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The derivation of time-dependent Schrödinger equations

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Abstract

Beginning with an entangled state of a time-independent (TI) quantum system coupled to its TI quantum environment, we show that a time-dependent Schrödinger equation (TDSE) for the quantum system alone can be derived in the limit that one of the environment variables becomes a classical variable. In the same limit the TI amplitude of the environment wavefunction becomes the TD amplitude of an eigenfunction expansion of the system TD wavefunction. Similarly, the phase of the TI environment wavefunction goes over into the TD phase of the system amplitude. By considering that more and more environment variables become successively classical, each provides a classical clock to give a multiple-time TDSE for the quantum system. Two examples of two-time TDSE given in the literature are derived. When all clocks are synchronized the multiple-time TDSE reduces to the usual one-time TDSE.

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1. Introduction

In three previous papers [8, 9, 12] a fundamental dissatisfaction with the conventional ‘derivations’ of the time-dependent Schrödinger equation (TDSE) given in quantum mechanics textbooks was expressed. Beginning with a time-independent Schrödinger equation (TISE) for a system and its environment an alternative derivation of the TDSE for the quantum system was given, motivated by the wish to provide a better-founded derivation than those currently accepted. Even though the TDSE is universally considered as more ‘fundamental’ than the TISE, there are difficulties with the conventional derivations and the related question of the meaning of the time–energy uncertainty relation. These points are discussed in detail

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in the previous papers, particularly in [12], but as an introduction to what follows will be recapitulated briefly here.

In 1926, Schrödinger [1] first derived the TISE from a variational principle and showed that quantization of energy can be formulated as an eigenvalue problem. The TISE applies to conservative time-independent Hamiltonians. He had great difficulty with the derivation of a TDSE, which can be applied to time-dependent Hamiltonians. Indeed, his first attempt in [2] specified a fixed energy E , did not contain \hbar and was of second order in the time derivative (by direct analogy with the wave equation of classical electrodynamics). However he recognized that to apply quantum mechanics to time-dependent Hamiltonians, in particular that of an atom in an external classical light field, he had to eliminate the fixed energy E from the problem. His first attempt to do this, involving real wavefunctions, resulted in an equation of fourth order in space derivatives and second order in the time derivative [3]. However, he quickly realized that by admitting complex wavefunctions he could derive the TDSE we know today, involving only a first time derivative. Nevertheless, his derivation begins with a time-independent Hamiltonian and only after eliminating the fixed energy could Schrödinger arbitrarily generalize to time-dependent Hamiltonians and consider the problem of an atom interacting with a classical light field (at that time the quantization of the electromagnetic field had not been achieved). Despite the success of this exercise, he was not satisfied with this TDSE and the accompanying complex wavefunction and writes in the last paragraph of his fourth 1926 communication [3], that the equation containing a first time derivative ‘... is only a surrogate for a real wave equation, probably of fourth order, in whose formulation in the non-conservative case I have not been successful’.

Since then the TDSE has come to be regarded as ‘the’ fundamental equation of quantum mechanics: the TISE being derived as a special case. Despite this, most textbooks follow Schrödinger’s route and consider first the TISE of a conservative system at fixed energy and suggest, by plausibility arguments, a TDSE which generally implies non-conservation of energy. The derivations fall into two categories, both beginning with time-independent Hamiltonians at fixed energy:

- (a) by analogy with the relationship between position and momentum, the energy in the TISE is replaced by $i\hbar\partial/\partial t$ on the grounds that energy and time are also classically conjugate variables. However, position and momentum are both Hilbert-space operators and then so is the Hamiltonian but $\partial/\partial t$ is a parametric differentiation. There is no Hilbert-space operator for time. Position, momentum and energy are probabilistic, time is certain.
- (b) a plane-wave spacetime wavefunction is assumed to describe the fixed-energy motion of a point particle, where the time-independent Hamiltonian is simply the kinetic energy operator without a potential. This function is a solution of the TDSE for this specific (time-independent) problem.

In both cases (a) and (b) the resulting TDSE contains a time-independent Hamiltonian but the equation is simply generalized, without proof, to apply to arbitrary time-dependent Hamiltonians.

Schrödinger in his 1926 papers and Born, Heisenberg and Jordan, in their famous 1926 paper [4] did not know how to quantize the electromagnetic field or a beam of charged particles. Hence, they used classical time-dependent fields to describe the interaction with the quantized atom. However, they realized from the outset that this was an approximation, valid only when the external classical field contains so much energy that it is unaltered by interaction with the quantized atom. Already in 1926 this approximation was rendered unnecessary by Born’s quantization of a particle beam [5] (incidentally the first example of a beam–atom entangled wavefunction is contained in this paper) and a few years later Dirac quantized the

electromagnetic field. This meant that all quantum transitions could be described by the TISE. Nevertheless the time dependence of a transition process is more intuitive to classical humans and the TDSE has many advantages. However, that it is an approximation, as recognized by the founding fathers, was first shown explicitly by Mott in 1931 [6], who considered the specific case of a plane-wave heavy-ion beam–atom interaction and showed that when the beam energy far exceeds the atomic excitation energies, Born’s TISE for the quantized beam–atom entangled wavefunction can be reduced to a TDSE for the atom alone, in which the beam ions move on a classical straight-line path. More importantly, Mott showed explicitly the origin of $\partial/\partial t$ in the TDSE as due to the beam motion. This aspect of the approximate nature of the TDSE appears to have been neglected and in [8] it was sought to re-emphasize this by generalizing Mott’s approach to derive a TDSE applicable to arbitrary external time-dependent interactions. That is, it is important to recognize that when time enters the Schrödinger equation in the form of a time-dependent interaction potential $H_I(t)$, the time is a classical variable arising from the solution of classical Maxwell, Newton (or equivalent) equations. From this point of view the TDSE is a mixed quantum-classical equation, the interaction potential $H_I(t)$ representing the interaction of a quantum system with an exterior classical time-dependent force.

