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# A shooting approximation to wavefunctions with harmonic amplitude

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**Abstract.** States which in the Schrödinger representation, have harmonic amplitudes or phases or both are discussed. The variational problem for the quantum mechanical action functional reduces to the solution of classical equations of motion by shooting methods, when the variation is restricted to wavefunctions whose phase satisfies the classical Hamilton-Jacobi equation. These wavefunctions have harmonic amplitude.

## 1. Introduction to 'harmonious' and 'coherent' states

Consider the quantum system for the potential  $V(\mathbf{x})$  which develops in time according to the Schrödinger equation

$$2m\mathrm{i}\hbar\partial\psi + \hbar^2\nabla^2\psi = 2mV(\mathbf{x},t)\psi. \tag{1.1}$$

The symbol  $\partial$  denotes partial differentiation with respect to t throughout this paper and the components of the vector  $\nabla$  are the derivatives with respect to the n variables x. The wavefunction solution

$$\psi(\mathbf{x}, t) \equiv a(\mathbf{x}, t) \exp(\mathrm{i}S(\mathbf{x}, t)/\hbar) \tag{1.2}$$

may equivalently be determined by the continuity equation

$$m\partial a^2 + \nabla \cdot (a^2 \nabla S) = 0 \tag{1.3}$$

coupled with

$$2m\partial S + (\nabla S)^2 + 2mV - \hbar^2 (\nabla^2 a)/a = 0$$
(1.4)

which we will call the quantum Hamilton-Jacobi equation.

$$V_a \equiv \frac{1}{2} \hbar^2 (\nabla^2 a) / ma \tag{1.5}$$

we call the 'quantum potential'  $V_q(\mathbf{x}, t)$ .

Among the many states in which we may prepare the quantum system there may be a set which we will call 'harmonious' states whose time development  $\psi(\mathbf{x}, t)$  have the property that  $a(\mathbf{x}, t)$  satisfies Laplace's equation

$$\nabla^2 a = 0 \tag{1.6}$$

and a set which we will call 'cohesive' states which have the property that S(x, t) satisfies Laplace's equation

$$\boldsymbol{\nabla}^2 \boldsymbol{S} = \boldsymbol{0}. \tag{1.7}$$

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These sets of states may be considered dual to each other. There may also be self-dual states for certain potentials.

Harmonious states thus have a probability density  $\rho(x, t)$ 

$$\rho = a^2 \tag{1.8}$$

which has no lumps at any time t and their phases S(x, t) satisfy the classical Hamilton-Jacobi equation

$$2m\partial S + (\nabla S)^2 + 2mV = 0. \tag{1.9}$$

For the case of the three-dimensional (n = 3) harmonic oscillator, for which

$$V(\mathbf{x}) = \frac{1}{2}m\omega^2 \mathbf{x} \cdot \mathbf{x} \tag{1.10}$$

the propagator or kernel is such a 'harmonious' state with a(x, t) a function of t alone

$$a^{2}(\mathbf{x}, t) = 1/\sin^{3}(\omega t)$$
 (1.11)

and

$$S(\mathbf{x}, t) = \frac{1}{2} m \omega [(\mathbf{x}^2 + \mathbf{x}_0^2) \cos \omega t - 2\mathbf{x} \cdot \mathbf{x}_0] / \sin \omega t$$
(1.12)

satisfies the classical Hamilton-Jacobi equation.

Cohesive states, on the other hand, have a probability density which remains unchanged as we move in time along any of the three-parameter family of paths x(y, t), which have the property that

$$\mathbf{x}'(\mathbf{y},t) = \nabla S(\mathbf{x},t)|_{\mathbf{x}=\mathbf{x}(\mathbf{y},t)} \qquad \mathbf{x}(\mathbf{y},0) = \mathbf{y}.$$
(1.13)

(Throughout this paper the prime ' denotes ordinary differentiation with respect to the argument t.) We will call such a path a 'quantum path'. There is a different 'quantum path' for each value of the three parameters y contained in  $\mathbb{R}^3$ . Thus if the probability density starts with a lump, this lump moves along the quantum path x(t) without dissipating:

$$m\partial a^2 + \nabla S \cdot \nabla a^2 = 0. \tag{1.14}$$

Since S(x, t) is not a solution of the classical Hamilton-Jacobi equation, x(t) is not a classical path (or ray). If it were, the state would be what is usually called a 'coherent' state, the state which most closely resembles a classical particle. The coherent states of the harmonic oscillator have

$$S(\mathbf{x}, t) = m\mathbf{x} \cdot \mathbf{x}'(t) \tag{1.15}$$

where x(t) satisfies the harmonic oscillator equation of motion. Thus the 'minimum uncertainty coherent' states (MUCS) (Nieto 1983) are also 'cohesive' states for the harmonic oscillator and

$$a(\mathbf{x},t) = \exp\left[-\frac{1}{2}m\omega(\mathbf{x}-\mathbf{x}(t))\cdot(\mathbf{x}-\mathbf{x}(t))/\hbar\right].$$
(1.16)

The lump is Gaussian and moves along the *classical* path x(t) without changing its shape.

In §2 we find exactly a family of 'cohesive' states for a class of systems whose *classical* equation of motion is of the form (Glauber 1966)

$$(\boldsymbol{\omega}\boldsymbol{x}(t) + \mathbf{i}\boldsymbol{m}\boldsymbol{x}'(t))' = f(\boldsymbol{\omega}\boldsymbol{x}(t) + \mathbf{i}\boldsymbol{m}\boldsymbol{x}'(t), t)$$
(1.17)

where f(z, t) is any function analytic in the complex variables z and continuous in t, and families of 'harmonious' and 'cohesive' states for the forced harmonic oscillator.

You will be unwilling to read this paper further unless the usefulness of these constructs is demonstrated. The simple harmonic oscillator has a three-parameter family of 'harmonious' states which together constitute the propagator or Green function from which the time development of all quantum mechanical wavefunctions of this system can be found exactly. The family of 'cohesive' states turns out to be the overcomplete set of MUCS. The knowledge of their time dependence again leads (Nieto 1983) to the solution of all quantum mechanical problems of the harmonic oscillator system. Section 3 shows that the time development of a given initial quantum state is found if the dynamical system has sets of 'harmonious' or 'cohesive' states in the following three cases.

(i) If the distribution, which is the limit of

$$G(\mathbf{x}, \mathbf{y}, t) = a(\mathbf{x}, \mathbf{y}, t) \exp(\mathrm{i}S(\mathbf{x}, \mathbf{y}, t)/\hbar)$$
(1.18)

as t approaches zero, gives  $\psi(x, 0)$  when convoluted with some  $C^x$  function. Here S(x, y, t) is a complete integral of the *classical* Hamilton-Jacobi equation (1.9) and a(x, y, t) satisfies the continuity equation (1.3) and Laplace's equation (1.6).

(ii) If the class of functions S(x, 0) is sufficiently extensive that a superposition of  $\psi(x, 0)$  can represent the initial state. Here  $\psi(x, t)$  is given by equation (1.2) with S(x, t) satisfying the *classical* Hamilton-Jacobi equation (1.9) with initial value S(x, 0).

(iii) If the initial state  $\psi(\mathbf{x}, 0)$  is a linear superposition of MUCS.

Such sets of states can only be found exactly for the harmonic oscillator but may be approximated by the methods of § 6.

In § 4 we extend the class of potentials for which exact 'harmonious' states and 'cohesive' states are found. There are potentials (§ 5) for which self-dual states may be found, i.e. states which are both 'harmonious' and 'cohesive'. For example, the plane-wave solution of Schrödinger's equation (1.1) for a constant potential satisfies both equation (1.6) and equation (1.7). For the two-dimensional case considered in § 5 we find potentials for which self-dual energy eigenstates exist, corresponding to each analytic function. Dual states are also found for a class of potentials in n dimensions.

