Time Dependence in Quantum Mechanics

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It is shown that the time-dependent equations (Schrödinger and Dirac) for a quantum system can be always derived from the time-independent equation for the larger object of the system interacting with its environment, in the limit that the dynamical variables of the environment can be treated semiclassically. The time which describes the quantum evolution is then provided parametrically by the classical evolution of the environment variables. The method used is a generalization of that known for a long time in the field of ion-atom collisions, where it appears as a transition from the full quantum mechanical perturbed stationary states to the impact parameter method in which the projectile ion beam is treated classically.

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I. INTRODUCTION

Originally Schrödinger [1] proposed his wave equation in time independent form as an eigenvalue equation for the time-independent Hamilton operator, i.e.

\[(E - H)\Psi = 0,\] (1)

the time-independent Schrödinger equation (TISE). Subsequently, this was generalized to consider quantum systems as being described by state vectors in Hilbert space and observables by Hermitian operators. Pairs of canonically conjugate operators satisfy Heisenberg commutation rules and thereby fulfill corresponding Heisenberg uncertainty relations. In a later paper [2] Schrödinger introduced a time-dependent Schrödinger equation (TDSE) and this version has found much wider application than the TISE even for time-independent Hamiltonians. On the one hand this is due to the technical reason that it is easier to solve the initial value problem of the TDSE than the boundary value problem of the TISE. On the other hand there is the deeper reason that our experience based on the classical world still conditions us to think in terms of physical processes proceeding from some initial state and developing in time to some final state. This is despite the fact that quantum mechanics teaches that the state \(\Psi\) of a closed system can be written as a time-independent superposition

\[\Psi = \sum_n c_n \Phi_n\] (2)

where \(\{x\}\) are the system variables. Notwithstanding the intuitive appeal of the TDSE there are several problems connected with its use, for example:

(A) Although many authors have contrived to define one [3], there is no simple obvious definition of a Hilbert space operator corresponding to time. The ”usual replacement”

\[E \rightarrow i\hbar \frac{\partial}{\partial t}\] (4)

is unusual in that \(E\) is the eigenvalue of the operator \(H\), but \(i\hbar \partial / \partial t\) is not the eigenvalue of an operator.

(B) Following from (A), there is no energy-time uncertainty relation, although time, as measured by clocks, is arguably an observable and countless books refer to the “energy-time” uncertainty relation.

(C) The TDSE admits time-dependent Hamiltonians. Time dependent potentials are often introduced in an ad hoc way and lead to non-Hermitian Hamiltonians. This implies a loss of norm of the quantum wavefunction, i.e. to an ad hoc loss of particles from the quantum system.

(D) The TDSE is simply postulated, with the tacit assumption that the parameter called time is to be identified with the classical time. There is no proof of this. For example, in the case that \(H_S\) is time-independent, corresponding to an isolated conservative system, the simple phase transformation

\[\tilde{\psi}_S(x,t) = \exp(i/\hbar E_S t)\psi_S(x)\] (5)

in [4] leads to the TISE

\[(E_S - H_S)\psi_S(x) = 0,\] (6)
where $E_S$ is well-defined as an eigenvalue of $H_S$. Clearly, in this procedure (or its inverse), the "time" $t$ merely appears as a mathematical parameter.

Here we will show that these difficulties can all be overcome in that the TDSE for a quantum system $S$ can be derived from the TISE for the larger object comprising the system $S$ and its quantum environment $E$. In the limit that the environment is so large (precisely what this means depends upon the object under discussion) that $E$ is practically unchanged in its interaction with $S$, it can be treated semiclassically. In this limit the variables of the environment undergo a time development described by classical equations involving a classical time parameter as measured by a clock. In the same approximation the system $S$ develops in time governed by the TDSE with an effective time-dependent Hamiltonian whose time dependence arises from the interaction with $E$ via the implicit time-dependence of the classical environment variables. In this way time always arises in quantum mechanics as an externally defined classical parameter and time-dependent Hamiltonians from the interaction with a classical environment. The most important example of the interaction of a quantum system $S$ with an environment is the act of observation or measurement, when time is defined by the classical (macroscopic) measuring device. Furthermore, since all measurements ultimately involve the detection of charged particles, photons, or heat (phonons) these are the types of environment we shall consider. Their classical motion is described by Newton or Maxwell equations and hence the time parameter introduced into the TDSE for the quantum system is identical with that entering the classical equations.