In the generalization of Mott’s analysis given in [8] it was shown how, beginning with a closed quantum composite at fixed energy described by a time-independent Schrödinger equation (TISE), the TDSE for a part of the composite (called the quantum system S) can be derived in the limit that the rest of the system (called the environment \mathcal{E}) becomes classical. Then the classical motion of the environment gives rise, via its kinetic energy operator, to the $\partial/\partial t$ term in the TDSE for the quantum system S and the time-independent interaction potential between system and environment becomes a time-dependent external potential $H_I(t)$ acting on the quantum system. In [9] this derivation was considered in detail for the case that $H_I(t)$ represents the interaction with a classical electromagnetic field as environment. It is also interesting to note, as discussed in detail in [12], that the method of derivation of the $\partial/\partial t$ operator in the time-dependent equation for matter fields in quantum gravity, beginning with the time-independent Wheeler–de Witt equation [7] is exactly the same as that employed by Mott and generalized in [8].

The derivation of the TDSE given in the above papers relies upon an adiabatic-like expansion of the total wavefunction of environment and system and leads directly to the TDSE for the system alone. Although this expansion is completely general, doubts have been raised to us that the derivation requires, and is limited to, the precise form of this expansion. To quell these doubts, we present here an alternative derivation beginning with a simple entangled wavefunction of system and environment. Although this does not lead directly to the TDSE, rather to coupled equations for the amplitudes of a basis set expansion of the TDSE, we feel the derivation is illuminating. Not only does the environment kinetic energy provide the $\partial/\partial t$ operator, as in the previous derivation, but the new approach shows explicitly how the time-independent amplitudes and phases of the environment wavefunctions transform directly into the time-dependent amplitudes and phases of the expansion co-efficients in the TDSE.

It should also be stressed that here we have the limited aim of showing that the TISE for system and environment reduces to the (norm-conserving but energy non-conserving) TDSE for the system alone. A more complete description of their interaction incorporating modern developments to describe decoherence, dissipation and time irreversibility requires a formulation in terms of density matrices and the Liouville equation, which allows more flexibility than the limitation to Schrödinger equations that is considered here.

Another aspect of time dependence in quantum mechanics is treated also in this paper. In [8] a single time variable arising from the classical motion of a many-dimensional environment

was defined. However, it is clear that any *single* classical variable, or a sequence of them, can be taken as the time-determining variables i.e. as external clocks. In particular it will be shown here that a hierarchy of clocks can be introduced to give multiple-time-dependent-Schrödinger equations (MTDSE). Such an equation is meaningful where two or more clocks perform different measurements on a quantum system so that two times are registered. An example of this, although derived by other means, is the clocked two-time SE of Sokolovski [10], where one clock monitors the overall time development and another the dwell time in a particular region of space only. Another example is the (t, t') method of Moiseyev and co-workers [11], where an additional time variable was introduced simply for mathematical convenience. Here we show that it can be derived by considering that two independent environment variables are used to provide two independent clocks. However, by generalizing the treatment of Moiseyev and co-workers [11] to multiple times, it will be shown how the MTDSE reduces to the normal one-time TDSE when all classical time variables are dependent (synchronization of clocks).

Finally, we show that it is not necessary to begin with a TISE for system plus environment in a given eigenstate, as assumed in [8]. Rather a linear superposition, or wavepacket in energy space, can be assumed as the initial total wavefunction. In short, the transition of the environment from quantum to classical behaviour will be considered more generally and from a different point of view than that given in [8, 9].

2. Time-dependent Schrödinger equations

In [8] a time variable was defined for a set of environment variables $R_i, i = 1, 2, \dots, N$ such that the time derivative appearing in the TDSE was derived as

$$\frac{d}{dt} = \sum_i \frac{1}{m_i} \frac{\partial W}{\partial R_i} \frac{\partial}{\partial R_i} = \sum_i \frac{dR_i}{dt} \frac{\partial}{\partial R_i}, \quad (1)$$

where W is the classical action of the environment, $\partial W/\partial R_i = P_i$ and m_i is the mass associated with the i th degree of freedom. Here we will consider the definition of multiple time variables and show how MTDSE occur naturally and reduce to the usual single-time TDSE under special conditions.

To begin we consider only a single environmental degree of freedom R and show how a Newtonian time is defined. First we generalize the derivation of [8] and also use a somewhat different method, employing initially a standard form of entangled system-environment wavefunction to show that one criterion for the introduction of classical time is the disentanglement of the environment (clock) from the remaining quantum system. This quantum system will be denoted by \mathcal{S} with totality of quantum variables denoted simply by $\{x\}$ with conjugate momenta $P_x = -i\hbar\partial/\partial x$. The environment \mathcal{E} will be considered to have a single quantum degree of freedom R whose transition to classical behaviour will give rise, through the interaction Hamiltonian $H_I(x, R)$, to a time dependence for \mathcal{S} . To illustrate the differences to the method of derivation given here, we give a brief summary of the method and results of [8]. In this approach we began with the total system $\mathcal{T} = \mathcal{E} \otimes \mathcal{S}$ in an eigenstate of total energy E with TISE

$$(H - E)\Psi(x, R) = 0. \quad (2)$$

Then to illustrate the explicit dependence of \mathcal{S} on the coupling with \mathcal{E} an ‘adiabatic-like’ expansion