Energy eigenstates can be cohesive for a reduced class of potentials

$$V(\mathbf{x}) = E - \frac{1}{2} (\nabla \times \mathbf{F} + \nabla \phi)^2 / m + \hbar^2 (\nabla^2 a) / a$$
(1.19)

where F(x) is any field and

$$\boldsymbol{\nabla}^2 \boldsymbol{\phi} = \boldsymbol{0}. \tag{1.20}$$

Finding the class of potentials which have harmonious energy eigenstates requires, however, the solution of a second-order partial differential equation which vitiates their usefulness in solving the Schrödinger equation (1.1). The dual energy eigenstates satisfy equations (1.6) and (1.7) and

$$\boldsymbol{\nabla} \boldsymbol{S} \cdot \boldsymbol{\nabla} \boldsymbol{a} = \boldsymbol{0} \tag{1.21}$$

so that, in two dimensions, a+iS is an analytic function of x+iy, independent of t. With this restriction the potential V(x) is given by

$$V = E - \frac{1}{2} (\nabla S)^2 / m.$$
(1.22)

It should be noted that harmonious states cannot be eigenstates of any operator corresponding to discrete eigenvalues. These require  $a^2(x, t)$  to be integrable and therefore zero at large distances. But harmonic a(x, t) zero at large distances is zero everywhere.

Approximations to the 'harmonious' states are given in § 6 for the general potential V(x). This involves finding a 'coherent set of natural motions' x(y, t) (Synge and Griffith 1970) for the particular potential which, for a given harmonic function a(x, t), satisfy a shooting condition:

$$a^{2}(\mathbf{x}(\mathbf{y}, +\infty), +\infty)J(\mathbf{y}, +\infty) = a^{2}(\mathbf{x}(\mathbf{y}, -\infty), -\infty)J(\mathbf{y}, -\infty)$$
(1.23)

where J(y, t) is the Jacobian of x(y, t). This differs from the WKB method (Morrette 1950) which requires initial conditions on both the position and momentum of the natural motion x(y, t). A similar approximation to 'harmonious' eigenfunctions corresponding to the continuum of energy eigenvalues is found in § 7.

The approximation to 'cohesive' states for the so-called 'harmonic potentials' is similar to the MUCS method (Nieto 1983).

## 2. Complete set of exact 'harmonious' and 'cohesive' states

Consider the quantum systems (Glauber 1966) for which the equation of motion for the Heisenberg quantum operators x(t) and p(t) can be written as

$$\boldsymbol{b}'(t) \equiv \boldsymbol{m}\boldsymbol{\omega}\boldsymbol{x}'(t) + \mathrm{i}\boldsymbol{p}'(t) = f(\boldsymbol{m}\boldsymbol{\omega}\boldsymbol{x}(t) + \mathrm{i}\boldsymbol{p}(t), t)$$
(2.1)

where f(z, t) depends on t and is an analytic function of the three complex variables z. This includes the harmonic oscillator as a special case. A MUCS |) (Nieto 1983) by definition satisfies

$$\boldsymbol{b}|\rangle = (\boldsymbol{m}\boldsymbol{\omega}\boldsymbol{x} + i\boldsymbol{p})|\rangle = (\boldsymbol{m}\boldsymbol{\omega}\langle\boldsymbol{x}\rangle + i\langle\boldsymbol{p}\rangle)|\rangle$$
(2.2)

where x and p are the coordinate and momentum operators in the Schrödinger representation.

If we choose the time-independent Heisenberg state to be a MUCS  $|\rangle$  the centroid of the Schrödinger wavefunction for this state follows the classical path

$$m\omega\langle \mathbf{x}(t)\rangle' + \mathrm{i}\langle \mathbf{p}(t)\rangle' = f(m\omega\langle \mathbf{x}(t)\rangle + \mathrm{i}\langle \mathbf{p}(t)\rangle, t)$$
(2.3)

since

$$f(\boldsymbol{m}\omega\boldsymbol{x}(t) + i\boldsymbol{p}(t), t)|\rangle = f(\boldsymbol{m}\omega\langle\boldsymbol{x}(t)\rangle + i\langle\boldsymbol{p}(t)\rangle, t)|\rangle.$$
(2.4)

The corresponding Schrödinger time-dependent state  $|t\rangle$  is defined by

$$(m\omega \mathbf{x} + \mathbf{i}\mathbf{p})|t\rangle = (m\omega \mathbf{x}(t) + \mathbf{i}\mathbf{p}(t))|\rangle \equiv \mathbf{b}(t)|\rangle$$
(2.5)

and

$$|0\rangle = |\rangle. \tag{2.6}$$

It follows that

$$\langle t | (\boldsymbol{b}^{+} - \langle \boldsymbol{b}^{+} \rangle) (\boldsymbol{b} - \langle \boldsymbol{b} \rangle) | t \rangle = \langle (\boldsymbol{b}^{+}(t) - \langle \boldsymbol{b}^{+}(t) \rangle) (\boldsymbol{b}(t) - \langle \boldsymbol{b}(t) \rangle) \rangle.$$
(2.7)

The time derivative to all orders of the function on the right-hand side of this equation may be constructed from equation (2.1) and its Hermitian adjoint. Equation (2.5) shows that at t = 0 the function and all its derivatives are zero. Thus the function is identically zero so

$$\langle t | (\boldsymbol{b}^{+} - \langle \boldsymbol{b}^{+} \rangle) (\boldsymbol{b} - \langle \boldsymbol{b} \rangle) | t \rangle \equiv 0.$$
(2.8)

The Schwartz inequality tells us that this equation can only be satisfied if  $|t\rangle$  is an eigenstate of  $b \equiv m\omega x + imp$ :

$$\boldsymbol{b}|t\rangle \equiv (\boldsymbol{m}\omega\boldsymbol{x} + \mathbf{i}\boldsymbol{p})|t\rangle = (\boldsymbol{m}\omega\langle\boldsymbol{x}(t)\rangle + \mathbf{i}\langle\boldsymbol{p}(t)\rangle)|t\rangle.$$
(2.9)

From this equation we can see that the Schrödinger wavefunction  $\langle \mathbf{x} | t \rangle$  satisfies the partial differential equation

$$\hbar \nabla \langle \mathbf{x} | t \rangle = (m\omega \langle \mathbf{x}(t) \rangle + i \langle \mathbf{p}(t) \rangle - m\omega \mathbf{x}) \langle \mathbf{x} | t \rangle$$
(2.10)

which has the solution

$$\langle \boldsymbol{x}|t\rangle = \exp\left[-\frac{1}{2}(m\omega\langle \boldsymbol{x}(t)\rangle + i\langle \boldsymbol{p}(t)\rangle - m\omega\boldsymbol{x})^{2}/\hbar m\omega\right].$$
(2.11)

The continuity equation (1.3) which may be rewritten using equation (2.9) in the form

$$(a^{2}(\langle \mathbf{x}(t)\rangle, t\rangle)' = 0$$
(2.12)

is satisfied by the modulus

$$a(\mathbf{x},t) = \exp\{\left[-\frac{1}{2}(m\omega\langle \mathbf{x}(t)\rangle - m\omega\mathbf{x})^2 + \frac{1}{2}\langle \mathbf{p}(t)\rangle^2\right]/\hbar m\omega\}.$$
 (2.13)

of this wavefunction since its phase

$$S(\mathbf{x}, t)/\hbar = 2\langle \mathbf{p}(t) \rangle \cdot (m\omega \langle \mathbf{x}(t) \rangle - m\omega \mathbf{x})/\hbar m\omega$$
(2.14)

satisfies Laplace's equation (1.6) and

$$m\langle \mathbf{x}(t) \rangle' = [\nabla S(\mathbf{x}, t)]_{\mathbf{x} = \langle \mathbf{x}(t) \rangle}.$$
(2.15)

We have used the fact that the operation of ip acting to the left on the eigenstates  $\langle x |$  of the operator x is just  $\hbar \nabla$ .

