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Quantum mechanics as a multidimensional Ermakov theory: I. Time independent systems

Robert A Lee

CSIRO Division of Chemical Physics, PO Box 160, Clayton Victoria, Australia 3168

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Abstract. In this paper we present a multidimensional Ermakov theory applicable to both separable and non-separable time independent quantum mechanical systems, the separability of the system being determined by the separability of the wavefunction in configuration space. A consequence of the theory is the existence of a new exact invariant for multidimensional quantum systems. In one dimension we show that this new invariant reduces to the well known Ermakov–Lewis invariant. Two applications of the theory are given. In the first case a new exact invariant is obtained for planar optical and particle channelling systems. In the second case we obtain the Ermakov invariants and electron ray path equations for the hydrogen atom.

1. Introduction

The simplest Ermakov system and the first one discovered (Ermakov 1880) and rediscovered in 1967 (Lewis 1967) is related to the properties of the one-dimensional harmonic oscillator with a time dependent frequency

$$\ddot{x} + \omega^2(t)x = 0 \tag{1}$$

where the dots denote derivatives with respect to t. The Ermakov invariant associated with (1) is given by

$$I = (x/\rho)^2 + c^{-2}[x\dot{\rho} - \rho\dot{x}]^2 \tag{2}$$

where c is a constant and $\rho(t)$ satisfies the auxiliary equation

$$\ddot{\rho} + \omega^2(t)\rho - c^2/\rho^3 = 0. \tag{3}$$

Equations (1)–(3) define an Ermakov system representation of the time dependent harmonic oscillator. Lewis and Riesenfeld (1969) have used the invariant given by (2) to construct an exact quantum theory of the time dependent harmonic oscillator based on the eigenstates of the operator form of I. Stimulated by this work, Hartley and Ray have applied the Ermakov technique to the study of more general time dependent systems, including the N-dimensional Schrödinger equation (Ray 1982, Hartley and Ray 1982a, b, Ray and Hartley 1982). It has also been shown that the Feynman propagator can be written in terms of the eigenfunctions of the invariant I (Khandekar and Lawande 1975). Stimulated by the above important applications, other workers have considered extensions of Ermakov theory to include nonlinear equations of motion (Ray and Reid 1979, 1980, Reid and Ray 1982) and studied the relationship between Ermakov invariants and the Lie and Noether symmetries of the

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equation of motion or corresponding Lagrangian (Lutzky 1978, Leach 1981a, b, Reid and Ray 1982). In quantum mechanics an Ermakov system may be established by noting the similarities between (1) and the time independent one-dimensional Schrödinger equation. That is, replacing $x(t)$ by $\Psi(x)$, $\omega(t)$ by $k(x)$ and $\rho(t)$ by $A(x)$, equations (1), (2) and (3) become respectively

$$\Psi'' + k^2(x)\Psi = 0 \tag{1'}$$

$$I = (\Psi/A)^2 + c^{-2}[\Psi A' - A\Psi']^2 \tag{2'}$$

$$A'' + k^2(x)A - c^2/A^3 = 0 \tag{3'}$$

where the primes denote derivatives with respect to x and k is the local wavenumber given by $k^2 = (2m/\hbar^2)(E - V(x))$. Equation (3') is known as the Milne equation (Milne 1930) and forms part of Milne's method of quantisation. In Milne's method the general solution of (1') can be expressed in the form

$$\Psi(x) = NA(x)\sin\left(c\int^x A^{-2}\,\mathrm{d}x - \delta\right) \tag{4}$$

where N and δ are arbitrary constants. The Milne quantisation condition follows from the requirement that the wavefunctions be bounded at both ends of the interval

$$c\int_{-\infty}^{\infty} A^{-2}\,\mathrm{d}x = n\pi \tag{5}$$

where n is a positive integer, the energy quantum number. The Milne method has received a revival of interest in recent years because of its superior numerical stability for $n \gg 1$ (Killingbeck 1980, Korsch *et al* 1981) and because of its close connection with standard WKB theory. The WKB approximation is obtained by neglecting the A'' term in (3') and restricting the limits on the integral in (5) to the classical turning points. The close connection between classical Ermakov theory and Milne's method of quantisation discussed above implies that there might exist a common physical interpretation which relates classical particle mechanics to quantum wave mechanics. We have recently explored this idea in the context of a theory of wave–particle duality based on the three-dimensional time independent Schrödinger equation (Lee 1982a) and in the relativistic case on the Klein–Gordon equation (Lee 1982d). When this theory was applied to the case of optical and particle channelling systems (Lee 1982b, c), where the eigenfunctions are separable functions of the longitudinal and transverse coordinates, we obtained a description which included an Ermakov system of equations of the form of (1'), (2'), (3'). In this case the Ermakov invariant played a bootstrapping role in connecting the dual representations of rays and waves.

The main purpose of this paper is to show that a similar result holds in the general case of a $3N$-dimensional non-separable quantum system of N particles where an Ermakov invariant will be shown to exist which bootstraps configuration space wavefunctions to configuration space quantum ray paths. This suggests a physical interpretation of the Ermakov invariant in the context of a theory of wave–particle duality.