In deriving a TDSE from the TISE of a composite system, we will follow closely the development of Briggs and Macek [4] who considered the particular case of a beam of ions (environment) interacting with a target atom (quantum system). In this particular case they showed how the initially time-independent equation for the coupled ion-atom reduces to a time-dependent equation for the atom alone, in the limit that the ion is considered to move along a classical trajectory. In fact the method is much older in origin in atomic collision physics and can be traced through the "perturbed stationary states" (PSS) method of Mott and Massey [5] to the original 1931 paper of Mott [6], where he showed the essential equivalence of the time-independent PSS and time-dependent impact parameter approaches in the limit of high beam velocities, with the time defined by the variables of the particle beam. The PSS method is a generalization of the adiabatic Born-Oppenheimer method as applied to stationary states of molecules. Interestingly, this method of molecular physics has become very popular recently in defining time in quantum gravity. Here time is introduced into the time-independent Wheeler-de Witt equation by treating gravitation semi-classically but the matter field quantum mechanically, in a procedure that is similar to that used in the case of atomic collisions [1].

Starting with the TISE of (1) for $E \otimes S$ we will derive the TDSE (3) for $S$. Thereby we will show that the parametric time derivative arises from the expectation values of the environment operators, thus resolving problem (A) and eliminating the need for the replacement (4). Similarly, we can show that the energy-time "uncertainty relation" for $S$ arises from true (operator based) uncertainty relation for $E$, explaining problem (B). Furthermore, it will be shown that the time-dependence of $H_S(t)$ arises in a well defined way from the interaction of $S$ with $E$ (problem (C)) and that the time which arises is precisely the time describing the classical motion of $E$ i.e. the classical environment provides the clock for the quantum system (problem (D)). The further approximation that the interaction of $S$ with $E$ can be neglected gives a time-independent Hamiltonian $H_S$ appropriate to a non-interacting (closed) quantum system and the TDSE (3) reduces to the new TISE (6) for $S$ alone.

It is clear that the procedure can now be continued in that $S$, described by the TISE (6), can be considered as composed of $S'$ and $E'$ to define time and a TDSE for $S'$. The extent to which the subdivision is valid depends on the accuracy with which the dynamics of $E'$ may be approximated (semi-)classically. More pragmatically, one might say that the position of the interface between the quantum and the classical worlds depends upon the degree of precision set (or achieved) by the measurement.

In section II the interaction of a quantum system with a material environment is considered. The TDSE is derived by generalizing the procedure due to Briggs and Macek [4] who considered the particular case of an atom interacting with a particle beam. Then it is shown how the energy-time uncertainty relation arises. In section III the general procedure is illustrated by the three generic examples of a system $S$ interacting with a particle beam or with a set of quantum oscillators (photons or phonons) as environment $E$. Finally, the same procedure can be applied to transform the time-independent Dirac equation (TIDE) into the time-dependent Dirac equation (TDDE). Here it is interesting to observe that the time component of the spacetime of the quantum system actually arises from the implicit time variation of the classical environment variables, i.e. again it is this variation that provides the clock for the quantum system.

## II. THE EMERGENCE OF TIME

We begin by decomposing the total Hamiltonian $H$ for the large object in (1) into

$$H = H_E + H_{ES} + H_S$$

(7)

with the Hamiltonians $H_E$ for the environment and $H_S$ for the quantum system. For convenience we assume a coordinate representation for $E$ with a standard form of
\[ H_\mathcal{E} = K + V_\mathcal{E} \] where the potential energy is a function of coordinates only, \( V_\mathcal{E} = V_\mathcal{E}(R) \) and the kinetic energy is written in mass scaled coordinates \( R = (R_1, R_2, \ldots) \) as a sum over all degrees of freedom, \( i = 1, \ldots, n \):
\[
K = -\frac{\hbar^2}{2M} \sum_i \frac{\partial^2}{\partial R_i^2}.
\] (8)

Almost all relevant environments can be cast into this form as will be illustrated in section III. In (7) \( H_{\mathcal{E}\mathcal{S}} \) describes the coupling between \( \mathcal{S} \) and \( \mathcal{E} \). However, as a consequence of the environment being "large" compared to the quantum system, the coupling is asymmetric in the sense that the state \( \chi \) of the environment \( \mathcal{E} \) depends negligibly on the variables \( \{x\} \) of the system \( \mathcal{S} \) while the system state \( \psi \) depends on the environment variables \( \{R\} \). Accordingly, we write the total wavefunction \( \Psi \) in (1) as
\[
\Psi(x, R) = \chi(R)\psi(x, R).
\] (9)

