On the derivation of the time-dependent equation of Schrödinger

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Abstract

Few have done more than Martin Gutzwiller to clarify the connection between classical time-dependent motion and the time-independent states of quantum systems. Hence it seems appropriate to include the following discussion of the origins of the time-dependent Schrödinger equation in this volume dedicated to him.

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I. INTRODUCTION

In all books which develop quantum mechanics from the Schrödinger equation it is considered that the time-dependent equation (TDSE) is more "fundamental" than the time-independent equation (TISE). In the TDSE

$$\left(H_{\mathcal{S}}(t) - i\hbar\frac{\partial}{\partial t}\right)\psi_{\mathcal{S}}(t) = 0 \tag{1}$$

for some quantum system S it is usually pointed out that time is a parameter, not enjoying the status of a quantum operator. However, it is almost never pointed out that the time occurring in $H_{\mathcal{S}}(t)$ *always* is a *classical* time arising from the classical time development (according to Newton or Maxwell equations) of external fields or material particles interacting with the quantum system. In this sense the TDSE is, from the outset, a mixed quantum-classical equation. Having postulated Eq. (1), the authors of standard quantum mechanics text books then discuss the special case of a time-independent Hamiltonian, when the solution of Eq. (1) can be written in the form

$$\psi_{\mathcal{S}}(t) = \phi_{\mathcal{S}}\exp\left(\frac{i}{\hbar}E_{\mathcal{S}}t\right) \tag{2}$$

to give the TISE

$$(H_{\mathcal{S}} - E_{\mathcal{S}})\phi_{\mathcal{S}} = 0. \tag{3}$$

The form of Eq. (3) enforces the assignment to the quantum system of a wavefunction oscillating in time. For example, to quote Feynman and Hibbs [1] "for this special solution the wavefunction oscillates with a definite frequency ... which corresponds, in classical physics, to the energy". That is, the student of quantum mechanics is asked to accept that all matter, even though in *stationary* quantum states described by Eq. (3), have wavefunctions which oscillate in time. This disturbing property is only slightly ameliorated by pointing out that in any expectation value of a measurable quantity the phase factor cancels to give a time-independent value. Surely, this suggests that the phase factor and indeed the time dependence in Eq. (2) is redundant? However, there is a more serious objection to the solution Eq. (2) and its Feynman-Hibbs interpretation. An oscillation *frequency* is, by definition, positive definite. However, the quantity $(E_{\mathcal{S}}/\hbar)$ is not absolutely defined and can take on any value, negative or positive, arbitrarily large, according to where the zero of energy is fixed.

As we will illustrate below, there are other serious problems in the derivation and application of the TDSE to isolated quantum systems. In a previous paper [2] we outlined an alternative point of view, well-known in atomic collision physics [3,4] from which to derive the TDSE, avoiding many ad hoc assumptions made in standard texts. In [2], hereafter referred to as paper I, the starting point is the TISE for a closed, energy conserving, quantum object comprised of two parts, called the system and the environment. In the limit that the environment can be treated classically, it provides a time variable with which to monitor the remaining quantum system whose development, as viewed from the environment, is governed by the TDSE for the system alone. This derivation shows explicitly that the origin of the classical time in $H_{\mathcal{S}}(t)$ is due to coupling with the classical environment, and that the parametric derivative $\frac{\partial}{\partial t}$ arises from the transition of environment variables from quantum to classical behaviour.

In this paper we return to this problem in order to clarify issues raised to us by several colleagues and to amplify certain aspects of the derivation given in paper I. In section II we give an historical account of the origins of the TDSE Eq. (1), since in our opinion this throws much light on the way in which this equation has been introduced in generations of quantum mechanics text books. In section III we discuss the attempts that have been made to remove the mixed classical-quantum nature of the TDSE by elevating time to a quantum variable, rather than a parameter. In turn these efforts have spawned a host of papers on the 'derivation' of an energy-time uncertainty relation and this problem is discussed also in section III. In section IV we present the derivation of the TDSE with a more careful description of the transition of the environment to classical behaviour than was given in paper I. In section V it is pointed out that a completely analogous procedure has been suggested for the introduction of time in a Schrödinger representation of quantum field theory including quantisation of both gravity and matter.

