reads

$$-(\partial_x^2 + \partial_y^2)\psi = i\partial_t\psi \tag{6}$$

and look for a preparatory moment to the associated one-dimensional problem:

$$-\partial_x^2 \psi = i \partial_t \psi \quad : \quad \psi(0, t) = \psi(1, t) = 0 \quad (\text{all } t) \quad (7.1)$$

The buzzing eigenfunctions are

$$\psi_n(x, t) = \sqrt{2} \sin[n\pi x] \cdot e^{-in^2\pi^2 t} \quad (7.2)$$

To set the probability density into motion one must superimpose two or more such functions. In the simplest instance one has

$$\psi_{mn}(x, t) = \cos \alpha \cdot \psi_m(x, t) + e^{i\beta} \sin \alpha \cdot \psi_n(x, t) \quad (7.3)$$

(here  $\alpha$  is a “mixing angle” and  $\beta$  a relative phase factor), giving

$$P_{mn}(x, t) \equiv |\psi_{mn}(x, t)|^2 = f_{mn}(x) + g_{mn}(x) \cos[\omega_{mn}(t - \delta)] \quad (7.4)$$

with  $\omega_{mn} = \pi^2(m^2 - n^2)$ . The oscillatory term arises as a cross term.<sup>1</sup>

Returning now to the 2D particle-in-a-square-box problem, from (6) we are led to buzzing eigenfunctions of form

$$\Psi_{mn}(x, y, t) = \psi_m(x, t) \cdot \psi_n(y, t) \quad (8)$$

Taking such functions in linear combinations of the factored form

$$\left[ \sum_m a_m \psi_m(x, t) \right] \cdot \left[ \sum_b b_b \psi_b(y, t) \right] = \sum_{m,n} a_m b_n \Psi_{mn}(x, y, t)$$

one is led to probability densities which, as products

$$P(x, y, t) = P(x, t) \cdot Q(y, t)$$

of independently oscillating factors, trace “quantum mechanical Lassajous figures.” This train of thought has recently been pursued, to brilliant effect, by Y. F. Chen, K. F. Huang & Y. P. Lan<sup>2</sup> in work which in several respects has much in common with the MPF paper. It serves MPF’s purpose to look, however, to simpler superpositions of the buzzing eigenfunctions  $\Psi_{mn}(x, y, t)$ . Specifically, they look to

$$\begin{array}{ll} \text{CASE I:} & \cos \alpha \cdot \Psi_{21}(x, y, t) + e^{i\beta} \sin \alpha \cdot \Psi_{12}(x, y, t) \\ \text{CASE II:} & \cos \alpha \cdot \Psi_{31}(x, y, t) + e^{i\beta} \sin \alpha \cdot \Psi_{13}(x, y, t) \\ \text{CASE III:} & \cos \alpha \cdot \Psi_{31}(x, y, t) + e^{i\beta} \sin \alpha \cdot \Psi_{12}(x, y, t) \end{array}$$

<sup>1</sup> Animations based upon (7.4) are very easy to produce with the assistance of *Mathematica* 6, and—especially when superimposed upon animations of the associated current  $J_{mn}(x, t)$ —serve very effectively in the classroom to underscore the point that, in quantum theory, motion is an interference effect.

<sup>2</sup> “Localizatiuon of wave patterns on classical periodic orbits in a square billiard,” *Phys. Rev. E* **66**, 046215 (2002) and “Quantum manifestations of classical periodic orbits in a square billiard: formation of vortex lattices,” *Phys. Rev. E* **66**, 066210 (2002).