Having defined the wavefunction of the system we can express what a "large" environment means in terms of an asymmetry condition. It defines and distinguishes, in the decomposition of \( H \), environment \( \mathcal{E} \) and system \( \mathcal{S} \) through the respective energy expectation values by
\[
\langle \chi | H_\mathcal{E} | \chi \rangle_R \equiv E_\mathcal{E} \equiv \langle \chi | U_\mathcal{S} | \chi \rangle_R.
\] (10)

where
\[
U_\mathcal{S}(R) = \langle \psi(x, R) | H - V_\mathcal{E} | \psi(x, R) \rangle_x.
\] (11)

A more detailed discussion of the requirements for the validity of (10) and a derivation of the form of \( U_\mathcal{S}(R) \) in (11) is given in the appendix, starting from a formally exact "entangled" wavefunction \( \Psi(x, R) = \sum_n \chi_n(R)\psi_n(x, R) \) for the complete object composed of system and environment. It will be shown there that the asymmetry condition (10) justifies a posteriori the form (11) of the wavefunction. As is well known from adiabatic approximations in other contexts a wavefunction of the form (11) can only be justified a posteriori if a condition such as (10) is fulfilled.

Backed by the asymmetry condition (10) and (11) we determine \( \chi \) from the eigenvalue equation
\[
(H_\mathcal{E} + U_\mathcal{S}(R) - E)\chi(R) = 0.
\] (12)

The term \( U_\mathcal{S} \) represents the very small influence \( \mathcal{S} \) has on the state of the environment. The environment is taken to be a large, quasiclassical system so that its state vector \( \chi \) can be approximated by a semiclassical wavefunction
\[
\chi(R) = A(R) \exp(iW/R),
\] (13)

where \( W(R, E) \) is the (time-independent) action of the classical Hamiltonian \( H_\mathcal{E} \).

Inserting (7) and (11) into (1) we get using (12)
\[
\chi \left[ U_\mathcal{S}(R) - H_\mathcal{S} - H_{\mathcal{E}\mathcal{S}} \right] \psi(x, R) = \frac{\hbar}{i} \sum_i C_i \frac{\partial}{\partial R_i} \psi(x, R),
\] (14)

where the operator \( C_i \) is given by
\[
C_i = \chi \left( \frac{\hbar}{2M} \frac{\partial}{\partial R_i} + \frac{\hbar}{M} \frac{\partial^2}{\partial R_i^2} + \frac{\partial A}{\partial R_i} + \frac{1}{M} \frac{\partial W}{\partial R_i} \right).
\] (15)

In accordance with the asymmetry condition (10) we have assumed that
\[
\langle H_{\mathcal{E}\mathcal{S}}, \chi \rangle = 0.
\] (16)

Note that (14) is an equation for the wavefunction \( \psi \) while \( \chi \) already fixed in (12) acts like a potential, i.e. an operator.

With the form of (13) for \( \chi \) we can write for the operator \( C_i \) of (15)
\[
C_i \approx \chi \frac{1}{M} \frac{\partial W}{\partial R_i} = \chi \frac{P_i}{M} = \chi \frac{dR_i}{dt}.
\] (18)

From this approximation for \( C_i \) emerges the classical time on the right hand side of (14) through
\[
\sum_i C_i \frac{\partial}{\partial R_i} = \chi \sum_i \frac{dR_i}{dt} \frac{\partial}{\partial R_i} = \chi \frac{d}{dt}.
\] (19)

Since the \( R_i \) are reduced to classical variables \( R_i(t) \) (14) can now be written
\[
(H_\mathcal{S} + H_{\mathcal{E}\mathcal{S}} - i\hbar \frac{\partial}{\partial t}) \psi(x, t) = 0
\] (20)