II. HISTORICAL DEVELOPMENT

It is not usually pointed out that, unlike the authors of most text books, Schrödinger derived first the TISE, not the TDSE. He used a variational argument [5]. This appears to us still the most simple and direct way to introduce quantisation. Although not quite the way of Schrödinger one proceeds from the classical relation for a closed system at energy E

$$H(p,q) = E \tag{4}$$

or constraint

$$(H - E) = 0 \tag{5}$$

to the quantum equivalent

$$\langle\psi|\hat{H}|\psi\rangle = E\langle\psi|\psi\rangle \tag{6}$$

or constraint

$$\langle\psi|(\hat{H} - E)|\psi\rangle = 0. \tag{7}$$

In the quantum constraint Eq. (7) all classical variables (p, q) from Eq. (4) are replaced by quantum operators $(\hat{p}, \hat{q})$. Variation of the state vector $\langle\psi|$ in Eq. (7) leads directly to the TISE

$$(\hat{H} - E)|\psi\rangle = 0 \tag{8}$$

This derivation requires only that we replace measured quantities by expectation values of the corresponding quantum operators.

Schrödinger had much more difficulty with the TDSE. Indeed it is very clear that he was looking for a second-order equation of form similar to the electromagnetic wave equation in which matter waves are described by time-dependent real wave amplitudes, exactly as the classical components of the electromagnetic field. In his second communication of 1926 [6], in which he introduces the TDSE, very clearly Schrödinger was influenced by the well-known analogy between wave optics and the Hamilton-Jacobi theory of classical mechanics and sought to deepen the analogy in formulating a wave theory for matter in which Hamiltonian classical mechanics would be the “geometric optics” limit. Hence his first suggested TDSE has the form

$$\Delta\psi - \frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2} = 0 \tag{9}$$

identical to the classical wave equation with the phase velocity u given by

$$u = E|\nabla W|^{-1} = E(2(E-V))^{-\frac{1}{2}} \tag{10}$$

where W is Hamilton’s characteristic action function. With Eq. (10) the TDSE appears as

$$\Delta\psi - \frac{2(E-V)}{E^2}\frac{\partial^2\psi}{\partial t^2} = 0 \tag{11}$$

and is clearly applicable to energy-conserving systems of total energy E. This equation, together with the TISE Eq. (8) in the form

$$\Delta\psi + \frac{2(E-V)}{\hbar^2}\psi = 0 \tag{12}$$

were introduced at the beginning of Schrödingers fourth 1926 communication [7] as the fundamental equations of the new mechanics. We note in passing that Eq. (11) does not contain $\hbar$! It is perhaps not uninteresting in the context of the present paper to remark that Schrödinger’s motivation in deriving an alternative TDSE to Eq. (11) was to eliminate the energy E from the equation, so making the equation applicable to non-conservative systems. In such systems Schrödinger considered that the time dependence arises from time-dependent potentials, in analogy to friction in classical mechanics. As a postulate, he introduced a time dependence $\exp(-iEt/\hbar)$ into the wavefunction so that Eq. (11) leads to Eq. (12) after time differentiation, i.e.

$$\frac{\partial^2\psi}{\partial t^2} = -\frac{E^2}{\hbar^2}\psi\,. \tag{13}$$

Since Eq. (12) is linear in E, elimination using Eq. (13) leads to a TDSE of *fourth* order. However, almost immediately Schrödinger saw that by admitting *complex* wavefunctions he could use

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi \tag{14}$$

to arrive at what we now call the TDSE

$$\begin{aligned} \Delta\psi - 2V\psi &= -2i\hbar\frac{\partial\psi}{\partial t} \\ \text{or}\quad (-\frac{1}{2}\Delta + V)\psi &= i\hbar\frac{\partial\psi}{\partial t} \end{aligned} \tag{15}$$

The complexity of the ensuing wavefunction was a problem for Schrödinger who in the last paragraph of [7] suggests that Eq. (15) is probably merely a surrogate for a fourth-order real wave equation applying to non-conservative systems. In section (4) we will return to this problem of why the wavefunction is complex. The first application of Eq. (15) in [7] was to the interaction of an atom with a classical electric field to give a time-dependent potential $V(t)$, a problem also considered in the famous 'Dreimännerarbeit' of Born, Heisenberg, and Jordan [8]. It is interesting that at this stage in the development of quantum mechanics it was not known how to quantise fields or even the free motion of particle beams. Hence, in both [7] and [8] they are considered as *external* sources perturbing the stationary atom. Nevertheless, and very important for the following, it was recognized that such a description is a *classical* treatment of the external source, valid when its energy is much greater than atomic energies. To quote the Dreimännerarbeit [8]

> "'In this sense one could, for example, treat the action of a strong alternating electromagnetic field on an atom entirely as the influence of an external force with neglect of the reaction, since the field energy can be regarded as infinitely large compared with that of the atom. The action of α-particles upon the electrons of an atom could also be regarded as an 'external force' as in classical theory..."

