Quantum Mechanics from an Equivalence Principle

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Abstract

The recent formulation of quantum mechanics from an equivalence principle challenges the standard interpretation of the quantum world. The reasoning behind this new formulation is investigated here, including its derivation of the Schrödinger equation. The example of the symmetric linear potential is taken, in order to verify that the energy levels derived from the new formalism are the same as those from the old, and to show the contrast between the classically predicted trajectories and the quantum trajectories derived using the Schrödinger equation. A general result for the energy levels of any possible potential is also shown.

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1 Introduction

Quantum mechanics is an unsatisfactory theory.

Not, that is, from the point of view of a practical physicist, working with the predictions of the theory from day to day. Applied with some good sense on scales from the subatomic to the cosmological, the theory makes statistical predictions accurate to a high degree, and is the basis for such wide ranging subjects as chemistry and condensed matter physics. A good record on anyone's terms.

But not when one looks deeper.

A theoretician, happy with the accurate predictions, may be unsatisfied with the domain of applicability, in particular its inherent incompatibility with another great theory of the twentieth century, general relativity. No adequate theory of quantum gravity has yet been established, and this can only be seen as a defect in the theory.

A mathematician, happy with the elegant form of Hilbert space, may be unsatisfied by the imprecise and seemingly arbitrary notions of measurement and wavefunction collapse. The jump of quantum measurement is not defined in the linear equations of the theory, but in an additional postulate, which has to rely on some good judgement in its application.

A philosopher, interested by the notions of uncertainty and determinism, may be unsatisfied that there is no agreement on the real meaning of theory. The quantum world is too murky.

These objections apply to both the relativistic theory and the non-relativistic theory. The relativistic theory increases the scope to include fields, but does not resolve these issues, and additionally introduces some problems of its own. Despite its long history, no real consensus has been reached on the answers to the problems in the non-relativistic theory, which will be the basis for this investigation.

There are two possible schemes to combat these problems with quantum theory. The first is of a 'wait and see' variety, to not worry about the interpretational difficulties now, but to hope that they will be solved or the solution to them clarified by the natural development of the theory. Schrodinger based his equation on plausibility arguments, rather than worrying about the foundations of the theory, and in this way the interpretational issues facing physics were changed completely. Dirac was a believer in this method of progress, 'expect[ing] developments in the theory which would make [the] problems look quite different. It would be a waste of time to worry overmuch about them now, especially since we get along very well in practice without solving them.'[1]

The second scheme looks differently at the development of new theory, saying that by examining the foundations of the present and either reforming or reinterpreting them, the development of the theory may be facilitated. Only by truly understanding quantum theory, that which Feynman denied anyone did by saying 'I think I can safely say that nobody today understands quantum physics', may its successors be found.

A notable example of this second scheme is the de Broglie-Bohm theory. Originated in 1927 and then developed by Bohm in the 1950s, this theory does what most students of quantum mechanics think impossible - introduce a theory of definite trajectories, in a perfectly valid manner, of which standard quantum mechanics is but the statistical result. The oddities of QM wave-particle duality is replaced by a definite particle under the influence (ie obeying deterministic equations at all times) of a guiding pilot-wave. The theory faces issues of its own, not least its 'cheap[ness]' according to Einstein and a myriad of other opponents. The pilot-wave theory was intended by de Broglie and Bohm as a starting point, a proof that trajectories and (non-local) hidden variables could be introduced into the theory without compromising its huge range of accurate predictions.

A recent development of the second scheme is Faraggi-Matone theory, based upon an 'equivalence principle'. Whilst having similarities in parts to de Broglie-Bohm theory, it cannot be viewed as an extension of it, but rather a re-examination once again of the foundations of general quantum theory.

The Schrödinger equation is usually seen as a postulate in itself, validated by its predictions rather than its derivation. But the Faraggi-Matone EP theory starts by deriving the time independent Schrodinger equation from the equivalence postulate [2]:

> For each pair W^a and W^b, there is a coordinate transformation such that $W^a(q) \to \tilde{W}^a(\tilde{q}) = W^b(\tilde{q})$.

This EP may initially look cryptic, but leads in a definite manner to the Schrodinger equation when non-relativistic approximations are taken. The derivation of the SE also sheds light on the significance of the terms contained therein: no use of the link between the wave function and probability is made, indeed the solutions are linked by a special transformation of co-ordinates to a system with vanishing energy. This transformation must exist according to the EP, giving constraints on the energy levels allowed (ie the SE with some special continuity conditions on the solutions), thus giving energy quantisation.

The important point, to be stressed again, is that none of the usual postulates of QM have been used, only the EP, and yet key predictions of standard QM have been made.

Yet the formulation is more ambitious: the derivation of the SE fits neatly in with classical Hamilton-Jacobi theory. The solutions to the SE and the transformations of co-ordinates are related to the action - not the classical action, but a quantum action involved in a quantum Hamilton-Jacobi equation which involves a quantum potential in addition to the normal potential. It is this classically unexpected quantum potential which leads to all quantum phenomena, but in contrast to de Broglie-Bohm, cannot be viewed as a guiding pilot-wave. In this way, using HJ theory, definite trajectories are introduced into quantum theory, meaning that a particle has a definite position in space at all times.

The theory goes further, with a natural extension to a relativistic formulation, and it also suggests possible links with fundamental interactions, including the origin of gravity. These are grand ambitions for any theory, so the first aim of this paper is to present an introduction to the theory, to present the careful reasoning behind it. The problems of QM are often neglected, assume to have been solved elsewhere at a prior time, relegating such notions of trajectories to past times.

However, this is not the case as has been seen with the de Broglie-Bohm theory, as well as this approach. The EP theory establishes some new foundations for QM, and can still produce many of the essential predictions of standard QM. To verify this agreement in predictions, a calculation is made using a non-standard potential - a symmetric linear potential. The classical calculation, made in Appendix B using classical HJ theory to demonstrate its applications, produces a parabolic trajectory, as can be easily pictured by considering constant forces and accelerations. The standard quantum calculation, not found in standard texts but shown in section 2, shows the use of Airy functions and the imposition of boundary conditions producing quantisation of energy levels, with the ground state not at zero energy. The quantum calculation using EP theory, in section 4, uses a vastly different method, including the utilisation of non-square integrable solution to the SE which are discarded in the standard calculation. However, the imposition of boundary conditions on the relevant quantities results once again in energy quantisation - to the same energy levels as before.

It is then shown in section 4 that the boundary conditions in the EP formulation on the function $w = \frac{\psi^D}{\psi}$, where ψ^D and ψ are linearly independent solutions to the SE, are actually equivalent to the imposition of square-integrability in the standard theory. So it has been verified that the new theory will predict the same energy levels as the standard theory for all potentials, for example the oft utilised simple harmonic oscillator.

The rest of the paper provides a background to this calculation. In order to properly understand the importance of the new interpretation, mainstream QM is examined in section 2. Then the SE, and conditions on solutions to it, are derived directly from the EP in sections 3 and 4. Further interesting applications are examined in section 5. The two appendices give further background - the first with some mathematics, specifically Wronskians and Schwarzian derivatives, and the second with Classical HJ theory. This gives insight into the theoretical foundations of classical theory, indicating the connections with the new use of HJ theory in QM.

2 Standard Quantum Mechanics

> 'There is no human knowledge which cannot lose its scientific character when men forget the conditions under which it originated, the question which it answered and the functions it was created to serve. A great part of the mysticism and superstition of educated men consists of knowledge which has broken loose from its historical moorings. (Benjamin Farrington [3])'

Quantum Mechanics (QM) is one of the most successful scientific theories in history, illuminating some of the darkest recesses of physics. It is difficult to overestimate its impact on modern science and the modern world. But despite its long history, QM still faces problems of interpretation and implementation, with many scientists practising this mysticism in interpreting it, while other valid scientific arguments are rejected for allegedly being mystical. QM is unsatisfactory in that it is still a controversial subject. There are many good references on the foundations of QM, from the mathematical [4] to the philosophical [5], so the aim here is to develop a little understanding in order to emphasise the contrast with the new EP formulation, and as such the discussion will be limited to the non-relativistic theory without fields.

2.1 The postulates and probability

> 'Physicists display an extraordinary confidence in the status of quantum mechanics coupled with a general reluctance to discuss its implications ... one finds there is not one Copenhagen interpretation [but in its place] a kind of umbrella under which a host of different, often contradictory positions coreside.[6]'

An introductory course to QM often utilises a set of postulates as the basis of the theory (similar to [7]):

> 1) The quantum state of a point particle in one dimension is represented by a complex-valued wave function $\psi(x)$ that can be normalised to one ie $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$.
>
> 2) Any physical quantity A that can be measured is represented by a linear differential operator $\hat{A}$ that acts on the wave functions and is self-adjoint.
>
> 3) The only possible result of measuring an observable is one of the eigenvalues of the operator that represents it.
>
> 4) Assuming no degeneracy and discrete eigenvalues, if the quantum state is $\psi(x)$, the probability that a measurement of A will yield a particular eigenvalue a_n is $|\alpha_n|^2$, where α_n are the coefficients in the expansion
>
> $$\psi(x) = \sum_{n=1}^{\infty} \alpha_n u_n(x)$$
>
> of the wave function as a linear combination of the normalised eigenfunctions of $\hat{A}(x)$.

