

On Wave Function Representation of Particles as Shock Wave Discontinuities

Babur M. Mirza

Department of Mathematics, Quaid-i-Azam University, 45320 Islamabad. Pakistan
Email: bmmirza2002@yahoo.com

Abstract In quantum theory particles are represented as wave packets. Shock wave analysis of quantum equations of motion shows that wave function representation in general and wave packet description in particular contain discontinuities due to a non-zero quantum force corresponding to quantum potential. The quantum force causes wave packet dispersion which results in the intersection of characteristic curves developing a shock discontinuity. Since quantum force vanishes for localized quantum density waves [1], it is thus established that localized quantum density waves form the only class of continuous wave representation of particles in quantum theory.

1 Introduction

Wave-particle duality is a central aspect of quantum processes. It is well known that the Schrödinger equation describes such a duality in the form of wave packets solutions, particularly with the Gaussian wave packets [2-5]. Wave packet solutions of the Schrödinger equation possess the property that even in the absence of an external potential they exhibit dispersion. Such a dispersion occurs at very short time scales, and is responsible interference of electron waves.

In quantum potential formalism, wave packet dispersion results from the tendency of quantum trajectories to accelerate away from each other. Quantum trajectories for a free Gaussian wave packet, given by $x(t) = u_0 t + x_0 \sqrt{1 + (\hbar t / 2m\sigma_0^2)^2}$, indicate that components of the wave packet starting off at close by yet different initial positions and initial speeds intersect after a short time, exhibiting a shock formation. Intersection of characteristics lines is a typical aspect of nonlinear systems. However, in quantum dynamics of wave packets, quantum trajectories are assumed to be non-crossing. In the following exact analysis of quantum wave packet dynamics we drop this assumption, and the complete nonlinear system is analyzed using general theory of Riemann invariants. This leads to the interesting result that quantum wave packets develop shock wave discontinuities immediately after their formation.

Beginning with the next Section, we investigate the existence of shock wave phenomenon in quantum hydrodynamic formulation of the Schrödinger wave equation. It is shown that for a general wave function solution of the Schrödinger equation a non-zero quantum force causes characteristics to intersect, hence generates shock wave discontinuities in a quantized system. Such discontinuities have a travelling wave form, and correspond to particle motion in the free particle case. We take the example of a Gaussian wave packet to calculate the position and time of formation of quantum shocks in Section 3, whereas Section 4 gives a summary of the main conclusions of the work and its relation to some recent experiments on electron waves.

2 Shock Wave Analysis

In the quantum potential approach, the general form of the wave function can be written as $\psi(\mathbf{r}, t) = R(\mathbf{r}, t) \exp iS(\mathbf{r}, t)/\hbar$. Then the time-dependent Schrödinger equation, with an external potential: $i\hbar\partial\psi(\mathbf{r}, t)/\partial t = -(\hbar^2/2m)\nabla^2\psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t)$ gives, after separating real and imaginary parts, the following equations

$$\frac{\partial\rho(\mathbf{r}, t)}{\partial t} + \nabla \cdot (\rho(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)) = 0, \quad (1)$$

$$\frac{\partial\mathbf{v}(\mathbf{r}, t)}{\partial t} + (\mathbf{v}(\mathbf{r}, t) \cdot \nabla) \mathbf{v}(\mathbf{r}, t) = -\frac{1}{m} \nabla(V(\mathbf{r}) + mQ(\mathbf{r}, t)). \quad (2)$$

where $Q(\mathbf{r}, t) = -(\hbar^2/2m^2 R(\mathbf{r}, t))\nabla^2 R(\mathbf{r}, t)$, and $\rho(\mathbf{r}, t) = R(\mathbf{r}, t)^2$. Equations (1) and (2) are the basic equations of quantum dynamics [6] in a fixed Eulerian frame, with respect to which the relative velocity of an element is $\mathbf{v}(\mathbf{r}, t)$.

We write the equation (1) and (2) as a single matrix equation, and keep to the one dimensional case only. Then equations (1) and (2) give,

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \rho_t \\ u_t \end{bmatrix} + \begin{bmatrix} u & \rho \\ Q_\rho & u \end{bmatrix} \begin{bmatrix} \rho_x \\ u_x \end{bmatrix} = 0. \quad (3)$$

where u is the component of the velocity \mathbf{v} along the x -direction. Here $\rho_t = \partial\rho/\partial t$ and $Q_\rho = \partial Q/\partial\rho$, etc.