Thus  $\psi(\mathbf{x}, t)$  with amplitude and phase given by equations (2.13) and (2.14), respectively, is a 'cohesive' state of the dynamical system equation (2.1).

A three-parameter family of 'harmonious' states for the forced harmonic oscillator with Lagrangian

$$L = \frac{1}{2}m\mathbf{x}' \cdot \mathbf{x}' - \frac{1}{2}m\omega^2 \mathbf{x} \cdot \mathbf{x} + \mathbf{f}(t) \cdot \mathbf{x}$$
(2.16)

can be found exactly using S(x, y, t) the complete integral of the *classical* Hamilton-Jacobi equation (1.9) as the phase:

$$S(\mathbf{x}, \mathbf{y}, t) \sin \omega t = \frac{1}{2} m \omega \{ (\mathbf{x} \cdot \mathbf{x} + \mathbf{y} \cdot \mathbf{y}) \cos \omega t - \mathbf{x} \cdot \mathbf{y} + \mathbf{x} \cdot \int^{t} f(\tau) \sin \omega \tau \, \mathrm{d}\tau - \mathbf{y} \cdot \int^{t} f(\tau) \sin \omega (t - \tau) \, \mathrm{d}\tau - \int^{t} \int^{\tau} \sin \omega (t - \tau) f(\tau) \cdot f(\sigma) \sin \omega \sigma \, \mathrm{d}\tau \, \mathrm{d}\sigma / m \omega$$
(2.17)

and

$$a(x, y, t) = \sin^{-3/2} \omega t$$
 (2.18)

as the amplitude.

A three-parameter family of cohesive states may be found for the same Lagrangian (2.16) by simply substituting the classical paths

$$m\omega \mathbf{x}(t) + \mathbf{i}\mathbf{p}(t) = (m\omega \mathbf{x}_0 + \mathbf{i}\mathbf{p}_0) \exp(-\mathbf{i}\omega t) - \mathbf{i} \int^t \mathbf{f}(\tau) \exp(-\mathbf{i}\omega(t-\tau)) d\tau$$
(2.19)

of this Lagrangian for  $\langle \mathbf{x}(\mathbf{y}, t) \rangle$  and  $\langle \mathbf{p}(\mathbf{y}, t) \rangle$  in equations (2.11), (2.13) and (2.14) which we will then distinguish by a prime. The modulus  $a(\mathbf{x}, t)$  of equation (2.13') and the phase  $S(\mathbf{x}, t)$  of equation (2.14') together satisfy the continuity equation (1.3). By virtue of the energy equation,  $S(\mathbf{x}, t)$  satisfies the *classical* Hamilton-Jacobi equation (1.9) which is equivalent to the *quantum* Hamilton-Jacobi equation (1.4) since  $a(\mathbf{x}, t)$ satisfies Laplace's equation (1.6). Thus  $a \exp(iS/\hbar)$  satisfies the Schrödinger equation (1.1).

A generalised 'cohesive' state is one for which

$$\nabla^2 S(\mathbf{x}, t) = 2mF'(t). \tag{2.20}$$

 $\psi(x, y, z, t) = \exp(F(t)) \exp\{i[mF'(t)(\alpha x^2 + \beta y^2 + \gamma z^2)/(\alpha + \beta + \gamma)$ 

$$+2m\phi(x, y, z, t)]/\hbar\}$$
 (2.21)

is such a state which is also 'harmonious' for the potential

$$-V(x, y, z, t) = mF''(\alpha x^{2} + \beta y^{2} + \gamma z^{2})/(\alpha + \beta + \gamma) + 2m\phi$$
  
+ 
$$2m[(F')^{2}(\alpha x + \beta y + \gamma z)/(\alpha + \beta + \gamma) + \nabla\phi] \qquad (2.22)$$

where  $\phi$  is linear in x, y, z. The phase S(x, y, z, t) of  $\psi(x, y, z, t)$  satisfies equation (2.20) and the *classical* Hamilton-Jacobi equation (1.9). The corresponding continuity equation for a(x, y, z, t) is satisfied by  $\exp(F(t))$ .

### 3. Exact 'classical' evolution

The time evolution of any state of a dynamical system which possesses 'harmonious' states ( $\S$  2) may be found as follows by 'classical' means.

(i) Suppose the set of 'harmonious' states may be parametrised by the n parameters y as

$$\psi(\mathbf{x}, \mathbf{y}, t) = a(\mathbf{x}, \mathbf{y}, t) \exp(\mathrm{i}S(\mathbf{x}, \mathbf{y}, t)/\hbar)$$
(3.1)

$$\boldsymbol{\nabla}^2 \boldsymbol{a}(\mathbf{x}, \mathbf{y}, t) = 0 \tag{3.2}$$

where the derivatives  $\nabla$  are with respect to x not y. Then S(x, y, t) is a complete integral of the *classical* Hamilton-Jacobi equation (1.9). a(x, y, t) is the harmonic solution (which by hypothesis exists) of ordinary differential equations

$$2m[\ln a(\mathbf{x}(\mathbf{y},t),\mathbf{y},t)]' = -[\nabla^2 S(\mathbf{s},\mathbf{y},t)]_{\mathbf{x}=\mathbf{x}(\mathbf{y},t)}$$
(3.3)

in terms of x(y, t) given by

$$mx'(y, t) = [\nabla S(x, y, t)]_{x = x(y, t)}$$
(3.4)

$$\boldsymbol{x}(\boldsymbol{y},\boldsymbol{0}) = \boldsymbol{y}.\tag{3.5}$$

$$\psi(\mathbf{x}, t) = \int \psi(\mathbf{x}, \mathbf{y}, t) f(\mathbf{y}) \, \mathrm{d}^n y \tag{3.6}$$

is also a solution of the Schrödinger equation (1.1) for this dynamical system, for any f(y) belonging to  $C^{\infty}$ . Thus any initial state which may be represented as

$$\psi(\mathbf{x},0) = \int \psi(\mathbf{x},\mathbf{y},0) f(\mathbf{y}) \,\mathrm{d}^n \mathbf{y}$$
(3.7)

where f(y) belongs to  $C^{\infty}$ , will have its time evolution given exactly by equation (3.6). Now  $\psi(x, y, 0)$  will not necessarily be a function, as the limit of  $\psi(x, y, t)$  as t approaches zero does not necessarily exist. Indeed for the forced harmonic oscillator equations (2.17) and (2.18) it clearly does not. However,  $\psi(x, y, 0)$  need only be a distribution (it is the Dirac distribution called the  $\delta$  function for the harmonic oscillator) which has meaning when convoluted with test functions from  $C^{\infty}$  in equation (3.6).

Only for the forced harmonic oscillator have we been able to find  $\psi(x, y, t)$  exactly 'harmonious' such that  $\psi(x, 0)$  may be *any* initial state. In § 6 'harmonious' states are approximated for general dynamical systems which boast such states.

(ii) Suppose that a set of 'harmonious' states  $\psi(\mathbf{x}, t)$  equation (1.2) exists for a dynamical system. Since  $a(\mathbf{x}, t)$  is harmonic,  $S(\mathbf{x}, t)$  is a solution of the *classical* Hamilton-Jacobi equation (1.9)

$$S(x(y, t), t) = \int^{t} L(x(y, \tau), x'(y, \tau)) d\tau + S(y, 0)$$
(3.8)

determined from  $S(\mathbf{x}, 0)$  by the solution  $\mathbf{x}(\mathbf{y}, t)$  of the ordinary differential equations of motion for the Lagrangian  $L(\mathbf{x}, \mathbf{x}', t)$  of the dynamical system. Then using this  $S(\mathbf{x}, t)$  we can determine  $a(\mathbf{x}, t)$  from  $a(\mathbf{x}, 0)$  by the system of ordinary differential equations (3.3), (3.4) and (3.5) equivalent to the continuity equation (1.3). Thus  $\psi(\mathbf{x}, t)$ is derived from  $\psi(\mathbf{x}, 0)$  by solving ordinary differential equations alone. The time development of an initial state which is a linear superposition of the  $\psi(\mathbf{x}, 0)$  will be the same linear superposition of the  $\psi(\mathbf{x}, t)$ .

