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Abstract. Starting from the time-independent Schrödinger equation for elastic scattering, a theory of wave–particle duality is developed which takes into account effects due to the quantum potential by means of a generalised ray equation. The duality between waves and particles is expressed in terms of two basic equations. Wave effects are described by a nonlinear amplitude equation which is coupled to a generalised ray equation that describes particle effects. The coupling between these two aspects of duality occurs by means of a function called the quantum expansion coefficient which describes the way in which a bundle of ray paths expand as the propagation distance increases.

For systems in which the phase of the one-body wavefunction is a separable function of its coordinates, we derive simplified forms for the ray equations. As an example we show how the theory may be used to calculate tunnelling ray paths in planar electron channelling. The reflected rays in this case originate from beyond the classical turning points, thereby demonstrating the existence of a Goos–Hänchen effect in electron channelling.

1. Introduction

Since the birth of wave mechanics in 1926 a considerable amount of effort has been invested in developing classical causal interpretations of Schrödinger's theory. The majority of these theories, apart from the statistical theories of Feynes (1952) and Nelson (1979), are based on the idea that the motion of the Schrödinger wave can be represented by a multitude of trajectories or rays.

Much of the motivation for these theories comes from the inability of Schrödinger's theory to explain wave–particle duality satisfactorily.

The duality problem manifests itself in several practical situations—most notably in the areas of particle channelling in crystals (Chadderton 1966) and the propagation of light in optical fibres.

In the case of particle channelling, where classical mechanics has proved to be very useful in describing the conditions necessary for channelling to exist (Chadderton 1970), there are problems related to the region of validity of classical mechanics and to how these conditions may be interpreted in terms of the standard wave theories of crystal diffraction (Cowley and Moodie 1957). More importantly, classical mechanics is incapable of describing tunnelling effects and other quantum phenomena which at present must be described by wave mechanics.

In the case of optical fibre propagation† we have a similar situation in the sense that all the current ray treatments of fibre propagation are based on geometric optics

† We are treating scalar optics on the same basis as time-independent wave mechanics because both situations are described by Helmholtz-type wave equations.

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(Mikaelian 1980) and are therefore incapable of predicting situations where tunnelling through the wall of the fibre becomes important (leaky modes and evanescent boundary wave propagation). Also, as geometric optics ignores wave effects completely, any refractive index profile (e.g. Mikaelian 1980) calculated to provide self-focusing of the propagating beam may be expected to lose its validity as the wavelength becomes increasingly finite—due to diffraction effects.

For these very practical reasons we have been motivated into developing a ray theory of wave propagation which reduces to geometric optics or classical mechanics in the limit of vanishing wavelength, and which for finite wavelengths reproduces all the results of scalar wave theory and wave mechanics. Most important of all, the theory is capable of describing tunnelling effects within a ray framework.

From a practical point of view all the existing ray theories of wave mechanics and optics are not very useful when it comes to trying to describe tunnelling effects. WKB theory (Dunham 1932) and Keller's geometric theory of diffraction (Keller 1978), for example, break down at caustics and the classical turning points. The main difficulty with the theories of Bohm (1952a, b), de Broglie (1930) and Takabayasi (1952, 1953) seems to be that they are unnecessarily over-restrictive in the way they link particle concepts such as momentum to wave concepts such as phase. In Bohm's and de Broglie's theories, for example, the gradient of the phase of the wavefunction is assumed to be equal to the particle momentum, in analogy with classical Hamilton–Jacobi theory.

In the theory developed in this paper, it is considered only that the ray paths are locally gauge invariant with respect to the original wave equation. By employing this principle of local gauge invariance of the ray path we obtain an alternative formulation of quantum mechanics in which wave–particle duality is given an explicit representation in terms of a generalised ray equation coupled to a nonlinear wave equation. The link between these two aspects of duality is provided by a function which we call the quantum expansion coefficient—in analogy with geometric optics where a function of similar form occurs (Kline and Kay 1965). The quantum expansion coefficient describes the way in which a bundle of ray paths expand, that is diffract.

We shall now discuss the development of this new theory.

2. Development of the theory

We start from the time-independent scalar wave equation

$$\nabla^2\psi + k^2(\boldsymbol{r})\psi = 0 \tag{1}$$

where in the case of quantum mechanics

$$k^2(\boldsymbol{r}) = (2m/\hbar^2)[E - V(\boldsymbol{r})] \tag{2}$$

where $V(\boldsymbol{r})$ is a real one-body potential.

In the scalar optics case $k^2 = k_0^2 n^2$ where $n(\boldsymbol{r})$ is a real refractive index distribution and k_0 is the vacuum wavenumber. We now develop the theory for the case of quantum mechanics. Very few changes are necessary for the scalar optics case which is discussed in another paper (Lee 1982).