The eigenvalues and eigenvectors for system (3) can be calculated from the characteristic equation

$$\det \begin{bmatrix} u - \lambda & \rho \\ Q_\rho & u - \lambda \end{bmatrix} = 0, \quad (4)$$

which gives

$$(u - \lambda)^2 - \rho Q_\rho = 0. \quad (5)$$

Thus the two eigenvalues $\lambda_{1,2}$ are

$$\lambda_{1,2} = u \pm \sqrt{\rho Q_\rho}. \quad (6)$$

According to Riemann theory of shock waves [7], these eigenvalues give the characteristic speed for families of characteristics C_+ and C_- . Thus we have

$$C_+ : \lambda = \frac{dx}{dt} = u + \sqrt{\rho Q_\rho} = \lambda_1, \quad (7)$$

$$C_- : \lambda = \frac{dx}{dt} = u - \sqrt{\rho Q_\rho} = \lambda_2, \quad (8)$$

and the corresponding eigenvectors are given by

$$\begin{bmatrix} M_r^1 \\ M_r^2 \end{bmatrix} = \begin{bmatrix} \pm\sqrt{\rho/Q_\rho} \\ 1 \end{bmatrix}. \quad (9)$$

In general, equations for characteristic lines for the system can be written as

$$X_\pm(t, t_0) = x(t_0) + \left(\frac{dx}{dt} \right)_{t=t_0} (t + t_0), \quad (10)$$

where $(dx/dt)_{t=t_0} = \lambda_r(t = t_0)$. For shocks to develop, characteristics (10) must intersect at some common point in space. This occurs if the slope of each characteristic increases with the initial time t_0 . In view of equations (7) and (8) this is the case provided $Q_\rho \neq 0$, that is, if the quantum force $\partial Q/\partial x$ does not vanish. Another way to state shock condition is to expand function $X_\pm(t, t_0)$ for $\delta t_0 \ll 1$ in the neighborhood of each characteristics as

$$X_\pm(t, t_0 + \delta t_0) \approx X_\pm(t, t_0) + \frac{\partial X_\pm(t, t_0)}{\partial t_0} \delta t_0, \quad (11)$$

then any two neighboring characteristics $X_\pm(t, t_0)$ and $X_\pm(t, t_0 + \delta t_0)$ intersect provided

$$\frac{\partial X_\pm(t, t_0)}{\partial t_0} = 0. \quad (12)$$

This is the shock condition for the system (3), which we shall use in the following to calculate the time of shock formation.

Having obtained the necessary (and sufficient) shock conditions (12), we can now explicitly determine the (travelling) shock wave solutions for the system (3). This is done in the Appendix, using Riemann invariants. These calculations show that the shock waves develop if the quantum force is non-zero, thus the phenomenon is of purely quantum nature. Since for a free Gaussian wave packet the quantum force is non-zero in general, this implies the existence of quantum shocks in the case of free Gaussian wave packets.

3 Quantum Shocks for the Case of a Gaussian Wave Packet

Gaussian wave packet solution to the Schrödinger equation for a free particle is given by the wave function

$$\psi(x, t) = \frac{1}{(2\pi s)^{3/4}} \exp\left(ik(x - u_0 t/2) - (x - u_0 t)^2 / 4s\sigma_0\right), \quad (13)$$

where u_0 is the uniform constant speed of the wave packet, and the measure of the spread $|s| = \sigma = \sqrt{\sigma_0^2(1 + (\hbar t/2m\sigma_0^2)^2)}$. Correspondingly, the amplitude and the phase functions are given by

$$R(x, t) = \frac{1}{(2\pi\sigma^2)^{3/4}} \exp\left[-(x - u_0 t)^2 / 4\sigma^2\right], \quad (14)$$

$$S(x, t) = \frac{-3\hbar}{2} \tan^{-1}\left(\frac{\hbar}{2m\sigma_0^2} t\right) + mu(x - u_0 t/2) + (x - u_0 t)^2 \frac{\hbar^2}{8m\sigma_0^2\sigma^2} t, \quad (15)$$

and the quantum potential is,

$$Q(x, t) = \frac{\hbar^2}{4m^2\sigma^2} \left(3 - \frac{(x - u_0 t)^2}{2\sigma^2}\right). \quad (16)$$

Using $u = (\partial S/\partial x)/m$, we obtain from equation (16) the speed of a wave packet element

$$u = u_0 + \frac{\hbar^2 t}{4m^2\sigma_0^2\sigma^2} (x - u_0 t). \quad (17)$$

hence by integration, the position of a wave packet component is

$$x(t) = u_0 t + x_0 \sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2}. \quad (18)$$

Here x_0 and u_0 denote the initial position and velocity of the wave components, respectively.