Here we emphasize that the time derivative is to be taken with \( \{x\} \) fixed since it arises from the derivative w.r.t. the independent (quantum) variables \( \{R\} \). Finally, a phase or gauge transformation
\[
\psi = \exp[\frac{i}{\hbar} \int_{-\infty}^t (U_\mathcal{S}(t'))dt']\tilde{\psi}
\] (21)

leads to the TDSE for the quantum system alone. To write it in a familiar form we might specify, although not necessary, \( H_{\mathcal{E}\mathcal{S}} = V(x, t) \), i.e. the interaction with the environment is expressed as a potential. Then we have from (20) and (21)
\[
(H_\mathcal{S} + V(x, t) - i\hbar \frac{\partial}{\partial t}) \tilde{\psi}(x, t) = 0.
\] (22)
Having accepted (23), the whole structure of time-dependent quantum mechanics, e.g., the transition to Heisenberg and interaction pictures, time-dependent perturbation theory etc., can be developed as usual. Indeed, Briggs and Macek show explicitly that, in the same approximations that lead to (22), the time-independent T-matrix element for the system plus environment reduces to a time-dependent transition amplitude for the system alone. Similarly, a precise consideration of the nature of the interaction $V(x, t)$ should allow one to derive the many variations of stochastic Schrödinger equations that have been proposed to model the interaction of a quantum system with an environment or measuring device.

One further observation must be made. This is the question of the “uncertainty relation” for energy and time. Since there is no canonical operator for time there is no uncertainty relation in the sense of Heisenberg. That quoted in many books arises from the basic property of the Fourier transform from energy space to time space in which time appears as a mathematical, rather than a mechanical (physical) variable. However, within the approximation of the environment as a classical object a time-energy relation for the quantum system can be derived from the uncertainty relation for the environment, since it is the position variable of the environment that defines the classical time. For any two operators related to the environment, one has

$$\Delta A \Delta B \geq \frac{1}{2i} \langle [A, B] \rangle_R. \tag{23}$$

In particular if $A = H_E$ and $B = R_i$, then

$$\Delta H_E \Delta R_i \geq \hbar/2 \frac{\langle P_i \rangle}{M}. \tag{24}$$

Now, in the classical limit for the environment variables, $\Delta R_i = v_i \Delta t$ and $v_i = P_i/M = \langle P_i \rangle/M$, so that we obtain

$$\Delta E_E \Delta t \geq \hbar/2. \tag{25}$$

However, from (12) and (13) $E = E_E + E_S$ where $E$ is the fixed total energy. Hence, $\Delta E_E = \Delta E_S$ and (23) becomes

$$\Delta E_S \Delta t \geq \hbar/2, \tag{26}$$

i.e. the energy-time uncertainty for the quantum system emerges from the fluctuations in the expectation values of the environment variables.

Note that for the derivation and application of this uncertainty relation it is necessary that the quantum system interacts with the environment through the potential $H_{ES}$. It is this interaction that leads to the uncertainty in the system energy $E_S$. In the same way the uncertainty in the time $\Delta t$ arises from the time development described by (22) where the time is the classical time defined by the classical time-development of the environment. Such energy-time relationships are to be distinguished from those usually postulated for the isolated quantum system alone, i.e. where the operators are those of the quantum system. In that case $H_{ES} = 0$ and the quantum systems satisfy the TISE (1). A time energy “uncertainty relation” then only arises by introduction of a mathematical time through Fourier transform of (1) to a “time” space. The uncertainties $\Delta E$ and $\Delta t$ then refer to the widths of Fourier distributions and the uncertainty relation to the inverse relation between them.

### III. SPECIFIC EXAMPLES

To illustrate the general approach of section II in more detail we will consider three examples which represent the most common ways in which quantum systems are probed and measured. First we will discuss the interaction of the quantum system with a particle beam, then we will describe the interaction with a ”bath” of oscillators, e.g. photons or phonons. Finally, we will show that also in a relativistic environment the time-dependent Dirac equation (TDDE) can be derived from the time-independent Dirac equation (TIDE) in a way analogous to the non-relativistic case.

#### A. A particle beam as environment

A particle beam of fixed momentum $\vec{P} = h\vec{K}$ interacting with a quantum system was considered by Briggs and Macek [1]. The asymmetry condition (9), necessary to separate environment and quantum system, is achieved when the beam kinetic energy $P^2/2M$ is much greater than than the energy differences $\Delta E_S$ in the system states populated as a result of the interaction. The (semi-)classical limit for the environment, necessary to justify (13), is reached when $\vec{P}$ is so large that the de Broglie wavelength is far shorter than the extent of the quantum system. In this case the WKB-wavefunction for a free beam-particle is the exact quantum solution. We may choose a coordinate system with the $z$–axis along the beam direction,

$$\chi(X, Y, Z) = (2\pi)^{-3/2} \exp(iP_2Z/h), \tag{27}$$

where $\vec{P} = (0, 0, P_Z)$ is the classical momentum of the beam. Since (13) is of the form (12), it leads directly to the emergence of time according to (13),

$$\frac{P_Z}{M} \frac{\partial}{\partial Z} = \frac{d}{dt} \frac{\partial}{\partial Z} = \frac{d}{dt}. \tag{28}$$