We now introduce the well known ansatz $\psi = A\exp(\mathrm{i}S/\hbar)$ where for $k^2 > 0$ $A(\boldsymbol{r})$ and $S(\boldsymbol{r})$ are real functions. The Schrödinger equation is then represented by the well

known equations

$$\nabla^2 S + 2\frac{\nabla A}{A}\cdot\nabla S = 0, \tag{3}$$

$$|\nabla S|^2 = 2m(E-V) + \hbar^2\frac{\nabla^2 A}{A} \equiv Q^2. \tag{4}$$

Bohm's, de Broglie's and Takabayasi's theories are based on the time-dependent form of these amplitude–phase relations.

We now introduce a ray representation according to the prescription

$$\nabla S = g(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}/\mathrm{d}\sigma \tag{5}$$

where $g(\boldsymbol{r})$ is an arbitrary gauge function and $\mathrm{d}\sigma$ is an element of arc length in a conformal metric.

We now define a point on a ray path in Cartesian coordinates by $\underline{r}(z)$ where z is the propagation coordinate and $\underline{r} = \hat{\imath}x + \hat{\jmath}y$. The gradient of the ray at $\underline{r}(z)$ is denoted by $\dot{\underline{r}}(z)$ where the dot denotes the total derivative with respect to z.

From (4) and (5) we therefore have

$$\frac{\mathrm{d}z}{\mathrm{d}\sigma} = \frac{Q}{g}\frac{1}{(1+\dot{\underline{r}}^2)^{1/2}}, \tag{6}$$

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\sigma} = \frac{Q}{g}\frac{\dot{\boldsymbol{r}}}{(1+\dot{\underline{r}}^2)^{1/2}} \equiv \frac{Q}{g}\hat{\boldsymbol{r}}, \tag{7}$$

$$\frac{\mathrm{d}g}{\mathrm{d}\sigma} = \frac{Q}{g}\frac{\dot{g}}{(1+\dot{\underline{r}}^2)^{1/2}}, \tag{8}$$

$$\frac{\mathrm{d}A}{\mathrm{d}\sigma} = \frac{Q}{g}\frac{\dot{A}}{(1+\dot{\underline{r}}^2)^{1/2}}. \tag{9}$$

Using equations (4)–(6) we obtain from (3) the result

$$\mathrm{d}/[\ln(A^2Q)]/\mathrm{d}z = -\nabla\cdot[\dot{\boldsymbol{r}}/(1+\dot{\underline{r}}^2)^{1/2}](1+\dot{\underline{r}}^2)^{1/2}. \tag{10}$$

Note that this result is independent of the gauge function $g(\boldsymbol{r})$.

Finally, integrating (10) using the definition of Q, we obtain the nonlinear wave equation

$$\nabla^2 A + k^2 A - \alpha^2\kappa^2 A^{-3} = 0 \tag{11}$$

where α is an integration constant and κ is given by

$$\kappa = \exp\left[-\int_{z_0}^{z}\nabla\cdot\left(\frac{\dot{\boldsymbol{r}}}{(1+\dot{\underline{r}}^2)^{1/2}}\right)(1+\dot{\underline{r}}^2)^{1/2}\,\mathrm{d}z\right]. \tag{12}$$

We call κ the quantum expansion coefficient since it describes the way in which a bundle of rays expand as a function of $\boldsymbol{r}$.

The ray equation is calculated from the extremisation of the action integral

$$L = \frac{\mathrm{d}S}{\mathrm{d}z} = \dot{\boldsymbol{r}}\cdot\nabla S = Q(1+\dot{\underline{r}}^2)^{1/2}, \qquad L = \frac{\hbar\alpha\kappa}{A^2}(1+\dot{\underline{r}}^2)^{1/2}, \tag{13}$$

$$S = \alpha\hbar\int_{z_0}^{z}\frac{\kappa}{A^2}(1+\dot{\underline{r}}^2)^{1/2}\,\mathrm{d}z'. \tag{14}$$

Hence, for $\kappa = \kappa(r)$ the quantum ray equation is given by

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{\kappa}{A^2}\hat{\dot{r}}\right) = [(\dot{r})^2]^{1/2}\nabla\left(\frac{\kappa}{A^2}\right). \tag{15}$$

An expression for the gradient of the phase of the wavefunction follows from equations (5), (7) and (11):

$$\nabla S = \hbar\alpha(\kappa/A^2)\hat{r}. \tag{16}$$

The time-independent quantum Hamilton–Jacobi equation is therefore given by

$$|\nabla S|^2 = \hbar^2\alpha^2\kappa^2/A^4. \tag{17}$$

From (12) and (16) we see that we can write the expansion coefficient in the form

$$\kappa = \exp\left[-\int \nabla\cdot\left(\frac{\nabla S}{|\nabla S|}\right)[(\dot{r})^2]^{1/2}\,\mathrm{d}z\right]. \tag{18}$$

Equations (11), (14), (15), (16), (17) and (18) form the basic set of equations for our time-independent theory of wave–particle duality.

It is important to emphasise here that this basic set of equations is independent of the gauge function $g(r)$. If we were to try and repeat this procedure starting from the time-dependent Schrödinger equation, we would find that the ray equations were *not* independent of the gauge function—even if we introduce a gauge function for the time coordinate as well. The earlier hidden variable theories of quantum mechanics based on the time-dependent Schrödinger equation (e.g. Bohm, de Broglie, Takabayasi, etc) are over-restrictive in the sense that they correspond to a particular choice of gauge function.