2. Configuration space quantum ray theory

Consider a quantum system of N identical particles interacting via a real scalar potential $V(\boldsymbol{X})$, where $\boldsymbol{X}$ is a $3N$-dimensional space vector. The time independent states of

the system are governed by the following $3N$-dimensional Schrödinger equation

$$\nabla^2\Psi + k^2(\boldsymbol{X})\Psi = 0 \tag{6}$$

where ∇ is the $3N$-dimensional gradient operator, $\Psi(\boldsymbol{X})$ is the configuration space wavefunction and $k^2(\boldsymbol{X}) = (2m/\hbar^2)[E - V(\boldsymbol{X})]$ where m is the mass of a particle.

We now write the wavefunction in the form $\Psi(\boldsymbol{X}) = A(\boldsymbol{X})\exp(\mathrm{i}S(\boldsymbol{X})/\hbar)$, substitute into (6) and separate real and imaginary parts to obtain the two well known equations

$$\nabla^2 S + 2(\nabla A/A)\cdot\nabla S = 0 \tag{7}$$

$$|\nabla S|^2 = \hbar^2 k^2 + \hbar^2\nabla^2 A/A. \tag{8}$$

We now develop the configuration space quantum ray representation by following a similar procedure to that employed in the one-particle case (Lee 1982a).

The ray representation is introduced according to the following prescription

$$\nabla S = g(\boldsymbol{X})\,\mathrm{d}\boldsymbol{X}/\mathrm{d}\sigma \tag{9}$$

where $g(\boldsymbol{X})$ is an arbitrary gauge function and $\mathrm{d}\sigma$ is an element of arc length in a conformal metric in the configuration space of the N-particle system. We now define a point on the ray path in configuration space by $\boldsymbol{X}(\mu)$ where μ is a continuously variable parameter. The derivative of $\boldsymbol{X}$ with respect to μ is denoted by $\dot{\boldsymbol{X}}$. From (8) and (9) we therefore have

$$\mathrm{d}\boldsymbol{X}/\mathrm{d}\sigma = (Q/g)\dot{\boldsymbol{X}}/|\dot{\boldsymbol{X}}| \equiv (Q/g)\dot{\boldsymbol{x}} \tag{10}$$

$$\mathrm{d}\mu/\mathrm{d}\sigma = (Q/g)1/|\dot{\boldsymbol{X}}| \tag{11}$$

$$\mathrm{d}g/\mathrm{d}\sigma = (Q/g)\dot{g}/|\dot{\boldsymbol{X}}| \tag{12}$$

$$\mathrm{d}A/\mathrm{d}\sigma = (Q/g)\dot{A}/|\dot{\boldsymbol{X}}| \tag{13}$$

where Q^2 is given by the RHS of (8) and the vertical bracket denotes the magnitude of the vector inside. From the above expressions and (7) we obtain the result

$$\mathrm{d}[\ln(A^2Q)]/\mathrm{d}\mu = -[\nabla\cdot\dot{\boldsymbol{x}}]|\dot{\boldsymbol{X}}|. \tag{14}$$

Finally integrating this expression and using the definition of Q we obtain the nonlinear wave equation

$$\nabla^2 A + k^2 A - \alpha^2\kappa^2 A^{-3} = 0 \tag{15}$$

where α is an integration constant and κ is the configuration space quantum expansion coefficient given by

$$\kappa = \exp\left(-\int^{\mu}[\nabla\cdot\dot{\boldsymbol{x}}]|\dot{\boldsymbol{X}}|\,\mathrm{d}\mu\right). \tag{16}$$

The configuration space quantum ray equation is given by the extremisation of the following action integral obtained from (9)–(15):

$$S(\mu) = \alpha\hbar\int^{\mu}(\kappa/A^2)|\dot{\boldsymbol{X}}|\,\mathrm{d}\mu. \tag{17}$$

Hence the N-particle quantum ray equation is given by

$$(\mathrm{d}/\mathrm{d}\tau)[(\kappa/A^2)\,\mathrm{d}\boldsymbol{X}/\mathrm{d}\tau] = \nabla(\kappa/A^2) \tag{18}$$

where $\mathrm{d}\tau = |\dot{\boldsymbol{X}}|\,\mathrm{d}\mu$ is an element of the configuration space ray path.

Equation (18) defines a set of $3N$ coupled ray equations describing the time independent interactions in the N-particle quantum system. There are two sources of these interparticle interactions: firstly the source due to the potential function $V(\boldsymbol{X})$. In the classical limit where the $\nabla^2 A$ term in (15) is neglected this interaction is still present and (18) reduces to the well known configuration space classical ray equations. In the absence of $V(\boldsymbol{X})$ these classical ray equations decouple into a set of $3N$ independent equations describing the straight line paths of N independent particles. However, in the exact quantum mechanical case where the $\nabla^2 A$ term in (15) is not neglected there is another source of interactions between the particles. This purely quantum interaction has the effect of causing the ray equations still to be coupled even in the absence of the potential function $V(\boldsymbol{X})$. The interesting thing about this quantum interaction is that it is independent of the separation between the particles and therefore represents the non-locality property of quantum phenomena. In a later paper we hope to explore the consequences of this non-local effect in more detail.