(iii) For a dynamical system which possesses a set of 'cohesive' states  $\psi(\mathbf{x}, t)$  given by equations (1.2) and (1.7), the time development of any initial state which is a linear superposition of  $\psi(\mathbf{x}, 0)$ , is the same linear superposition of  $\psi(\mathbf{x}, t)$ . However, we can establish the (over)completeness of  $\psi(\mathbf{x}, 0)$  (Moyal 1949) and the exact cohesiveness of  $\psi(\mathbf{x}, t)$ , i.e.  $S(\mathbf{x}, t)$  is harmonic in  $\mathbf{x}$  for all t only in the special case of the harmonic oscillator.

#### 4. Potentials which have harmonious or cohesive states

The following potential has a harmonious state

$$V(x, t) = -\partial S(x, t) - \frac{1}{2} (\nabla S(x, t))^2 / m$$
(4.1)

where

$$S(\mathbf{x},t) = \boldsymbol{\delta}(t) \cdot \mathbf{x} + l(t)(\boldsymbol{\beta} \cdot \mathbf{x})^2 + n(t)(\boldsymbol{\gamma} \cdot \mathbf{x})^2 + b(t)/\boldsymbol{\beta} \cdot \mathbf{x}$$
(4.2)

and  $\beta$  and  $\gamma$  are constant orthogonal *n* vectors such that

either 
$$\boldsymbol{\beta} \cdot \boldsymbol{\delta}(t) = 0$$
 or  $b(t) = 0$ . (4.3)

The harmonious state is given by

$$\psi(\mathbf{x}, t) = a(\mathbf{x}, t) \exp[\mathrm{i}S(\mathbf{x}, t)/\hbar]$$
(4.4)

and

$$a(\mathbf{x}, t) = g(t) + \boldsymbol{\alpha}(t) \cdot \mathbf{x} + k(t)(\boldsymbol{\beta} \cdot \mathbf{x})(\boldsymbol{\gamma} \cdot \mathbf{x}).$$
(4.5)

Equation (4.4) satisfies the Schrödinger equation (1.1) provided that a(x, t) and S(x, t) satisfy the continuity equation (1.3), since a(x, t) is harmonic and S(x, t) satisfies the

classical Hamilton-Jacobi equation (1.9). The continuity equation implies that the functions g(t),  $\alpha(t)$  and k(t) are determined by the following differential equations:

$$mk' + 3k(l\boldsymbol{\beta} \cdot \boldsymbol{\beta} + n\boldsymbol{\gamma} \cdot \boldsymbol{\gamma}) = 0$$
(4.6)

$$m\alpha' + 2n\gamma(\gamma \cdot \alpha) + 2l\beta(\beta \cdot \alpha) = -k[\gamma(\delta \cdot \beta) + \beta(\delta \cdot \gamma)]$$
(4.7)

$$mg' + g(l\beta \cdot \beta + n\gamma \cdot \gamma) = -\alpha \cdot \delta$$
(4.8)

with, additionally for the case  $b(t) \neq 0$ , the initial conditions

$$\boldsymbol{g}(0) = \boldsymbol{0} \tag{4.9}$$

$$\boldsymbol{\beta}(\boldsymbol{\alpha}(0) \cdot \boldsymbol{\beta}) - \boldsymbol{\alpha}(0)(\boldsymbol{\beta}^2) = \boldsymbol{0}. \tag{4.10}$$

Thus

$$k(t) \equiv k(0)(L(t)N(t))^{3/2}$$
(4.11)

$$\boldsymbol{\alpha}(t) \equiv -\boldsymbol{\beta}L(t) \int^{t} (k(t)\boldsymbol{\delta}(t) \cdot \boldsymbol{\gamma}/L(t)) dt + (\boldsymbol{\alpha}(0) \cdot \boldsymbol{\beta})\boldsymbol{\beta}(L(t) - 1) + (\boldsymbol{\alpha}(0) \cdot \boldsymbol{\gamma})\boldsymbol{\gamma}(N(t) - 1) + \boldsymbol{\alpha}(0)$$
(4.12)

$$g^{2}(t) = g^{2}(0)L(t)N(t) - 2L(t)N(t) \int^{t} (\boldsymbol{\alpha} \cdot \boldsymbol{\delta}(\tau)/L(\tau)N(\tau)) d\tau \qquad (4.13)$$

where we have written

$$L(t) = \exp\left(-2\boldsymbol{\beta} \cdot \boldsymbol{\beta} \int^{t} l(t) \, \mathrm{d}t/m\right)$$
(4.14)

$$N(t) = \exp\left(-2\gamma \cdot \gamma \int^{t} n(t) \, \mathrm{d}t/m\right). \tag{4.15}$$

The potential

$$V(\mathbf{x},t) = \partial S(\mathbf{x},t) - (\nabla S(\mathbf{x},t))^2 - \hbar^2 \nabla^2 a(\mathbf{x},t) / a(\mathbf{x},t)) / 2m$$
(4.16)

has an exact 'cohesive' state if S(x, t) is harmonic in x and a(x, t) is constructed in terms of an arbitrary function g(y) as follows.

Find the solutions x(y, t) of the equations

$$m\mathbf{x}'(\mathbf{y},t) = [\nabla S(\mathbf{x},t)]_{\mathbf{x}=\mathbf{x}(\mathbf{y},t)} \qquad \mathbf{x}(\mathbf{y},0) = \mathbf{y}.$$
(4.17)

Define  $a(\mathbf{x}, t)$  by

$$a(\mathbf{x}(\mathbf{y}, t), t) = g(\mathbf{y}) \qquad \text{for all } t. \tag{4.18}$$

Equation (4.16) shows that  $S(\mathbf{x}, t)$  satisfies the quantum Hamilton-Jacobi equation (1.4). For  $\psi = a \exp(iS/\hbar)$  to be a solution of the Schrödinger equation (1.1), a and S must satisfy the continuity equation (1.3) which may be rewritten

$$m\partial a^2 + \nabla S \cdot \nabla a^2 = a^2 \nabla^2 S \tag{4.19}$$

or since S(x, t) is harmonic in x

$$(a(x(y, t), t))' = 0$$
(4.20)

using equations (4.17) and (1.7). Clearly a(x, t), defined by equation (4.18), satisfies equation (4.20) for arbitrary g(y).

I have no proof that a 'harmonious' or 'cohesive' state *exists* for a given potential in general, except where they are explicitly found for the particular cases in § 2 and the less physically relevant classes given here and in § 5.

### 5. Self-dual states

The plane wave states are self-dual

$$\psi(\mathbf{x}, t) = \exp(\mathrm{i}\mathbf{k} \cdot \mathbf{x}) \tag{5.1}$$

in which the amplitude a(x, t) being constant satisfies Laplace's equation as does the phase.

In two-dimensional space there are many more self-dual states. If f(x+iy) is any analytic function of its complex argument and

$$f(x+iy) \equiv a(x, y) + iS(x, y)$$
(5.2)

then both a(x, y) and S(x, y) satisfy Laplace's equation (1.6) in two dimensions. The lines of constant a(x, y) and S(x, y) are everywhere perpendicular. Thus a(x, y) is constant in the direction  $\nabla S(x, y)$  so the continuity equation (1.3) is satisfied by a(x, y) with

$$S(x, y, t) = S(x, y) - Et.$$
 (5.3)

This S(x, y, t) satisfies the *classical* Hamilton-Jacobi equation (1.4) for the time-independent potential

$$V(x, y) = E - (\nabla S(x, y))^2 / 2m.$$
(5.4)

We have, however, only found a particular energy eigenstate, namely that corresponding to eigenvalue E for this potential.