In order to obtain a gauge invariant time-dependent theory of wave–particle duality, it is necessary to start from a wave equation which is symmetric in the order of the space and time derivatives. In a later paper, we hope to develop such a theory starting from the Klein–Gordon equation and show how it leads to a system of mechanics based on local masses.

We now consider the classical limit of our time-independent theory.

3. The classical limit

One of the most interesting properties of equation (11) is the way it mirrors the approach to the classical limit. Consider the Lagrangian density corresponding to this equation:

$$L = \tfrac{1}{2}[(\nabla A)^2 - \alpha^2\kappa^2\phi(A)], \tag{19}$$

$$\phi(A) = p^2A^2 + A^{-2}, \tag{20}$$

where $p = k/\alpha\kappa$. The minimum points of the potential wells occur at

$$A_0 = \pm(\alpha\kappa\hbar)^{1/2}/[2m(E-V)]^{1/4}. \tag{21}$$

Substituting this value of 'A' into the generalised ray equation (15) gives

$$\frac{\mathrm{d}}{\mathrm{d}z}\{[2m(E-V)]^{1/2}\hat{\boldsymbol{r}}\}=[(\dot{\boldsymbol{r}})^2]^{1/2}\nabla[2m(E-V)]^{1/2} \tag{22}$$

which is just the well known classical ray equation for elastic propagation.

Hence, the classical limit corresponds to the minimum points of the Lagrangian density potential function of the nonlinear amplitude equation.

The semiclassical wavefunction corresponding to the classical ray equation (22) follows from equations (21) and (14):

$$\psi_{\mathrm{c}}=\pm\frac{(\alpha\kappa\hbar)^{1/2}}{[2m(E-V)]^{1/4}}\exp\left(\frac{\mathrm{i}}{\hbar}\int_{\tau_0}^{\tau}[2m(E-V)]^{1/2}\,\mathrm{d}\tau\right) \tag{23}$$

where $\mathrm{d}\tau=(1+\dot{\boldsymbol{r}}^2)^{1/2}\,\mathrm{d}z$ is an element of Cartesian arc length.

Apart from the constant α, which can be removed by renormalising the wavefunction, equation (23) is just the first-order multidimensional WKB wavefunction as given by Ranfagni (1977). Multidimensional WKB wavefunctions have been shown to be particularly useful in constructing semiclassical treatments of elastic and inelastic atomic collision processes (Bates and Holt 1966, Chen and Watson 1968, Bates and Crothers 1970). The semiclassical theory of Bates and colleagues is particularly useful for calculating excitation cross sections with greater accuracy than standard impact parameter methods. It might be expected that the accuracy of these semiclassical theories could be further improved, particularly for low-velocity scattering, if the usual classical atomic trajectories were replaced by quantum trajectories. We hope to investigate this in detail in a later paper.

4. Straight rays

Straight ray solutions of the quantum ray equations (15) and (16) may be obtained in cases where the amplitude and phase functions, A and S, are functions of a single variable, γ.

If $S=S(\gamma)$, then we have, applying Jeffery's method (Jeffery 1981) to the present problem,

$$\nabla S=\nabla\gamma\,\mathrm{d}S/\mathrm{d}\gamma, \tag{24}$$

$$\nabla\cdot\left(\frac{\nabla S}{|\nabla S|}\right)=\frac{\nabla^2\gamma}{|\nabla\gamma|}-\frac{\nabla\gamma}{|\nabla\gamma|^2}\cdot\nabla|\nabla\gamma|. \tag{25}$$

Now $\mathrm{d}\gamma=\nabla\gamma\,\mathrm{d}\boldsymbol{r}=\nabla\gamma\dot{\boldsymbol{r}}\,\mathrm{d}z=|\nabla\gamma|\,|\dot{\boldsymbol{r}}|\cos\theta\,\mathrm{d}z$. For $S=S(\gamma)$, $\nabla\gamma$ is in the same direction as $\dot{\boldsymbol{r}}$ since $Q\dot{\boldsymbol{r}}(1+\dot{\boldsymbol{r}}^2)^{1/2}=(\mathrm{d}S/\mathrm{d}\gamma)\nabla\gamma$. Therefore $\theta=0$ and $|\dot{\boldsymbol{r}}|\,\mathrm{d}z=\mathrm{d}\tau=\mathrm{d}\gamma/|\nabla\gamma|$.

$$\therefore\qquad \kappa(\gamma,\gamma_0)=\exp\left[-\int_{\gamma_0}^{\gamma}\left(\frac{\nabla^2\gamma'}{|\nabla\gamma'|^2}-\frac{\mathrm{d}}{\mathrm{d}\gamma'}\ln|\nabla\gamma'|\right)\mathrm{d}\gamma'\right],$$

$$\therefore\qquad \kappa(\gamma,\gamma_0)=\frac{|\nabla\gamma|}{|\nabla\gamma_0|}\exp\left(-\int_{\gamma_0}^{\gamma}\frac{\nabla^2\gamma'}{|\nabla\gamma'|^2}\,\mathrm{d}\gamma'\right). \tag{26}$$