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**ILLUSTRATIVE CASE I** By use of *Mathematica* 6's `Manipulate` command one can easily achieve the freedom to range freely in parameter space. But MPF elect, for unexplained reasons, to (in effect) set  $\alpha = \arccos \frac{2}{3}$  and  $\beta = \arctan 2$ , giving

$$\begin{aligned} \cos \alpha &= \frac{2}{3} \\ e^{i\beta} \sin \alpha &= \frac{1+2i}{3} \end{aligned}$$

whence

$$\Psi(x, y, t) = \frac{2}{3}\Psi_{21}(x, y, t) + \frac{1+2i}{3}\Psi_{12}(x, y, t) \tag{10}$$

The resulting expressions for  $P(x, y, t)$ ,  $J_x(x, y, t)$ ,  $J_y(x, y, t)$ ,  $\mathbf{Arg}(x, y, t)$ ,  $V_x(x, y, t)$ ,  $V_y(x, y, t)$  and  $\Omega(x, y, t)$  are too complicated to merit rendering on the printed page, are best consigned to the mind/memory of *Mathematica* and displayed graphically. 3D display of  $P(x, y, 0)$ —my Figure 1—suggests, and calculation confirms, that

$$P\left(\frac{1}{2}, \frac{1}{2}, t\right) = 0 \quad : \quad \text{all } t$$

The probability current  $\mathbf{J}(x, y, 0)$  circulates around that point (my Figure 3), and so does the velocity field  $\mathbf{V}(x, y, 0)$  (my Figure 4).<sup>3</sup> The singularity at  $(\frac{1}{2}, \frac{1}{2})$  marks the end of a branch cut in displays of the phase of  $\Psi(x, y, 0)$  (my Figures 5 & 6). The vorticity is found (my Figure 7) to vanish *except* at the singularity:

$$\Omega(x, y, 0) = 2\pi \delta\left(x - \frac{1}{2}, y - \frac{1}{2}\right)$$

To expose the more clearly the source of the phenomena displayed in the figures, MPF suggest that we look to be behavior of  $\Psi$  in the immediate neighborhood of the singularity (*i.e.*, of the point where  $\Psi$  vanishes). *Mathematica*'s `Series` command supplies

$$\Psi\left(\frac{1}{2} + dx, \frac{1}{2} + dy, t\right) = -\frac{3}{8}e^{-i5\pi^2 t} \left[ dx + \left(\frac{1}{2} + i\right)dy \right] + \dots$$

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<sup>3</sup> To gain *Mathematica*'s graphic cooperation I adopted a modified definition of the velocity field:

$$\mathbf{V} = \frac{\mathbf{J}}{P} \quad \mapsto \quad \frac{\mathbf{J}}{P + 0.000001}$$

**ILLUSTRATIVE CASE II** MPF elect, for unexplained reasons, to (in effect) set  $\alpha = \frac{\pi}{4}$  and  $\beta = \frac{\pi}{2}$ , giving

$$\begin{aligned}\cos \alpha &= \frac{1}{\sqrt{2}} \\ e^{i\beta} \sin \alpha &= i \frac{1}{\sqrt{2}}\end{aligned}$$

whence

$$\Psi(x, y, t) = \frac{1}{\sqrt{2}}\Psi_{31}(x, y, t) + i \frac{1}{\sqrt{2}}\Psi_{13}(x, y, t) \quad (11)$$

Working from (11), we construct Figures 8 & 9, the form of which lead us to conjecture/verify that

$$\Psi\left(\frac{1}{3}, \frac{1}{3}, t\right) = \Psi\left(\frac{1}{3}, \frac{2}{3}, t\right) = \Psi\left(\frac{2}{3}, \frac{1}{3}, t\right) = \Psi\left(\frac{2}{3}, \frac{2}{3}, t\right) = 0 \quad : \quad \text{all } t$$

There are in this case four singularities, four symmetrically-placed vortices within the box. Expansion about the zeros of the wave function

$$\begin{aligned}\Psi\left(\frac{1}{3} + dx, \frac{1}{3} + dy, t\right) &= 3\sqrt{\frac{3}{2}}e^{-i10\pi^2 t}(-dx - i dy) + \dots \\ \Psi\left(\frac{1}{3} + dx, \frac{2}{3} + dy, t\right) &= 3\sqrt{\frac{3}{2}}e^{-i10\pi^2 t}(-dx + i dy) + \dots \\ \Psi\left(\frac{2}{3} + dx, \frac{1}{3} + dy, t\right) &= 3\sqrt{\frac{3}{2}}e^{-i10\pi^2 t}(+dx - i dy) + \dots \\ \Psi\left(\frac{2}{3} + dx, \frac{2}{3} + dy, t\right) &= 3\sqrt{\frac{3}{2}}e^{-i10\pi^2 t}(+dx + i dy) + \dots\end{aligned}$$

exposes primitive local approximations to the phase (see my Figure 11) that, when spliced together, account for the intricate structure shown in Figure 10.