5) The state function evolves in time according to the time-dependent Schrodinger equation, where the Hamiltonian operator is obtained from the classical energy expression by replacing the momentum and position by their corresponding operators.

These postulates can be extended from a wave function representation to a more abstract vector space and to encompass more dimensions and particles, but the basic wave function is illustrative here. Schrödinger initially interpreted the wave function as representing the density of matter in some way, and it was only with Born that the idea of a probability wave, giving the likelihood of finding a particle at a position, came into use [8]. So the wave function is inherently tied to the notion of probability and hence when its norm squared is integrated over all space or all possibilities, the result must be unity. In calculations, this connection with probability is used to discard divergent solutions, which would otherwise make it impossible to normalize the wave function, thus resulting in the usual two independent solutions to a second order ordinary differential equation being reduced to just the one (see section 7.1). For example, in the standard series solution of the simple harmonic oscillator, the series has to terminate to stop the full solution diverging as x increases, thus producing the Hermite polynomials and equi-spaced energy levels. This reduction to a single solution is not a result of the SE itself, but of the interpretation placed upon it.

A pragmatic use of the postulates results in a very successful theory, pragmatic being when there is a clear line between the microscopic quantum world and the macroscopic experimental apparatus (a rather difficult line to draw for a cosmologist). A large array of key phenomena are accounted for in this manner, including the quantisation of energy levels and quantum tunnelling into classically forbidden regions, as long as the probabilities in the predictions are taken to refer to the relative frequencies of measurements taken a sufficiently large number of times. The theory is so successful that any new theory must agree with the predictions of the old to a very high degree of precision, almost to the extent of it being inconceivable that the new would be any different from the old. For example, the addition of a non-linear term to the SE would have to be within such small upper limits, it would run into problems of its own.

2.2 The symmetric linear potential

As an example of the use of quantum mechanics, the symmetric linear potential will be taken. This is an unusual potential, not usually found in the literature but which is illustrative of the steps taken in following through a calculation. The discarding of solutions which are not normalizable, due to the incompatibility with the probability interpretation of the wave function, is especially clear.

The Schrödinger equation for the potential as shown in Figure 1 is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha|x|\psi = E\psi \tag{2.1}$$

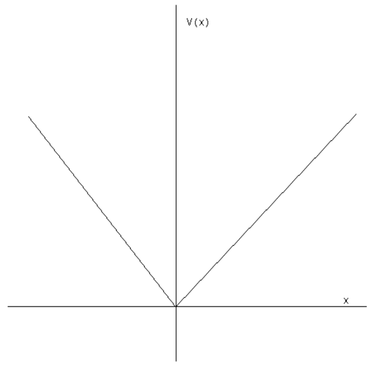

Figure 1: The symmetric linear potential

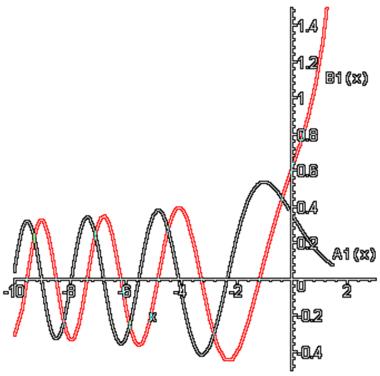

Figure 2: The Airy functions Ai(x) and Bi(x)

For $x > 0$, the substitution $y = \beta(\alpha x - E)$ where $\beta^3 = \frac{2m}{\hbar^2\alpha^2}$, produces

$$\frac{d^2\psi}{dy^2} - y\psi = 0 \tag{2.2}$$

This equation can be solved by a series solution:

$$\psi = \sum_{n=0}^{\infty} a_n y^n$$

producing the recursion relation

$$\frac{a_{n+3}}{a_n} = \frac{1}{(n+2)(n+3)}$$

The general solution of equation (2.2) is $\psi = Af(y) + Bg(y)$, where $f(y) = 1 + \frac{y^3}{6} + \frac{y^6}{180} + \cdots$ and $g(y) = y + \frac{y^4}{12} + \frac{y^7}{504} + \cdots$. These series converge for all y.

The equation 2.2 can also be recognised as the Airy equation, with two linearly independent solutions given by $Ai(y)$ and $Bi(y)$[9], as shown in Figure 2. The general solution in terms of these solutions is

$$\psi_{x>0} = A_1 Ai\left[\beta(\alpha x - E)\right] + B_1 Bi\left[\beta(\alpha x - E)\right]$$

For $x < 0$, the equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha x\psi = E\psi$$

The substitution $y = \beta(-\alpha x - E)$ leads to the same Airy equation, giving the general solution for $x < 0$ as

$$\psi_{x<0} = A_2 Ai\left[\beta(-\alpha x - E)\right] + B_2 Bi\left[\beta(-\alpha x - E)\right]$$

The boundary conditions of the problem must now be imposed:

1) At $x = 0$, $V(x)$ is continuous and so ψ and ψ' at least must also be continuous.

2) The solution must satisfy $\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$, ie any divergent solutions for $x \to \pm\infty$ must be discarded.

The Bi functions are divergent as $x \to \infty$, so condition 2) results in $B_1 = B_2 = 0$. Condition 1) implies the two equations:

$$A_1 Ai(-\beta E) = A_2 Ai(-\beta E) \tag{2.3}$$
$$A_1 Ai'(-\beta E) = -A_2 Ai'(-\beta E) \tag{2.4}$$

with the prime denoting differentiation with respect to x. Therefore,

$$\text{If } A_1 \neq -A_2 \Rightarrow Ai'(-\beta E) = 0$$

$$\text{If } A_1 = -A_2 \Rightarrow Ai(-\beta E) = 0$$

For the first case, as the zeros of Ai and Ai' do not coincide, $A_1 = A_2$. If $Ai(z) = 0$ for $z = -\gamma_i$ and $Ai'(z) = 0$ for $z = -\delta_i$, then:

$$E = \frac{\gamma_i}{\beta} \text{ or } E = \frac{\delta_i}{\beta}$$

The first few wave functions are plotted in figure 3. As the first zero of either $Ai(z)$ or $Ai'(z)$ is below zero, the ground state energy is greater than zero. Successive solutions in increasing energy can be seen to be alternative even and odd, with all solutions of definite parity as the potential is symmetric.

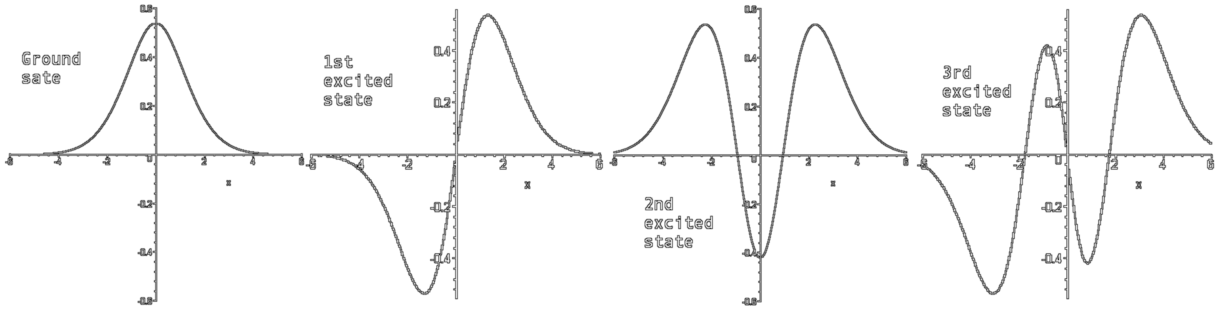

Figure 3: Wave functions for the lowest energy states for the symmetric linear potential

2.3 Further analysis

Application of the pragmatic theory has yielded a quantized energy spectrum for the symmetric linear potential, as it does for other potentials like the potential well and simple harmonic oscillator. But further analysis of the theory is necessary, as the postulates stated above are not necessarily the only ones which would make an accurate prediction for the energy levels of the symmetric linear potential (indeed, the EP calculation made later is direct evidence of that). Furthermore, this interpretation gives very little clue to the meaning, sense or world view of the theory.

The analysis depends on the judgement of whether or not the wave function is complete - whether it and its statistical predictions are the most complete description of the system possible. Einstein answered this question in the negative, seeing the statistical nature of QM as a result of the incompleteness of the wave function, whilst at the same time accepting the statistical predictions as valid.

> 'I am, in fact, firmly convinced that the essentially statistical character of contemporary quantum theory is solely to be ascribed to the fact that this (theory) operates with an incomplete description of physical systems.'[5]

If the wave function is judged as incomplete, one or more hidden variables may fill the gap to provide a complete description.