For $A = A(\gamma)$ the amplitude equation (11) takes the form

$$\frac{d^2A}{d\gamma^2} + \frac{\nabla^2\gamma}{|\nabla\gamma|^2}\frac{dA}{d\gamma} + \frac{k^2(\gamma)}{|\nabla\gamma|^2}A - \alpha^2\frac{\kappa^2(\gamma, \gamma_0)}{|\nabla\gamma|^2}A^{-3} = 0. \tag{27}$$

Hence for 'A' to be a function only of the single variable γ we must have

$$\nabla^2\gamma = f(\gamma), \tag{28}$$

$$|\nabla\gamma|^2 = g(\gamma), \tag{29}$$

where $f(\gamma)$ and $g(\gamma)$ are yet to be determined.

Equations (28) and (29) have been studied by Collins (1976) who has shown that without loss of generality $g(\gamma)$ may be put equal to a constant and that the only real variable solutions in three dimensions are of the following forms.

(i) $f(\gamma) = 0$ and $\gamma = lx + my + nz + B$ where $l^2 + m^2 + n^2 = L^2$ and B is a constant.

(ii) $f(\gamma) = 1/\gamma$ and $\gamma = [(x - x_1)^2 + (y - y_1)^2]^{1/2}$ with rotations and translations between x, y and z. x_1 and y_1 are constants.

(iii) $f(\gamma) = 2/\gamma$ and $\gamma = [(x - x_1)^2 + (y - y_1)^2 + (z - z_1)^2]^{1/2}$ where x_1, y_1 and z_1 are constants.

In the context of our theory these solutions correspond to plane, cylindrical and spherical wavefronts respectively. The corresponding quantum expansion coefficients, amplitude equations and phase functions are given by the following.

(i) Plane wavefronts ($\kappa(\gamma, \gamma_0) = 1$):

$$L^2\, d^2A/d\gamma^2 + k^2(\gamma)A - \alpha^2A^{-3} = 0, \tag{30}$$

$$S(\gamma) = S_0 + \frac{\hbar\alpha}{L}\int_{\gamma_0}^{\gamma}\frac{d\gamma'}{A^2(\gamma')}. \tag{31}$$

(ii) Cylindrical wavefronts ($\kappa(\gamma, \gamma_0) = \gamma_0/\gamma$):

$$\frac{d^2A}{d\gamma^2} + \frac{1}{\gamma}\frac{dA}{d\gamma} + k^2(\gamma)A - \alpha^2\left(\frac{\gamma_0}{\gamma}\right)^2A^{-3} = 0, \tag{32}$$

$$S(\gamma) = S_0 + \alpha\gamma_0\hbar\int_{\gamma_0}^{\gamma}\frac{d\gamma'}{\gamma' A^2(\gamma')}. \tag{33}$$

(iii) Spherical wavefronts ($\kappa(\gamma, \gamma_0) = (\gamma_0/\gamma)^2$):

$$\frac{d^2A}{d\gamma^2} + \frac{2}{\gamma}\frac{dA}{d\gamma} + k^2(\gamma)A - \alpha^2\left(\frac{\gamma_0}{\gamma}\right)^4A^{-3} = 0, \tag{34}$$

$$S(\gamma) = S_0 + \alpha\gamma_0^2\hbar\int_{\gamma_0}^{\gamma}\frac{d\gamma'}{\gamma'^2A^2(\gamma')}. \tag{35}$$

The ray paths corresponding to these solutions may be calculated from (16). From (16) we have

$$\frac{dx}{dz} = \frac{\partial S}{\partial x}\Big/\frac{\partial S}{\partial z}, \tag{36}$$

$$\frac{dy}{dz} = \frac{\partial S}{\partial y}\Big/\frac{\partial S}{\partial z}, \tag{37}$$

$$\frac{dx}{dy} = \frac{\partial S}{\partial x} \Big/ \frac{\partial S}{\partial y}. \tag{38}$$

It is a simple matter to verify that these expressions satisfy the ray equation (15) exactly.

From equations (36), (37) and (38) we obtain the following expressions for the ray paths.

(i) Plane wavefront rays:

$$\frac{dx}{dz} = \frac{l}{n}, \qquad \frac{dy}{dz} = \frac{m}{n}, \qquad \frac{dx}{dy} = \frac{l}{m}. \tag{39}$$

(ii) Cylindrical wavefront rays:

$$dx/dy = (x - x_1)/(y - y_1). \tag{40}$$

(iii) Spherical wavefront rays:

$$\frac{dx}{dz} = \frac{x - x_1}{z - z_1}, \qquad \frac{dy}{dz} = \frac{y - y_1}{z - z_1}, \qquad \frac{dx}{dy} = \frac{x - x_1}{y - y_1}. \tag{41}$$

Hence in all cases the ray paths are straight lines perpendicular to the surfaces of constant phase which are planes, cylinders and spheres respectively—corresponding to planar, cylindrical and spherical equipotential surfaces.