An expression for the gradient of the phase of the configuration space wavefunction follows from (9), (10) and (15):

$$\nabla S = \alpha\hbar(\kappa/A^2)[\mathrm{d}\boldsymbol{X}/\mathrm{d}\tau]. \tag{19}$$

The configuration space quantum eikonal equation is therefore given by

$$|\nabla S|^2 = \alpha^2\hbar^2\kappa^2/A^4. \tag{20}$$

From the above expressions it can be seen that the N-particle quantum expansion coefficient can also be written in the form

$$\kappa = \exp\left(-\int \nabla \cdot (\nabla S/|\nabla S|)\,\mathrm{d}\tau\right). \tag{21}$$

From (19) and (21) it can be seen that $\nabla \cdot (A^2 \nabla S) = 0$ and therefore, from applying Gauss's theorem to a thin 'tube' of rays connecting two wavefronts at τ_0 and τ, it can be seen that the expansion coefficient can be written in the form $\kappa(\tau) = \kappa(\tau_0)\,\mathrm{d}\Sigma_0/\mathrm{d}\Sigma = \kappa(\tau_0)J^{-1}[\partial X_i(\tau)/\partial X_j(\tau_0)]$ where $\mathrm{d}\Sigma_0$ and $\mathrm{d}\Sigma$ are the 'areas' of wavefronts cutting the ray 'tube' at τ_0 and τ and $J[\partial X_i(\tau)/\partial X_j(\tau_0)]$ is the Jacobian of the mapping from τ_0 to τ. Equations (15)–(21) define the configuration space quantum ray representation of the N-particle time independent Schrödinger equation and are a natural generalisation of the one-particle case considered in an earlier paper (Lee 1982a). In § 3 we shall show how these equations may be used to define the configuration space quantum Ermakov invariant.

3. The Ermakov invariant

The main reason for believing in the existence of an Ermakov invariant for N-particle systems is that (6) and (15) are just multidimensional equivalents to (1′) and (3′) respectively. The only difference is that (15) requires for its complete solution the solution of a set of generalised ray equations given by (18).

To find the configuration space equivalent of (2′) consider (17) which can be rewritten in the form

$$S(\boldsymbol{X}_0, \tau) = \alpha\hbar \int^{\tau} (\kappa/A^2)\,\mathrm{d}\tau \tag{22}$$

where $\boldsymbol{X}_0$ is an initial point for one particular configuration space quantum ray path given by solving (15) and (18) for $\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{X}_0, \tau)$.

Two linearly independent solutions of (6) are now given in the ray representation by

$$\Psi_1(\boldsymbol{X}_0, \tau) = A(\boldsymbol{X}_0, \tau) \cos\left(\alpha \int^{\tau} [\kappa(\boldsymbol{X}_0, \tau)/A^2(\boldsymbol{X}_0, \tau)]\, \mathrm{d}\tau \right) \tag{23}$$

$$\Psi_2(\boldsymbol{X}_0, \tau) = A(\boldsymbol{X}_0, \tau) \sin\left(\alpha \int^{\tau} [\kappa(\boldsymbol{X}_0, \tau)/A^2(\boldsymbol{X}_0, \tau)]\, \mathrm{d}\tau \right) \tag{24}$$

where $A(\boldsymbol{X}_0, \tau) = A(\boldsymbol{X}(\boldsymbol{X}_0, \tau))$. The solutions Ψ_1 and Ψ_2 obviously satisfy the following Wronskian relation

$$\Psi_1(\mathrm{d}\Psi_2/\mathrm{d}\tau) - \Psi_2(\mathrm{d}\Psi_1/\mathrm{d}\tau) = \alpha\kappa. \tag{25}$$

It is now obvious that the following function is a constant in the configuration space of the N-particle system:

$$I = [\Psi/A]^2 + (\alpha\kappa)^{-2}[\Psi(\mathrm{d}A/\mathrm{d}\tau) - A(\mathrm{d}\Psi/\mathrm{d}\tau)]^2 \tag{26}$$

where $\Psi = a\Psi_1 + b\Psi_2$ and a and b are arbitrary constants independent of τ. The invariance of I can be checked by substituting (23) and (24) into (26) to obtain $I = a^2 + b^2$. The above expression is the configuration space Ermakov invariant and (6), (26) and (15) define a multidimensional Ermakov system.

In the one-dimensional case where $\mathrm{d}\tau = \mathrm{d}x$, $A = A(x)$ and $\Psi = \Psi(x)$ the quantum expansion coefficient given by (16) or (21) reduces to unity. Therefore (6), (26) and (15) reduce to (1′), (2′) and (3′) respectively, thus proving that the multidimensional Ermakov system contains the one-dimensional system as a special case as we would expect. In § 4 we shall consider a more interesting application of the above theory to the case of planar channelling systems.

Before proceeding to this case, however, the following points should be mentioned.