$$\Psi(x, R) = \sum_n \chi_n(R)\psi_n(x, R) \quad (3)$$

was used, where χ_n are wavefunctions of the environment in different states and ψ_n are corresponding wavefunctions of the quantum system \mathcal{S} . Then, when the environment becomes sufficiently large, the changes in the state of the system, described by different wavefunctions ψ_n , do not affect the state of the environment significantly. This allows the expansion (3) to be approximated by the single channel form

$$\Psi(x, R) \sim \chi(R)\psi(x, R). \tag{4}$$

Note that in this approximation the environment and the system are still entangled due to the interaction term H_I in the total Hamiltonian

$$H_T = H_E(R) + H_S(x) + H_I(x, R). \tag{5}$$

Specific examples of ‘environment’ considered in [8, 9] are a beam of charged particles or an electromagnetic field providing an interaction with a target molecule, atom or nucleus as quantum system. The state of the environment (e.g. beam or field) is now defined by the single-channel equation (see equation (14) of [8])

$$(H_E + U_S(R) - E)\chi(R) = 0, \tag{6}$$

where U_S is an effective potential provided by the quantum system. It is shown that when $\chi(R)$ is approximated by a semi-classical wavefunction with phase $W(R)$ given by Hamilton’s characteristic action function, time enters from the definition of a *classical* momentum and velocity i.e.

$$P(R) = \frac{\partial W}{\partial R} = M \frac{dR}{dt}, \tag{7}$$

where M is the environment mass. Then, to lowest order in \hbar , the $\partial/\partial t$ operator acting on $\psi(x, R(t))$ is shown to arise from the environment (clock) kinetic energy operator $-(\hbar^2/2M)\partial^2/\partial R^2$ acting on the product equation (4). The TDSE for the quantum system \mathcal{S} alone becomes

$$\left(H_S(x) + H_I(x, t) - i\hbar \frac{\partial}{\partial t} \right) \psi(x, t) = 0. \tag{8}$$

A further paper [12] contains a discussion of why we believe this derivation to be better-founded than that given in textbooks, where, as explained above, the TDSE is simply introduced in an ad hoc way from a plausible but nevertheless unfounded generalization of *time-independent* systems at fixed energy.

Here we present an alternative more general derivation of equation (8) which shows that it is not necessary to assume the ‘adiabatic-like’ expansion equation (3).

To see this we begin again with expansion equation (3). However, clearly one can expand the x dependence of the functions $\psi_n(x, R)$ further in any fixed complete set $\phi_k(x)$ i.e.

$$\psi_n(x, R) = \sum_k c_{nk}(R)\phi_k(x) \tag{9}$$

or,

$$\Psi(x, R) = \sum_n \sum_k \chi_n(R)c_{nk}(R)\phi_k(x)$$

i.e.,

$$\Psi(x, R) = \sum_k \mathcal{K}_k(R)\phi_k(x), \tag{10}$$

where,

$$\mathcal{K}_k(R) = \sum_n \chi_n(R)c_{nk}(R). \tag{11}$$

The expansion equation (10) is now in the usual form describing an entangled state of environment \mathcal{E} with system \mathcal{S} . Hence one sees that the form equation (3) implies no restriction on validity since it is connected to equation (10) by a linear transformation. Only the matrix elements arising in the TISE are different in the two bases. Nevertheless, as we now show, the form equation (10) gives a direct correspondence between the time-independent environment wavefunctions and the time-dependent amplitudes and phases of a basis-set expansion of the TDSE for the quantum system.

The total Hamiltonian is given by equation (5) where $H_{\mathcal{E}}$ and $H_{\mathcal{S}}$ are those of environment and system respectively. Substitution of the expansion equation (10) and the Hamiltonian equation (5) in the TISE equation (2) and projection on one of the set $\phi_k(x)$ leads to

$$\sum_k \langle \phi_l | H_{\mathcal{E}} + H_{\mathcal{S}} + H_I - E | \phi_k \rangle \mathcal{K}_k(R) = 0 \quad (12)$$

a set of coupled equations for the environment wavefunctions $\mathcal{K}_k(R)$. If we choose the expansion basis $\phi_k(x)$ to be orthonormal then the coupled equations become

$$(H_{\mathcal{E}} - E)\mathcal{K}_l(R) + \sum_k \langle \phi_l | H_{\mathcal{S}} + H_I | \phi_k \rangle \mathcal{K}_k(R) = 0 \quad (13)$$

showing that the different \mathcal{K}_k are mixed by the back-coupling of the quantum system on the environment. We write the exact \mathcal{K}_k functions as

$$\mathcal{K}_k(R) = c_k(R) \exp \left\{ \frac{i}{\hbar} W_k(R) \right\}, \quad (14)$$

where the functions W_k are chosen real and fixed (see below) but, unlike the usual expansion of this form, c_k are in general complex functions. With

$$H_{\mathcal{E}} = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial R^2} + V_{\mathcal{E}}(R)$$

this transformation leads to the coupled equations,

$$\begin{aligned} & \left[\frac{1}{2M} \left(\frac{\partial W_l}{\partial R} \right)^2 - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial R^2} + V_{\mathcal{E}}(R) - E \right] c_l - \left[\frac{i\hbar}{2M} c_l \frac{\partial^2 W_l}{\partial R^2} + \frac{i\hbar}{M} \frac{\partial c_l}{\partial R} \frac{\partial W_l}{\partial R} \right] \\ & + \sum_k \langle \phi_l | H_{\mathcal{S}} + H_I | \phi_k \rangle c_k(R) \exp \left\{ -\frac{i}{\hbar} (W_l - W_k) \right\} = 0. \end{aligned} \quad (15)$$

At this stage the coupled equations are exact and represent the TISE of equation (A.3).