**ILLUSTRATIVE CASE III** MPF assign to  $\alpha$  and  $\beta$  the same values as in the preceding case, so study

$$\Psi(x, y, t) = \frac{1}{\sqrt{2}}\Psi_{31}(x, y, t) + i \frac{1}{\sqrt{2}}\Psi_{12}(x, y, t) \quad (12)$$

From Figure 12 one is led to the observations that

$$\Psi\left(\frac{1}{3}, \frac{1}{2}, t\right) = \Psi\left(\frac{2}{3}, \frac{1}{2}, t\right) = 0 \quad : \quad \text{all } t$$

and

$$\begin{aligned}\Psi\left(\frac{1}{3} + dx, \frac{1}{2} + dy, t\right) &= 3\sqrt{2}e^{-i10\pi^2 t} \left( -dx - i \frac{e^{i5\pi^2 t}}{\sqrt{3}} dy \right) + \dots \\ \Psi\left(\frac{2}{3} + dx, \frac{1}{2} + dy, t\right) &= 3\sqrt{2}e^{-i10\pi^2 t} \left( +dx - i \frac{e^{i5\pi^2 t}}{\sqrt{3}} dy \right) + \dots\end{aligned}$$

We are, on these grounds, not surprised when graphic display of the  $\mathbf{J}$ -field reveals two symmetrically-placed counterrotating vortices—what MJF call a “vortex dipole.” Surprises do, however, emerge when one looks to *animated*

representations of  $P(x, y, t)$  and  $\mathbf{J}(x, y, t)$ , which MPF try not very successfully to do. Those figures oscillate, with period  $\tau = \frac{2}{5\pi}$ . One finds (Figure 13) that the  $\mathbf{J}$ -field abruptly reverses sign twice per period, and that at the moments of reversal ( $t = \frac{1}{4}\tau, \frac{3}{4}\tau$ ) it globally vanishes. This it does because the wave function becomes momentarily real

$$\begin{aligned}\Psi(x, y, \frac{1}{4}\tau) &= \sqrt{2}(-\sin[3\pi x]\sin[\pi y] + \sin[\pi x]\sin[2\pi y]) \\ \Psi(x, y, \frac{3}{4}\tau) &= \sqrt{2}(-\sin[3\pi x]\sin[\pi y] - \sin[\pi x]\sin[2\pi y])\end{aligned}$$

Which it does for the curious reason (Figure 14) that at those times its phase assumes the value  $+\pi$  on one sector of the square, the value  $-\pi$  on another sector, and vanishes on the remainder of the square. 3D representations of the phase are, at other times, surprisingly intricate (Figures 15 & 16).

**1. Summary.** Relatively little attention is paid to probability current, and still less to the *phase* of the wave function, in the standard introductory quantum texts. Nor is it often remarked how intricately related

$$\text{probability current} = (\hbar/m)(\text{probability density}) \cdot \nabla(\text{phase})$$

those two concepts are. Mahoney, Paganin & Faulkner have undertaken to remedy that omission, which is arguably a useful thing to do. And they have demonstrated that the two-dimensional box problem is rich enough to permit such issues to be explored in a relatively simple way, which is in itself a valuable observation. I find, however, that MPF pursue their objective in a way which manages in several different ways to blunt the force of what they have to say.