The Copenhagen interpretation is an example of the much more common completeness school. There are a large number of variations on the Copenhagen view, but a central issue in all is that the whole entity must be considered, the apparatus and the observed quantum system. There is little sense in referring to the quantum system on its own without specifying the equipment being used to make measurements on it, thus making the simultaneous reference to complementary attributes such as position and momentum meaningless as both cannot be simultaneously measured. The need for classical language to describe the world is reflected in the apparatus being regarded as in a classical realm, so that unequivocal statements can be made about readings and results, although this does leave a hazy distinction as to where the apparatus / system divide actually lies.

An example of an alternative interpretation, this time of the incompleteness school, is the de Broglie-Bohm approach. The statistical predictions of QM are left unchanged, but the assertion that this disallows definite trajectories is rejected. Indeed, Bohm used this approach as a counter example to prove that the many theorems that hidden variables were disallowed by QM were flawed. A good introduction to the formalism used can be found by Holland [10], and Bell also argues the case [5]. The only hidden variable introduced is the position, so different initial positions give different final positions. All measurements really come down to measurements of position, for example in the Stern-Gerlach experiment the spin of a particle is 'measured' by its deflection in a magnetic field. The central idea is that of the pilot-wave: the particle follows a definite path in space, being guided by a quantum potential / pilot-wave. It is the nature of this quantum potential which gives rise to the unusual quantum behaviour, as the classical prejudice that a particle in field-free space must move in a straight line must be left behind. But even though a particle may have a definite position and momentum, these cannot be measured directly as the imposition of apparatus changes the quantum potential. This results in one of the theory's greatest weaknesses, its inability to be experimentally verified as the stand out feature of trajectories cannot be measured. Many a physicist reject its ideas by the oft referenced Occam's razor: 'Entia non sunt multiplicanda praeter necessitatem'[8].

Many a comparison is made between the multitude of interpretations of QM and the very fixed interpretation of relativity. The theories of relativity are loosely based on single principles, the principle of relativity or Einstein's equivalence principle. Compared to these, the axioms of QM seem like an ad hoc collection of rules to make a theory work, even though extremely well at that. This in itself is evidence that QM is still a work in progress, and if QM could be based or derived from a single principle then the problems of interpretation and implementation would all fall into place. The Faraggi-Matone theory of QM from an equivalence principle does this and the derivation of the Schrodinger equation sheds a different light on the problems of interpretation.

3 The Equivalence Postulate

3.1 From CM, through GR, to an EP

The HJ equation in classical mechanics (CM) is derived by considering a change of variables, a canonical transformation of coordinates and momenta, to a system with a vanishing Hamiltonian (see section 8). This vanishing Hamiltonian implies constant coordinates and momenta in this new frame, but other physical comments are difficult to relate to due to the mixing of coordinates and momenta inherent in the transformation of form:

$$Q = Q(q, p, t) \text{ and } P = P(q, p, t)$$

In [11], it is suggested to look at the transformation in a different manner, to ask if a similar transformation exists if p (and t) are treated as dependent variables on q. It should first be noted that the action S is itself not the transformation of variables, only the 'generator' of it. The explicit form of the transformation

$$Q = Q(q)$$

cannot be found, even if the solution to the equations of motion have been found, as the question itself is nonsensical in this framework: the Q is a point / constant, so the mapping to a continuous q cannot be produced.

So when p is treated as a dependent variable, $p = \frac{\partial S_0}{\partial q}$, the transformation to the free frame cannot be found. In [11], this is noted to be the result of the privilidged nature of the rest frame in CM, as a coordinate transformation can link all frames except the rest frame. But what if we search for a formulation which does not exhibit this privilidged rest frame? From this question arises the formulation of an equivalence principle, similar to that Einstein used as the basis for general relativity, a new EP that insists that transformations between all frames of differing $W(q) = V(q) - E$ must exist.

Einstein's first statement of his Equivalence Principle (EP) was in his 1911 paper

> 'We arrive at a very satisfactory interpretation of this law of experience, if we assume that the systems K and K' are physically equivalent, that is, if we assume that we may as well regard the system K as being in a space free from gravitational fields, if we then regard K as uniformly accelerated.'[12]

This, taken in a stronger form, means that 'in any and every local Lorentz frame, anywhere and anytime in the universe, all the laws of physics must take on their familiar ... forms'[12]. Whilst General Relativity (GR) may not be deduced directly from this statement, it does seem to be the only metric theory that embodies this EP completely. From this follows the geometric interpretation of gravity and the curved spacetime phenomenon. Nearly a century later, the EP is either worshiped as a great foundation of physics or eschewed as merely a statement that proved useful in the original formulation of GR. However, a re-examination of the EP, formulated in a different fashion but still following the original sentiment, can prove fruitful.

If two separate and distinct physical systems are governed by the same physical laws, then a potential function should be able to be transformed from one to the other by a simple coordinate transformation. This suggests the following strong formulation of an equivalence principle:

> For each pair W^a and W^b, there is a coordinate transformation such that $W^a(q) \rightarrow \tilde{W}^a(\tilde{q}) = W^b(\tilde{q})$[2].

where $W(q) = V(q) - E$, $V(q)$ being the potential function and E the energy.

An immediate result of this principle is that a coordinate transformation can be found connecting any system with one of vanishing energy, the $W(q) = 0$ system. This, as discussed before, will be explicitly shown to be incompatible with the classical stationary Hamilton-Jacobi equation (CSHJE). But first a note should be made of the contrast between this EP and that of Einstein. In GR, a coordinate transformation can balance a gravitational field at a point, making the geometry locally flat ie at a point and the infinitesimal area around it. But this new EP applies globally, not just applying to curvature at a point, but to all potentials in all space.[13] In GR, this is impossible as the space metric is independent of the coordinate system used. But the new formulation has a different approach.

3.2 Applying the EP

The EP relies only on the existence of a potential function, a value for the energy of the system, and a coordinate transformation between systems. There are two aspects to the derivation of the Quantum Stationary Hamilton-Jacobi equation (QSHJE): the first is the connection with classical theory, and modifications of equations contained therein; the other is the properties of $W(q)$ itself, which must hold for the EP to be satisfied. These two aspects, though not entirely independent, lead to two inter-dependent routes to the QSHJE.

3.2.1 Modifying the CSHJE

Classical mechanics has a large sphere of applicability, so it seems natural to start from classical equations of motion and add extra terms to account for quantum behaviour. The most notable example of this is in de Broglie-Bohm theory when the quantum motion can be expressed in terms of Newton's 2nd law with an extra term or in an HJ framework also with an extra term [10].

Use of the reduced action S_0 is made in classical mechanics, where S_0 satisfies the CSHJE (see section 8):

$$\frac{1}{2m}\left(\frac{dS_0}{dq}\right)^2 + W(q) = 0$$

where $W(q) = V(q) - E$.

The transformations considered here will be 'v-transformations', which are locally invertible coordinate transformations defined by:

$$q \rightarrow \tilde{q} = v(q) \text{ AND } \tilde{S}_0(\tilde{q}) = S_0(q(\tilde{q}))$$

It is this last statement about the transformation of $S_0(q)$ that fixes the transformational properties of $W(q)$ and leads directly to the derivation of the Quantum Stationary Hamilton Jacobi Equation and the Schrodinger Equation.

But first is the question of whether the CSHJE is compatible with the EP. The CSHJE must hold for all choices of generalised coordinates q. Therefore, under a coordinate transformation, $W(q)$ must transform in the same manner as $\left(\frac{dS_0}{dq}\right)^2$, ie homogeneously as a quadratic differential.

$$\Rightarrow \tilde{W}(\tilde{q}) = f(\tilde{q})W(q)$$

where $f(\tilde{q}) = \left(\frac{dq}{d\tilde{q}}\right)^2$

However, no homogeneous transformation can connect $\tilde{W} = 0$ to $W \neq 0$. Therefore, the EP is incompatible with the CSHJE as it stands.

A solution to this conundrum is to add an extra term to the CSHJE:

$$\frac{1}{2m}\left(\frac{dS_0}{dq}\right)^2 + W(q) + Q(q) = 0 \tag{3.1}$$

where Q(q) is a 'quantum potential'. There are conditions on this equation - it must reduce to the classical equation in a suitable limit, it must be consistent under v-transformations, and it must satisfy the EP. The identity 7.11 in section 7.2.3:

$$\left(\frac{dS_0}{dq}\right)^2 = \frac{\beta^2}{2}\left(\{e^{\frac{2i}{\beta}S_0}, q\} - \{S_0, q\}\right)$$

where $\{S_0, q\}$ is the Schwarzian Derivative of S_0 with respect to q and β is a dimensional constant), produces

$$W(q) + Q(q) = \frac{\beta^2}{4m}\left[\left(-\{e^{\frac{2i}{\beta}S_0}, q\} + \{S_0, q\}\right)\right]$$

A natural solution to this would be to identify $W(q)$ with the expression $-\frac{\beta^2}{4m}\{e^{\frac{2i}{\beta}S_0}, q\}$ and Q(q) with $\frac{\beta^2}{4m}\{S_0, q\}$. This satisfies all the properties necessary, and can be shown to be unique [11]. This gives the QSHJE

$$W(q) = -\frac{\beta^2}{4m}\{e^{\frac{2iS_0}{\beta}}, q\} \tag{3.2}$$

or equivalently:

$$\frac{1}{2m}\left(\frac{dS_0}{dq}\right)^2 + V(q) - E + \frac{\beta^2}{4m}\{S_0, q\} = 0 \tag{3.3}$$

3.2.2 Properties of the potential

By analysing the transformation properties of $W(q)$, the expression for W(q) can be derived without any reference to the Hamilton-Jacobi framework. The physics of the EP may be obscured by deriving the expression with reference to the reduced action.