(i) The usual configuration space representation of the wavefunctions is obtained from the ray path wavefunctions given by (23) and (24) by simply inverting the mapping relations $\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{X}_0, \tau)$ to obtain $\boldsymbol{X}_0 = \boldsymbol{X}_0(\boldsymbol{X}, \tau)$ and substituting the result into $\Psi(\boldsymbol{X}_0, \tau)$ to obtain $\Psi(\boldsymbol{X})$. Alternatively we can solve (15)–(21) explicitly for κ and τ as functions of $\boldsymbol{X}$ and substitute the results into (23) and (24) to obtain $\Psi_1(\boldsymbol{X})$ and $\Psi_2(\boldsymbol{X})$. This method will be demonstrated in § 4.

(ii) The classical limit of the theory is obtained by evaluating the amplitude function $A(\boldsymbol{X})$ at the minimum point of the Lagrangian density potential function of (15). The method is described in Lee (1982a). The result is that the quantum ray equation (18) reduces to the usual N-particle classical ray equation and the wavefunctions reduce to N-particle WKB wavefunctions with the Ermakov invariant given by (26) remaining unchanged.

(iii) Quantisation of the above theory is achieved by requiring the wavefunction to be single valued. In this way we obtain the quantisation condition

$$\alpha \oint (\kappa/A^2)\, \mathrm{d}\tau = 2n\pi \tag{27}$$

where $n = 0, \mp 1, \mp 2$, etc, and the integral is taken around a closed path in configuration space. It is interesting to note that the above expression is very similar in structure to the Einstein quantisation condition (Einstein 1917) and can be put into exact

correspondence if we identify $\boldsymbol{P} = \alpha\hbar(\kappa/A^2)[\mathrm{d}\boldsymbol{X}/\mathrm{d}\tau]$ as a generalised configuration space momentum. In this case (27) assumes the Einstein form

$$\oint \boldsymbol{P} \cdot \mathrm{d}\boldsymbol{X} = nh.$$

In a later paper we hope to study the implications of this quantisation condition in more detail.

4. One-particle planar separable systems

In the case of one-particle planar separable systems as represented by planar optical and particle channelling systems (Lee 1982d, b), where the eigenfunctions are only a function of the transverse coordinate x, the phase of the wavefunction is given by $S/\hbar = l_3 z + f(x)$. The quantity l_3 denotes the longitudinal wavenumber of the channelling particle. The function $f(x)$ is determined by substituting this expression for $S(x, z)$ into the two-dimensional forms of (15)–(21) with $A = A(x)$ and $\mathrm{d}\tau^2 = \mathrm{d}x^2 + \mathrm{d}z^2$ and requiring self consistency between the resulting expressions. In this way the following results are obtained:

$$\kappa = \Lambda_0[1 + (l_3/(\alpha\Lambda_0))^2 A^4]^{1/2} \tag{28}$$

$$S/\hbar = l_3(z - z_0) \mp \alpha\Lambda_0 \int^x A^{-2}(x)\,\mathrm{d}x \tag{29}$$

where Λ_0 is a constant dependent upon the initial conditions and z_0 is an initial z point.

The continuum wavefunctions corresponding to (23) and (24) are therefore given by

$$\Psi_1(x, z) = A(x)\cos\left(l_3(z - z_0) \mp \alpha\Lambda_0 \int^x A^{-2}\,\mathrm{d}x\right) \tag{30}$$

$$\Psi_2(x, z) = A(x)\sin\left(l_3(z - z_0) \mp \alpha\Lambda_0 \int^x A^{-2}\,\mathrm{d}x\right) \tag{31}$$

and (15) reduces to the following equation for the amplitude function $A(x)$:

$$\mathrm{d}^2A/\mathrm{d}x^2 + k_\perp^2(x)A - \alpha^2\Lambda_0^2 A^{-3} = 0 \tag{32}$$

where $k_\perp^2(x) = (2m/\hbar^2)[E_\perp - V(x)]$. $E_\perp$ is the transverse energy of the propagating quanta and is related to the total energy E according to $E_\perp = E - \hbar^2 l_3^2/(2m)$.

In the case of planar one-particle systems the configuration space Schrödinger equation given by (6) reduces to

$$\nabla^2\Psi + (k_\perp^2 + l_3^2)\Psi = 0 \tag{33}$$

where Ψ is any linear combination of Ψ_1 and Ψ_2 and ∇ is the two-dimensional gradient operator operating in the x, z plane. Since the phase function is a separable function of x and z we may take appropriate linear combinations of Ψ_1 and Ψ_2 and write the planar wavefunctions in the form $\Psi(x, z) = \Phi(x)\exp(\mathrm{i}l_3 z)$ where $\Phi(x)$ is a standing wave solution and obeys the following one-dimensional equation:

$$\mathrm{d}^2\Phi/\mathrm{d}x^2 + k_\perp^2(x)\Phi = 0. \tag{34}$$

The planar ray equation obtained from (19) is given by

$$z = z_0 \mp (l_3/(\alpha\Lambda_0)) \int^x A^2(x)\,dx \tag{35}$$

where the amplitude function is related to the two linearly independent solutions of (34) according to the relation

$$A = [\Phi_1^2 + \Phi_2^2]^{1/2}. \tag{36}$$

The two linearly independent solutions Φ_1 and Φ_2 are given by

$$\Phi_1(x) = A(x)\cos\left(\alpha\Lambda_0 \int^x A^{-2}\,dx\right) \tag{37}$$

$$\Phi_2(x) = A(x)\sin\left(\alpha\Lambda_0 \int^x A^{-2}\,dx\right). \tag{38}$$

Note that because these solutions satisfy the Wronskian relation $\Phi_1(d\Phi_2/dx) - \Phi_2(d\Phi_1/dx) = \alpha\Lambda_0$ only one of these functions can satisfy the boundary conditions and asymptote to zero as x goes to plus or minus infinity.