*i)* The introductory paragraph wanders very far from the authors' chosen topic, in support of a point ("There is something compelling about things that swirl and spin") that hardly needs reinforcement. It adds more than two thirds to the length of the bibliography, and most of those citations have no place in an already overlong paper of avowedly pedagogical intent. Curiously absent from this introductory grab bag is any reference to Descartes, or to Kelvin's vortex atoms. Or to Helmholtz, who initiated the serious study of vortices (1858). The introduction to Iwo Bialynicki-Birula, *et al*, "Motion of vortex lines in quantum mechanics," Phys. Rev. A, **61**, 032110 (2000) seems to me to provide an effective model of how MPF might better have set their discussion into motion.

*ii)* The equations most basic to the paper (my equations (2), (3) and (4)) are presented only at the end of the MPF paper, where they appear as equations (39) and (40), buried in the text of the Problems (§5). [In that regard: several of the papers I have recently been asked to referee have had problem sets attached. Perhaps it has become an editorial policy of AJP to encourage this innovation, but is my own opinion that, while I expect now and again to encounter points that "will be left as an exercise for the reader," enumerated problem sets seem to me to be almost invariably inappropriate.]

*iii)* Readers who attempt to reproduce or to extend the details presented in the paper will certainly make essential use of *Mathematica* or of some equivalent

resource. That being the case, references (§3.B) to how space and time variables are to be discretized are quite unnecessary, irrelevant, pointlessly distracting. As are indications (§3.A; Problems 4 and 5) of how the reader is to go about developing the first-order Taylor expansion of a function.

*iv)* So intensely computational must be any attempt to make detailed sense of the paper (which might most suitably be published in the computational counterpart of AJP, if such a thing existed) that it seems misleading not to note that fact, and a wasted opportunity not to draw upon it. Readers who consign the computational burden to *Mathematica* will find it very easy—and highly informative—to range around in parameter space, and to animate all the figures. They should be explicitly encouraged to do so. The graphic results of such an exercise are certain to be highly effective in the lecture hall.

*v)* The point of the Taylor expansions (a topic pursued in distracting detail in MPF’s equations (13) through (27)) was evidently to establish simple instances of the “polynomial vortex” concept introduced in connection with MPF’s equation (2). The authors do not attempt to elaborate upon this concept; the references which they cite are unlikely to be found in many/most undergraduate libraries, and the web provides no clear assistance in this regard. Introduction of the “polynomial vortex” can therefore be dismissed as an off-putting distraction, quite inessential to the main thrust of the paper.

*vi)* The density plots favored by the authors are, as I think I have quite convincingly demonstrated, invariably much less informative than the figures produced by *Mathematica*’s `Plot3D` command—particularly since the 3D figures produced by *Mathematica6* can be rotated, viewed from an angle.

*vii)* It is my opinion that MPF tend generally to get bogged down in elementary details, with the consequence that their writing too often lacks sharply incisive clarity.

**2.** Any respect in which the paper is not *technically* correct has escaped my notice.

**3.** It is my feeling that if the authors had kept their intended audience more clearly in mind they would have written in a more tightly focused way, stripped of all grand allusions (as in the introduction) and distracting generality: if the essential point is illustrated clearly the generalizations will be evident to all intended readers.

**4.** Though I take exception to some of the authors’ expository choices, their command of English grammar, *etc.* cannot be faulted.

**5.** The figures could easily—and (I have argued) should—be made much more vividly informative.

**6.** The references reflect the inappropriate and distracting extravagance of the introductory remarks, and a presumption that the reader has ready access to a well-equipped research library. Additional reference might usefully be made to papers by Bialynicki-Birula *et al*, of which one was cited previously, and

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to Chapter 13 (“Topics in quantum hydrodynamics: the stress tensor and vorticity”) in Robert E. Wyatt, *Quantum Dynamics with Trajectories: An Introduction to Quantum Hydrodynamics* (Springer, 2005).

7. My overall recommendation is **Revise and Resubmit**, where I understand “revise” to mean “shorten/sharpen/illustrate more effectively.”

8. I would expect the revised paper to be of substantial interest to instructors of Griffiths-level undergraduate quantum mechanics courses—especially those who (like me) make heavy in-class use of *Mathematica* or of comparable software. I have experimented, and found that *Mathematica* 6 makes quick/smooth work of all the calculations and animations in question.