#### B. A quantized field as environment

In the second example the environment comprises a collection of quantum oscillators with mode frequencies
much greater than that of the system fermion relativistic mass neglected. In this case the classical limit will be where the energies are such that pair production can be neglected of two fermions whose spins are uncoupled and where the derivation simple we restrict ourselves to a quantum observation (TIDE) for system plus environment becomes a time-dependent equation for femions, i.e. how a time-independent Dirac equation can be written formally as in (1) with the Hamiltonian whose elements are now defined as, $H = \hbar \dot{\vec{P}} + \vec{V} = \hbar \dot{\vec{P}} + \vec{V} = \hbar \dot{\vec{P}} + \vec{V}$. The potentials $V, V$ are potentials acting separately on environment and system particles, respectively and can be neglected in what follows, i.e. we consider two free fermions interacting through a coupling Hamiltonian $H_{\xi S}$. The total wavefunction $\psi$ is then written as in \ref{eq:psi} but is now a product of a spinor $\chi(\vec{R})$ representing the spin state of $\xi$ and a spinor $\psi(\vec{x}, \vec{R})$ representing the spin state of the system but depending parametrically on the space variables of the environment. The analogue of (14) now becomes

$$\chi(E_{\xi} - E + H_{S} + H_{\xi S}) - c\alpha_{\xi}E_{\xi}\psi(\vec{x}, \vec{R}) = 0.$$  

However, the operator $c\alpha_{\xi}$ is just the velocity operator $\vec{v}$ which for positive energy solutions has the form $c^{2}\vec{P}_{\xi}/E_{\xi}$.

For free motion the exact solution is the same as the semiclassical one. However, Jensen and Bernstein \cite{Jensen1960} have shown that even when potentials as in (34a) and (34b) are retained, in lowest order semiclassical approximation the form of the velocity operator is unchanged. Then, in this limit, with $E_{\xi} = Mc^{2}$ one has

$$\vec{P}_{\xi}/M = \vec{v}_{\xi} = \frac{d\vec{R}}{dt}.$$  

so that (35) becomes

$$[H_{S} + H_{\xi S} - i\hbar \vec{v}_{\xi}\nabla_{R}]\psi(\vec{x}, \vec{R}(t)) = U_{S}\psi(\vec{x}, \vec{R}(t))$$  

or

$$[H_{S} + H_{\xi S} - i\hbar \frac{\partial}{\partial t}]\psi(\vec{x}, t) = U_{S}(t)\psi(\vec{x}, t).$$  

With the phase transformation (21) one has

$$[H_{S} + H_{\xi S} - i\hbar \frac{\partial}{\partial t}]\psi(\vec{x}, t) = 0,$$

the time dependent Dirac equation. Here, it is interesting to note that the time coordinate of the quantum system spacetime arises from the space coordinate of the classical environment.

\section*{C. An example of relativistic dynamics}

Finally, we consider how the relativistic generalization of the transition from the TISE to TDSE occurs for femions, i.e. how a time-independent Dirac equation (TIDE) for system plus environment becomes a time-dependent Dirac equation for the system. To keep the derivation simple we restrict ourselves to a quantum object of two fermions whose spins are uncoupled and where the energies are such that pair production can be neglected. In this case the classical limit will be where the relativistic mass $M$ of the environment fermion becomes much greater than that of the system fermion $m$. The TIDE can be written formally as in (1) with the Hamiltonian whose elements are now defined as,

$$H_{\xi} = c\alpha_{\xi}\vec{P}_{\xi} + V_{\xi}(\vec{R}) + \beta Mc^{2}, \quad (34a)$$

$$H_{S} = c\alpha_{S}\vec{P}_{S} + V_{S}(\vec{x}) + \beta smc^{2}. \quad (34b)$$

The potentials $V_{\xi}, V_{S}$ are potentials acting separately on environment and system particles, respectively and can be neglected in what follows, i.e. we consider two free fermions interacting through a coupling Hamiltonian $H_{\xi S}$. The total wavefunction $\psi$ is then written as in (1)

$$\begin{align*}
\psi(x, Q) &= \chi(Q)\psi(x, Q). \quad (32)
\end{align*}$$

Substitution of $\Psi$ into (1) leads as before to (14). The quasiclassical field limit now exists for the operator $C_{2}$ in (14) to the replacement

$$C_{2} = \frac{P_{2}}{m_{2}}\chi \to \chi \frac{dQ_{2}}{dt} \quad (33)$$

where $Q_{2}(t)$ is now a classical field amplitude. Since (33) is of the same form as (18) time emerges as in (19) and the TDSE is established for the case of a quasi-classical field as environment.