As in [8], a classical time now is introduced by considering that the environment is so massive or has such high energy that it can be treated classically and the quantum variable R becomes a classical time-dependent variable $R(t)$, parametrized by a classical time t . Although not necessary, it will make the subsequent analysis more transparent if at this stage we take ϕ_l to be the eigenstates of the Hamiltonian $H_{\mathcal{S}}$, with eigenenergies ϵ_l . The first step in the transition to a classical environment is to disentangle the quantum environment \mathcal{E} from the quantum system \mathcal{S} . This is achieved by neglecting the back-coupling, via the interaction matrix elements $\langle \phi_l | H_I | \phi_k \rangle$, of the changes in state of the quantum system on the environment. The condition for the neglect of back-coupling is that the interaction matrix elements, of dimension of energy, are negligibly small compared to the energy of the environment so that changes in the quantum system state do not perceptibly influence the environment motion. In the semi-classical limit the defining terms for the motion of the environment are those independent of \hbar in equation (15) i.e. the action function W_l satisfies the classical Hamilton–Jacobi (H–J) equation

$$\frac{1}{2M} \left(\frac{\partial W_l}{\partial R} \right)^2 + V_{\mathcal{E}}(R) - (E - \epsilon_l) = 0. \quad (16)$$

This equation can be solved to give the classical action

$$W_l(R) = \int^R \sqrt{2M[E - \epsilon_l - V_{\mathcal{E}}(R')]} dR' \tag{17}$$

and to define the classical time t_l via the equation

$$\frac{\partial W_l}{\partial R} = P_l = M \frac{dR}{dt_l}, \tag{18}$$

where $P_l(R)$ is the classical momentum function of the environment. Note that equation (17) defining W_l as the classical action is equivalent to making the WKB approximation for the phase of the exact environment wavefunction $\mathcal{K}_k(R)$ in equation (14).

For the purposes of this paper, unlike [8, 9], we wish to consider that the environment is a (classical) clock used to specify a time (from equation (18)) as

$$t_l(R) = M \int^R \frac{dR'}{\partial W_l / \partial R'}. \tag{19}$$

Various types of clock are discussed in [13]. The simplest, called the perfect clock, is one in which a particle of mass M moves in a straight line with constant momentum. This is equivalent to putting $V_{\mathcal{E}}(R) = 0$ in equation (17) and avoids the difficulty of the possibility of turning points at which $E - \epsilon_l = V_{\mathcal{E}}(R)$, where the WKB approximation breaks down (that this breakdown causes no difficulty in principle is demonstrated in [9] where the specific case of a quantum oscillating environment, classically a pendulum clock, is considered). For the linear perfect clock equation (19) becomes

$$\begin{aligned} t_l(R) &= \int^R dR' \sqrt{2M(E - \epsilon_l)} \\ &= R \sqrt{2M(E - \epsilon_l)}. \end{aligned} \tag{20}$$

This is the last vestige of the influence of the quantum system in one of its eigenstates ϕ_l with energy ϵ_l on the classical motion of the clock. However, clearly if E is an energy of classical dimensions, to justify the WKB approximation it must be far greater than any energy fluctuations arising from the quantum system. Hence we can put

$$t_l \approx t = \frac{R}{\sqrt{2ME}} = \frac{R}{v} \quad \forall l, \tag{21}$$

where

$$v = \frac{dR}{dt} \tag{22}$$

is the constant classical velocity of the clock whose energy is $E = Mv^2/2 = P^2/2M$.

With the validity of the H-J equation (16) for the classical clock (environment \mathcal{E}) we return to equation (15), which now reads

$$-\frac{\hbar^2}{2M} \frac{\partial^2 c_l}{\partial R^2} - \left[\frac{i\hbar}{2M} c_l \frac{\partial^2 W_l}{\partial R^2} + \frac{i\hbar}{M} \frac{\partial c_l}{\partial R} \frac{\partial W_l}{\partial R} \right] + \sum_k \langle \phi_l | H_I | \phi_k \rangle c_k(R) \exp \left\{ -\frac{i}{\hbar} (W_l - W_k) \right\} = 0 \tag{23}$$

defining the dynamics of the quantum system as the environment changes its state. The first term $(-\hbar^2/2M)\partial^2 c_l/\partial R^2$ is proportional to what is known as the ‘quantum potential’ in Bohmian mechanics [14]. It is highly oscillatory in the classical short wavelength limit and is of second order in \hbar as $\hbar \rightarrow 0$. Hence it can be neglected so long as the second derivative of c_l is not of the order of \hbar^{-2} . Indeed the neglect of this quantum potential can

be seen as a condition for the validity of the TDSE. If it is not negligible one has to consider the corrections explicitly. The first term in square brackets in equation (23) is only of first order in \hbar but involves the second derivative of the slowly varying classical action. Hence this term can be neglected since the classical momentum does not vary appreciably over atomic dimensions. Indeed, for the perfect clock with free motion this term is identically zero i.e. $\partial^2 W/\partial R^2 = \partial P/\partial R = 0$. The second term in square brackets is the time-defining term for the quantum system, since

$$\frac{i\hbar}{M} \frac{\partial c_l}{\partial R} \frac{\partial W_l}{\partial R} = i\hbar \frac{\partial c_l}{\partial R} \frac{dR}{dt} = i\hbar \frac{\partial c_l(t)}{\partial t}. \quad (24)$$