Now there are two different types of Ermakov invariants for this system corresponding to the two different types of wavefunctions given by (30), (31) and (37), (38). The first invariant is obtained by eliminating $k_\perp^2(x)$ between (32) and (34) and integrating to obtain an invariant of the form of (2′) with Φ replacing Ψ and $c = \alpha\Lambda_0$. The main feature of this particular constant of the motion is that it represents a standing wave invariant, being a function of the standing wave solutions (37) or (38) of (33). Further discussion on this standing wave invariant and its application to planar optical channelling can be found in Lee (1982c).

The second type of Ermakov invariant is the multidimensional Ermakov invariant and corresponds to the propagating wave solutions of (33) given by the expressions (30) and (31). These propagating solutions correspond to waves travelling in the $+x$ or $-x$ directions as represented by the + and − signs in (30) and (31) corresponding to the + and − ray paths given by (35). As shown in the appendix, these + and − ray paths are just the paths of constructive interference in the total wave fields of the + and − propagating waves. An expression for the propagating wave Ermakov invariant may be obtained from (26), (28) and (35) and the Cartesian metric interval expression $d\tau^2 = dx^2 + dz^2$. The result is

$$I_p = (\Psi/A)^2 + (\Lambda_0/\alpha)^2(A/\kappa)^4[d(\Psi/A)/dx]^2 \tag{39}$$

where $\Psi(x, z)$ is any linear combination of propagating wavefunctions satisfying (33) and $d/dx = \partial/\partial x + (dz/dx)\partial/\partial z$. The corresponding expression for the standing wave Ermakov invariant is given by

$$I_s = (\Phi/A)^2 + (\alpha\Lambda_0)^{-2}A^4[d(\Phi/A)/dx]^2. \tag{40}$$

The main difference between these two expressions lies in the presence of the expansion coefficient in the propagating wave case. This is just what we would expect since propagating waves correspond to bundles of propagating quantum ray paths which expand due to diffraction effects.

A physical interpretation of these invariants is suggested by expressing the amplitude function in terms of the gradient of the ray path function according to (35) and

substituting the result into (39) and (40) to obtain

$$I_p^* = \Psi^2(dz/dx)\{(dx/dz)^2 + l_3^{-2}[1+(dz/dx)^2]^{-2}[d/dx \ln(\Psi(dx/dz)^{1/2})]^2\} \tag{41}$$

$$I_s^* = \Phi^2(dz/dx)\{(dx/dz)^2 + l_3^{-2}[d/dx \ln(\Phi(dx/dz)^{1/2})]^2\} \tag{42}$$

where $I_p^* = \mp(\alpha\Lambda_0/l_3)I_p$ and $I_s^* = \mp(\alpha\Lambda_0/l_3)I_s$. Hence the Ermakov invariants have the meaning of differential conservation laws relating the gradient properties of the paths of constructive interference to properties of the channelling wavefunctions. In this sense they can be interpreted as wave–particle duality invariants and used as auxiliary boundary conditions when determining wave and ray properties of optical and particle channelling systems.

This idea can be extended to more complicated geometries than the simple planar system considered in this section. In Lee (1982b) we derived the ray path equations and Ermakov invariants for an optical fibre system. In § 5 a similar procedure will be adopted to derive the electron ray paths and Ermakov invariants for the hydrogen atom.

5. The hydrogen atom as a quantum Ermakov system

In the case of one-particle systems the form of equations (15)–(21) remains unchanged but the arc length element reduces to $d\tau^2 = dx^2 + dy^2 + dz^2$. The resulting theory was discussed in Lee (1982a). The aim here is to apply this theory to the case of the hydrogen atom and derive the corresponding Ermakov invariants and electron ray path equations.

For the hydrogen atom it is easily shown by an application of the three-space form of (15)–(21) that for a separable amplitude function of the form $A_{lkj}(r, \theta) = M_{lk}(r)N_{lj}(\theta)$ and a separable phase function of the form $\hbar^{-1}S_{lkj}(r, \theta, \phi) = \pm m_{lk}(r) \pm n_{lj}(\theta) + j\phi$ the nonlinear amplitude equation (15) separates into the following radial and angular Milne type equations:

$$d^2M_{lk}/d\mu^2 + (2/\mu)\, dM_{lk}/d\mu + \alpha_{lk}M_{lk} - \mu^{-4}M_{lk}^{-3} = 0 \tag{43}$$

$$(1-\nu^2)\, d^2N_{lj}/d\nu^2 - 2\nu\, dN_{lj}/d\nu + \beta_{lj}N_{lj} - \varepsilon_{lj}\gamma_{lj}N_{lj}^{-3} = 0 \tag{44}$$

where

$$\alpha_{lk} = -1 + (2k/\mu) - l(l+1)/\mu^2 \qquad \beta_{lj} = l(l+1) - j^2/(1-\nu^2)$$

$$\gamma_{lj} = [\Gamma(l+j+1)/\Gamma(l-j+1)]/(1-\nu^2) \equiv \varepsilon_{lj}/(1-\nu^2).$$

In these expressions Γ denotes the gamma function, l is the angular momentum quantum number, k is the energy quantum number and j is the magnetic quantum number. Also $\nu = \cos(\theta)$ and $\mu = rZ/(ka_0)$ where Z is the nuclear charge and a_0 is the radius of the first Bohr orbit.

