The Born-Oppenheimer Approach to the Matter-Gravity System and Unitarity

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Abstract

The Born-Oppenheimer approach to the matter-gravity system is illustrated in a simple minisuperspace model and the corrections to quantum field theory on a semiclassical background exhibited. Within such a context the unitary evolution for matter, in the absence of phenomena such as tunnelling or other instabilities, is verified and compared with the results of other approaches. Lastly the simplifications associated with the use of adiabatic invariants to obtain the solution of the explicitly time dependent evolution equation for matter are evidenced.
The Born-Oppenheimer (BO) approach has been extensively applied to composite systems, such as molecules, which involve two mass, or time, scales [1]. Such an approach has also been suggested for the matter-gravity quantum system [2] in order to generalize the suggestion that matter follows semiclassical gravity adiabatically [3] (in the quantum mechanical sense). The plausibility of such an approach relies on the fact that the mass scale of gravity is the Planck mass which is much greater than that of normal matter. Thus one may consider the matter variables as the "fast" degrees of freedom whereas the "slow" ones are the gravitational variables. This is in analogy with the case of molecules where one considers the intermolecular distance to be the slow degree of freedom and the electron coordinates to be the fast ones.

The purpose of this note is to briefly illustrate and compare the diverse approaches [4, 5, 6] with a particular emphasis on a possible violation of unitarity in the evolution of the matter system. For this it will be sufficient to consider a Friedmann-Robertson-Walker (FRW) line element:

\[ ds^2 = -dt^2 + a^2(t)g_{ij}dx^i dx^j = a^2(\eta) \left(-d\eta^2 + g_{ij}dx^i dx^j\right) \]  

(1)

where \( g_{ij} \) is the metric for a three-space of constant curvature \( k \) (which we shall always take equal to 1) and we have introduced a conformal time \( \eta \). We shall consider a matter-gravity action given by:

\[ S = \int d\eta \left[ -\frac{1}{2}m^2 \dot{a}^2 - m^2 V + L^M(a, \phi) \right] \]  

(2)

where a dot denotes a derivative with respect to \( \eta \), \( m \) is the Planck mass, \( m^2 V \) the gravitational potential [7] and \( L^M \) the matter (\( \phi \)) Lagrangian which is allowed to depend on \( a \) but not \( \dot{a} \). From the above one obtains a classical Hamiltonian:

\[ H = -\frac{\pi_a^2}{2m^2} + m^2 V(a) + H^M(a, \phi) \]  

(3)

where \( \pi_a = -m^2 \dot{a} \), \( H^M \) is the matter Hamiltonian (which does not depend on \( \pi_a \)) and the classical Hamiltonian constraint is \( H = 0 \). We note that the momentum constraint (diffeomorphism invariance on a space-like three-surface) is automatically satisfied in this minisuperspace model.

On quantising one obtains a Wheeler-DeWitt (WDW) equation [8]:
\[ \hat{H} \Psi(a, \phi) \equiv \left( \frac{\hbar^2}{2m^2} \frac{\partial^2}{\partial a^2} + m^2 V(a) + \hat{H}^M \right) \Psi(a, \phi) = 0 \]  \hspace{1cm} (4)

where \( \Psi \) is a function of \( a \) and \( \phi \) and describes both gravity and matter. Subsequently one makes a BO decomposition of \( \Psi \) as:

\[ \Psi(a, \phi) = \psi(a) \chi(a, \phi) \hspace{1cm} (5) \]

where \( \chi(a, \phi) \) is not further separable. Coupled equations of motions for \( \chi \) and \( \psi \) may then be obtained by first substituting the above decomposition into eq. (4) and contracting with \( \chi^* \) obtaining [2]:

\[
\left[ \frac{\hbar^2}{2m^2} \frac{\partial^2}{\partial a^2} + m^2 V \right. \\
\left. + \frac{\langle \chi | \hat{H}^M | \chi \rangle}{\langle \chi | \chi \rangle} \right] \psi = -\frac{\hbar^2}{2m^2} \langle \chi | \hat{\mathcal{D}}^2 | \chi \rangle \psi = \\
\frac{\hbar^2}{2m^2} \frac{1}{\langle \chi | \chi \rangle} \left\{ \langle \chi | \partial_a \left[ 1 - \frac{\langle \chi | \chi \rangle}{\langle \chi | \chi \rangle} \right] \partial_a \rangle \right\} \psi
\hspace{1cm} (6)
\]

where we have introduced covariant derivatives:

\[ D \equiv \frac{\partial}{\partial a} + iA; \quad \bar{D} \equiv \frac{\partial}{\partial a} - iA \hspace{1cm} (7) \]

with [9]:

\[ A \equiv -i \langle \chi | \frac{\partial}{\partial a} \chi \rangle = -i \langle \frac{\partial}{\partial a} \rangle \hspace{1cm} (8) \]

and a scalar product:

\[ \langle \chi | \chi \rangle \equiv \int d\phi \chi^*(a, \phi) \chi(a, \phi) \hspace{1cm} (9) \]

where the integral is over the different matter modes.