Since by the above analysis the characteristics along which each wave packet component travels must intersect, we determine the location of the quantum shock in this case. Using equations (7) and (8), the equation of characteristic is given by

$$X_{\pm}(t, t_0) = x(t_0) + \left(u \pm \sqrt{\rho Q_{\rho}}\right)_{t=t_0} (t + t_0). \quad (19)$$

Then from the shock condition (12), we have

$$x'(t_0) + \frac{d\left(u \pm \sqrt{\rho Q_{\rho}}\right)_{t=t_0}}{dt_0} (t + t_0) - \left(u \pm \sqrt{\rho Q_{\rho}}\right)_{t=t_0} = 0. \quad (20)$$

Substituting for Q , u , and x from equations (16), (17) and (18) respectively, and then taking $t_0 = 0$ we have, after some simplification,

$$t_s = \frac{-8m^2\sigma_0^4}{\hbar^2 x_0} \left(u_0 \pm \sqrt{\frac{\hbar^2}{16\sigma_0^3}}\right), \quad (21)$$

and therefore, from equations (7) and (8),

$$x_s = \left(u_0 \pm \sqrt{\frac{\hbar^2}{4\sigma_0^3}}\right) t_s. \quad (22)$$

Equations (21) and (22) give the time and position for the quantum shock associated with the Gaussian wave packet (13).

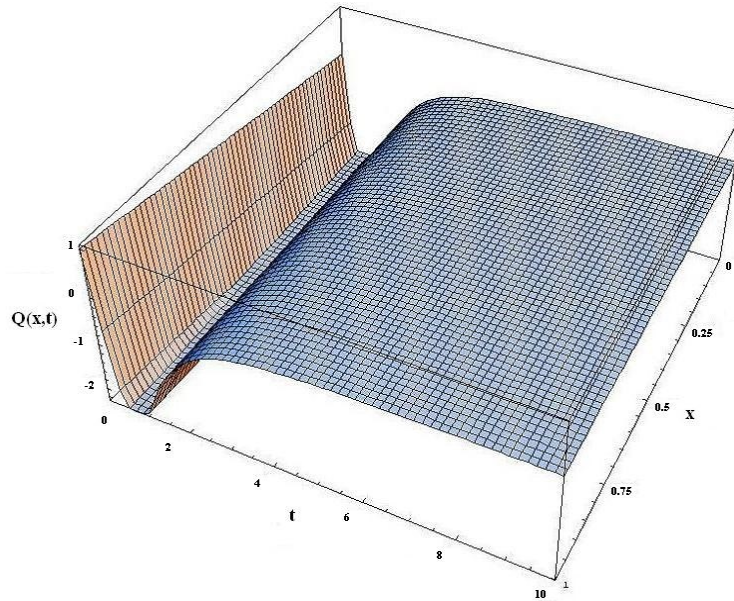


Figure 1. Quantum force for the Gaussian wave packet (13), with \hbar , m , σ_0 unity, and $u_0 = 10$ units.

4 Conclusions

The analysis presented in this paper shows that if in any region of space the quantum force tends to increase, a shock-like situation will develop. This must be so, since slope of the characteristics (19) then increases, causing characteristic curves to intersect. This was explicitly shown for the case of Gaussian wave packets, where the quantum force is equal to $\hbar^2(x - u_0t)/4m\sigma(t)^4$; which although decreasing first, then increases, and eventually attains a constant limit as $x \rightarrow \infty$ and $t \rightarrow \infty$ (Fig. 1). This indicates that the quantum force causes the wave packet to burst rather than spread smoothly.

If the relative velocity of the Gaussian wave packet and the lab frame coincides, quantum shock occurs at time $t_s = \sqrt{4m^2\sigma_0^{13}/\hbar^2x_0^2}$, and position $x_s = \sqrt{m^2\sigma_0^{10}/x_0^2}$, travelling with the speed x_s/t_s . Equation (22) shows that this speed differs from the classical formula by a constant $\hbar/(2\sigma_0^{3/2})$ due to wave packet dispersion.