Thus, for the quantum system, in the semi-classical limit for the environment, equation (23) simplifies to

$$\sum_{k \neq l} \langle \phi_l | H_I(x, t) | \phi_k \rangle c_k(t) \exp \left\{ -\frac{i}{\hbar} (W_l - W_k) \right\} = i\hbar \frac{\partial c_l(t)}{\partial t}. \quad (25)$$

To derive time-dependent phase factors, first we define the phase factor in equation (25) as

$$\Phi \equiv \exp \left\{ -\frac{i}{\hbar} (W_l - W_k) \right\}. \quad (26)$$

The classical action function W_l is given in equation (17) as

$$W_l(R) = \int^R [2M(E - V_{\mathcal{E}}(R') - \epsilon_l)]^{\frac{1}{2}} dR'. \quad (27)$$

Now we take the limit that the classical kinetic energy $E - V_{\mathcal{E}}(R')$ is always much larger than the quantum energy ϵ_l . Then we can expand

$$W_l(R) = \int^R (2M)^{\frac{1}{2}} [E - V_{\mathcal{E}}(R')]^{\frac{1}{2}} \left(1 - \frac{1}{2} \epsilon_l [E - V_{\mathcal{E}}(R')]^{-1} \right) dR'. \quad (28)$$

Clearly the first term on the rhs of (28), which is the classical action of the environment (clock) uninfluenced by the state of the quantum system, cancels out in equation (26), leaving

$$\Phi \equiv \exp \left\{ -\frac{i}{\hbar} (\epsilon_l - \epsilon_k) \frac{1}{2} (2M)^{\frac{1}{2}} \int^R [E - V_{\mathcal{E}}(R')]^{-\frac{1}{2}} dR' \right\}. \quad (29)$$

However, the classical momentum is defined by

$$P(R) = [2M(E - V_{\mathcal{E}}(R))]^{\frac{1}{2}} = M \frac{dR}{dt} \quad (30)$$

so that the classical time is

$$t = M \int^R [2M(E - V_{\mathcal{E}}(R'))]^{-\frac{1}{2}} dR'. \quad (31)$$

Substitution into (29) gives

$$\Phi \equiv \exp \left\{ -\frac{i}{\hbar} (\epsilon_l - \epsilon_k) t \right\}, \quad (32)$$

which is the usual quantum-mechanical phase difference. Therefore, we can write equation (25) as

$$\sum_{k \neq l} \langle \phi_l | H_I(x, t) | \phi_k \rangle c_k(t) \exp \left\{ -\frac{i}{\hbar} (\epsilon_l - \epsilon_k) t \right\} = i\hbar \frac{\partial c_l(t)}{\partial t}. \quad (33)$$

From equation (33) one sees that the quantum variable R is transformed to a classical time parameter t (via equation (21)) and a part of the environment's kinetic energy (the motion of the clock) provides the $\partial/\partial t$ operator. The amplitudes of the time-independent environment wavefunctions go over into time-dependent occupation amplitudes for the various quantum system eigenstates and the classical action provides the usual time-dependent phase factors on these amplitudes. Thus there is a complete reduction of the time-independent quantum environment to providing a classical time dependence for the remaining quantum system.

It is trivial to show that equation (33) is entirely equivalent to the TDSE

$$\left(H_S + H_I(x, t) - i\hbar \frac{\partial}{\partial t} \right) \psi_S(x, t) = 0 \quad (34)$$

for the quantum system alone, with the expansion

$$\psi_S(x, t) = \sum_k c_k(t) \phi_k(x) \exp\left(-\frac{i}{\hbar} \epsilon_k t\right) \quad (35)$$

in eigenstates of H_S . Substitution of equation (35) in equation (34) and projection onto $\phi_l \exp(-i\epsilon_l t/\hbar)$ gives

$$\sum_{k \neq l} \langle \phi_l | H_I(x, t) | \phi_k \rangle c_k \exp\left\{-\frac{i}{\hbar} (\epsilon_l - \epsilon_k) t\right\} = i\hbar \frac{\partial c_l(t)}{\partial t} \quad (36)$$

i.e. exactly equation (33) and therefore the TDSE equation (34) expanded in eigenfunctions of H_S . Note that the interaction potential H_I , which is neglected in the motion of the classical environment becomes a time-dependent external potential for the quantum system. However, when the environment is simply a clock, monitoring the time of the quantum system, it is clear that the clock should not disturb the system noticeably. Then the effect of the clock interaction on the quantum system can be neglected, the system Hamiltonian becomes time-independent and equation (34) reduces to the 'usual' one-time TDSE

$$\left(H_S(x) - i\hbar \frac{\partial}{\partial t} \right) \psi_S(x, t) = 0. \quad (37)$$

This derivation illustrates the role of measurement of a quantum system by a classical environment in providing a scale for time: The TDSE is a mixed quantum-classical equation. It is clear that this usual form of the TDSE is an approximation valid only when the disturbance by the act of time measurement is vanishingly small. Then the initial state, or initial linear combination of states, propagates in time according to equation (37) only by accumulating a time-dependent phase. There are no transitions between states. In the more general case where the interaction Hamiltonian (interaction with the environment) is not negligible but, as in the case of a particle beam or a laser pulse, goes to zero for large negative and positive times, the system will begin in some initial state and propagate in time according to equation (34) with transitions to some linear combination of final states.