On now multiplying eq. (6) by \( \chi \) and subtracting it from eq. (4) one obtains:

\[
\psi \left( \hat{H}^M - \langle \hat{H}^M \rangle \right) \chi + \frac{\hbar^2}{m^2} (D\psi) \bar{D} \chi = -\frac{\hbar^2}{2m^2} \psi \left( \bar{D}^2 - \langle \bar{D}^2 \rangle \right) \chi = \\
-\frac{\hbar^2}{2m^2} \psi \left[ \left( \frac{\partial^2}{\partial a^2} - \langle \frac{\partial^2}{\partial a^2} \rangle \right) - 2 \langle \frac{\partial}{\partial a} \rangle \left( \frac{\partial}{\partial a} - \langle \frac{\partial}{\partial a} \rangle \right) \right] \chi \hspace{1cm} (10)
\]
and we note that the r.h.s. of eqs. (6) and (10) are related to fluctuations, that is they consist of an operator acting on a state minus its expectation value with respect to that state, and in the BO (or adiabatic) approximation they are neglected.

In order to better understand our equations it is convenient to consider the following form for the gravitational wavefunction:

\[ \psi \equiv e^{-i \int^a A \, d' \psi} \approx \frac{1}{N} e^{-i \int^a A \, d' + \frac{i}{\hbar} S_{\text{eff}}} \]  

where \( N \) (which is related to the Van Vleck determinant [3, 4]) and \( S_{\text{eff}} \) are real. On neglecting fluctuations in eq. (6), in the semiclassical limit for gravity \( S_{\text{eff}} \) will satisfy the following gravitational Hamilton-Jacobi equation [10]:

\[ \frac{1}{2m^2} \left( \frac{\partial S_{\text{eff}}}{\partial a} \right)^2 + m^2 V + \langle \hat{H}^M \rangle = 0 \]  

which includes the back reaction of matter through the average matter Hamiltonian. We note \( \frac{\partial S_{\text{eff}}}{\partial a} = -m^2 \dot{a} \) and in the classical limit also for matter one obtains the classical Einstein equation.

On substituting into eq. (10) one obtains:

\[ \left( \hat{H}^M - i\hbar \frac{\partial}{\partial \eta} \right) e^{-i \int^\eta \langle \hat{H}^M \rangle \, d\eta' - i \int^a \langle \hat{H} \rangle \, da' A} \chi = \]

\[ - \frac{\hbar}{2m^2} e^{-\frac{i}{\hbar} \int^\eta \langle \hat{H}^M \rangle \, d\eta' - i \int^a \langle \hat{H} \rangle \, da' A} \left[ - \frac{\partial}{\partial a} D + \frac{1}{2} \left( \frac{\partial}{\partial a} \right)^2 \right] \chi \]

where we have introduced the time derivative through \( i\hbar \frac{\partial}{\partial \eta} \equiv -i \frac{\hbar}{m^2} \frac{\partial S_{\text{eff}}}{\partial a} \frac{\partial}{\partial a} \). We note that on neglecting the r.h.s. of eq. (13), corresponding to the semiclassical limit for gravity and the adiabatic (or BO) approximation, one obtains the usual evolution equation for matter (Schwinger-Tomonaga or Schrödinger). Thus it is natural to identify the matter wave function in the above as [11]:

\[ \chi_s \equiv e^{-\frac{i}{\hbar} \int^\eta \langle \hat{H}^M \rangle \, d\eta' - i \int^a \langle \hat{H} \rangle \, da' A} \chi = e^{-\frac{i}{\hbar} \int^\eta \langle \hat{H}^M \rangle \, d\eta'} \tilde{\chi} \]

since in the above mentioned limits it becomes the usual Schrödinger wave function.