\section*{IV. SUMMARY}

We began our considerations with a time independent stationary state of a complete object comprising system and environment. The semiclassical treatment of the environment $E$ with the requirement that its own state and energy to zeroth order are unaffected by the quantum system $S$, has led to a TDSE for this system in which the quantum variables of the environment are replaced by classical variables. The interaction with the environment then appears as explicitly time-dependent and the motion of the environment provides a time derivative which monitors the development of the quantum system. If the interaction with the environment is ignored i.e. the quantum system is closed, then time is reduced to a mere mathematical variable and can be removed entirely by the simple phase transformation (1) leading to the TISE of (1). Note, however, that it is inconsistent
to put \( V(x,t) = H_{ES} \) in (22) to zero in order to obtain a TDSE of the form of (9), which is simply postulated. Were \( H_{ES} \) zero, the TDSE (22) cannot be derived, since the Hamiltonian (3) is then fully separable in \( x \) and \( R \) and instead of the approximation (9) one has an exact solution of the form \( \Psi(x,R) = \chi(R)\psi(x) \). This has the consequence that system and environment are fully decoupled implying that the environment can no longer provide time for the system. Formally, one can see this from the uncertainty relation (24). As \( H_{ES} \rightarrow 0 \), the energy exchange between environment and system vanishes and \( \mathcal{E} \) and \( \mathcal{S} \) separately become isolated without uncertainty in their respective energy. Hence, in (24) with \( \Delta E_S \rightarrow 0 \) we get \( \Delta t \rightarrow \infty \). In this sense time arises and is meaningful for a quantum system only when interaction with a quasi-classical external environment defines a clock (e.g. an oscillator) with which the time development is monitored.

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**APPENDIX A:**

In the following we will show under what approximations and with which consequences an exact or "entangled" wavefunction,

\[
\Psi(x,R) = \sum_n \chi_n(R)\psi_n(x,R) \tag{A1}
\]

for the large object described by the Hamiltonian \( H \) in (9), leads to the product wavefunction (10). This form of the wavefunction describes a state of \( H = H_E + H_S + H_{ES} \) if the system \( S \) and the environment \( \mathcal{E} \) are weakly coupled under the asymmetry condition (10). Without loss of generality we may assume the \( \psi_n \) to be orthonormal for each \( R \), i.e. \( \langle \psi_n|\psi_m \rangle = \delta_{nm} \), where here and in the following brackets (|) denote integration over system variables \( x \) only.

We first proceed exactly as in the Born-Oppenheimer, or better, perturbed stationary states (PSS) approximation of molecular physics (9) where (A1) is substituted in \( H_E + H_S + H_{ES} - E|\Psi \rangle = 0 \) and a projection is made unto a particular state \( \psi_m \) to give

\[
\sum_n \langle \psi_m|H_E + H_S + H_{ES} - E|\psi_n \rangle \chi_n = 0 \tag{A2}
\]

Making use of the explicit form of \( H_E \) given in (8) we see that (A2) describes a state \( \chi_m \) of the environment ’closely coupled’ to all other states \( \chi_n \):

\[
H_E \chi_m + \sum_n \langle \psi_m|H_S + H_{ES}|\psi_n \rangle \chi_n = E \chi_m
\]

This is the full quantum equation for the environment whose states \( \chi_m \) are mixed by the "back-coupling" from the system. The first set of coupling terms on the l.h.s. of (A3) are called potential couplings and usually the \( \psi_n \) are chosen to diagonalize these terms. The remaining terms are the ”dynamical couplings”, since their off-diagonal matrix elements describe changes in the state of the quantum system induced by the motion of the environment. Clearly, in order to fulfill the conditions that we demand for separation of environment and system, it is necessary that all off-diagonal couplings are small, i.e. the environment is insensitive to changes in the state of the system. Then (A3) reduces to the single-channel equation

\[
(H_E + E_m(R) - E)\chi_m(R) = \sum_i \langle \psi_m|\partial R_i |\psi_i \rangle \frac{\hbar^2}{2M} \partial R_i \chi_m
\]

where

\[
E_m(R) = \langle \psi_m|H_S + H_{ES} - \sum_i \frac{\hbar^2}{2M} \partial^2 R_i |\psi_m \rangle. \tag{A5}
\]