Dual states in three dimensions can be found in a similar manner using

$$f(z + ix \cos \tau + iy \sin \tau) \equiv a(x, y, z) + iS(x, y, z)$$
(5.5)

for some  $\tau$ .

We now seek time-dependent dual states  $a(\mathbf{x}, t) \exp(iS(\mathbf{x}, t)/\hbar)$ .

(1) If S(x, t) is linear in x

$$S(\mathbf{x}, t) = m\boldsymbol{\beta}(t) \cdot \mathbf{x}$$
(5.6)

then the continuity equation (1.3) becomes

$$\partial a(\mathbf{x}, t) + \boldsymbol{\beta}(t) \cdot \boldsymbol{\nabla} a(\mathbf{x}, t) = 0.$$
 (5.7)

Therefore for  $\beta$  constant

$$a(\mathbf{x}, t) = a(\boldsymbol{\beta} \cdot \mathbf{x} - \boldsymbol{\beta} \cdot \boldsymbol{\beta} t, 0)$$
(5.8)

and the requirement that a(x, t) be harmonic in x for all t implies that a(x, 0) is linear in x. Therefore

$$a(\mathbf{x}, t) = \boldsymbol{\beta} \cdot \mathbf{x} - \boldsymbol{\beta} \cdot \boldsymbol{\beta} t.$$
(5.9)

(2) If  $\nabla S(x, t)$  is linear in x, then

$$\nabla S(\mathbf{x}, t) = m\beta(t)\mathbf{x} + m\beta(t)$$
(5.10)

where  $\mathbf{x}, \boldsymbol{\beta}(t)$  and  $\nabla S(\mathbf{x}, t)$  are *n*-column vectors.  $\boldsymbol{\beta}(t)$  is an  $n \times n$  matrix which must be traceless if  $S(\mathbf{x}, t)$  is to be harmonic. The continuity equation (1.3) becomes

$$a'(\mathbf{x}, t) + \mathbf{x}^{T} \boldsymbol{\beta}(t) \nabla a(\mathbf{x}, t) + \boldsymbol{\beta}(t) \cdot \nabla a(\mathbf{x}, t) = 0.$$
(5.11)

If a(x, t) is linear in x, then

$$\boldsymbol{\nabla}\boldsymbol{a}(\boldsymbol{x},t) = \boldsymbol{\alpha}(t) \tag{5.12}$$

which is a function of t only and equation (5.11) becomes

$$\boldsymbol{\alpha}'(t) + \boldsymbol{\beta}(t)\boldsymbol{\alpha}(t) = 0 \tag{5.13}$$

$$g'(t) + \alpha(t) \cdot \beta(t) = 0 \tag{5.14}$$

where

$$a(\mathbf{x}, t) = \boldsymbol{\alpha}(t) \cdot \mathbf{x} + \boldsymbol{g}(t). \tag{5.15}$$

(3) If the component of  $\nabla S(\mathbf{x}, t)$  parallel to  $\nabla a(\mathbf{x}, t)$  is  $mk(t)\nabla a(\mathbf{x}, t)$  then the continuity equation (1.3) becomes

$$a'(\mathbf{x}, t) + k(t) |\nabla a(\mathbf{x}, t)|^2 = 0.$$
(5.16)

If a(x, t) is linear, equation (5.15), this becomes

$$g'(t) + k(t)\boldsymbol{\alpha}(t) \cdot \boldsymbol{\alpha}(t) = 0$$
(5.17)

$$\boldsymbol{\alpha}'(t) = 0. \tag{5.18}$$

(4) There are some dual states among those given by equation (4.2) when b(t) = 0and  $\beta$ ,  $\gamma$ , l(t) and m(t) are chosen so that

$$\boldsymbol{\nabla}^{2}[l(t)(\boldsymbol{\beta}\cdot\boldsymbol{x})^{2}+\boldsymbol{m}(t)(\boldsymbol{\gamma}\cdot\boldsymbol{x})^{2}]=0.$$
(5.19)

(5) We also have the special dual states

$$a(\mathbf{x}, t) = \boldsymbol{\alpha} \cdot \mathbf{x} + \alpha(t) \exp(\boldsymbol{\alpha} \cdot \mathbf{x}) \sin(\boldsymbol{\beta} \cdot \mathbf{x} + \boldsymbol{\phi})$$
(5.20)

$$S(\mathbf{x}, t) = \boldsymbol{\beta} \cdot \mathbf{x} + \boldsymbol{\beta}(t) \exp(\boldsymbol{\alpha} \cdot \mathbf{x}) \cos(\boldsymbol{\beta} \cdot \mathbf{x} + \boldsymbol{\phi})$$
(5.21)

where

$$\boldsymbol{\alpha} \cdot \boldsymbol{\beta} = \boldsymbol{\alpha} \cdot \boldsymbol{\alpha} - \boldsymbol{\beta} \cdot \boldsymbol{\beta} = 0. \tag{5.22}$$

## 6. Approximate method for finding 'harmonious' states

A general variation of the wavefunction

$$\psi(\mathbf{x}, t) = a(\mathbf{x}, t) \exp(\mathrm{i}S(\mathbf{x}, t)/\hbar)$$
(6.1)

in the action functional

$$I = \int \left[ \frac{1}{2} \mathrm{i}\,\hbar (\psi^+ \partial \psi - \partial \psi^+ \psi) - \frac{1}{2}\,\hbar^2 \nabla \psi^+ \cdot \nabla \psi / m - V \psi^+ \psi \right] \mathrm{d}^n x \,\mathrm{d}t \tag{6.2}$$

gives the Schrödinger equation (1.1) as its exact Euler-Lagrange equation. The exact solutions of the Schrödinger equation (1.1) which extremise I will not for general potentials be 'harmonious' states. Our approximation will be to extremise I over the

restricted set of wavefunctions (6.1) for which S(x, t) satisfies the classical Hamilton-Jacobi equation (1.9). Since

$$\delta I = \frac{1}{2} \int \delta S[\partial a^2 + \nabla \cdot (a^2 \nabla S)/m] d^n x dt$$
$$-\int \delta a \{ a[\partial S - \frac{1}{2} (\nabla S)^2/m + V] - \hbar^2 \nabla^2 a \} d^n x dt$$
(6.3)

the independent variation of a(x, t) is extremised by any harmonic function a(x, t), since the square bracket in (6.3) is zero by hypothesis.

The restriction of the set of functions S(x, t) contained in  $L^2(\mathbb{R}^{n+1})$  over which I is to be extremised is given in terms of an arbitrary function  $\beta(y)$  contained in  $L^2(\mathbb{R}^n)$  as follows:

$$S(x, t) = (S_0(x, y, t) + \beta(y))_{y = y(x, t)}$$
(6.4)

where y(x, t) is the solution of the *n* algebraic equations

$$\partial_t [S_0(\mathbf{x}, \mathbf{y}, t) + \boldsymbol{\beta}(\mathbf{y})] = 0 \tag{6.5}$$

where  $\partial_i$  is the partial derivative with respect to  $y_i$  and  $S_0(x, y, t)$  is a complete integral of the *classical* Hamilton-Jacobi equation (1.9). Incidentally y(x, t) is the inverse, for each t, of x(y, t) the 'coherent' set of classical paths (Synge and Griffith 1970):

$$y(x(y, t), t) = y \qquad \text{for all } t. \tag{6.6}$$

S(x, t) is a solution of equation (1.9) for any arbitrary function  $\beta(y)$  since using equations (6.4) and (6.5)

$$\nabla S(\mathbf{x}, t) = (\nabla S_0(\mathbf{x}, \mathbf{y}, t))_{\mathbf{y} = \mathbf{y}(\mathbf{x}, t)}$$
(6.7)

$$\partial S(\mathbf{x}, t) = (\partial S_0(\mathbf{x}, \mathbf{y}, t))_{\mathbf{y} = \mathbf{y}(\mathbf{x}, t)}$$
(6.8)