It is easily verified that $M_{lk} = (R_{lk}^2 + T_{lk}^2)^{1/2}$ where R_{lk} and T_{lk} are the two linearly independent solutions of the radial Schrödinger equation, while $N_{lj} = (P_{lj}^2 + Q_{lj}^2)^{1/2}$ where P_{lj} and Q_{lj} are the two linearly independent associated Legendre functions. Now since R_{lk}, T_{lk} and P_{lk}, Q_{lk} satisfy the Wronskian relations

$$R_{lk}(dT_{lk}/d\mu) - T_{lk}(dR_{lk}/d\mu) = 1/\mu^2 \tag{45}$$

$$P_{lj}(dQ_{lj}/d\nu) - Q_{lj}(dP_{lj}/d\nu) = (-1)^j\gamma_{lj} \tag{46}$$

it is readily apparent that $R_{lk} \pm iT_{lk} = M_{lk}\exp(\pm im_{lk})$ and $P_{lj} \pm iQ_{lj} = N_{lj}\exp(\pm in_{lj})$

where the radial and angular phase functions are given by

$$m_{lk} = \int^{\mu} \mathrm{d}\mu/[\mu^2 M_{lk}^2(\mu)] \tag{47}$$

$$n_{lj} = (-1)^j[\Gamma(l+j+1)/\Gamma(l-j+1)] \int^{\nu} \mathrm{d}\nu/[(1-\nu^2)N_{lj}^2(\nu)]. \tag{48}$$

The simplest method for obtaining the orbit equations is now to utilise the fact that for separable systems the solutions of the general quantum ray equations are given by the ratios of the derivatives of the separable phase functions. This was proved in Lee (1982a). Employing this method we obtain the following exact equations for the electron ray paths in the hydrogen atom:

$$\int^{\mu} M_{lk}^2(\mu)\,\mathrm{d}\mu = (-1)^j[\Gamma(l-j+1)/\Gamma(l+j+1)] \int^{\nu} N_{lj}^2(\nu)\,\mathrm{d}\nu \tag{49}$$

$$\phi = \phi_0 + j(-1)^j[\Gamma(l-j+1)/\Gamma(l+j+1)] \int^{\nu} [N_{lj}^2(\nu)/(1-\nu^2)]\,\mathrm{d}\nu. \tag{50}$$

From the above expressions it can be seen that the $j=0$ states correspond to planar orbits.

In the classical limit, corresponding to the minimum points of the Lagrangian density potential functions of the radial and angular Milne equations, the ray equations reduce to the elliptical orbits of the old quantum theory. These elliptical orbits are given by $\mu = l(l+1)/\{k+[(k^2-l(l+1))]^{1/2}\sin(\theta-\theta_0)\}$ and are obtained from the present theory by neglecting the second derivative terms in (43) and (44).

In order to obtain some idea of how wave aspects affect the orbit it is interesting to look at the next semiclassical approximation. This is obtained by taking the classical limit of the radial Milne equation and the exact solution of the angular Milne equation. The resulting orbit or constructive interference path is given by

$$\mu = l(l+1)\Big/\left[k+(k^2-l(l+1))^{1/2}\sin\left(C_{lj}\int^{\nu} N_{lj}^2(\nu)\,\mathrm{d}\nu\right)\right]$$

where $C_{lj} = (l(l+1))^{1/2}(-1)^j\Gamma(l-j+1)/\Gamma(l+j+1)$. Hence the elliptical orbit of the old quantum theory is modified by the addition of wave-like aberrations to the θ dependence of the orbit. For j not equal to 0 this aberrated elliptical orbit rotates in the ϕ direction according to (50).

The Ermakov invariants for the hydrogen atom are obtained from this theory by making use of (43) and (44) and the corresponding radial and angular Schrödinger equations given by

$$\mathrm{d}^2R_{lk}/\mathrm{d}\mu^2 + (2/\mu)\,\mathrm{d}R_{lk}/\mathrm{d}\mu + \alpha_{lk}R_{lk} = 0 \tag{51}$$

$$(1-\nu^2)\,\mathrm{d}^2P_{lj}/\mathrm{d}\nu^2 - 2\nu\,\mathrm{d}P_{lj}/\mathrm{d}\nu + \beta_{lj}P_{lj} = 0. \tag{52}$$

The radial Ermakov invariant is obtained by eliminating α_{lk} between (43) and (51) and integrating the result to find

$$I_{lk} = (R_{lk}/M_{lk})^2 + \mu^4[M_{lk}(\mathrm{d}R_{lk}/\mathrm{d}\mu) - R_{lk}(\mathrm{d}M_{lk}/\mathrm{d}\mu)]^2. \tag{53}$$

Similarly, the angular Ermakov invariant is obtained by eliminating β_{lj} between (44) and (52) and integrating the result to find

$$J_{lj} = (P_{lj}/N_{lj})^2 + \gamma_{lj}^{-2}[N_{lj}(\mathrm{d}P_{lj}/\mathrm{d}\nu) - P_{lj}(\mathrm{d}N_{lj}/\mathrm{d}\nu)]^2. \tag{54}$$

The set of equations (43), (51) and (53) defines the radial Ermakov system of the hydrogen atom while the set of equations (44), (52) and (54) defines the corresponding angular Ermakov system.