The EP implies that a transformation of coordinates can be made to a free system with vanishing energy ie to $W(q) = 0$. As shown above, this cannot be done by only homogeneous terms in the transformation.

$$q \to \tilde{q}(q) \text{ and } W \to \tilde{W}(\tilde{q})$$

$$\text{ie Equivalence Principle } \Rightarrow \tilde{W}(\tilde{q}) = f(\tilde{q})W(q) + (q; \tilde{q})$$

where $(q; \tilde{q})$ is the inhomogeneous term. An example would be for $q = q_0$, the coordinate system corresponding to the system with vanishing energy, $W(q_0) = 0$. This gives

$$\tilde{W}(\tilde{q}) = 0 + (q_0; \tilde{q})$$

$$\Rightarrow W(q) = (q_0; q)$$

Therefore, the EP implies that the allowed expression for $W(q)$ is exactly the inhomogeneous term in the transformation.

The homogeneous transformation properties of $W(q)$ are given by the function $f(\tilde{q})$. In the previous section, $W(q)$ was found to transform as a quadratic differential due to the invariance of S_0. But the expressions in the HJ equation are argued from their own principles: $\left(\frac{dS_0}{dq}\right)^2$ appears because the expression for T, the kinetic energy, in classical mechanics is $\frac{p^2}{2m}$ or $T = T(v^2)$. In Landau and Lifshitz[14], an argument is made for the classical Lagrangian L to be $L = L(v^2)$ for an inertial frame with homogeneous and isotropic space and time. With the same classical considerations of homogeneity and isotropy, the transformation for $W(q)$ (the homoegeneous part) must be as a quadratic differential:

$$f(\tilde{q}) = \left(\frac{dq}{d\tilde{q}}\right)^2$$

So the transformational properties of $W(q)$ and $S_0(q)$ result from the same physical arguments. This is a very non-relativistic reasoning, so perhaps a relativistic derivation would depart here, with a different transformation for $W(q)$, and then another consideration for non-inertial, non-homoegeneous and non-isotropic space.

But for the present, this gives an expression for the transformation of $W(q)$:

$$W^b(q^b) = \left(\frac{dq^a}{dq^b}\right)^2 W^a(q^a) + (q^a; q^b) \tag{3.4}$$

A similar expression can be made for $W^a(q^a)$ in terms of $W^b(q^b)$:

$$W^a(q^a) = \left(\frac{dq^b}{dq^a}\right)^2 W^b(q^b) + (q^b; q^a) \tag{3.5}$$

Substituting 3.4 in 3.5, and that $\left(\frac{dq^a}{dq^b}\right)^2 \left(\frac{dq^b}{dq^a}\right)^2 = 1$, gives

$$(q^b; q^a) = -\left(\frac{dq^b}{dq^a}\right)^2 (q^a; q^b)$$

This can be seen to be identical to the property of the Schwarzian derivative (from equation 7.9):

$$\{y, x\} = -\left(\frac{dy}{dx}\right)^2 \{x, y\}$$

Using

$$W^b(q^b) = \left(\frac{dq^c}{dq^b}\right)^2 W^c(q^c) + (q^c; q^b)$$

in 3.5, and substituting 3.4 in the resulting expression, gives the cocycle condition:

$$(q^a; q^c) = \left(\frac{dq^b}{dq^c}\right)^2 \left[(q^a; q^b) - (q^c; q^b)\right] \tag{3.6}$$

This is identical to the chain rule property of the Schwarzian derivative (from equation 7.10):

$$\{x, z\} = \left(\frac{dy}{dz}\right)^2 [\{x, y\} - \{z, y\}]$$

It can also be shown that $(\tilde{q}; q)$ is invariant under a Mobius transformation of $\tilde{q}$:

The inhomogeneous term of the transformation shares many properties of the Schwarzian derivative, the most important of which is its invariance under Möbius transformations. It can be shown [13] that the cocycle condition in equation 3.6 uniquely determines the Schwarzian derivative, up to a multiplicative factor, a global constant and a coboundary term. Therefore, as before in equation 3.2

$$W(q) = -\frac{\beta^2}{4m}\{q^0, q\} \tag{3.7}$$

where q^0 is the trivialising coordinate corresponding to the system with W=0.

3.3 Deriving the Schrödinger Equation

Deriving the Schrödinger Equation from equation 3.7 is a simple matter of using the properties of the Schwarzian derivative. As shown in section 7.2.4, the SD is intimately connected to 2nd order differential equations and ratios of their independent solutions. These properties imply the equation

$$y'' - \frac{2m}{\beta^2} W(q) y = 0 \tag{3.8}$$

$$\Rightarrow -\frac{\hbar^2}{2m} y'' + V(q) y = E y \tag{3.9}$$

where $q_0(q) = \frac{y_1(q)}{y_2(q)}$, $y_1(q)$ and $y_2(q)$ being two linearly independent solutions of equation 3.8 and β has been identified as $\hbar$. As the Schwarzian derivative is invariant up to a Möbius transformation, the general form of q^0 (ie $y(q)$) is

$$q^0(q) = \frac{A y_1(q) + B y_2(q)}{C y_1(q) + D y_2(q)}$$

From the identification $w = \frac{\psi^D}{\psi}$, a solution to the SE can be expressed as

$$y(q) = \frac{1}{\sqrt{S_0'}} \left(Ae^{-\frac{i}{\hbar}S_0} + Be^{\frac{i}{\hbar}S_0} \right)$$

This is in contrast to the de Broglie / Bohm approach, where the wave function was identified as [10]:

$$y(q) = Re^{\frac{i}{\hbar}S_0}$$

This has important implications, as when ψ is proportional to a real function (as for bound states), the result is not that S_0=const, which would violate the EP.

3.4 Relativistic extension

In [11], the basic relativistic version of the Schrödinger equation, the Klein-Gordon equation, is derived by changing from the non-relativistic expression $W(q) = V(q) - E$ to the relativistic version:

$$W_{rel}(q) = \frac{1}{2mc^2} \left[m^2c^4 - (V - E)^2 \right]$$

However, it should also be possible to derive the relativistic equation via the original method. If one insists that $(W(q))^2$ transforms as a quadratic differential with an inhomogeneous term, then the same derivation will result in:

$$\{q^0, q\} = \alpha \left((V - E)^2 + \gamma \right) \tag{3.10}$$

Considering the transformational properties of $W(q) = V(q) - E$ may tell us more than just changing the expression for $W(q)$. Equation 3.10 is related, in a similar manner to before, to the second order differential equation:

$$\frac{d^2y}{dq^2} + \frac{\alpha}{2} \left((V - E)^2 + \gamma \right) y = 0$$

which is compatible with the Klein-Gordon equation:

$$-c^2\hbar^2 \frac{d^2\phi}{dq^2} + (m^2c^4 - E^2 + 2EV - V^2)\phi = 0$$

Further relativistic considerations are made in [13], where higher dimensional Euclidean and Minkowskian spaces are shown to have a cocyle condition, with the relativistic quantum Hamilton-Jacobi equation applying in these more general situations.

4 Conditions on solutions to the SE and applications of the formalism

The derivation of the Schrödinger equation (SE) from a first principle is an achievement in itself, but it is certainly not the end of the story. As shown in section 2, the key results of Quantum Mechanics (QM) do not blindly follow from the SE, and other postulates are needed to impose conditions on the solutions. These postulates are usually founded on a pragmatic probabilistic interpretation—thus discarding any troubling infinities or divergent solutions.

Thus far, however, no use of the probabilistic interpretation has been used, as this formulation is supplanting the previous mathematically precise but physically hazy axioms. The Equivalence Principle on its own can be shown to imply all conditions necessary to derive a quantised energy spectrum, and other quantum phenomena.