 $(\nabla$  has components  $\nabla_i$  the partial derivative with respect to  $x_i$  distinguished from  $\partial_i$  the partial derivative with respect to  $y_i$ , here and later). Indeed  $S(\mathbf{x}, t)$  is the general solution of the *classical* Hamilton-Jacobi equation (1.9). The variation in  $S(\mathbf{x}, t)$  consequent on a variation of the arbitrary function  $\beta(\mathbf{y})$  is

$$\delta S(\mathbf{x},t) = (S_0(\mathbf{x},\mathbf{y},t) + \boldsymbol{\beta}(\mathbf{y}) + \delta \boldsymbol{\beta}(\mathbf{y}))_{\mathbf{y} = \mathbf{y}(\mathbf{x},t) + \delta \mathbf{y}} - (S_0(\mathbf{x},\mathbf{y},t) + \boldsymbol{\beta}(\mathbf{y}))_{\mathbf{y} = \mathbf{y}(\mathbf{x},t)}$$
(6.9)

where  $y(x, t) + \delta y(x, t)$  is the solution of

$$\partial_{\mu}(S_0(\mathbf{x}, \mathbf{y}, t) + \boldsymbol{\beta}(\mathbf{y}) + \boldsymbol{\delta}\boldsymbol{\beta}(\mathbf{y})) = 0.$$
(6.10)

Therefore using equation (6.5)

$$\delta S(\mathbf{x}, t) = \delta \beta(\mathbf{y}(\mathbf{x}, t)) \tag{6.11}$$

to lowest order in small quantities. Thus for any given harmonic a(x, t)

$$\delta I = \int \delta \beta(\mathbf{y}(\mathbf{x}, t)) [\partial a^2 + \nabla \cdot (a^2 \nabla S) / m] d^n x dt$$
(6.12)

$$= \int \delta \boldsymbol{\beta}(\boldsymbol{y}) [\partial a^2 + \boldsymbol{\nabla} \cdot (a^2 \boldsymbol{\nabla} \boldsymbol{S}) / \boldsymbol{m}]_{\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{y}, t)} J(\boldsymbol{y}, t) \, \mathrm{d}^n \boldsymbol{y} \, \mathrm{d}t$$
(6.13)

where J(y, t) is the Jacobian of the transformation x(y, t) from x to y

$$J(\mathbf{y}, t) = |\partial_{i} x_{j}|. \tag{6.14}$$

Since  $\delta \beta(y)$  is an arbitrary variation

$$0 = \int \left[ m \partial a^2(\mathbf{x}, t) + \nabla \cdot (a^2(\mathbf{x}, t)) \cdot \nabla S_0(\mathbf{x}, t) \right]_{\mathbf{x} = \mathbf{x}(\mathbf{y}, t)} J(\mathbf{y}, t) \, \mathrm{d}t \tag{6.15}$$

$$= \int (ma^{2}(\mathbf{x}(\mathbf{y},t),t)J(\mathbf{y},t))' \,\mathrm{d}t$$
 (6.16)

where we have used

$$m\mathbf{x}'(\mathbf{y}, t) = (\nabla S(\mathbf{x}, t))_{\mathbf{x}=\mathbf{x}(\mathbf{y}, t)}$$
(6.17)

from which it follows that

$$m[\ln J(y, t)]' = [\nabla^2 S(x, t)]_{x = x(y, t)}.$$
(6.18)

In deriving equation (6.18) from (6.17) we have used the fact that

$$\partial \ln \det A(t) = \operatorname{tr} A^{-1}(t) \partial A(t)$$
 (6.19)

for a matrix A(t) with elements  $A_{0k}$ , and have taken  $A_{ik}$  to be  $\partial_i x_i$  so that its determinant, equation (6.14), is J(y, t) and

$$\partial A_{ik} \equiv \partial \partial_k x_i = \partial_k x_i' = \partial_k x_j \nabla_i \nabla_j S / m \tag{6.20}$$

using equation (6.17).

Equation (6.17) requires proof. Since x(y, t) is the solution of equation (6.5), then

$$(\partial_t S_0(\mathbf{x}, \mathbf{y}, t))_{\mathbf{x} = \mathbf{x}(\mathbf{y}, t)} = \partial_t \boldsymbol{\beta}(\mathbf{y})$$
(6.21)

is independent of t and therefore

$$0 = \partial \partial_{\mu} \beta(\mathbf{y}) \tag{6.22}$$

$$=\partial[(\partial_t S_0(\mathbf{x}, \mathbf{y}, t))_{\mathbf{x}=\mathbf{x}(\mathbf{y}, t)}]$$
(6.23)

$$= \mathbf{x}'(\mathbf{y}, t) \cdot [(\nabla \partial_i S_0(\mathbf{x}, \mathbf{y}, t))_{\mathbf{x} = \mathbf{x}(\mathbf{y}, t)}] + [(\partial \partial_i S_0(\mathbf{x}, \mathbf{y}, t))_{\mathbf{x} = \mathbf{x}(\mathbf{y}, t)}].$$
(6.24)

However, differentiating the classical Hamilton-Jacobi equation (1.9) with respect to  $y_i$  gives

$$\boldsymbol{m}\partial\partial_{t}\boldsymbol{S}_{0}(\boldsymbol{x},\boldsymbol{y},t) + \boldsymbol{\nabla}\boldsymbol{S}_{0}(\boldsymbol{x},\boldsymbol{y},t) \cdot \boldsymbol{\nabla}\partial_{t}\boldsymbol{S}_{0}(\boldsymbol{x},\boldsymbol{y},t) = 0$$
(6.25)

so equation (6.24) becomes

$$[\nabla \partial_{i} S_{0}(\mathbf{x}, \mathbf{y}, t)]_{\mathbf{x} = \mathbf{x}(\mathbf{y}, t)} \cdot (m\mathbf{x}'(\mathbf{y}, t) - [\nabla S_{0}(\mathbf{x}, \mathbf{y}, t)]_{\mathbf{x} = \mathbf{x}(\mathbf{y}, t)}) = 0$$
(6.26)

and this system of n algebraic equations or  $n \times n$  matrix equation has the unique solution

$$mx'(y, t) = [\nabla S_0(x, y, t]_{x=x(y,t)}$$
(6.27)

using equation (6.6), if the determinant of its matrix is non-zero. A zero value for the determinant of the matrix  $\nabla \partial S_0$  would imply that not all of the momenta  $\nabla_i S_0$  could be varied independently, contrary to the hypothesis that  $S_0$  is a complete integral of the *classical* Hamilton-Jacobi equation (1.9). Equation (6.17) follows from equation (6.27) using equation (6.7).

Equation (6.16) means that for all y the 'shooting' equation

$$a^{2}(\mathbf{x}(\mathbf{y},+\infty),+\infty)J(\mathbf{y},+\infty) = a^{2}(\mathbf{x}(\mathbf{y},-\infty),-\infty)J(\mathbf{y},-\infty)$$
(6.28)

must be satisfied by  $S(\mathbf{x}, t)$  which is related to J by equation (6.18). We have shown that the wavefunction equation (6.1) with  $S(\mathbf{x}, t)$  restricted to satisfy the *classical* Hamilton-Jacobi equation (1.9) minimises, subject to that restriction, the action functional I equation (6.2) iff  $a(\mathbf{x}, t)$  is harmonic for all t and  $S(\mathbf{x}, t)$  satisfies equation (6.28).

If we take the action I as the natural measure of the error in any approximate solution of the Schrödinger equation, the wkb method which puts no restriction on which solution of the classical Hamilton-Jacobi equation is to be used as phase, is improved upon here where we chose precisely that solution which serves to minimise the error I. As the price for this improved accuracy only 'harmonious' state solutions may be found even though a given system may not possess such states. However, the wkb method will itself be inaccurate if the state is not approximately 'harmonious'.