5. Rays corresponding to plane curves

The next class of solutions we consider are those solutions corresponding to ray paths which are plane curves and correspond to phase functions which are separable functions of the propagation and transverse coordinates.

Expressions for the ray paths are obtained by substituting into the general expression for the expansion coefficient separable forms for the phase function in terms of unknown functions and then solving for the unknown functions self-consistently.

For example, consider the case where the equipotential surfaces are planar and are of the form $V = V(\gamma)$ where $\gamma = l_1 x + l_2 y = \underline{l} \cdot \underline{r}$. We wish to find the ray paths corresponding to the case

$$A = A(\gamma), \qquad S/\hbar = l_3 z + f(\gamma), \tag{42}$$

where l_3 is the longitudinal wavevector and $f(\gamma)$ is an unknown function.

$$\nabla \cdot (\nabla S/|\nabla S|) = l_3^2 \underline{l}^2 f''/[l_3^2 + (\underline{l}f')^2]^{3/2} \tag{43}$$

where the primes correspond to derivatives with respect to γ.

From (16) we have

$$\frac{dx}{dz} = \frac{l_1}{l_3} f', \qquad \frac{dy}{dz} = \frac{l_2}{l_3} f'. \tag{44}$$

The element of Cartesian arc length is therefore given by

$$d\tau = \frac{[l_3^2 + (\underline{l}f')^2]^{1/2}}{\underline{l}^2 f'} d\gamma. \tag{45}$$

Substituting (43) and (45) into the general expression (18) for the expansion coefficient and performing the integration by a change of variable, we obtain

$$\kappa = \Lambda_0[l_3^2/\underline{l}^2 + (f')^2]^{1/2}/f' \tag{46}$$

where the constant Λ_0 is given by

$$\Lambda_0 = f_0'/[l_3^2/\underline{l}^2 + (f_0')^2]^{1/2}. \tag{47}$$

f_0 and f_0' are the value of the function and its first derivative at the initial ray point x_0, y_0.

The unknown function $f(\gamma)$ is now determined from equations (17), (42) and (46). The result is

$$\frac{df}{d\gamma} = \frac{\alpha}{|\underline{l}|}\Lambda_0 \frac{1}{A^2}. \tag{48}$$

From (47) and (48) we therefore have

$$df/d\gamma|_0 = \pm[(\alpha^2/\underline{l}^2)A^{-4}(\gamma_0) - l_3^2/\underline{l}^2]^{1/2}. \tag{49}$$

The expansion coefficient, phase function and amplitude equation now take the forms

$$\kappa = [\Lambda_0^2 + (l_3^2/\alpha^2)A^4]^{1/2}, \tag{50}$$

$$\frac{S(\gamma, z)}{\hbar} = l_3 z + \frac{\alpha}{|\underline{l}|}\Lambda_0 \int_{\gamma_0}^{\gamma} \frac{d\gamma'}{A^2(\gamma')}, \tag{51}$$

$$d^2A/d\gamma^2 + U(\gamma)A - \beta^2 A^{-3} = 0, \tag{52}$$

where

$$U(\gamma) = (k^2(\gamma) - l_3^2)/\underline{l}^2, \qquad \beta^2 = (\alpha^2/\underline{l}^2)\Lambda_0^2, \qquad \Lambda_0 = \pm(1 - l_3^2 A_0^4/\alpha^2)^{1/2}.$$

Finally, the equation for the ray paths follows from equations (44) and (48):

$$Z = Z_0 + \frac{l_3}{\alpha|\underline{l}|\Lambda_0}\int_{\gamma_0}^{\gamma} A^2(\gamma')\,d\gamma'. \tag{53}$$

Hence, the ray paths are curves in the z, γ plane.

Equations (50), (51), (52) and (53) are an appropriate set of equations for studying planar elastic channelling in crystals. In a later section we shall show how these equations may be used to calculate tunnelling ray paths in parabolic channelling.

For cylindrical equipotential surfaces we may calculate a corresponding set of planar ray path functions. The procedure followed is similar to the previous case except that in this case γ is replaced by ρ where $\rho = (x^2 + y^2)^{1/2}$. The expansion coefficient, phase function and amplitude equation are easily calculated and are given by

$$\kappa(\rho, \rho_0) = [\Gamma_0^2/\rho^2 + (l_3^2/\alpha^2)A^4]^{1/2}, \tag{54}$$

$$\frac{S(\rho, z)}{\hbar} = l_3 z + \alpha\Gamma_0 \int_{\rho_0}^{\rho} \frac{d\rho'}{\rho' A^2(\rho')}, \tag{55}$$

$$\frac{d^2A}{d\rho^2} + \frac{1}{\rho}\frac{dA}{d\rho} + U(\rho)A - \frac{\varepsilon^2}{\rho^2}A^{-3} = 0, \tag{56}$$

where Γ_0, ε and $U(\rho)$ are respectively given by

$$\Gamma_0 = \pm\rho_0[1-(l_3^2/\alpha^2)A^4(\rho_0)]^{1/2}, \tag{57}$$

$$\varepsilon = \alpha\Gamma_0, \tag{58}$$

$$U(\rho) = k^2(\rho) - l_3^2. \tag{59}$$

The corresponding ray path function is given by

$$Z = Z_0 + \frac{l_3}{\alpha\Gamma_0}\int_{\rho_0}^{\rho} \rho' A^2(\rho')\,\mathrm{d}\rho'. \tag{60}$$

The above set of equations form an appropriate set for the study of meridional rays propagating through systems with cylindrical equipotential surfaces.