To summarize, Schrödinger saw the TISE as the fundamental equation of wave mechanics, deriving it from a variational principle. The TDSE was introduced in an ad hoc way with the aim of describing quantum systems subject to a time-varying perturbation. It was clear to all the founding fathers of quantum theory that such an external perturbation arises from a *classical* treatment of an external environment. Within a few years after 1926, techniques to quantise external electromagnetic fields and particle beams were developed. Following work of Born, in 1931 Mott [3] described the impact of α-particles on atoms by treating both atom *and* beam quantum-mechanically with the TISE. Then he showed that for a high energy beam he could describe its motion classically resulting in a time-dependent Hamiltonian and TDSE for the atom alone. The generalisation of this derivation of the TDSE given in paper I removes the necessity to postulate a $\exp(-iEt/\hbar)$ dependence as done by Schrödinger and, we feel, belatedly completes the development of the TDSE from the TISE, which was begun in his monumental 1926 papers.

In modern quantum mechanics text books little reference is made to Schrödinger's order of development or to his difficulties with the TDSE. Rather the TDSE is simply presented as the *fundamental* equation of wave mechanics from which the TISE (and hence a wavefunction with the $\exp(-iEt/\hbar)$ factor) is derived as a special case for time-independent Hamiltonians. No mention is made of the fact that time is entering only from a classical interacting environment or that the TDSE does not correspond to energy conservation (the fundamental equation of wave mechanics violates the fundamental principle of physics).

The 'derivations' of the TDSE given in text books fall into the three main categories given below (the specific books quoted are to be taken as exemplary only).

1) The TDSE is simply postulated (Cohen-Tannoudji et.al. [9], Eder [10]). Here one can raise the objections to the TDSE described above plus the fact that, unlike the postulated TISE Eq. (8), the immediate connection of the TISE with classical mechanics is not obvious.

2) The correspondence principle is invoked to re-write the classical equation Eq. (5) as

$$\left(H(-i\hbar\nabla_q, \vec{q}) - i\hbar\frac{\partial}{\partial t}\right)\psi = 0 \tag{16}$$

i.e. the correspondence

$$\vec{p} \rightarrow -i\hbar\nabla_q \tag{17a}$$

$$E \to i\hbar \frac{\partial}{\partial t} \tag{17b}$$

is assigned (Messiah [11]). Clearly this is somewhat problematic in that E is a fixed energy in Eq. (5) but the derived Eq. (16) applies to systems without fixed energy. Somewhat better perhaps is the assignment (Roman [12])

$$H \to -i\hbar \frac{\partial}{\partial t}\,, \tag{18}$$

i.e. treating the r.h.s of Eq. (18) as an operator (Bransden and Joachain [13]). However, then one has the problem that, unlike Eq. (17a) where p and q are both operators, H is an Hilbert-space operator but t is merely an external parameter.

3) One makes plausible that a free matter wave has the form of the plane wave solution of a classical wave equation i.e.

$$\psi \sim \exp[i\vec{k}\vec{r} - i\omega t] \tag{19}$$

to remark that for $E = \hbar\omega = \hbar^2 k^2/2m$, this is a solution of the TDSE

$$\left(-\frac{\hbar^2}{2m}\Delta - i\hbar\frac{\partial}{\partial t}\right)\psi = 0 \tag{20}$$

for free motion (with constant energy E!). Then it is postulated that the equation must also be valid in the general case where a time-dependent potential appears in the Hamiltonian. This approach is used by very many text books. Its origin lies of course in Eq. (19) being the solution of the classical wave equation for a plane wave without dispersion. Then the dispersion relation $\omega = (\hbar/2m)k^2$ leads directly to Eq. (20). Note that this argument is based entirely on the properties of an energy-conserving system with fixed energy E.

To summarize, all derivations of the TDSE presented in quantum mechanics books known to us proceed according to one of the three methods listed above, all of which rely on loose correspondence-principle or other plausibility arguments. There is no precise explanation of the origin of a time-dependent Hamiltonian or specification of the type of quantum system to which the TDSE applies.

III. THE TIME OPERATOR, QUANTUM TIME AND THE TIME-ENERGY UNCERTAINTY RELATION

The clear recognition by Born, Heisenberg and Jordan [8], also discussed in the introduction, that time enters the quantum Hamiltonian only when some external system is approximated by classical behaviour appears to have been rapidly forgotten. The TDSE assumed the mantle of the fundamental, wholly quantum dynamical equation. Nevertheless, over the last seventy-odd years many physicists have been uncomfortable with the way time is introduced into quantum mechanics and the fact that $\vec{x}$ and $\vec{p}$ are Hilbert-space operators but t is apparently not. One strategy has been to revise the theory so that t is also elevated to the status of an operator i.e. to use Dirac's designation [14], to change time from a c-number to a q-number.