If we were to lift the restriction and permit a general phase and amplitude, even lower values of I could be obtained by letting

$$a^{2}(\mathbf{x}(\mathbf{y},t),t)J(\mathbf{y},t) = a^{2}(\mathbf{x}(\mathbf{y},-\infty),-\infty)J(\mathbf{y},-\infty)$$
(6.29)

for all y and t, and letting S(x, t) satisfy the quantum Hamilton-Jacobi equation (1.4). These are coupled equations for S(x, t) and a(x, t) equivalent to the exact Schrödinger equation (1.1), since using equation (6.18) we see that equation (6.29) is another way of writing the continuity equation (1.3).

Though the wavefunction may belong to the set of harmonious states at t = 0 the *true* quantum-mechanical time development will in general take it outside this set. Thus S(x, t) satisfying the *classical* Hamilton-Jacobi equation (1.9) and the shooting equation (6.28) for harmonic a(x, t) does not in general give exact solutions of the Schrödinger equation (1.1) via equation (1.2).

The approximate time-dependent harmonious state for an arbitrary harmonic function a(x, t) is the exact solution of a variational problem: the minimisation of I subject to the restriction mentioned above. However, this variational problem is equivalent to a set of *ordinary* differential equations: the classical equations of motion

$$[\boldsymbol{\nabla}_{\mathbf{x}'}L]' - \boldsymbol{\nabla}L = 0 \tag{6.30}$$

where  $\nabla_{x'}$  is the derivative with respect to x' and L(x, x') is the Lagrangian of the system

$$L(\mathbf{x}, \mathbf{x}') = \frac{1}{2}m\mathbf{x}' \cdot \mathbf{x}' - V(\mathbf{x}).$$
(6.31)

The solutions x(y, t) for each y in  $\mathbb{R}^n$  form a coherent (Synge and Griffiths 1970) set of natural motions. The S(x, t) to which these are related by equation (6.17) is then given by

$$S(\mathbf{x}(\mathbf{y},t),t) = \int^{t} L(\mathbf{x}(\mathbf{y},t),\mathbf{x}'(\mathbf{y},t)) \,\mathrm{d}t.$$
(6.32)

The Jacobian J(y, t) may be derived from x(y, t) using equation (6.14). The initial and final  $(t = +\infty)$  conditions imposed to determine the solution are

$$\mathbf{x}(\mathbf{y},\mathbf{0}) = \mathbf{y} \tag{6.33}$$

and equation (6.28). For scattering problems, where information is given about the time-dependent states at  $t = \pm \infty$ , over a large region in x, this can be an advantage over the WKB method which imposes a condition on both the initial position and momentum of the classical path.

The solution of the classical equations of motion subject to the initial condition (6.33) and the shooting condition (6.29) is found numerically by the 'shooting' method,

as follows. Let the  $\mathbb{R}^n$  coordinate and momentum spaces be replaced by a grid of physically close points y and v respectively. We take our grid spacing to be our unit although it represents physically very small distances. Let x(y, v, t) be the solution of the classical equations of motion with initial conditions

$$\mathbf{x}(\mathbf{y}, \mathbf{v}, 0) = \mathbf{y} \tag{6.34}$$

$$\boldsymbol{x}'(\boldsymbol{y}, \boldsymbol{v}, \boldsymbol{0}) = \boldsymbol{v} \tag{6.35}$$

and the components of the matrix A(y, v, t) be given by

$$A_{ij}(y, v, t) = x_i(y + e_j) - x_i(y)$$
(6.36)

where  $x_i$  is the *i* component of x and  $y + e_i$  is the grid point adjacent to y in the positive *i* direction.

For general v the quantity

$$F(\mathbf{y}, \mathbf{v}) = a(\mathbf{x}(\mathbf{y}, \mathbf{v}, +\infty), +\infty) \det A(\mathbf{y}, \mathbf{v}, +\infty)$$
$$-a(\mathbf{x}(\mathbf{y}, \mathbf{v}, -\infty), -\infty) \det A(\mathbf{y}, \mathbf{v}, -\infty)$$
(6.37)

will not be zero as required by equation (6.28). The Newton-Raphson method replaces v by  $v + \sum e_i \varepsilon_i$  which makes  $F(y, v + \sum e_i \varepsilon_i)$  closer to zero if  $\varepsilon_i$  are the solutions of the linear equations

$$\sum F_i(\boldsymbol{y}, \boldsymbol{v})\boldsymbol{\varepsilon}_i = -F(\boldsymbol{y}, \boldsymbol{v}) \tag{6.38}$$

where

$$F_i(\mathbf{y}, \mathbf{v}) = F(\mathbf{y}, \mathbf{v} + \mathbf{e}_i) - F(\mathbf{y}, \mathbf{v}).$$
(6.39)

The repeated iteration required to find a v which zeros F(y, v) for each y makes this method more involved than the WKB method.

If the method is applied to the harmonic oscillator potential we find *exact* 'harmonious' states:

$$\psi(\mathbf{x}, \mathbf{y}, t) = \sin^{-3/2} \omega t \exp\{\frac{1}{2} m \omega [(\mathbf{x}^2 + \mathbf{y}^2) \cos \omega t - 2\mathbf{x} \cdot \mathbf{y}]/\hbar \sin \omega t\}$$
(6.40)

for every value of the variational parameters y.

I have not found numerically an exact 'harmonious' state for any other physically relevant system. The solutions to equation (6.29) for  $t = +\infty$  which we find are indeed 'harmonious' states, and moreover are the 'harmonious' states which give the least error *I*. However, to give an *exact* solution of the Schrödinger equation, equation (6.29) would have to be satisfied for all t not just at  $t = +\infty$ . The task may be more successfully pursued by those with access to even a few 'transputers'. A single 'transputer' can operate for a given y, v without communication to solve the ordinary differential equations and establish  $x(y, v, \pm\infty)$ . The result from the 'transputers' labelled  $(y, v), (y + e_j, v), (y, v + e_i)$  and  $(y + e_j, v + e_i)$  are communicated to the system which is to solve equation (6.38).

### 7. Approximate method for finding 'harmonious' energy eigenstates

These  $\psi(x) = a(x) \exp(iS(x)/\hbar)$  must be energy eigenstates corresponding to continuous eigenvalues. For

$$\int \psi^+ \psi \, \mathrm{d}^n x = \int a^2(\mathbf{x}) \, \mathrm{d}^n x \tag{7.1}$$

is supposed finite for discrete eigenvalues and infinite (Dirac  $\delta$  function) for continuous eigenvalues. But if finite, a(x) must be zero at large distances. But the only solution of Laplace's equation which is zero at large distances is

$$a(\mathbf{x}) \equiv 0. \tag{7.2}$$

The argument which shows that  $\psi(x)$  minimises the action functional

$$I = \int \left[ \frac{1}{2} \hbar^2 \nabla \psi^+(\mathbf{x}) \cdot \nabla \psi(\mathbf{x}) / m + (V(\mathbf{x}) - E) \psi^+ \psi \right] \mathrm{d}^n \mathbf{x}$$
(7.3)

over arbitrary a(x) and S(x) restricted to satisfy

$$\frac{1}{2}(\nabla S(\mathbf{x}))^2 / m = (V(\mathbf{x}) - E)$$
(7.4)

provided  $a(\mathbf{x})$  is harmonic and  $a^2(\mathbf{x}(y, \pm \infty) J(y, \pm \infty))$  are equal, is exactly the same as that of § 6 with  $S(\mathbf{x}, t)$ ,  $a(\mathbf{x}, t)$ ,  $\beta(y)$ ,  $S_0(\mathbf{x}, \mathbf{y}, t)$  and  $\mathbf{x}(y, t)$  replaced by  $S(\mathbf{x})$ ,  $a(\mathbf{x})$ ,  $\beta(y)$ ,  $S_0(\mathbf{x}, \mathbf{y}, E)$  and  $\mathbf{x}(y, \tau)$  and  $\vartheta$  operating on anything replaced by multiplication by zero. Having made such replacements we shall distinguish the equation numbers with a prime '.  $S_0(\mathbf{x}, \mathbf{y}, E)$  in terms of n-1 arbitrary constants y is the complete integral of equation (7.4) up to the additive constant. That  $\mathbf{x}(y, \tau)$ , the solution of the n-1algebraic equations (6.5'), satisfies

$$m\mathbf{x}'(\mathbf{y},\tau) = [\boldsymbol{\nabla} S(\mathbf{x})]_{\mathbf{x}=\mathbf{x}(\mathbf{y},\tau)}$$
(7.5)

does, however, require a separate proof as follows.