The final example of a system with planar ray paths is provided by the case of central potential scattering. In this case we have $A_l(r,\theta) = M_l(\mu)N_l(\nu)$ where $\mu = r(2mE)^{1/2}/\hbar$, $\nu = \cos\theta$ and $M_l(\mu)$ and $N_l(\nu)$ satisfy the following radial and angular amplitude equations:

$$\begin{aligned} &\frac{\mathrm{d}^2M_l}{\mathrm{d}\mu^2} + \frac{2}{\mu}\frac{\mathrm{d}M_l}{\mathrm{d}\mu}\left(1 - V(\mu) - \frac{l(l+1)}{\mu^2}\right)M_l - \frac{1}{\mu^4}M_l^{-3} = 0, \\ &(1-\nu^2)\frac{\mathrm{d}^2N_l}{\mathrm{d}\nu^2} - 2\nu\frac{\mathrm{d}N_l}{\mathrm{d}\nu} + l(l+1)N_l - \frac{1}{1-\nu^2}N_l^{-3} = 0, \end{aligned} \tag{61}$$

where l is the angular momentum quantum number and $V(\mu)$ is a real one-body potential in dimensionless units.

It is easily verified that $M_l = (R_l^2 + T_l^2)^{1/2}$ where R_l and T_l are the two linearly independent solutions of the radial Schrödinger equation, while $N_l = (P_l^2 + Q_l^2)^{1/2}$ where P_l and Q_l are the linearly independent solutions of Legendre's equation.

Now, since R_l, T_l and P_l, Q_l satisfy the Wronskian relations

$$R_l\,\mathrm{d}T_l/\mathrm{d}\mu - T_l\,\mathrm{d}R_l/\mathrm{d}\mu = 1/\mu^2, \qquad P_l\,\mathrm{d}Q_l/\mathrm{d}\nu - Q_l\,\mathrm{d}P_l/\mathrm{d}\nu = 1/(1-\nu^2), \tag{62}$$

it is easily shown that $R_l + \mathrm{i}T_l = M_l\exp(\mathrm{i}m_l)$ and $P_l + \mathrm{i}Q_l = N_l\exp(\mathrm{i}n_l)$ where the radial and angular phase functions are given by

$$m_l(\mu) = \int_{\mu_0}^{\mu} \mathrm{d}\mu/[\mu^2 M_l^2(\mu)], \qquad n_l(\nu) = \int_{\nu_0}^{\nu} \mathrm{d}\nu/[(1-\nu^2)N_l^2(\nu)], \tag{63}$$

where μ_0, ν_0 defines an initial point. The total phase function corresponding to a scattering state of angular momentum l is therefore given by $S_l(r,\theta) = m_l(\mu) + n_l(\nu)$.

We now substitute this expression for the total phase function and the corresponding expression for the total amplitude function $A_l(r,\theta) = M_l(\mu)N_l(\nu)$ into the polar coordinate form of the ray path relation (16). We then obtain two equations which when substituted into each other to eliminate the expansion coefficient and integrated result in the following ray path relation:

$$\int_{\mu_0}^{\mu} M_l^2(\mu)\,\mathrm{d}\mu = \int_{\nu_0}^{\nu} N_l^2(\nu)\,\mathrm{d}\nu. \tag{64}$$

Equation (64) is the desired quantum ray relation for central potential scattering. The self-consistency of this result can be checked by substituting equation (11) into the mod square of equation (16) to obtain $\nabla^2 A + (k^2(r) - \hbar^{-2}|\nabla S|^2)A = 0$. It is then easy

to show that the amplitude function $A_l = M_l N_l$ and the phase function $S_l = m_l + n_l$ satisfies this equation exactly.

To conclude this section, we note that it is a simple matter to check that in each of the above three examples of planar ray paths the corresponding classical limit ray paths are given by the minimum point in the Lagrangian density potential function of the appropriate amplitude equations.

We shall now give a simple application of the theory in the area of particle channelling in crystals.

6. Tunnelling rays in parabolic channelling

Consider the case of an electron channelling in a planar harmonic oscillator potential of the form

$$V(x) = U_1 x^2 - B \tag{65}$$

where U_1 and B are constants. This type of potential has been suggested by Pantell and Swent (1979) as an appropriate potential for the study of thermal effects in the planar channelling of 56 MeV electrons in the ⟨110⟩ direction in silicon. The quantum ray paths, wavefunctions and eigenvalues are calculated as follows.