A similar analysis can be applied to the case of Airy beams [8], and to the recently observed leviton structures [9], where limits on electron interferometry has been reduced to the attosecond scale [10,11]. For quantum density soliton waves, representing particle-like localization, such discontinuities do not form, since quantum force in this case is identically zero. This result also has implications for the problem of equivalence principle in quantum theory [12].

Acknowledgments. Thanks are due to Editor Prof. C. Corda of *Theoretical Physics* for article submission invitation.

References

1. B. M. Mirza, *Mod. Phys. Lett. B* **28** 1450253 (2014) .
2. N. Lee, et.al., *Science* **332**, 330 (2011).
3. V. Krueckl and T. Kramer, 2009 *New J. Phys.* **11**, 093010 (2009).
4. J. Billy, et al., *Nature* **453**, 891 (2008).
5. R. E. Wyatt , C. J. Trahan, *Quantum Dynamics with Trajectories* (Springer-Verlag, New York, 2005).
6. V. E. Madelung, *Z. Physik.* **40**, 322 (1926); L. de Broglie, *Electrons et Photons, Report au Ve Conseil Physique Solvay* (Gauthier-Villiers, Paris, 1930); D. Bohm, *Phys. Rev.* **85**, 166 (1952).

7. R. Courant and R. Friedrichs, *Supersonic Flows and Shock Waves* (Springer-Verlag, New York, 1985).
8. N. Voloch-Bloch, et.al., *Nature* **494**, 331 (2013).
9. J. Dubois, et al. *Nature* **502**, 659 (2013).
10. M. Holler, et.al., *Phys. Rev. Lett.* **106**, 123601 (2011).
11. T. Remetter, et.al., *Nature Physics* **2**, 323 (2006).
12. B. M. Mirza, in preparation.

APPENDIX: Riemann Invariants and the Shock Wave Solution

To obtain the Riemann invariants for the system (3), we take a linear combination of the equations (3) with coefficients being the components of the eigenvectors (9), this gives:

$$(\rho_t + u\rho_x + \rho u_x) \pm \sqrt{\rho/Q_\rho} (u_t + Q_\rho \rho_x + uu_x) = 0. \quad (\text{A1})$$

Since $(\partial\rho/\partial\eta) / (\pm\sqrt{\rho/Q_\rho}) = (\partial u/\partial\eta)$, it follows that

$$\frac{\partial u}{\partial\rho} = \pm\sqrt{\frac{Q_\rho}{\rho}}, \text{ and } \frac{\partial\rho}{\partial u} = \pm\sqrt{\frac{\rho}{Q_\rho}}. \quad (\text{A2})$$

Then substituting for $u_x = u_\rho \rho_x = \pm\sqrt{Q_\rho/\rho} \rho_x$, and $\rho_x = \rho_u u_x = \pm\sqrt{\rho/Q_\rho} u_x$, into equation (A1) we have

$$(\rho_t + (u \pm \sqrt{\rho Q_\rho}) \rho_x) \pm \sqrt{\rho/Q_\rho} (u_t + (u \pm \sqrt{\rho Q_\rho}) u_x) = 0, \quad (\text{A3})$$

and using equations (7) and (8):

$$d(u \pm F(\rho)) = 0, \text{ where } F(\rho) = \int \sqrt{Q_\rho/\rho} d\rho. \quad (\text{A4})$$

Integrating we have the two constants (Riemann invariants), A and B along the characteristics:

$$u + F(\rho) = A(\xi), \text{ along } \Gamma_1 \text{ with parameter } \xi = x + \lambda t, \quad (\text{A5})$$

$$u - F(\rho) = B(\eta), \text{ along } \Gamma_2 \text{ with parameter } \eta = x - \lambda t. \quad (\text{A6})$$

Thus eliminating u and $F(\rho)$, we have the solution for $u(x, t)$ and $\rho(x, t)$:

$$u(x, t) = A(x + \lambda t) + B(x - \lambda t), \quad (\text{A7})$$

$$F(\rho) = A(x + \lambda t) - B(x - \lambda t). \quad (\text{A8})$$

which can be easily verified as a (traveling) shock wave solution to the system (3). We notice in the above analysis that if the quantum force is zero, then the shock speeds λ_1 and λ_2 equal the speed u .