Since  $x(y, \tau)$  is the solution of equation (6.5'), then

$$[\partial_i S_0(\mathbf{x}, \mathbf{y}, \tau)]_{\mathbf{x} = \mathbf{x}(\mathbf{y}, \tau)} = \partial_i \boldsymbol{\beta}(\mathbf{y})$$
(7.6)

is independent of  $\tau$  and therefore differentiating with respect to  $\tau$  (indicated by  $\partial$  in this section) yields

$$0 = \partial \partial_{y} \beta(y) \tag{7.7}$$

$$=\partial([\partial_{y}S_{0}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{E})]_{\boldsymbol{x}=\boldsymbol{x}(\boldsymbol{y},\tau)})$$
(7.8)

$$= \mathbf{x}'(\mathbf{y}, \tau) \cdot ([\nabla \partial_1 \mathbf{S}_0(\mathbf{x}, \mathbf{y}, E)]_{\mathbf{x}=\mathbf{x}(\mathbf{y}, \tau)}).$$
(7.9)

This system of n-1 algebraic equations or  $(n-1) \times n$  matrix equation determines the ratios of the *n* unknowns  $\mathbf{x}'(y, \tau)$  for non-zero determinant  $|\nabla_i \partial_j S_0|$  where *i* runs over any n-1 of the *n* possible indices and *j* runs over 1 to n-1. If any of these determinants were zero this would imply that n-1 of the momenta  $\nabla S_0(\mathbf{x})$  could not be varied independently contrary to the hypothesis that  $S_0$  is a complete integral. Now  $[\nabla S_0(\mathbf{x}, y, E)]_{\mathbf{x}=\mathbf{x}(y,\tau)}$  satisfies the same n-1 equations as  $\mathbf{x}'(y, \tau)$  as may be seen by differentiating the classical Hamilton-Jacobi equation (7.4) with respect to  $y_i$  to give

$$[\boldsymbol{\nabla} S_0(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{E}) \cdot \boldsymbol{\nabla} \partial_{\boldsymbol{y}} S_0(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{E})]_{\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{y}, \tau)} = 0.$$
(7.10)

Thus

$$f(y,\tau)\mathbf{x}'(y,\tau) = [\nabla S_0(\mathbf{x}, y, E)]_{\mathbf{x} = \mathbf{x}(v,\tau)}$$
(7.11)

$$= \left[ \nabla S(\mathbf{x}) \right]_{\mathbf{x} = \mathbf{x}(\mathbf{y}, \tau)} \tag{7.12}$$

and  $f(y, \tau)$  is the proportionality factor. Since  $\tau$  is an arbitrary parameter parameterising each of the paths  $x(y, \tau)$  it may be changed to any function of  $\tau$  on each path. Let us therefore choose the parameter  $\tau$  for each path so that

$$\frac{1}{2}m\mathbf{x}'(y,\tau) \cdot \mathbf{x}'(y,\tau) - V(\mathbf{x}, y, \tau) = E$$
(7.13)

then  $f(y, \tau)$  is determined by equations (7.13), (7.4) and (7.12) to be *m* and therefore equation (7.5) follows from equation (7.12).

The harmonic oscillator is an inappropriate example to use in this case as all its energy eigenvalues are discrete. Indeed these states in the Schrödinger representation, far from being harmonic have, for the lowest-energy state, for example,

$$a(\mathbf{x}) = \exp(-\frac{1}{2}m\omega\mathbf{x} \cdot \mathbf{x}/\hbar) \tag{7.14}$$

which gives  $\hbar^2(\nabla^2 a)/ma$  equal to  $V(\mathbf{x})$  (equation (1.10)), rather than negligible compared to  $V(\mathbf{x})$ , in equation (1.4) thus allowing the  $\nabla S$  term to be zero as it should be since the phase of the lowest-energy eigenfunction is constant.

The hyperbolic paths of the Coloumb potential together with an a(x) independent of x do furnish an example where the positive energy states are approximated by  $\psi(x) = a \exp(iS(x)/\hbar)$ 

$$S(\mathbf{x}(y,t)) = \int^{t} L(\mathbf{x}(y,\tau),\mathbf{x}'(y,\tau)) \,\mathrm{d}\tau$$
(7.15)

where  $L(\mathbf{x}, \mathbf{x}')$  is the Lagrangian for the Coulomb potential.

## 8. Conclusions

The dual constructs 'harmonious' and 'cohesive' states discussed in this paper are of interest in their own right if they may be realised even approximately for a dynamical system. The 'harmonious' probability distributions have no lumps and require no quantum potential  $V_q$  (equation (1.5)) for their classical description. A lump in a 'cohesive' probability distribution, however, sticks together even when classical forces tend to pull it apart. These concepts readily generalise. The probability density of a generalised harmonious state for which a(x, t) satisfies the Helmholtz equation

$$\nabla^2 a(\mathbf{x}, t) = 2mk^2(t)a(\mathbf{x}, t)/\hbar^2$$
(8.1)

has wavelike lumps but no soliton lumps. The probability density of a generalised cohesive state which has

$$\nabla^2 S(\mathbf{x}, t) = 2mF'(t) \tag{8.2}$$

is scaled by exp(-2mF(t)) but keeps its shape as we move along the quantum path.

'Harmonious' states can be found approximately corresponding to each a(x, t) harmonic in x for all t, by solving by 'shooting' methods, the classical equations of motion with conditions (6.28) and (6.33). These minimise the quantum action functional I equation (6.2) with respect to variations over wavefunctions whose phase satisfies the *classical* Hamilton-Jacobi equation (1.9). If  $\psi(x, y, t)$  are an *n*-parameter family of 'harmonious' states corresponding to the family of harmonic functions a(x, y, t), the family of phases S(x, y, t) constitute a complete integral of the *classical* Hamilton-Jacobi equation (1.9).

The limit  $\psi(x, y, 0)$  of  $\psi(x, y, t)$  as t approaches zero gives a distribution which when convoluted with  $C^{\infty}$  functions spans our space of initial states. The time evolution of these initial states will be the  $C^{\infty}$  function convoluted with  $\psi(x, y, t)$ .

'Cohesive' states of the harmonic oscillator are minimal uncertainty coherent states which are over-complete and although not orthogonal may be used as any other representation in quantum mechanics. 'Cohesive' states for general potentials which are not *like* the harmonic oscillator (Nieto 1983) are not easily approximated. The variation of I with respect to wavefunctions in two dimensions with a phase

$$S = \sum^{\pm} \alpha_n(t) \,^{\pm} S_n(\mathbf{x}) \tag{8.3}$$

where  ${}^{\pm}S_n(x)$  are the two harmonics which are homogeneous of degree *n*, leads to the *quantum* Hamilton-Jacobi equation (1.4) together with the infinite set of equations

$$\iint \left\{ \partial a^2 + \nabla \cdot (a^2 \nabla S) \right\} \,^{\pm} S_n(\mathbf{x}) \, \mathrm{d}^2 \mathbf{x} = 0 \tag{8.4}$$

which do not provide a useful alternative approximation procedure.

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