One may now search for eventual violations of unitary evolution for matter by considering:
\[
\int \chi^* \chi s \, d\phi = \int d\phi \left[ \chi^* i \hbar \frac{\partial}{\partial \eta} \chi s - c.c. \right] = \int d\phi \left\{ \chi^* \left( \hat{\mathcal{H}}^M - \frac{\hbar^2}{m^2} \partial \log N \partial a \bar{D} + \frac{\hbar^2}{2m^2} (\bar{D}^2 - \langle \bar{D}^2 \rangle) \right) \chi - c.c. \right\} = \int d\phi \left\{ \left[ \langle \chi | \hat{\mathcal{H}}^M | \chi \rangle - \frac{\hbar^2}{m^2} \partial \log N \partial a \langle \chi | \bar{D} \rangle \right] \chi - c.c. \right\} = 0 , \]

where we observe that \( \langle \bar{D} \rangle \), \( \langle (\bar{D}^2 - \langle \bar{D}^2 \rangle) \rangle \) are zero and we have assumed \( \langle \hat{\mathcal{H}}^M \rangle \) is real. Thus unless one considers non Hermitian Hamiltonians (or the presence of tunneling phenomena leading to instabilities) there is no violation of unitarity. We note that in our approach, wherein we identified the gravitational and matter wave functions and equations of motion, one could envisage the presence of instabilities both in matter and gravitation and such that they compensate in the composite system [12].

Let us now compare our results with those of others. One approach [4] consists of expressing \( \Psi \) as:

\[
\Psi = e^{i\mathcal{S}} \]

and expanding \( S \) in powers of \( m^2 \):

\[
S = m^2 S_0 + S_1 + \frac{1}{m^2} S_2 + \mathcal{O} \left( \frac{1}{m^4} \right)
\]

\[
= \left[ m^2 S_0(a) + \frac{1}{m^2} \sigma_2(a) \right] + \left[ S_1(a,\phi) + \frac{1}{m^2} \eta_2(a,\phi) \right] + \mathcal{O} \left( \frac{1}{m^4} \right) . \]

This allows one to rewrite \( \Psi \) in the following factorized form:

\[
\Psi \approx \left( \frac{1}{N_K} e^{i S_0/m^2 S_0 + \frac{1}{m^2} \sigma_2} \right) \left( N_K e^{i S_1/m^2 + \frac{1}{m^2} \eta_2} \right) \equiv \tilde{\psi}_K \tilde{x}_K \]

where \( N_K \) is also related to the Van Vleck determinant. We may now tentatively identify the above \( \tilde{\psi}_K \) and \( \tilde{x}_K \) with our \( \tilde{\psi} \) (eq. (11)) and \( \tilde{x} \) (eq. (14)) which satisfy:

\[
\left( \frac{\hbar^2}{2m^2} \frac{\partial^2}{\partial a^2} + m^2 V + \langle \hat{\mathcal{H}}^M \rangle \right) \tilde{\psi} = -\frac{\hbar^2}{2m^2} \frac{\langle \bar{D}^2 \rangle}{\langle \tilde{x} | \tilde{x} \rangle} \tilde{\psi}
\]

and:
\[
\left( \tilde{H}^M - \langle \tilde{H}^M \rangle \right) \tilde{\chi} + \frac{\hbar^2}{m^2} \frac{\partial \ln \tilde{\psi}}{\partial a} \frac{\partial \tilde{\chi}}{\partial a} = - \frac{\hbar^2}{2m^2} \left( \frac{\partial^2}{\partial a^2} \frac{\langle \tilde{\chi} | \frac{\partial^2}{\partial a^2} | \tilde{\chi} \rangle}{\langle \tilde{\chi} | \tilde{\chi} \rangle} \right) \tilde{\chi}
\]

(20)

Indeed, on substituting \( \tilde{\psi}_K \) and \( \tilde{\chi}_K \) for \( \tilde{\psi} \) and \( \tilde{\chi} \) into eqs. (19) and (20) and retaining terms to \( O(m^2) \), \( O(m^0) \), \( O(m^{-2}) \), one obtains from (19):

\[
- \frac{1}{2} S_0'' + V = 0
\]

(21)

\[
- \hbar i \frac{N''_K}{N_K} S_0' + \hbar i S_0'' = \langle \tilde{H}^M \rangle_0 = 0
\]

(22)

\[
\frac{\hbar^2}{2} \left( \frac{2N''_K}{N_K} - \frac{2S_0' \sigma_2'}{\hbar^2} - \frac{N''_K}{N_K} \right) + \langle \tilde{H}^M \rangle_2 = - \frac{\hbar^2}{2} \langle \tilde{D}^2 \rangle_0
\]