4.1 Continuity conditions

The EP implies the existence of the Quantum Stationary Hamilton Jacobi Equation 3.2 and the Schrödinger equation 3.9. Further, the EP implies that the only permissible w's are those that allow the derived equations to exist, where $w(q) = q_0(q) = \frac{\psi^D}{\psi}$ with ψ and ψ^D being independent solutions to the SE. The main conditions come from the existence of the Schwarzian Derivative in:

$$\{w, q\} = \frac{-4m}{\hbar^2} W(q)$$

The definition of the SD is

$$\{w, z\} = \left(\frac{w''}{w'}\right)' - \frac{1}{2}\left(\frac{w''}{w'}\right)^2$$

which is undefined if $w' = 0$, so $w \neq$ const. The obvious conditions on w are [11]:

$w \neq$const, $w \in C^2(R)$, and $\partial_q^2 w$ differentiable on R

But there is a further condition on the continuity of the function w. As explained further in [11], the SD exhibits symmetry under inversion, so the QSHJE can also be derived in the form:

$$\{w, q^{-1}\} = -\frac{4m}{\hbar^2} q^4 W(q)$$

So the continuity of the function w at 0 then maps to continuity at $\pm\infty$. This means that the function must be continuous on the extended real line, including the points at ∞. This translates as the condition:

$$\begin{aligned} w(-\infty) &= w(+\infty) \text{ for } w(-\infty) \neq \pm\infty && (4.1) \\ OR &= -w(+\infty) \text{ for } w(-\infty) = \pm\infty && (4.2) \end{aligned}$$

4.2 Example of implementing the continuity conditions

The continuity conditions in equation 4.1 and 4.2 seem very different from the conditions imposed by the probability interpretation. It would seem unlikely that predictions of energy levels made by the new formalism would coincide with those of the old, so an explicit calculation is necessary to see whether the predictions are compatible.

4.2.1 The linear potential

The linear potential was solved using the standard quantum mechanical formalism in section 2.2 The square integrability was used at an early stage to discard any solutions involving $Bi(y)$, which considerably simplified the problem. When using the new formalism, however, this simplification is not allowed - the continuity conditions at infinity have to be applied instead.

The beginning of the calculation is similar to that in section 2.2. Using a suitable substitution , the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha|x|\psi = E\psi$$

is reduced to the Airy equation, $\frac{d^2\psi}{dy^2} - y\psi = 0$, giving rise to a general solution in terms of Airy functions:

$$\psi_{x>0} = A_1 Ai\left[\beta(\alpha x - E)\right] + B_1 Bi\left[\beta(\alpha x - E)\right]$$

$$\psi_{x<0} = A_2 Ai\left[\beta(-\alpha x - E)\right] + B_2 Bi\left[\beta(-\alpha x - E)\right]$$

Due to the invariance of the Schwarzian derivative with respect to Möbius transformations, any linear combination of solutions can be taken. As the potential is symmetric, a simplifying route is to take one solution as an even function of x, and the dual solution to be odd, guaranteeing that ψ and ψ^D are linearly independent.

$$\psi_{x>0} = AAi\left[\beta(\alpha x - E)\right] + BBi\left[\beta(\alpha x - E)\right]$$

$$\psi_{x<0} = AAi\left[\beta(-\alpha x - E)\right] + BBi\left[\beta(-\alpha x - E)\right]$$

$$\psi^D_{x>0} = CAi\left[\beta(\alpha x - E)\right] + DBi\left[\beta(\alpha x - E)\right]$$

$$\psi^D_{x<0} = -\left(CAi\left[\beta(-\alpha x - E)\right] + DBi\left[\beta(-\alpha x - E)\right]\right)$$

Continuity conditions at $x = 0$ for ψ, $\frac{d\psi}{dx}$, ψ^D and $\frac{d\psi^D}{dx}$ give

$$\begin{aligned}
AAi(-\beta E) + BBi(-\beta E) &= AAi(-\beta E) + BBi(-\beta E) && (4.3)\\
\alpha\beta AAi'(-\beta E) + \alpha\beta BBi'(-\beta E) &= -\alpha\beta AAi'(-\beta E) - \alpha\beta BBi'(-\beta E) && (4.4)\\
CAi(-\beta E) + DBi(-\beta E) &= -CAi(-\beta E) - DBi(-\beta E) && (4.5)\\
\alpha\beta CAi'(-\beta E) + \alpha\beta DBi'(-\beta E) &= \alpha\beta CAi'(-\beta E) + \alpha\beta DBi'(-\beta E) && (4.6)
\end{aligned}$$

Equations 4.4 and 4.5 imply

$$AAi'(-\beta E) + BBi'(-\beta E) = 0$$

$$CAi(-\beta E) + DBi(-\beta E) = 0$$

The other condition to impose is of continuity on the extended real line of $w = \frac{\psi^D}{\psi}$.

$$w_{x>0} = \frac{CAi\left[\beta(\alpha x - E)\right] + DBi\left[\beta(\alpha x - E)\right]}{AAi\left[\beta(\alpha x - E)\right] + BBi\left[\beta(\alpha x - E)\right]}$$

$$w_{x<0} = \frac{-\left(CAi\left[\beta(\alpha x - E)\right] + DBi\left[\beta(\alpha x - E)\right]\right)}{AAi\left[\beta(\alpha x - E)\right] + BBi\left[\beta(\alpha x - E)\right]}$$

As x increases, $Ai(x)$ approaches zero, and $Bi(x)$ increases. Therefore

$$lim_{x\to\infty} w = \frac{D}{B}$$

$$lim_{x\to-\infty} w = -\frac{D}{B}$$

Therefore, for

$$\begin{aligned} w(-\infty) = &\quad w(+\infty) \text{ for } w(-\infty) \neq \pm\infty \\ OR &\quad -w(+\infty) \text{ for } w(-\infty) = \pm\infty \end{aligned}$$

to hold, either $\frac{D}{B} = 0$ and so $D = 0$ or $\frac{D}{B} = \pm\infty$ giving $B = 0$.

$$D = 0 \Rightarrow Ai(-\beta E) = 0$$

$$B = 0 \Rightarrow Ai'(-\beta E) = 0$$

These are the same conditions as equations 2.3 and 2.4 in section 2. This shows that in this case the condition of w being continuous on the extended real line gives the same result as imposing the square integrability of the solution to the Schrödinger equation.

4.3 Proving the two formalisms give the same result

The symmetric linear potential example has produced the same energy levels for the new formalism as for the old. It has also been explicitly shown in [11] that this same correspondence applies in the case of the potential well and the SHO, but it is not necessary to show this result for each possible potential. A general result can be proven.

There are two stages to the general proof - to show that if a normalisable solution exists to the SE, then the EP is satisfied, and then to show that if none exists, then the EP is not satisfied. In this way, the imposition of the continuity on the extended real line that follows directly from the EP is shown to be equivalent to imposing the existence of a normalisable solution.

4.3.1 Normalisable solutions satisfy the EP

Take an energy value that has a solution to the Schrodinger equation which is normalisable, and call this solution y_1 and the other solution y_2. The results in section 7.1 tell us some properties of this second solution, given that the first must approach 0 at $\pm\infty$, specifically that the solution y_2 must diverge at $\pm\infty$. A general solution for this energy value is:

$$\psi = Ay_1 + By_2$$

with the dual solution being

$$\psi^D = Cy_1 + Dy_2$$

giving

$$w = \frac{Cy_1 + Dy_2}{Ay_1 + By_2}$$

As $x \to \pm\infty$, the normalisable solution approaches zero and so becomes negligible in comparison with the diverging solution.

$$\Rightarrow \lim_{x\to\pm\infty} = \frac{D}{B}$$

This obviously satisfies the continuity conditions:

$$w(-\infty) = w(+\infty) \text{ for } w(-\infty) \neq \pm\infty \tag{4.7}$$

as long as $B \neq 0$. If $B = 0$ then

$$\lim_{x\to\pm\infty} w = \frac{Dy_2}{Ay_1}$$

Using equation 7.3,

$$\frac{y_2}{y_1} = \int_0^x \frac{du}{y_1^2(u)}$$

As $y_1(u)$ approaches 0 as $u \to \pm\infty$, this integral obviously diverges for $x \to \pm\infty$, but as the denominator is always positive, the $x \to +\infty$ will give a positive answer, and the $x \to -\infty$ will give a negative answer, thus satisfying the continuity condition

$$w(-\infty) = -w(+\infty) \text{ for } w(-\infty) = \pm\infty \tag{4.8}$$

So, if there is a normalisable solution, then it satisfies the EP.

4.3.2 A non-normalisable solution does not satisfy the EP

As shown in section 7.1, if one solution to the Schrodinger equation approaches zero in a $x \to +\infty$ limit, then the other must diverge. The same applies for the $x \to -\infty$ limit, but the approaching zero solutions for these two limits may not belong to the same overall solution. If they do, then a normalisable solution is the result, but if they don't then one solution will approach 0 at the negative limit but diverge at the positive, and the other will diverge at the negative and approach zero at the positive - and no normalisable solution exists.

Take y_1 as diverging at $+\infty$, vanishing at $-\infty$ and y_2 vanishing at $+\infty$, diverging at $-\infty$. The ratio

$$w = \frac{y_2}{y_1}$$

has limits

$$\lim x \to +\infty = 0$$

$$\lim x \to -\infty = \pm\infty$$

This cannot be continuous on the extended real line, and so the EP is not satisfied.

This is a wonderful result, meaning that the new formalism will produce the same results as the old. The Hilbert space structure relies on using the normalisable solutions to the SE and other eigenvalue equations, but this rederives the applicability of these solutions.

5 Further consequences of the EP

The standard result of the quantisation of energy levels hold for the new formulation. But there is more to add - in the derivation of the QSHJE and the SE, references to classical HJ theory were made and similarities noted. This connection can be used to explain some old phenomena as well as introduce some dramatically different ideas to QM.