The fundamental algebra of q-numbers distinguishing them from c-numbers is of course their non-commutivity as, for example,[1]

$$[\hat{x}_i, \hat{p}_i] = i\hbar \tag{21}$$

On the basis that H and t are canonically-conjugate variables, as are $\vec{x}$ and $\vec{p}$, it was sought to introduce a time operator $\hat{t}$, such that

$$[\hat{H}, \hat{t}] = i\hbar \tag{22}$$

Pauli raised a fundamental objection to the existence of such a relation by pointing out that the eigenvalue spectrum of $\hat{H}$ is bounded from below but that of $\hat{t}$ apparently not [15]. Despite this, prominent authors made suggestions for the definition of $\hat{t}$. For example, in 1961 Aharonov and Bohm [16] used the classical relation between t, x and p for a particle of mass m

$$t = \frac{mx}{p} \tag{23}$$

to suggest

$$\hat{t} = \frac{m}{2}(\hat{p}^{-1}\hat{x} + \hat{x}\hat{p}^{-1}), \tag{24}$$

the non-commutivity forcing the symmetrisation of the expression. As recently as 1996, Grot et al. [17] suggested the more compact form

$$\hat{t} = \frac{m}{2}(\hat{p}^{-1/2}\hat{x}\hat{p}^{-1/2}) \tag{25}$$

The main drawback of such operators is that they are singular in p-space, surely a shameful attribute for such a blatantly non-singular quantity as time? Later, we will use the classical relation Eq. (23) to introduce time into quantum mechanics as a classical quantity without the need to invoke q-numbers such as Eq. (24) or Eq. (25).

The most famous corollary of Eq. (21) is the proof of the uncertainty relation

$$\Delta x_i \Delta p_i \geq \hbar/2 \tag{26}$$

first derived by Heisenberg [18] on the basis of matrix mechanics. Heisenberg himself postulated the existence of a similar relationship for energy and time

$$\Delta E \Delta t \sim \hbar \tag{27}$$

based on their classical conjugate relationship. The origin of Eq. (26) is the general statement linking the uncertainty in the expectation values of any two non-commuting observables A and B, i.e.

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[1] In this section a caret will distinguish operators from c-numbers.

$$\Delta A \Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle| \tag{28}$$

The absence of a time operator has left generations of students, and the authors of texts on quantum theory, bemused as to the origin of Eq. (27). As in the derivation of the TDSE, most authors resort to the plausibility argument based on E and t as classically conjugate variables (e.g., Roman [12]). However, others do attempt to link the relation Eq. (27) to the act of measurement using arguments first put forward by Mandelstam and Tamm [19] described below. Although we believe this to be the correct point of view, it still requires the TDSE for its proof, as do all the methods listed below. In paper I we gave a derivation based on the TISE, using only the fundamental operator relation Eq. (28).

Over the years there have been many attempts to ’clean-up’ the derivation of the time-energy relation from the TDSE. Some of the derivations are listed here simply to demonstrate, by the variety of these derivations, the fundamental difficulty of defining the role of time in quantum mechanics, see [20,21] and references therein).

1. Energy wavepackets

   In this approach one forms wavepackets bounded in time from an integral over eigenstates of different energy, with an arbitrarily chosen weight function. The relation Eq. (27) then arises from the mathematical property of Fourier transforms of bounded functions in frequency and time

   $$\Delta\omega\Delta t \sim 1$$

   and hence, in quantum mechanics

   $$\Delta E\Delta t \sim \hbar$$

2. Time-dependent perturbation theory

   In 1931, Peierls and Landau [22] considered a quantum system subjected to a constant perturbation and derived the probability of performing an inelastic transition of energy change ΔE as

   $$P(t) \sim \frac{\sin^2(\frac{\Delta E t}{\hbar})}{(\Delta E)^2} \tag{29}$$

   The width of this function as ΔE is varied gives the uncertainty relation Eq. (27). This derivation is clearly based on an open system and the use of first-order perturbation theory limits the applicability.

3. From the position-momentum uncertainty relation

   Many books start from Eq. (26) for a closed system and use the relation for a free particle of mass m

   $$\Delta E = \frac{\partial E}{\partial p}\Delta p = v\Delta p \tag{30}$$

   and define $\Delta t = \Delta x/v$ to obtain

   $$\Delta x\Delta p = \Delta E\Delta t \geq \hbar/2 \tag{31}$$

Not only does this method rely upon free motion, it is also required to introduce the concept of velocity, a classical quantity alien to a quantum system.