The Ermakov invariants given by (53) and (54) have been expressed in terms of the functions $R_{lk}(\mu)$ and $P_{lj}(\nu)$ and not in terms of linear combinations of R_{lk} and T_{lk} or P_{lj} and Q_{lj}. The reason for this is that in the case of the hydrogen atom the second linearly independent solutions of the radial and angular Schrödinger equations are in general unbounded functions and therefore do not lend themselves to a probability interpretation. It is for this reason that no use is made of these functions in the usual wave mechanical treatment of the hydrogen atom. However, in the present theory these unbounded solutions have been given a physical interpretation because the ray equations given by (49) and (50) depend on both the radial and angular probability functions R_{lk}^2 and P_{lj}^2 and the corresponding unbounded functions T_{lk}^2 and Q_{lj}^2. The Ermakov invariants (53) and (54) then have the meaning of duality invariants in the sense that they involve radial and angular probability amplitudes coupled to radial and angular electron ray path functions M_{lk} and N_{lj}.

Finally it should be mentioned that although we have implicitly employed Schrödinger's method of quantisation for obtaining the integer values of l, k and j this is not strictly necessary. An alternative and equivalent procedure is to apply Milne's method to the radial, angular and azimuthal phase functions. The resulting quantisation conditions then assume forms analogous to the quantisation conditions of the old quantum theory. However, these Milne quantisation conditions are exact, because instead of employing classical radial and angular momentum functions they employ local radial and angular momentum functions defined in terms of Milne amplitudes.

6. Conclusions

In this paper we have developed a representation of time independent quantum mechanics as a multidimensional Ermakov system. The theory is applicable to both separable and non-separable quantum systems, the separability of the system being determined by the separability of the N-particle wavefunction in configuration space. The mathematical representation of the theory consists of a $3N$-dimensional nonlinear wave equation (equation (15)) coupled to a set of $3N$ coupled generalised ray equations (equation (18)). Quantisation of the theory is achieved by means of a configuration space path integral condition (equation (27)). An interesting feature of the theory is the existence of a new exact configuration space invariant (equation (26)) which has the form of a generalised Ermakov invariant.

In one dimension we showed that this new configuration space invariant reduces to the well known Ermakov–Lewis invariant. Two applications of the theory were then given. In the first case a new exact invariant was obtained for planar optical and particle channelling systems. It was also shown here that the quantum ray paths in the system corresponded exactly to the paths of constructive interference in the total channelling wave field. In the second case we obtained the Ermakov invariants and electron ray path equations for the hydrogen atom. As in the channelling case, the Ermakov invariants were found to have the meaning of duality invariants in the sense of bootstrapping properties relating to the wave and particle aspects of the quantum system. In a later paper it is hoped to extend this theory to the case of time dependent systems.

Appendix. Quantum rays as constructive interference paths

The total planar channelling wave field in the x, z plane is given by

$$\Psi(x, z) = \sum_n a(k_{\perp n})\Phi(k_{\perp n}, x) \exp(\mathrm{i}l_3(z - z_0)) \tag{A1}$$

where $a(k_{\perp n})$ is the probability amplitude for the excitation of the channel mode $\Phi(k_{\perp n}, x)$ and $k_{\perp n}^2 = k_\perp^2(x) + (2m/\hbar^2)V(x)$. The excitation amplitude is related to the initial wavefunction at the entrance face of the channel according to the expression

$$a(k_{\perp n}) = \int_{-\infty}^{+\infty} \Phi_n(x)\Psi(x, z_0)\,\mathrm{d}x. \tag{A2}$$

The mode functions obey equation (34) with the subscript n added to Φ.

$\Phi_n(x)$ is a standing wave and is therefore given by the sum of a wave travelling in the $+x$ direction and a wave travelling in the $-x$ direction as shown by (37) and (38). Therefore $\Psi(x, z) = \frac{1}{2}(\Psi_+(x, z) + \Psi_-(x, z))$ where Ψ_+ and Ψ_- correspond to waves travelling in the $+x$ and $-x$ directions respectively. It follows that

$$\Psi_{+-}(x, z) = \sum_n a(k_{\perp n})A_n \exp(\mathrm{i}S_{+-}/\hbar) \tag{A3}$$

where the phase function S_{+-} is given by (29).