5.1 Tunnelling

A key quantum phenomenon is that of tunnelling, when a particle is able to penetrate a potential barrier which would be classically forbidden. In standard QM, this is explained by the exponential decay of the wave function outside a potential well for a particle 'confined' to that well. This gives a non-zero probability of finding the particle outside the well. But this explanation has to be re-examined with the new formulation.

From the modified HJ equation 3.3, the origin of tunnelling is obvious.

$$\frac{1}{2m}\left(\frac{dS_0}{dq}\right)^2 + W(q) + \frac{\beta^2}{4m}\{S_0, q\} = 0$$

Classically, $Q(q) = 0$ so when $W(q) > 0$ then

$$\left(\frac{dS_0}{dq}\right)^2 < 0$$

giving a complex momentum $p = \frac{dS_0}{dq}$ which is not allowed. But if $Q(q) < 0$, then even in classically forbidden regions where the potential barrier is greater than the energy of the particle, it may still be that

$$\left(\frac{dS_0}{dq}\right)^2 > 0 \tag{5.1}$$

and the particle can reach that point. As $Q(q)$ depends on S_0, there is no fixed limiting value to it, so equation 5.1 can hold for any q, resulting in no forbidden regions.

5.2 Conjugate variables

The previous section utilised the identification in HJ theory that $p = \frac{\partial S_0}{\partial q}$, where p is the conjugate momentum. A basic example is that of a free particle, with the Schrodinger equation

$$\frac{d^2\psi}{dx^2} = 0$$

giving

$$\psi = Ax + B$$

$$\psi^D = Cx + D$$

Thus

$$e^{\frac{2i}{\hbar}S_0} = \frac{Ax+B}{Cx+D}$$

$$\Rightarrow S_0 = \frac{\hbar}{2i} ln\left(\frac{Ax+B}{Cx+D}\right)$$

This gives an expression for the conjugate momentum as

$$p = \frac{\hbar}{2i}\left[\frac{AD-BC}{(Ax+B)(Cx+D)}\right]$$

The A, B, C and D come from the invariance of the SD under a Mobius transformation (see section 7.2.1). As $AD - BC \neq 0$ from the definition of the transformation, this expression can be simplified [11] to

$$p_0 = \pm\frac{\hbar l_1}{(x+l_2)^2 + l_1^2}$$

where $l_1 \neq 0$ and $l_2 \neq 0$. A similar treatment can be given for a general state [11], which also introduces two independent variables. In a way, these can be considered the hidden variables of the formulation.

5.3 Time parametization

It is very well having expressions for the reduced action and the conjugate momentum, but in order to find proper trajectories time has to be introduced. In section 8.3, it is noted for a special case that

$$t - t_0 = \frac{\partial S_0}{\partial E}$$

This is known as Jacobi's theorem. In classical mechanics this coincides with the identification $p = m\frac{dq}{dt}$, but they do not coincide for the quantum version of the HJ equation. The latter identification does not lead to expected results, such as the free particle being at rest, but Jacobi's theorem provides a better choice.

Using this, it is possible to construct definite trajectories depending on a couple of hidden variables. The example of the symmetric linear potential has

$$\begin{aligned} e^{\frac{2i}{\hbar}S_0} &= \frac{CAi[\beta(\alpha x - E)]}{AAi[\beta(\alpha x - E)] + BBi[\beta(\alpha x - E)]} \text{ for } Ai[-\beta E] = 0 \\ &= \frac{CAi[\beta(\alpha x - E)] + DBi[\beta(\alpha x - E)]}{AAi[\beta(\alpha x - E)]} \text{ for } Ai'[-\beta E] = 0 \end{aligned}$$

From this, a complicated expression for $t - t_0$ can be found, but some features can be seen without the explicit expression. It is obvious that this deviates from the parabolic paths derived for the classical case in section 8.4. It differs also in a fundamental way from the calculation in section 2.2, where trajectories are a priori rejected. This new EP formulation gives definite trajectories, but classically unexpected ones due to the effects of the quantum potential.

6 Conclusion

Quantum mechanics is an unsatisfactory theory.

But that is not to say that quantum theory has not been hugely successful over the century of its existence. As we look forward to the future of physics, a new theory needs to take the place of existing quantum mechanics as the framework of the rest of the subject, circumventing any cognitive repression of radical new ideas.

The new EP theory relies on many ideas, new and old, drawing on mainstream QM, Einstein's work on GR and de Broglie-Bohm theory. The derivation of the SE from the EP in section 3.3 is the first success of the theory, but it is not limited to that. Indeed, in [13] the derivation of the relativistic quantum HJ equation is shown to be more natural, with the time-dependent SE emerging only in the non-relativistic approximation.

The SE is used in the new formulation in a seemingly very different way from a mainstream probability interpretation, so finding the same energy levels being predicted is an important result, as shown explicitly here for the symmetric linear potential. This result has also been shown to be general for all potentials. The EP theory has further consequences when applied in an HJ framework, including the introduction of definite trajectories and hidden variables. This adds another strand to the longstanding debate over hidden variables in QM.

There are a huge number of further consequences left unexplored here, such as the connection with Legendre transformations, and the possible position for the Planck length in the theory suggesting an intimate connection with gravity. Indeed, as noted in [13], just because the formulation works in one dimension, it does not mean that the extension to higher dimensions will immediately follow. But this extension to higher dimensions has been made [13].

The EP theory certainly does not have all the answers to the problems of QM. But it does suggest a new approach to solving these problems, and throws up some interesting questions of its own. Quantum theory has certainly not heralded the end of physics, and the dramatically different route taken by the EP theory shows that we are likely still only at the beginning.

7 Appendix A - Mathematical background

7.1 Wronskians and linearly independent solutions

A Wronskian is defined as

$$W(y_1, y_2) = y_1 \frac{dy_2}{dx} - y_2 \frac{dy_1}{dx} \tag{7.1}$$

which can also easily be expressed as the determinant of a matrix. Their most common property is that if W vanishes over the entire interval from $-\infty$ to $+\infty$ then y_1 and y_2 are multiples of each other. They can be used to show very general properties about solutions to some ordinary differential equations.

7.1.1 Obtaining a 2nd solution

A 2nd order homogeneous linear ordinary differential equation is of form:

$$y'' + p(z)y' + q(z)y = 0 \tag{7.2}$$

Two linearly independent solutions to this equation are y_1 and y_2. Differentiation of the Wronskian gives

$$\begin{aligned} W' &= y_1 y_2'' - y_2 y_1'' \\ &= -y_1 \left[p(z)y_2' + q(z)y@2\right] + y_2 \left[p(z)y_1' + q(z)y_1\right] \\ &= -Wp(z) \end{aligned}$$

using the expressions for y'' from equation 7.2. Integrating this gives an expression for W in terms of $p(z)$. The Schrodinger equation is of the form of equation 7.2, with $p(z) = 0$, giving W as a constant.

Using expression 7.1 for W and rearranging gives

$$\frac{W}{y_1^2} = \frac{y_2'}{y_1} - \frac{y_1' y_2}{y_1^2} = \frac{d}{dz}\left(\frac{y_2}{y_1}\right)$$

Integrating this with respect to z and using a constant for W as for the Schrodinger equation gives

$$y_2 = y_1 \int \frac{1}{y_1^2} dz \tag{7.3}$$

7.1.2 Limits of solutions to the Schrodinger equation

The Schrodinger equation is of the form

$$y'' + [E - U(x)]\, y = 0 \tag{7.4}$$

and the situation we are interested in is that $E - U(x) < 0$ for $x > x_0$ ie the particle is confined by the potential. The symmetric linear potential is obviously of this type as it tends to ∞ as x increases. The same reasoning as that applied here can be used to find similar conclusions about the limit at $-\infty$.

Two linearly independent solutions are y_1 and y_2 as before, but here these are of a particular form: $y_1(x_0) = 1$, $y_1'(x_0) = 0$, $y_2(x_0) = 0$, $y_2'(x_0) = 1$. A general solution can be expressed in terms of these functions:

$$y = \alpha y_1 + \beta y_2$$

and so $y(x_0) = \alpha$ and $y'(x_0) = \beta$.

Some properties of y_1 and y_2 can be seen from the equation. As $y(x_0) > 0$ and $E - U(x) < 0$ for $x > x_0$, $y_1'' > 0$ for $x > x_0$ (using equation 7.4), so y_1 will tend to ∞ as x increases from x_0. A similar argument applies to y_2, except that y'' starts at 0 at x_0, but as $y'(x_0) > 0$ at x_0, y increases and so y'' increases.

As both y_1 and y_2 increase to ∞ as x increases, there is only one possibility for an expression for a solution to the Schrodinger equation which does not diverge similarly. Define $u(x) = \frac{y_1}{y_2}$, and take the limit of $u(x)$ as $x \to \infty$ as C.

$$\begin{aligned} y &= y_1 - C y_2 && (7.5) \\ &= (u(x) - C)\, y_2 && (7.6) \end{aligned}$$

If the factor in front of y_2 goes to 0 quicker than y_2 goes to ∞, then we have found a solution which does not diverge. A more detailed treatment in [15] shows this to be the case, but it can be seen from the expression 7.3: the ratio $\frac{y_1}{y_2}$ will tend to its limit faster than y_2 itself.