4. From the ’true’ uncertainty relation

   In 1945, Mandelstam and Tamm [19] introduced a derivation based on the operator relation Eq. (28). With $\hat{B} = \hat{H}$ one has

   $$\Delta A \Delta E \geq \frac{1}{2} |\langle [\hat{A}, \hat{H}] \rangle| \tag{32}$$

   Using the TDSE, one then proves that

   $$\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{A}, \hat{H}] \rangle \tag{33}$$

   to define a time interval

   $$\Delta t = \Delta A \left| \frac{d\langle \hat{A} \rangle}{dt} \right|^{-1} \tag{34}$$

   Then, from Eq. (32), one has

   $$\Delta t \Delta E \geq \hbar/2 \, .$$

   Although based on Eq. (28), this result is also a little unsatisfactory since the definition of Δt, and hence the uncertainty ΔE in the energy of the quantum system, appears to depend upon some arbitrary other observable A.

5. From the moments of time

   Wigner in 1972 [23] suggested that one define moments of the time distribution defined as

   $$\langle t^n \rangle = \frac{\int_{-\infty}^{\infty} |\psi(x,t)|^2 t^n dt}{\int_{-\infty}^{\infty} |\psi(x,t)|^2 dt} \tag{35}$$

   and than constructed the time uncertainty

   $$\Delta t = (\langle t^2 \rangle - \langle t \rangle^2)^{\frac{1}{2}} \tag{36}$$

   to derive the energy-time uncertainty relation from the TDSE. This method has the difficulty that the moments are in principle position-dependent and they do not necessarily correspond to convergent integrals.

6. From the density matrix

   Eberly and Singh [24], in 1973 proceeded from the TDSE to arrive at a Liouville equation for the density operator $\hat{\rho}$ i.e.

   $$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] \tag{37}$$

They then showed that the stationarity of the ensemble is proportional to $\Delta(\frac{d\rho}{dt})$ and used this to define a time uncertainty

$$\Delta t \sim \left[\Delta\left(\frac{d\rho}{dt}\right)\right]^{-1} \tag{38}$$

They then derived the time-energy uncertainty by use of Eq. (37).

There have been many other derivations published, using variants of the above methods [21,25]. The plethora of proofs points to the uncertain position occupied by the time-energy uncertainty relation in standard quantum mechanics. We suggest that the problem is the failure to recognise that the TDSE, on which the above proofs are based, is a mixed quantum-classical equation and that ΔE, like Δp and Δx is a property of the system but Δt is fixed by the external environment and is not a property of the system itself. From this point of view we feel that treatments interpreting Δt as the time taken for a measurement (the intrusion of a classical measuring apparatus into the quantum system) are the valid ones. Similar remarks can be made concerning the numerous attempts to define quantum times e.g. dwell times, lifetimes, tunnelling times, arrival times. Whilst doubtless a useful practical concept for the description of the results of measurements made with macroscopic devices, time, as velocity, is basically a concept alien to quantum mechanics. As shown in paper I, time enters only when the measuring device becomes so large that it can be treated to good enough approximation as an object obeying classical mechanics.

IV. THE DERIVATION OF THE TDSE FROM THE TISE

In paper I it was shown how the TDSE for a quantum system arises from the TISE for the larger object of system plus environment in the limit that the environment becomes large enough to be treated classically. In this section we present a more detailed derivation of the TDSE with the aim of showing how the initially entangled state of system and environment becomes gradually disentangled in the limit that the back-coupling of the system on the environment can be neglected. This occurs at various levels of semi-classical approximation. One aspect of the back-coupling that will be emphasized is the occurrence of generalized 'vector potentials', one element of which are the geometric phases in the environment wavefunction $\chi_n(R)$.

The TISE for the quantum object comprising a system S and its environment $\mathcal{E}$ is written

$$\begin{aligned} H\Psi &= E\Psi \\ \text{i.e.}\quad (H_{\mathcal{E}} + H_{\mathcal{S}} + H_I)\Psi &= E\Psi \end{aligned} \tag{39}$$

where H_I represents the interaction between S and $\mathcal{E}$. The total wavefunction can be expanded

$$\Psi(x,R) = \sum_m \chi_m(R)\psi_m(x,R) \tag{40}$$

where {x} and {R} are system and environment variables respectively. The environment Hamiltonian is $H_{\mathcal{E}} = K + V_{\mathcal{E}}$ with

$$K = -\frac{\hbar^2}{2M}\sum_i \frac{\partial^2}{\partial R_i^2} = -\frac{\hbar^2}{2M}\nabla_R^2 \tag{41}$$

a form that is appropriate to environments consisting of charged particles or quantized fields (photons or phonons).