We now convert the previous summation into an integral by means of the Poisson summation formula

$$\sum_n f_n = \sum_\nu \exp(-\mathrm{i}\nu\pi) \int f(\varepsilon - \tfrac{1}{2}) \exp(2\pi\mathrm{i}\nu\varepsilon)\,\mathrm{d}\varepsilon. \tag{A4}$$

In this case f_n is given by

$$f_n = a(k_{\perp n})A_n \exp(\mathrm{i}S_{+-}/\hbar). \tag{A5}$$

Equation (A3) may now be written in the form

$$\Psi_{+-}(x, z) = \sum_\nu \exp(-\mathrm{i}\nu\pi)I_\nu(x, z) \tag{A6}$$

where $I_\nu(x, z)$ is a phase integral given by

$$I_\nu(x, z) = \int a(k_\perp(\varepsilon - \tfrac{1}{2}))A(\varepsilon - \tfrac{1}{2}) \exp(\mathrm{i}\Omega_{+-})\,\mathrm{d}\varepsilon. \tag{A7}$$

The phase function Ω_{+-} is given by

$$\Omega_{+-} = 2\pi\nu\varepsilon + l_3(\varepsilon)(z - z_0) \pm \alpha\Lambda_0 \int^x A^{-2}(x, \varepsilon - \tfrac{1}{2})\,\mathrm{d}x. \tag{A8}$$

To obtain the paths of constructive interference we apply the method of stationary phase to the integral given by (A7). The paths of constructive interference are therefore given by

$$\partial\Omega_{+-}/\partial\varepsilon = 0. \tag{A9}$$

From (A8) and (A9) we have

$$2\pi\nu + (\partial l_3/\partial\varepsilon)(z - z_0) \pm \int^x (\partial(\alpha\Lambda_0 A^{-2})/\partial\varepsilon)\,\mathrm{d}x = 0. \tag{A10}$$

Now from (32) we have

$$\partial(\alpha\Lambda_0 A^{-2})/\partial\varepsilon = -l_3\,\partial l_3/\partial\varepsilon(A^2/\alpha\Lambda_0). \tag{A11}$$

Substituting this expression into (A10) we obtain the following expression for the constructive interference paths:

$$z_\nu(\varepsilon, x) = z_{0\nu}(\varepsilon) \pm (l_3/\alpha\Lambda_0)\int^x A^2(\varepsilon, x)\,\mathrm{d}x \tag{A12}$$

where $z_{0\nu}(\varepsilon) = z_0 - 2\pi\nu/(\partial l_3/\partial\varepsilon)$ and ν is an integer. The quantity $D = 2\pi/(\partial l_3/\partial\varepsilon)$ gives the periodicity of the ray in the channel. The transverse reflection point χ is then given by

$$\partial\varepsilon/\partial l_3 = [2l_3/(\pi\alpha\Lambda_0)]\int^\chi A^2(\varepsilon, x)\,\mathrm{d}x. \tag{A13}$$

The difference between χ and the x value of the classical turning point gives the x direction Goos–Hanchen shift. The corresponding longitudinal Goos–Hanchen shift is given by the difference between the z value corresponding to χ and the z value of the classical turning point.

Equation (A12) is of exactly the same form as (35). Hence, at least in the channelling case, quantum ray paths are equivalent to paths of constructive interference in the total wave field of the channelling particle. Since classical rays are WKB approximants to quantum rays one reason for the success of the classical theory of channelling is now apparent. Classical channelling theory is just a quasi-particle approximation to the exact wave mechanical theory. The quasi-particle in this case is just a little lump of probability following the quantum trajectory of the channelling particle.

References

Einstein A 1917 *Verhandlungen der Deutschen Physikalischen Gesellschaft* **19** 82–92
Ermakov V P 1880 *Univ. Izv. Kiev* **20** no 9, 1
Hartley J G and Ray J R 1982a *Phys. Rev.* D **25** 382
—— 1982b *Phys. Rev.* A **25** 2873
Khandekar D C and Lawande S V 1975 *J. Math. Phys.* **16** 384
Killingbeck J 1980 *J. Phys. A: Math. Gen.* **13** L231
Korsch H J, Laurent H and Mohlenkamp R 1981 *J. Phys. B: At. Mol. Phys.* **14** 4213
Leach P G L 1981a *Phys. Lett.* **84A** 161
—— 1981b *J. Math. Phys.* **22** 465
Lee R A 1982a *J. Phys. A: Math. Gen.* **15** 2761
—— 1982b *Opt. Acta* **29** 569
—— 1982c *Appl. Phys.* A **29** 81
—— 1982d *Rad. Eff. Lett.* **68** 113
Lewis H R 1967 *Phys. Rev. Lett.* **18** 510
Lewis H R and Riesenfeld W B 1969 *J. Math. Phys.* **10** 1458
Lutzky M 1978 *Phys. Lett.* A **68** 3
Milne W E 1930 *Phys. Rev.* **35** 863
Ray J R 1982 *Phys. Rev.* A **26** 729
Ray J R and Hartley J G 1982 *Phys. Lett.* A **88** 125
Ray J R and Reid J L 1979 *J. Math. Phys.* **20** 2054
—— 1980 *Nuovo Cimento* **59A** 134
Reid J L and Ray J R 1982 *J. Phys. A: Math. Gen.* **15** 2751