Firstly, the nonlinear amplitude equation for the planar potential case (equation (52) with $l_2 = 0$) is transformed into dimensionless form by a simple change of variable. The resulting equation is given by

$$\mathrm{d}^2F/\mathrm{d}\xi^2 - (a + \tfrac{1}{4}\xi^2)F - (2/\pi)F^{-3} = 0 \tag{66}$$

where 'a', F and ξ are given by

$$a = -(m/2U_1\hbar^2)^{1/2}(E_\perp + B), \qquad A = \{\pi\alpha^2\hbar/[4\Lambda_0^2(2mU_1)^{1/2}]\}^{1/4}F \equiv C_0F,$$
$$\xi = (8mU_1/\hbar^2)^{1/4}x,$$

where $E_\perp$ is the transverse energy of the channelling particle.

The linear base equation—that is the amplitude equation without the F^{-3} term—is now of a standard form, the solutions being given by parabolic cylinder functions. In order to solve nonlinear equations of this form it is necessary to find two independent solutions of the linear base equation (Milne 1930, Pinney 1950).

The solution of the nonlinear equation is now given by

$$F(a, \xi) = [U^2(a, \xi) + V^2(a, \xi)]^{1/2} \tag{67}$$

where $U(a, \xi)$ and $V(a, \xi)$ are the parabolic cylinder functions (Abramowitz and Stegun 1965).

The calculation of the phase function and the standard wavefunction is now quite straightforward. The phase function is given by

$$S/\hbar = \zeta \pm (2/\pi)^{1/2} \int_{\xi_0}^{\xi} [U^2(a, \xi) + V^2(a, \xi)]^{-1}\, \mathrm{d}\xi \tag{68}$$

where $\zeta = l_3 Z$. The standard wavefunction is therefore given by

$$\psi_\pm(a, \xi, \zeta) = C_0\, \mathrm{e}^{\mathrm{i}\zeta}(U^2 + V^2)^{1/2} \exp\left(\pm \mathrm{i}(2/\pi)^{1/2} \int_{\xi_0}^{\xi} \frac{\mathrm{d}\xi}{U^2 + V^2}\right). \tag{69}$$

Now, since the parabolic cylinder functions obey the Wronskian relation

$$W\{U, V\} = (2/\pi)^{1/2}, \tag{70}$$

we can perform the integration and write the wavefunction in the form

$$\psi_{\pm}(a, \xi, \zeta) = C_0 \exp[\mathrm{i}(s_0 + \zeta)][U(a, \xi) \pm \mathrm{i}V(a, \xi)] \tag{71}$$

where $s_0 = \tan^{-1}[V(a, \xi_0)/U(a, \xi_0)]$.

Now, since the original Schrödinger equation is a linear equation, the determination of the physical eigenfunctions (that is, the wavefunctions which incorporate the boundary conditions) is just given by linear combinations of the standard wavefunctions.

In this particular case, we require a wavefunction which asymptotes to zero at $x = \pm\infty$. Therefore, the physical eigenfunctions are given by $U(a, \xi)$ since $V(a, \xi)$ diverges as $x \to \pm\infty$.

$$\Psi(a, \xi, \zeta) = \psi_+(a, \xi, \zeta) + \psi_-(a, \xi, \zeta) = 2C_0 \exp[\mathrm{i}(s_0 + \zeta)]U(a, \xi). \tag{72}$$

Now, $U(a, \xi)$ will only have the correct asymptotic behaviour and approach zero as $\xi \to \pm\infty$ if the parameter 'a' is restricted to having only negative half-integer values. For $a = -(n + \frac{1}{2})$ where n is a positive integer the parabolic cylinder function $U(a, \xi)$ is related to the Hermite polynomials according to the relation

$$U(-[n + \tfrac{1}{2}], \xi) = 2^{-n/2} \exp(-\xi^2/4) H_n(\xi/\sqrt{2}). \tag{73}$$

The eigenfunctions are therefore given by

$$\Psi_n(\xi, \zeta) = N_n \exp[\mathrm{i}(s_0 + \zeta)] \exp(-\xi^2/4) H_n(\xi/\sqrt{2}) \tag{74}$$

where the normalisation constant $N_n (= 2^{1-n/2} C_0)$ determines the parameter α from the condition

$$\int_{-\infty}^{\infty} \Psi_n^* \Psi_n \, \mathrm{d}x = 1. \tag{75}$$

From the half-integer condition on the parameter 'a', we obtain the eigenvalue relation

$$E_n = (n + \tfrac{1}{2})\hbar\omega - B, \qquad n = 0, 1, 2, 3, \ldots, \tag{76}$$

where $\omega = (2U_1/m)^{1/2}$ is the frequency constant.