3. Multiple-time Schrödinger equations

Clearly, the process of transition of a quantum variable to a classical time-determining parameter can now be continued for successively more variables to derive MTDSE. To illustrate the derivation of MTDSE, the further sub-division of the quantum system will be made as shown in figure 1, i.e. $\mathcal{S} = \mathcal{E}' \otimes \mathcal{S}'$, corresponding to taking one of the variables $\{x\}$ as defining a new environment with degree of freedom R' ,

$$\{x\} = \{x'\} \oplus R'. \quad (38)$$

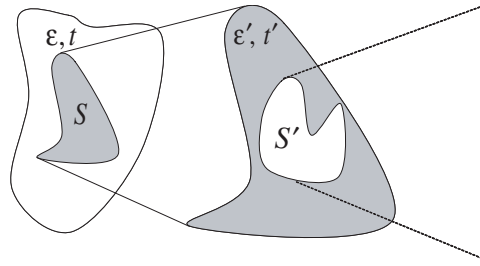


Figure 1. Illustrating the successive movement of the quantum/classical boundary as selected variables become classical.

Then we can write equation (34) explicitly, dropping the S from the wavefunction, as

$$\left[H_{S'} + H_{\mathcal{E}'} + H_I(x', R', t) - i\hbar \frac{\partial}{\partial t} \right] \psi(x', R', t) = 0, \quad (39)$$

where H_I now includes the interaction between S' and \mathcal{E}' . Note that this is the starting point of the analysis of Aharonov and Bohm [15] in their classic paper on the boundary, often referred to simply as the ‘cut’, between classical and quantum behaviour.

Equation (39) is the ‘usual’ TDSE for the quantum system S with time defined by classical motion of the variable $R(t)$. The key observation here is that the transition of quantum variables R to classical $R(t)$ and the transition of the corresponding quantum kinetic energy to a $\partial/\partial t$ differential can also be made in equation (39) with respect to the variable R' , leading to the ‘two-time’ TDSE

$$\left[H_{S'} + H_I(x', R'(t'), t) - i\hbar \frac{\partial}{\partial t'} \right] \psi(x', R'(t'), t) = i\hbar \frac{\partial}{\partial t} \psi(x', R'(t'), t), \quad (40)$$

or simply,

$$\left[H_{S'} + H_I(x', t', t) - i\hbar \frac{\partial}{\partial t'} \right] \psi(x', t', t) = i\hbar \frac{\partial}{\partial t} \psi(x', t', t). \quad (41)$$

Here, there really are two time derivatives i.e. two clocks measuring different times t and t' given by

$$t = \int \frac{dR}{\dot{R}} \quad \text{and} \quad t' = \int \frac{dR'}{\dot{R}'}. \quad (42)$$

The $\partial/\partial t$ derivative is taken with R' and x' fixed but the $\partial/\partial t'$ derivative only with x' fixed. The variable x' is many-dimensional, so that the process of moving the cut to include fewer quantum and more classical variables can be continued. Then more classical clocks, each with its own time variable τ_n and partial derivative will be introduced i.e. one obtains for the general case

$$[H_S(x) + H_I(x, \tau_1, \tau_2, \dots, \tau_n)] \psi(x, \tau_1, \tau_2, \dots, \tau_n) - i\hbar \sum_n \frac{\partial}{\partial \tau_n} \psi(x, \tau_1, \tau_2, \dots, \tau_n) = 0, \quad (43)$$

where $H_S(x)$ is the Hamiltonian of the quantum system remaining after n variables have been placed on the classical side of the cut and $\{x\}$ now represents the remaining quantum variables. H_I is the total interaction of the classical environment with the quantum system. This is the fundamental multiple-time-dependent Schrödinger equation (MTDSE). We now derive two examples of this general formula, obtained in the literature using different methods.

4. Two examples of the MTDSE

As the first example we derive the so-called t, t' method which is a case of the TDSE with two time variables. In a series of papers [11], Moiseyev and co-workers have pointed out the usefulness of a two-time (t, t') TDSE which reduces to the usual one-time TDSE in the limit $t' = t$. In these papers the variable t' and the associated $i\hbar\partial/\partial t'$ factor in the TDSE were introduced as a mathematical device; by extending the Hilbert space by introduction of the t' variable methods used for time-independent Hamiltonians can be employed. However, here we have seen that the MTDSE, equation (43), arises from the successive transition of quantum variables to classical variables, retaining terms to lowest order in \hbar . For example for $n = 2$, taking t to be the perfect clock, and to conform to the development in [11], putting $H(x, t') = H_S + H_I(x, t')$, i.e. neglecting any t dependence of the total Hamiltonian, we have

$$i\hbar \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial t'} \right) \psi(x, t', t) = H(x, t')\psi(x, t', t) \tag{44}$$

which is exactly equation (9) of Peskin and Moiseyev [11]. In that paper they also show that

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial t'} \right) \psi(x, t', t) \Big|_{t'=t} = \frac{\partial \tilde{\psi}(x, t)}{\partial t}, \tag{45}$$

where

$$\tilde{\psi}(x, t) = \psi(x, t', t) \Big|_{t'=t} \tag{46}$$

and satisfies the one-time TDSE

$$i\hbar \frac{\partial \tilde{\psi}(x, t)}{\partial t} = H(x, t)\tilde{\psi}(x, t). \tag{47}$$

Implicitly the procedure used in going from equation (44) to equation (47) to define a single common time is used in equation (1) which is the definition of time given in [8]. That is, if one first specifies a separate time t_i for each variable R_i , then equation (1) reads

$$\frac{d}{dt} = \sum_i \frac{dR_i}{dt_i} \frac{\partial}{\partial R_i} = \sum_i \frac{d}{dt_i}.$$

Then repetition of the procedure of equation (45) and equation (46), i.e. $t_i = t \forall i$, leads to the one-time SE of equation (47).