The more detailed treatment in [15] yields the more complete conclusion:

> i) there is one solution of equation 7.4 which approaches 0 as x approaches infinity, at least as rapidly as e^{-Mx}.
>
> ii) all the other solutions to equation 7.4 tend towards infinity as x increases, at least as rapidly as e^{Mx}.

7.2 The Schwarzian Derivative

The Schwarzian Derivative (SD) is a simple expression involving first, second and third derivatives of a function with respect to a specific variable, and enjoys some interesting properties which result in its use in a wide range of physics and mathematics. The SD of w with respect to z, $\{w, z\}$ is defined as

$$\{w, z\} = \left(\frac{w''}{w'}\right)' - \frac{1}{2}\left(\frac{w''}{w'}\right)^2 \qquad (7.7)$$

The properties involving real functions find an application in the study of chaotic systems [16] and the SD also has extensive use in complex analysis [17]. These properties include invariance under linear fractional transformations, some simple chain rule-like relations and an interesting connection to particular 2nd order linear differential equations.

7.2.1 Invariance under linear fractional transformation

A good example of the appearance of the SD is the consideration of a function that would be invariant under a linear fractional transformation / Mobius transformation, that is under a transformation of form

$$W : w \to \frac{Aw + B}{Cw + d}$$

where w and W are functions of z. Differentiation of the expression for W gives

$$W' = \frac{((Cw + D)A - (Aw + B)C)w'}{(Cw + D)^2} = \frac{(AD - BC)w'}{(Cw + D)^2}$$

where the prime denotes differentiation with respect to z. Differentiation of the logarithm produces

$$(\ln W')' = \frac{W''}{W'} = \frac{w''}{w'} - \frac{2Cw'}{Cw + D}$$

$$\Rightarrow \left(\frac{W''}{W'}\right)' = \left(\frac{w''}{w'}\right)' - \frac{2Cw''}{Cw + D} + \frac{2C^2w'^2}{(Cw + D)^2}$$

$$\left(\frac{W''}{W'}\right)^2 = \left(\frac{w''}{w'}\right)^2 + \frac{4Cw''}{Cw + D} - \frac{4C^2w'^2}{(Cw + D)^2}$$

From this, it is obvious that

$$\left(\frac{W''}{W'}\right)' - \frac{1}{2}\left(\frac{W''}{W'}\right)^2 = \left(\frac{w''}{w'}\right)' - \frac{1}{2}\left(\frac{w''}{w'}\right)^2$$

Using the definition of the SD (equation 7.7), this has shown that the SD is invariant under any linear fractional transformation.

$$\{w, z\} = \{W, z\}$$

This may often be seen as the defining property of the SD.

7.2.2 Chain rule

When using standard derivatives, be it ordinary or partial, the chain rule is very useful in simplifying statements when changes of variables are being used. A similar rule for the SD is also useful.

Application of the chain rule for ordinary differentiation on a function $h = h(x)$ where $x = x(y)$ gives:

$$\frac{dh}{dx} = \frac{dy}{dx}\frac{dh}{dy}$$

$$\frac{d^2h}{dx^2} = \frac{d^y}{dx^2}\frac{dh}{hy} + \left(\frac{dy}{dx}\right)^2\frac{d^2h}{dy^2}$$

$$\frac{d^3h}{dx^3} = \frac{d^3y}{dx^3}\frac{dh}{dy} + \frac{d^2y}{dx^2}\frac{dy}{dx}\frac{d^2h}{dy^2} + 2\frac{dy}{dx}\frac{d^2y}{dx^2}\frac{d^2h}{dy^2} + \left(\frac{dy}{dx}\right)^3\frac{d^3h}{dy^3}$$

By substituting these expressions into the definition of the SD (7.7), a simple chain rule is produced:

$$\{h(x), x\} = \left(\frac{dy}{dx}\right)^2 \{h(y), y\} + \{y(x), x\} \tag{7.8}$$

A similar expression for $h = h(y)$ is found for $y = y(x)$:

$$\{h(y), y\} = \left(\frac{dx}{dy}\right)^2 \{h(x), x\} + \{x(y), y\}$$

Substituting this back into (7.8) gives

$$\{y, x\} = -\left(\frac{dy}{dx}\right)^2 \{x, y\} \tag{7.9}$$

This gives an alternate expression for the chain rule:

$$\{h(x), x\} = \left(\frac{dy}{dx}\right)^2 (\{h(y), y\} - \{x, y\}) \tag{7.10}$$

7.2.3 A simple application of the chain rule

By using exponentials, the square of an ordinary derivative can be expressed as the difference between two SDs.

Let $h(x) = e^{\alpha y(x)}$.

$$\Rightarrow \{h(x), x\} = \left(\frac{dy}{dx}\right)^2 \{e^{\alpha y}, y\} + \{y, x\}$$

$\{h(y), y\}$ can be simply evaluated to give $-\frac{\alpha^2}{2}$, thus giving

$$\left(\frac{dy}{dx}\right)^2 = \frac{2}{\alpha^2} \left[\{y, x\} - \{e^{\alpha y}, x\}\right] \tag{7.11}$$

7.2.4 Connection with 2nd order linear ordinary differential equations

The SD also appears when considering some linearly independent solutions to a particular subset of 2nd order DEs. An equation of form:

$$\frac{d^2 y}{dz^2} + p(z) y = 0 \tag{7.12}$$

has a first solution $u_1(z)$. Another solution of the form $u_2(z) = u_1(z) w(z)$ can be found, as long it has certain properties:

$$\frac{d^2}{dz^2}(u_1 w) + p(z) u_1 w = 0$$

$$\Rightarrow u_1 w'' + 2u_1' w' + w\left[u_1'' + p(z) u_1\right] = 0$$

Therefore, the product is a solution as long as

$$\frac{w''}{w'} = -2\frac{u_1'}{u_1}$$

Differentiating this gives

$$\left(\frac{w''}{w'}\right)' = -2\frac{u_1''}{u_1} + 2\frac{(u_1')^2}{u_1^2} = 2p(z) + \frac{1}{2}\left(\frac{w''}{w'}\right)^2$$

$$\Rightarrow \{w, z\} = 2p(z) \tag{7.13}$$

$w = \text{const}$ cannot be a solution to (7.13), as the SD of a constant vanishes, and so the new solution $u_2 = wu_1$ must be a linearly independent solution of equation (7.12). This statement can be reversed, to say that a solution w to equation (7.13) involving the SD can be expressed as a ratio between two linearly independent solutions of the 2nd order linear DE (7.12). A more thorough argument can be found at [17].

8 Appendix B: An introduction to Classical HJ theory

Hamilton-Jacobi (HJ) theory is an elegant expression of classical mechanics. The development from Newton's laws, through Lagrangian and Hamiltonian formulations, to HJ theory provides deep insight into the foundations of the subject. Classic expositions of the subject include Goldstein [18] and Landau and Lifshitz [14], so here only some key points, pertaining to its extension in the application of the EP, will be illustrated, especially the retrieval of trajectories from the differential equation.

8.1 Lagrangian and Hamiltonian formulations

Classical mechanics is deterministic - if 'all the coordinates and velocities are simultaneously specified ... the state of the system is completely determined and ... its subsequent motion can, in principle, be calculated.' [14]. The starting point of this calculation is a principle of least action, whose applicability is a result of its compatibility with Newton's laws, rather than its mysterious physical content.

> The motion of the system from time t_1 to time t_2 is such that the line integral
>
> $$S = \int_{t_1}^{t_2} L dt$$
>
> where $L = T - V$, has a stationary value for the actual path of the motion[18].

where T is the kinetic energy and V is the potential energy. This statement, and application of the calculus of variations, directly leads to Lagrange's equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i} \text{ for all coords } q_i (i = 1, 2 \ldots) \tag{8.1}$$

Arguments of homogeneity and isotropy of space and time [14] and compatibility with Newton, lead to specific expressions for T and V.

Compatibility of equations 8.1 with or equivalence to Newton's laws, with the covariance of the equations with respect to change of coordinates, means that equations 8.1 apply under any suitable generalised coordinate system.

The Hamiltonian formulation of the laws of mechanics arise from a Legendre transformation - ie a change of independent variables from q_i and $\dot{q}_i$ to q_i and p_i, where $p_i = \frac{\partial L}{\partial \dot{q}_i}$ is the generalised momentum. The transformation

$$H(p, q, t) = \sum p_i \dot{q}_i - L \tag{8.2}$$

leads to Hamilton's equations of motion:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \text{ and } \dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{8.3}$$

These, like Lagrange's equations and Newton's second law, are differential equations which can, in principle, be solved for the trajectory of the particle or system state $q_i = q_i(t)$ for $i = 1, 2 \ldots$.