Substitution of the expansion Eq. (40) into Eq. (39) and projection onto a state $\psi_n(x, R)$ leads to the coupled TISE for the environment wavefunctions χ_m i.e.

$$\sum_m \langle\psi_n| - \frac{\hbar^2}{2M}\nabla_R^2|\psi_m\rangle\chi_m(R) + V_{\mathcal{E}}\chi_n(R) + \sum_m \langle\psi_n|H_{\mathcal{S}} + H_I|\psi_m\rangle\chi_m(R) = E\chi_n(R) \tag{42}$$

where integration is over system variables {x} only. The ’potentials’

$$\mathcal{E}_{mn}(R) = \langle\psi_m|H_{\mathcal{S}} + H_I|\psi_n\rangle \tag{43}$$

depending upon the state of the quantum system provide energy surfaces which decide the state of the environment. The rest of the coupling occurs in the kinetic energy terms and can be conveniently written as

$$\langle\psi_m| - \frac{\hbar^2}{2M}\nabla_R^2|\psi_n\rangle\chi_n = -\frac{\hbar^2}{2M}\sum_k(\delta_{mk}\nabla_R + \langle\psi_m|\nabla_R|\psi_k\rangle)(\delta_{kn}\nabla_R + \langle\psi_k|\nabla_R^2|\psi_n\rangle)\chi_n \tag{44}$$

Defining

$$A_{mn}(R) = i\hbar\langle\psi_m|\nabla_R|\psi_n\rangle, \tag{45}$$

Eq. (42) can be written formally as

$$\sum_m \left[\frac{1}{2M}(\underline{\underline{P}}^2)_{nm} + \mathcal{E}_{nm}(R)\right]\chi_m + V_{\mathcal{E}}\chi_n(R) = E\chi_n(R) \tag{46}$$

where,

$$\underline{\underline{P}} = -i\hbar(\underline{\underline{1}}\nabla_R - \frac{i}{\hbar}\underline{\underline{A}}) = (\underline{\underline{1}}P_R - \underline{\underline{A}}) \quad \text{or} \quad P_{ij} = (\delta_{ij}P_R - A_{ij}) \tag{47}$$

This is exact, the notation being chosen to emphasize that the kinematic coupling $\underline{\underline{\mathrm{A}}}$ appears as a vector potential. One notes that back-coupling from the system to the environment occurs not only through the vector potential but explicitly through the potentials $\mathcal{E}_{mn}(R)$.

The companion set of equations to Eq. (46) for the system wavefunctions is

$$\begin{aligned}\sum_m \chi_m(R)\Bigg[H_{\mathcal{S}} + H_I(x,R) - \left(E - V_{\mathcal{E}}(R) + \frac{1}{\chi_m}\frac{\hbar^2}{2M}\nabla_R^2\chi_m\right) - \frac{\hbar^2}{2M}\nabla_R^2 \\ - \frac{1}{\chi_m}\frac{\hbar^2}{M}\nabla_R\chi_m\cdot\nabla_R\Bigg]\psi_m(x,R) = 0\end{aligned} \tag{48}$$

which gives an effective equation for each state of the quantum system.

The key approximation in disentangling Eq. (46) and Eq. (48) is to consider that the environment becomes so large that changes in the system, i.e. the variation of the matrix elements $\mathcal{E}_{mn}(R)$ and $A_{mn}(R)$, has no appreciable effect on its dynamics. The first stage in this approximation scheme, equivalent to a first-order perturbation theory is to neglect in Eq. (46) all off-diagonal matrix elements, to give

$$\left[\frac{1}{2M}\left(P_R - A_{nn}(R)\right)^2 + V_{\mathcal{E}}(R) + E_n(R)\right]\chi_n(R) = E\chi_n(R), \tag{49}$$

where $E_n(R) = \mathcal{E}_{nn}(R)$. In this approximation, there is simply a different effective potential energy surface deciding the state of the environment coupled to each state of the quantum system. The vector potential A_{nn}, giving rise to a geometric phase, is zero for real wavefunctions $\psi_n(x,R)$ or, since now diagonal, can be incorporated in the definition of an effective environment momentum operator.

The next level of approximation is to use a semi-classical approximation for each $\chi_n(R)$ i.e., one writes

$$\chi_n(R) = a_n(R)\exp(iW_n(R)/\hbar) \tag{50}$$

with

$$\nabla_R W_n = \vec{P}_n \tag{51}$$

where the classical momentum $\vec{P}_n$ and position $\vec{R}_n$ are decided by Hamilton's equations

$$\frac{d}{dt}\vec{P}_n = -\nabla_R H = -\nabla_R(V_{\mathcal{E}} + E_n) \tag{52a}$$

$$\frac{d}{dt}\vec{R}_n = \nabla_P H \tag{52b}$$

For the standard kinetic energy $\vec{P}^2/2M$ we use, one obtains from Eq. (52b) that $\vec{P}_n = Md\vec{R}_n/dt$. It is at this level of approximation that time first enters quantum mechanics, since to leading order in $\hbar$ we can write, with Eq. (50)

$$\frac{\hbar}{iM}\nabla_R\chi_n = \frac{\chi_n}{a_n}\frac{\hbar}{iM}\nabla_R a_n + \chi_n\frac{1}{M}\nabla_R W_n \approx \chi_n\frac{d\vec{R}_n}{dt} \tag{53}$$