As a second example we derive the ‘clocked’ Schrödinger equation. By analogy to the case of the diffusion equation in the classical theory of Brownian motion, Sokolovski [10] has derived a two-time Schrödinger equation, called the ‘clocked’ SE. This is of the form, in one dimension,

$$i\hbar \frac{\partial}{\partial t} \psi(x, t, \tau) = H_p \psi(x, t, \tau) - i\hbar \Theta_{ab}(x) \frac{\partial}{\partial \tau} \psi(x, t, \tau), \tag{48}$$

where $\Theta_{ab}(x) = 1$ for $a \leq x \leq b$ and zero otherwise. The function $\psi(x, t, \tau)$ is interpreted as the probability amplitude for the particle, as the quantum system with Hamiltonian $H_S = H_p(x)$, to have spent duration τ in $[a, b]$ prior to time t . It is claimed that this equation goes beyond the SE and cannot be derived from it: the derivation of Sokolovski employing a path integral formalism is suggested to provide insights into quantum motion not provided by the Schrödinger approach. However, we see that our two-time TDSE equation (41) is precisely of the general form of the clocked SE of Sokolovski. To see the connection we must begin with a modified equation (40) in which the potential interaction H_I is neglected. Then the clock which is to be defined by the transition of the quantum variable R to classical $R(\tau)$ is represented by the Hamiltonian H_C . To conform with Sokolovski’s time measurement,

this clock is only on, i.e. measuring time, when the particle represented by the Hamiltonian $H_p(x)$ is in the x -region $[a, b]$. Hence, we write the one-time TDSE

$$i\hbar \frac{\partial}{\partial t} \psi(x, t, R) = [H_p(x) + H_{\mathcal{E}}(R)\Theta_{ab}(x)]\psi(x, t, R). \quad (49)$$

Then by repeating the analysis leading to equation (10) we obtain the two-time TDSE

$$i\hbar \frac{\partial}{\partial t} \psi(x, t, R(\tau)) = H_p \psi(x, t, R(\tau)) - i\hbar \Theta_{ab}(x) \frac{\partial}{\partial \tau} \psi(x, t, R(\tau)) \quad (50)$$

or simply,

$$i\hbar \frac{\partial}{\partial t} \psi(x, t, \tau) = H_p \psi(x, t, \tau) - i\hbar \Theta_{ab}(x) \frac{\partial}{\partial \tau} \psi(x, t, \tau), \quad (51)$$

which is equation (48). When integrating this equation we must regard the reading of the time τ to be taken from the point at which the particle enters the region $[a, b]$ i.e. τ measures the dwell time in the region.

Note that equation (45) which reduces the two-time TDSE to the one-time TDSE, relies upon the fact that $\partial t' / \partial t = 1$ when $t' = t$. Hence, from our point of view, this step corresponds to a synchronization of the two clocks so that they show the same time. Then of course one only needs the single reference clock. Plainly this is also so in the case that *all* the clocks in the MTDSE are synchronized. Then equation (43) reduces to the one-time TDSE. This is not the case however with Sokolovski's clocked SE since here the two clocks perform different tasks. One clock monitors the overall time t development of the quantum particle, the other monitors the time spent in a particular region via the $\Theta_{ab}(x)$ factor in equation (51). In this case the two-time TDSE does not reduce to the one-time TDSE and this will be so for the MTDSE if all clocks monitor different times i.e. perform different measurements.

5. Conclusions

Beginning with an eigenstate (or a linear superposition of eigenstates) of a quantum composite of environment and observed system described by a TISE we have derived the TDSE for the system. The essential step is the disentanglement of environment and system by the use of a semi-classical wavefunction, involving Hamilton's characteristic classical action function, for the environment. This approximation is valid in the limit that the environment energy is so large that it is unaffected by changes in state of the quantum system. This also allows a single velocity function, independent of the quantum system state, and hence a well-defined time, to be associated with the motion of each environment degree of freedom. Such a degree of freedom then can function as a clock to monitor the time development of the quantum system. By considering that more and more quantum variables are transferred to the classical side of the cut we derive MTDSE involving multiple-time derivatives. When all times are on an equal footing, the clocks can be synchronized to reduce the MTDSE to the usual one-time TDSE. In this way the coupled time-independent equations for the entangled state of environment and system reduce to coupled equations for the time-development of the system alone. The amplitudes of the environment wavefunction become the time-dependent amplitudes for the system eigenstates and the phases of the environment wavefunctions provide time-dependent phases for the system. This is somewhat analogous to the derivation of time-dependent transition amplitudes for scattering states in ion-atom collisions from the full time-independent T-matrix elements, as given in Briggs and Macek [17].

It is shown that two examples of two-time TDSE introduced already in the literature are special cases of our general procedure. The first is the (t, t') method of Moiseyev and

co-workers. It is interesting that in their method t' is introduced mathematically 'as an additional *co-ordinate*' [10], so that in equation (44) the operator

$$H(x, t') - i\hbar \frac{\partial}{\partial t'} \quad (52)$$

can be viewed as a time-independent operator, since the time t does not appear. In our derivation t' really is an additional co-ordinate of the environment. In fact, by going one step back in our derivation one can write equation (44) as

$$\left[H(x, R') - i\hbar \dot{R}' \frac{\partial}{\partial R'} - i\hbar \frac{\partial}{\partial t} \right] \psi(x, R', t) = 0. \quad (53)$$

Since, for a perfect clock \dot{R}' is constant one can equally well put it to unity and use R' as an additional co-ordinate. Equation (53) is identical to the equation derived by Aharonov and Bohm. They also showed that the two time derivatives can be combined to one, essentially by identifying t' with t as in the (t, t') method. Indeed, as mentioned in the introduction, the first to show that the term $\dot{R}'\partial/\partial R'$, arising from the quantum kinetic energy of a degree of freedom R , can provide the $\partial/\partial t$ operator in the TDSE was Mott in 1931 [6].