The dynamical coupling involving the second derivatives \( \partial^2 R_i \) has been incorporated formally in \( E_m(R) \). However, in connection with the semiclassical approximation for \( \chi_m \) which must be made to derive the TDSE for the system, it is consistent to neglect this term. This is shown explicitly in section II in the reduction of the operator \( C_i \). Note that this forces a choice of the environment such that the major \( R \)-dependence is contained in the \( \chi_m \) and the \( \psi_m \) are slowly varying functions of \( R \). Then, since

\[
\langle \psi_m|\partial^2 R_i |\psi_m \rangle = \sum_n |\langle \psi_m|\partial R_i |\psi_n \rangle|^2, \tag{A6}
\]

the requirement that the term on the l.h.s. of this equation is small ensures that the off-diagonal dynamical couplings in (A3) are also small.

If the \( \psi_m \) can be chosen real, the dynamical coupling terms on the r.h.s of (A4) vanish. If the \( \psi_m \) are complex, these terms give rise only to geometric (or Berry) phases that can be accounted for by a phase transformation of the \( \chi_n \). Effectively, then (A4) reduces to the eigenvalue equation

\[
(H_E + E_m(R) - E)\chi_m(R) = 0 \tag{A7}
\]

for the state of the environment when the quantum system is in the state \( \psi_m \). Note that the environment is still coupled to the system in that the different states of the system provide separate potential surfaces \( E_m(R) \) for the
motion of the environment. The complete independence of the environment from the precise state of the system is achieved in the approximation that the differences in the $E_m(R)$ can be replaced by an average potential leading to a common $R$ dependence for all $\chi_m(R)$, i.e., $\chi_m = a_m \chi$, where the $a_m$ are constants. This gives the simplified form of (A1)

$$\Psi(x, R) = \chi(R) \sum_n a_n \psi_n(x, R) \equiv \chi(R) \psi(x, R) \quad (A8)$$

corresponding to the ansatz of (9). Similarly (A7) becomes identical to (12), where the averaged potential $U_S$ of (11) assumes the form

$$U_S(R) = \langle \psi | H - V_E(R) | \psi \rangle = \sum_m |a_m|^2 E_m(R) \quad (A9)$$

with $E_m(R)$ from (A5).

Note that the product ansatz (A8) ((9) of the text) and the environment equation (12) evaluated in the lowest order WKB approximation lead directly to the TDSE (22) for the quantum system. The analysis of this appendix shows how the environment must be chosen “large enough” so that it is insensitive to the back-coupling from the system. This insensitivity is necessary to derive an effective TDSE from the TISE for the composite object of system coupled to environment.

[1] E. Schrödinger, Ann. der Phys. 79, 361 (1926).
[2] E. Schrödinger, Ann. der Phys. 81, 109 (1926).
[3] Y. Aharonov and D. Bohm, Phys. Rev. 122, 1649 (1961); D. H. Kobe and V. C. Aguilera-Navarro, Phys. Rev. A 50, 933 (1994); D. T. Pegg, Phys. Rev. A 58, 4307 (1998).
[4] J. S. Briggs and J. H. Macek, Adv. At. Mol. Phys. 28, 1 (1991).
[5] N. F. Mott and H. S. W. Massey, Theory of Atomic Collisions, (Oxford Univ. Press: Oxford 1965).
[6] N. F. Mott, Proc. Camb. Phil. Soc. 27, 553 (1931).
[7] R. Brout and G. Venturi, Phys. Rev. D 39, 2436 (1989); D. P. Datta, Mod. Phys. Lett. 8, 191 (1993); J. B. Barbour, Phys. Rev. D 47, 5422 (1993); T. Brotz and C. Kiefer, Nucl. Phys. B 475, 339 (1996).
[8] J. D. Björken and S. D. Drell, Relativistic Quantum Mechanics, (McGraw Hill: New York 1964).
[9] R. V. Jensen and I. B. Bernstein, Phys. Rev. A 29, 282 (1984).