For the system $\mathcal{S}$ the equations coupled to Eq. (49) read now

$$\sum_m \chi_m\left[H_{\mathcal{S}} + H_I(x,R) - E_m(R) - \frac{\hbar^2}{2M}\nabla_R^2 - \frac{d\vec{R}_m}{dt}\cdot\nabla_R\right]\psi_m(x,R) = 0 \tag{54}$$

In paper I it was shown that the term $(\hbar^2/2M)\nabla_R^2$ in Eq. (54) involving higher-order gradient couplings can be neglected in comparison with

$$i\hbar\frac{d\vec{R}_n}{dt}\nabla_R = i\hbar\frac{d}{d\tau_n} \tag{55}$$

Hence Eq. (54) becomes

$$\sum_m \chi_m\left[H_{\mathcal{S}} + H_I(x,\tau_m) - E_m(\tau_m) - i\hbar\frac{\partial}{\partial\tau_m}\right]\psi_m(x,\tau_m) = 0 \tag{56}$$

where now the quantum R dependence has been replaced by a classical time dependence.

In the approximation represented by equations Eq. (51) and Eq. (56), the environment moves classically but its motion and hence the interaction time with the quantum system is still governed by the state of the quantum system. This is the last vestige of a quantum influence on the environment. It is removed in the limit that the environment becomes fully disentangled from the quantum system and therefore can function as an external clock reading a unique time. This is achieved in the approximation that Eq. (50) becomes

$$\chi_n(R) = a_n \exp(iW(R)/\hbar) \tag{57}$$

valid if the variations in the potentials E_n in Eq. (52a) are negligible compared to $V_{\mathcal{E}}$. Then we get from Eq. (57) the unique time derivative

$$\nabla_R W = M\frac{d\vec{R}}{dt} \tag{58}$$

Recognising that the terms $E_m(t)$ in Eq. (56) can be removed by a purely time-dependent phase transformation and writing $\psi_{\mathcal{S}}(x) = \sum_n a_n \psi_n(x)$ Eq. (56) becomes

$$\left[H_{\mathcal{S}} + H_I(x,t) - i\hbar\frac{\partial}{\partial t}\right]\psi_{\mathcal{S}}(x,t) = 0 \tag{59}$$

the TDSE of Eq. (1) for the quantum system alone. This completes the disentanglement of the environment from the system; the environment's dynamics is defined by classical equations of motion unperturbed by changes in the state, e.g. the energy, of the quantum system. Conservation of energy has been abandoned at the price of introducing a unique time. This is consistent with the derivation of the energy-time uncertainty relation given in paper I. By contrast, the quantum system interacts with the environment through $H_I(x,t)$ and thereby can emit or absorb energy. As a result of this interaction, its change of state can be monitored by the environment clock. Note that this interaction, however small, is crucial, since were it zero then the time dependence can be transformed away, the quantum system is closed and the TDSE Eq. (59) becomes the TISE Eq. (3).

Another aspect of quantum theory 'illuminated' by the above derivation is the question as to why the wavefunction is a complex function. As intimated in the introduction, Schrödinger had initially some difficulty with this point and discussions persist up to recent times [26]. The necessity for complexity is usually explained as due to the factor 'i' in the term $ih\frac{\partial}{\partial t}$ of the TDSE. However, we argue that this term only arises in a classical approximation to the environment. When this approximation is not made, the environment remains quantal and there appears no reason that the solution to the TISE should not be real. Examination of our derivation shows that the origin of the factor 'i' in the TDSE lies in our semi-classical approximation for the environment

$$\chi(R) \sim a(R)\exp(iW(R)/\hbar) \tag{60a}$$

Why is a complex solution necessary? The answer can be seen most simply by taking the environment to be a single massive particle of constant momentum $\vec{K}$ (no back-coupling from the quantum system, as we require). Then the semi-classical approximation Eq. (60a) becomes exact and we have, for motion in the Z direction

$$\chi(R) = \exp(\pm iKZ) \tag{60b}$$

Hence one sees that this function, which is an eigenfuntion of the momentum operator, is the origin of the factor 'i' (the simple form Eq. (60b) is exactly that used by Mott [3] in his original derivation). That such a phase-matching of the *real* solutions $\sin(KZ)$ and $\cos(KZ)$ is necessary is very nicely discussed by Merzbacher [27]. Thus we would argue that the origin of the complexity of wavefunctions arises not from the TDSE but from the construction of eigenfunctions of the $\hat{p}$ operator in the TISE. It is the expression of our ability to distinguish between motion to the left or to the right ($\pm K$ in Eq. (60b)) or expansion from contraction in the case of spherical waves. It is also significant in this connection that what is usually called 'time reversal' invariance in quantum mechanics is in fact the property of the system under momentum reversal.