Sokolovski derived a two-time TDSE using a path integral formalism and intimated thereby that the path integral approach contains elements of dynamics not describable in Schrödinger mechanics. However, that the clocked SE is derivable in the Schrödinger picture has been demonstrated already in [16]. The analysis given here shows also that the clocked SE is simply a special case of the MTDSE.

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Appendix

Here we show that is not necessary to assume that \mathcal{T} is described by a single eigenstate $\Psi(x, R)$. Although we believe that practically this latter assumption is always admissible, since the total energy

$$E = E_{\mathcal{E}} + E_{\mathcal{S}} \quad (A.1)$$

is dominated by $E_{\mathcal{E}}$ as the environment becomes classical, nevertheless we sketch the more general derivation since it has been suggested to us that the assumption of a single eigenvalue equation (equation (2)) and the adiabatic-like expansion equation (3) represent severe restrictions on the derivation of the TDSE given in [8] and on the generality of our approach. Accordingly we begin with \mathcal{T} represented by a superposition of eigenstates

$$\Psi(x, R) = \sum_m b_m \Psi_m(x, R) \quad (A.2)$$

obeying the generalized TISE

$$H\Psi(x, R) = \sum_m b_m E_m \Psi_m(x, R) \quad \text{or} \quad \sum_m b_m (H - E_m) \Psi_m(x, R) = 0$$

with eigenenergies E_m . Since each eigenfunction propagates independently in energy space one can consider each separately i.e. consider

$$(H - E_m)\Psi_m(x, R) = 0, \quad (\text{A.3})$$

which is the TISE defining one of the eigenstates of \mathcal{T} . We expand

$$\Psi_m(x, R) = \sum_k \mathcal{K}_{mk}(R)\phi_k(x)$$

and substitute in equation (A.3). The analysis then follows exactly the steps leading to equation (33) to give

$$\sum_{k \neq l} \langle \phi_l | H_I(x, t) | \phi_k \rangle c_{mk}(t) \exp \left\{ -\frac{i}{\hbar}(\epsilon_l - \epsilon_k)t \right\} = i\hbar \frac{\partial c_{ml}}{\partial t}. \quad (\text{A.4})$$

The assumption (A.2) is that the total system is in a linear superposition of quantum states. Clearly, in order for such quantum coherence to be relevant, the variations in E must be at the quantum level, e.g. of the order of variations in the ϵ_l . However, in the classical limit the (macroscopic) total energy can be considered constant to within quantum fluctuations. This implies that one defines a *unique* time for the motion of the classical system, independent of m , i.e.

$$t = R/v, \quad (\text{A.5})$$

where $v = P/M$ is the classical constant velocity of the perfect clock. Then, with the definition

$$a_j(t) = \sum_m b_m c_{mj}(t) \quad (\text{A.6})$$

the TISE equation (A.3), via equation (A.5), reduces to

$$\sum_{k \neq l} \langle \phi_l | H_I(x, t) | \phi_k \rangle a_k(t) \exp \left\{ -\frac{i}{\hbar}(\epsilon_l - \epsilon_k)t \right\} = i\hbar \frac{\partial a_l(t)}{\partial t} \quad (\text{A.7})$$

which is identical to equation (33).

References

- [1] Schroedinger E 1926 *Ann. Phys., Lpz.* **79** 361
- [2] Schroedinger E 1926 *Ann. Phys., Lpz.* **79** 489
- [3] Schroedinger E 1926 *Ann. Phys., Lpz.* **81** 109
- [4] Born M, Heisenberg W and Jordan P 1926 *Z. Phys.* **35** 557
- [5] Born M 1926 *Z. Phys.* **38** 803
- [6] Mott N F 1931 *Proc. Camb. Phil. Soc.* **27** 553
- [7] Kiefer C 1997 *Time, Temporality, Now* ed H Atmanspacher and E Ruhnau (Berlin: Springer) p 227
- [8] Briggs J S and Rost J M 2000 *Eur. Phys. J. D* **10** 311
- [9] Braun L, Strunz W T and Briggs J S 2004 *Phys. Rev. A* **70** 033814
- [10] Sokolovski D 1995 *Phys. Rev. A* **52** R5–8
Sokolovski D 1997 *Phys. Rev. Lett.* **79** 4946
- [11] Peskin U and Moiseyev N 1993 *J. Chem. Phys.* **99** 4590
Peskin U, Kosloff R and Moiseyev N 1994 *J. Chem. Phys.* **100** 9716
Moiseyev N 1994 *J. Chem. Phys.* **101** 9716
Moiseyev N, Chrysos M and Lefebvre R 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 2599
- [12] Briggs J S and Rost J M 2001 *Found. Phys.* **31** 693
- [13] Briggs J S 2004 *Nonadiabatic Transition in Quantum Systems* ed V I Osherov and L I Ponomarev (Chernogolovka: Inst. of Problem of Chem. Phys.) p 69
- [14] Bohm D and Hiley B J 1993 *The Undivided Universe* (London: Routledge)
- [15] Aharonov Y and Bohm D 1961 *Phys. Rev.* **122** 1649
- [16] Boonchui S, Sa-yakanit V and Srirakool W 2006 *Phys. Rev. A* **73** 012108
- [17] Briggs J S and Macek J 1990 *Adv. Atom. Mol. Opt. Phys.* **28** 1