8.2 Changes of coordinates

When solving problems, changes of coordinates which simplify the problem can be used extensively, especially transformations which make a particular variable constant in time. But in the Hamiltonian formulation, general transformations of form

$$Q_i = Q_i(q_i, p_i, t) \text{ and } P_i = P_i(q_i, p_i, t)$$

will not in general retain the form of Hamilton's equations. Transformations which do keep the form are called 'canonical transformations'.

Hamilton's equations can be derived directly from the variational principle:

$$\delta S = \delta \int \left(\sum p_i \dot{q}_i - H \right) dt = 0 \tag{8.4}$$

So, Hamilton's equations will apply is equation 8.4 also applies in the new coordinates:

$$\delta S = \delta \int \left(\sum P_i \dot{Q}_i - K \right) dt = 0 \tag{8.5}$$

where K is the new Hamtiltonian. After a little examination, it can be seen that this can only be the case if the two expressions under the integral only differ by a total derivative $\frac{dF}{dt}.dt$.

$$\Rightarrow \sum P_i \dot{Q}_i - K + \frac{dF}{dt} = \sum p_i \dot{q}_i - H$$

$$\Rightarrow dF = \sum p_i dq_i - \sum P_i dQ_i + (K - H)dt$$

$$\Rightarrow \frac{dF}{dq_i} = p_i \ , \ \frac{dF}{dQ_i} = -P_i \ , \ \frac{\partial F}{\partial t} = K - H \tag{8.6}$$

where F is known as the generating function of the transformation.

A particularly simple set of variables, coordinates and momenta, would be for all Q_i and P_i to be constant in time.

$$\dot{Q}_i = \frac{\partial K}{\partial P_i} = 0 \text{ and } \dot{P}_i = -\frac{\partial K}{\partial Q_i} = 0$$

Therefore, up to an additive constant, which is physically irrelevant, $K = 0$. Using this new set of coordinates and vanishing Hamiltonian in the last part of equation 8.6 gives:

$$H(q_i, \frac{\partial F}{\partial q_i}, t) + \frac{\partial F}{\partial t} = 0 \tag{8.7}$$

- a partial differential equation in n+1 variables. Further analysis shows that the function F is in fact the action S up to an additive constant:

$$S = \int \left(\sum P_i \dot{Q}_i - K + \frac{dF}{dt} \right) dt$$

$$\Rightarrow S = \int P_i dQ_i + F = F + c$$

as $dQ_i = 0$ at the end points.

This gives the full Hamilton Jacobi equation:

$$H\left(q_i, \frac{\partial S}{\partial q_i}, t\right) + \frac{\partial S}{\partial t} = 0 \tag{8.8}$$

where S is both the action and the generating function of a canonical transformation to variables which are constant in time.

8.2.1 Other forms of the HJ equation

In some simple situations, other forms of the HJ equation may crop up. For example, if the Hamiltonian does not explicitly depend on t (as the system is conservative), the substitution $S = S_0 - Et$ yields the stationary Hamilton-Jacobi equation:

$$H\left(q_i, \frac{\partial S_0}{dq_i}, t\right) = E \tag{8.9}$$

The Hamiltonian may also take a standard form

$$\begin{aligned} H &= T + V \\ &= \frac{1}{2m}p^2 + V \\ &= \frac{1}{2m}(\text{grad}S_0)^2 + V \end{aligned}$$

giving a Stationary Hamilton Jacobi equation of form

$$\frac{1}{2m}\left(\text{grad}S_0\right)^2 + V = E \tag{8.10}$$

8.3 Solving for trajectories

The HJ equation is a partial differential equation for the action S in n+1 variables, and so the full solution will have n+1 arbitrary constants. However, as S itself is not explicitly contained in the equation, only its derivatives, one of these constants will only be additive and so can be discarded as it will not affect the physics.

Solution of the HJ equation gives S as a function of the coordinates, time and these n independent constants of integration, $\alpha_1, \alpha_2 \ldots$:

$$S = S(q_1, q_2 \ldots, \alpha_1, \alpha_2 \ldots, t)$$

Without losing generality [18], these constants can be taken as the constant momenta in the reference frame with zero Hamiltonian. When $F = F(q_i, Q_i, t)$, it has been shown that $P_i = -\frac{\partial F}{\partial Q_i}$. It can also be shown that when F is expressed as $F = F(q_i, P_i, t)$:

$$Q_i = \frac{\partial F}{\partial P_i} = \frac{\partial S}{\partial \alpha_i}$$

As the Q_i are also constant, and to clarify are expressed as constants β_i, we now have a set of n equations relating q_i and t which can be solved for each $q_i = q_i(\alpha_i, \beta_i, t)$, which is a solution to the problem.

When S can be expressed as $S = S_0 - Et$, where E is a constant, E can be identified as one of the constant momenta as well as the total energy of the system. A particularly simple example is a 1-dimensional system, where the constant coordinate Q is $\frac{\partial S}{\partial E}$:

$$\frac{\partial S}{\partial E} = \frac{\partial S_0}{\partial E} - t = \beta$$

$$\Rightarrow t - t_0 = \frac{\partial S_0}{\partial E} \tag{8.11}$$

8.4 The linear potential

The linear symmetric potential

$$\begin{aligned} V(q) &= \alpha q \text{ for } q > 0 \\ &= -\alpha q \text{ for } q < 0 \end{aligned}$$

and a Stationary HJ equation of form

$$\frac{1}{2m}\left(\frac{\partial F_0}{\partial q}\right)^2 + V(q) = E$$

gives

$$\begin{aligned} \frac{\partial F_0}{\partial q} &= (2m)^{\frac{1}{2}} (E - \alpha q)^{\frac{1}{2}} \text{ for } q > 0 \\ &= (2m)^{\frac{1}{2}} (E + \alpha q)^{\frac{1}{2}} \text{ for } q < 0 \end{aligned}$$

Integration of this gives

$$\begin{aligned} F_0 &= -\frac{(2m)^{\frac{1}{2}}}{\alpha} . \frac{2}{3}(E - \alpha q)^{\frac{3}{2}} + k_1 \text{ for } q > 0 \\ &= \frac{(2m)^{\frac{1}{2}}}{\alpha} . \frac{2}{3}(E + \alpha q)^{\frac{3}{2}} + k_1 \text{ for } q < 0 \end{aligned}$$

Continuity of F_0 at $q = 0$ gives the integration constants $k_1 = -k_2 = \frac{2\sqrt{2m}}{3\alpha}E^{\frac{3}{2}}$, implying an expression for F itself as:

$$\begin{aligned} F &= \frac{2\sqrt{2m}}{3\alpha}\left[E^{\frac{3}{2}} - (E - \alpha q)^{\frac{3}{2}}\right] - Et \text{ for } q > 0 \\ &= \frac{2\sqrt{2m}}{3\alpha}\left[(E + \alpha q)^{\frac{3}{2}} - E^{\frac{3}{2}}\right] - Et \text{ for } q < 0 \end{aligned}$$

Use of equation 8.11 gives

$$\begin{aligned} \beta + t &= \frac{\sqrt{2m}}{\alpha}\left[E^{\frac{1}{2}} - (E - \alpha q)^{\frac{1}{2}}\right] \text{ for } q > 0 \\ &= \frac{\sqrt{2m}}{\alpha}\left[(E + \alpha q)^{\frac{1}{2}} - E^{\frac{1}{2}}\right] \text{ for } q < 0 \end{aligned}$$

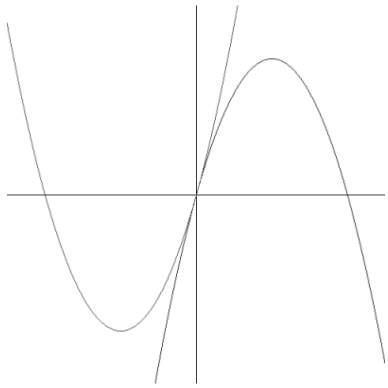

Figure 4: Trajectory for particle subjected to symmetric linear potential

Rearrangement of this gives an expression for q in terms of t and the two constants of integration E and β:

$$\begin{aligned} q &= \frac{1}{\alpha}\left(E - \left[E^{\frac{1}{2}} - \frac{\alpha}{\sqrt{2m}}(\beta + t)\right]^2\right) \text{ for } q > 0 \\ &= \frac{1}{\alpha}\left(\left[E^{\frac{1}{2}} + \frac{\alpha}{\sqrt{2m}}(\beta + t)\right]^2 - E\right) \text{ for } q < 0 \end{aligned}$$

These two parabolas with sample values for the constants are illustrated in Figure 4.

However, the condition on continuity imposed by the HJ equation is not just on F_0, but on F itself. This leads to conditions being placed on the solution every time the $q = 0$ axis is crossed, which results in these parabolas being translated sideways to create a repeating oscillation.

This solution was obvious from the start: the linear potential results from a constant force, resulting in constant acceleration, resulting in the parabolas found so often in basic mechanics problems involving gravity. There are no dissipative forces, so these parabolas join at $q = 0$ to form an infinite oscillation in time.

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