The above relations for the eigenvalues and eigenfunctions of the harmonic oscillator are of course well known. What is not known though is that corresponding to this set of eigenvalues and eigenfunctions is a set of eigenrays. The eigenrays for the planar harmonic oscillator are determined from equations (53) and (67) and are given by

$$\zeta_n(\xi) = \zeta_{0n} + C_1 \int_{\xi_0}^{\xi} [U^2(-n - \tfrac{1}{2}, \xi) + V^2(-n - \tfrac{1}{2}, \xi)] \, \mathrm{d}\xi \tag{77}$$

where $C_1 = l_3^2(\pi\hbar^2/16mU_1)^{1/2}$ and ξ_0, ζ_{0n} is the starting point of the ray in the channel.

The eigenrays for parabolic channelling are plotted by numerically integrating the above equation using a table of parabolic cylinder functions (e.g. Abramowitz and Stegun 1965). As an example we have plotted the ray paths for the first excited state ($n = 1$). The ray paths are plotted in figure 1 (for one cycle) together with the corresponding classical (first-order WKB) ray path. In the quantum case we obtain

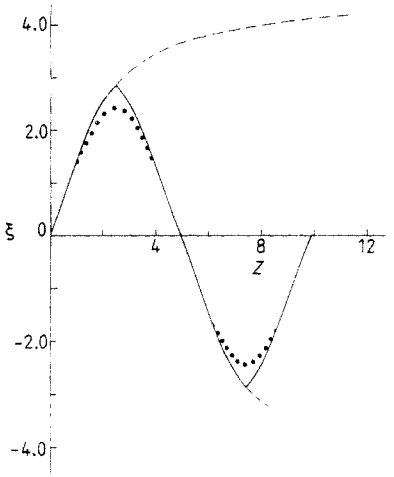

Figure 1. Electron ray paths ($n = 1$) in parabolic channelling. $Z_1 = \int_0^{\xi} F^2(-1.5, \xi')\, d\xi'$. $Z_1 = \zeta_1/C_1$, · · · classical ray path, - - - - - - quantum tunnelling ray path, ——— quantum reflected ray path.

tunnelling rays as well as reflected rays—reflection taken from the ζ point corresponding to the classical turning point in order for the exact ray path to match the WKB ray path away from the turning point. The inability of classical mechanics to describe tunnelling effects is probably best understood from figure 2 which shows a plot of the integrand of equation (77) for $n = 1$ in both the quantum and classical cases. As can be seen, the classical integrand diverges at the turning point. Higher-order WKB theory also diverges here because all the higher-order terms have the same singularity structure as the lowest-order term. On the other hand, the quantum integrand is well behaved (non-singular) at the turning point and therefore tunnelling through the caustic can occur.

The shapes of the quantum and classical curves (ray paths and integrands) are only similar if we are far enough away from the turning points. This is just what

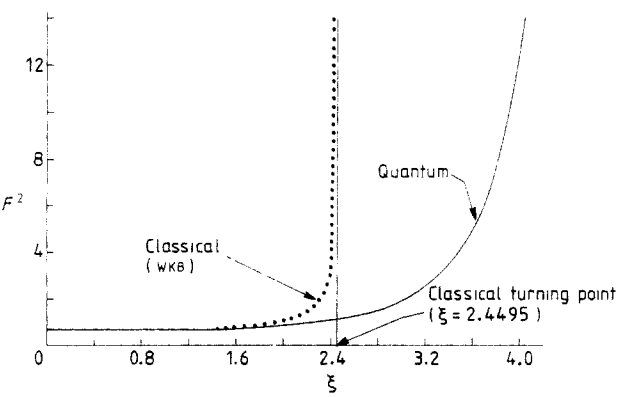

Figure 2. Plots of the quantum (———) and classical (· · · · ·) integrands of equation (77) for the first excited state of the harmonic oscillator ($n = 1$; $F^2(-1.5, \xi)$).

would be expected from a simple WKB analysis. The advantage of this new theory though is that we are able to calculate the ray paths not just in the WKB region, but in every region of space, including the turning points.

Note that the reflected rays in figure 1 originate from beyond the classical turning points. This provides theoretical evidence for the existence of a Goos–Hänchen effect in planar electron channelling (Goos and Hänchen 1947). This effect is well known in optics (Lotsch 1970) and has also been suggested for matter waves (Renard 1964), but does not seem to have been considered for the case of channelling.

7. Conclusions

In this paper, we have developed a theory of quantum ray equations appropriate to one-body non-relativistic elastic propagation. The theory treats wave effects and particle effects in a symmetric fashion and therefore may be regarded as a theory of wave–particle duality.

It must be stressed here that the ray paths given by the theory are not physical ray paths in the sense of being physically measurable—just as the wavefunctions given by wave mechanics are not physical fields (according to the Copenhagen interpretation). Physical reality can only be applied to a statistical ensemble of ray paths in accordance with the statistical interpretation of the wavefunction. By this we mean that corresponding to each eigenstate of a dynamical system is an eigenray path through which the power flows. Therefore, just as it is impossible to predict which eigenstate the system will be in, so it is impossible to predict which eigenray the particles of the system will follow—hence diffraction. Therefore our theory of duality is completely consistent with the Copenhagen interpretation of quantum mechanics—we are not trying to ascribe a classical causal or deterministic interpretation to quantum mechanics.

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