V. THE TDSE IN QUANTUM GRAVITY

There is an approach to quantum field theory in which *functional* Schrödinger equations appear, i.e. wave functionals which depend on field functions. Apart from this, the equations resemble Schrödinger equations of ordinary quantum mechanics. This approach has been much used in the field of quantum gravity [28]. There one attempts to quantise gravity in a way in which the classical limit produces the field equations of general relativity. One begins with the 'Hamiltonian constraint' of general relativity

$$H = 0 \tag{61}$$

and writes an operator version as the Wheeler-deWitt equation of quantum gravity

$$\hat{H}\psi = 0 \tag{62}$$

The analogy to the quantisation of the classical constraint Eq. (5) to give the TISE of quantum mechanics Eq. (8) is complete. The remarkable thing is that Eq. (62) does not contain time. How one recovers the time to enter the classical four-dimensional space-time is known as 'the problem of time in quantum gravity' (a very readable account is given by Kiefer [29]). An even more remarkable thing is that the solution to this problem is to proceed exactly as is done in atomic and molecular physics ([28,30] and as has been done in section IV, to reduce the TISE for a composite system to the TDSE for a part of the system whereby the remaining part has been treated semi-classically. In atomic physics the quantum part is the electronic motion and the motion of the heavy nuclei provides the classical time. In the general case of section IV (see paper I) the quantum system has a classical time provided by the large environment. In the case of quantum gravity, matter fields in the universe are the quantum objects and the gravitational field is treated in a semi-classical limit. As in section IV, back-coupling of matter fields on the gravitational three-metric is neglected and ψ is factorised

$$\psi(\mathcal{G}, \phi) \approx \chi(\mathcal{G})\psi(\phi, \mathcal{G}) \tag{63}$$

where $\mathcal{G}$ denotes gravitational and ϕ matter fields. This corresponds exactly to the single-channel version of Eq. (40). One sees that the gravitational field plays the role of the environment and the matter field ϕ that of the quantum system.

Time arises when, exactly as in equation Eq. (50), the functional χ is approximated semi-classically

$$\chi(\mathcal{G}) = a(\mathcal{G}) \exp\left(\frac{i}{\hbar} W(\mathcal{G})\right) \tag{64}$$

where the functional W obeys the Hamilton-Jacobi equations for the gravitational field alone (which are equivalent to the Einstein equations of classical general relativity). The operator $\hat{H}$ in Eq. (62) contains the gravitational field operator and the operator $\hat{H}_m$ of the matter fields. Substitution of Eq. (63) and Eq. (64) into the TISE Eq. (62) then leads to the TDSE for the matter fields alone i.e.

$$i\hbar \nabla W \cdot \nabla \psi \equiv i\hbar \frac{\partial \psi}{\partial t} \approx H_m \psi \tag{65}$$

again in complete analogy to Eq. (55).

One sees that the time entering the functional TDSE for the quantum fields arises from a classical description of the ’environment’ and the time parameter is that arising in the classical field equations for this environment.

VI. CONCLUSIONS

We have presented a derivation of the time-dependent equation of Schrödinger. This derivation, unlike those presented in quantum mechanics text-books but in the spirit of Schrödinger’s original approach to the problem, acknowledges that time enters quantum mechanics only when an external force on the quantum system is considered classically. Starting from a fully time-independent formulation of quantum mechanics (the TISE) we systematically derive the TDSE for a quantum system, with appropriate effective time-dependent Hamiltonian, in the approximation that the environment is treated semi-classically.

Our derivation relies on the assumption of a closed object comprising system plus environment. Only when the state of the environment is completely disentangled from that of the quantum system does a unique classical time parameter, a clock, for that system appear. Our supposition that this is how time always arises in quantum theory is supported by the observation that this is precisely how time enters the functional Schrödinger equation of quantum gravity. Here, the time-independent functional Schrödinger equation for quantised space and matter (the whole universe) reduces to an effective functional TDSE for matter fields only, in the limit that the gravity field (the background environment for the quantised matter fields) is treated semi-classically. Apart from the replacement of wavefunctions by wave-functionals, the methods of derivation in the two cases are identical.

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