(23)

where a prime denotes a derivative with respect to \( a \). Eqs. (21), (22) and (23) are respectively the equations \( O(m^2) \), \( O(m^0) \), \( O(m^{-2}) \) and by \( \langle \tilde{H}^M \rangle_0 \), \( \langle \tilde{D}^2 \rangle_0 \) and \( \langle \tilde{H}^M \rangle_2 \) we mean the corresponding terms of \( O(m^0) \) and \( O(m^{-2}) \) respectively. Analogously from eq. (20) one obtains:

\[
H_0^M - \langle \tilde{H}^M \rangle_0 + \hbar i S_0' \left( \frac{N'_K}{N_K} + \frac{iS'_1}{\hbar} \right) = 0
\]

(24)

\[
\left( H_2^M - \langle \tilde{H}^M \rangle_2 \right) - \hbar^2 \frac{N'_K}{N_K} \left( \frac{N'_K}{N_K} + \frac{iS'_1}{\hbar} \right) - S_0' \eta_2 =
\]

\[
\frac{\hbar^2}{2} \left( \langle \tilde{D}^2 \rangle_0 - \frac{N''_K}{N_K} - \frac{iS''_1}{\hbar} + \frac{S''_1}{\hbar^2} - 2 \frac{iS''_1}{\hbar} \frac{N'_K}{N_K} \right)
\]

(25)

to \( O(m^0) \) and \( O(m^{-2}) \) respectively (where we have defined the c-number \( H^M \) by \( \tilde{H}^M \chi_K = H^M \chi_K \)). On comparing the two \( O(m^0) \) equations and eliminating \( \langle \tilde{H}^M \rangle_0 \) one obtains:

\[
H_0^M + \frac{i\hbar S_0''}{2} - S_0'S_1' = 0
\]

(26)

which agrees with the corresponding equation obtained on substituting for \( \Psi \) directly in the WDW equation (4) [4]. Similarly on composing the two \( O(m^{-2}) \) equations one can eliminate \( \langle \tilde{H}^M \rangle_2 + \frac{\hbar^2}{2} \langle \tilde{D}^2 \rangle_0 \) obtaining:

\[
-S_0' \eta_2' + H_2^M - S_0' \sigma_2' + i \frac{S''_1}{2} \hbar - \frac{S''_1}{2} = 0
\]

(27)
again in agreement with the corresponding expression obtained directly from the WDW equation [4]. Thus eqs. (26) and (27) confirm our identification of $\tilde{\psi}_k$ and $\tilde{\chi}_k$ with $\tilde{\psi}$ and $\tilde{\chi}$ respectively.

The above equations (24) and (25) then lead to the following expression for eq. (13):

$$\left\{ \left( H_0^M + \frac{1}{m^2} H_{-2}^M \right) - i\hbar \frac{\partial}{\partial \eta} \right\} e^{-\frac{i}{\hbar} \int^\eta (\hat{H}^M)_{00} \frac{1}{m^2} (\hat{H}^M)_{-2} d\eta'} \tilde{\chi}_K =$$

$$\frac{h^2}{m^2 N_K} \left( \frac{N_K'}{N_K} + i S_1' \right) \tilde{\chi}_K +$$

$$\frac{h^2}{2m^2} \left( \frac{\langle \xbar{\chi} \frac{\partial}{\partial a} \xbar{\chi} \rangle_0}{\langle \xbar{\chi} \xbar{\chi} \rangle_0} - \frac{N_K'}{N_K} - i \frac{S_1'}{\hbar} + \frac{S_1'^2}{\hbar^2} - 2 i \frac{S_1' N_K'}{N_K} \right) \tilde{\chi}_K$$

(28)

where we now have $\chi_{Ks} \equiv e^{-\frac{i}{\hbar} \int^\eta (\hat{H}^M)_{00} \frac{1}{m^2} (\hat{H}^M)_{-2} d\eta'} \tilde{\chi}_K$. Note that $\langle \chi | \bar{D} | \chi \rangle = \langle \tilde{\chi} | \frac{\partial}{\partial a} | \tilde{\chi} \rangle = 0$ now becomes (see also eq. (24)):

$$\langle \tilde{\chi} | \frac{\partial}{\partial a} | \tilde{\chi} \rangle = \int d\phi \left[ \chi_K^* \left( \frac{N_K'}{N_K} + i \frac{S_1'}{\hbar} + i \frac{\eta_2'}{m^2 \hbar} \right) \chi_K \right] = 0.$$  

(29)

One may now check, as in eq. (15), whether a violation of unitarity occurs, obtaining on using eqs. (28) and (29):

$$i\hbar \frac{\partial}{\partial \eta} \int \chi_{Ks}^* \chi_{Ks} d\phi = i\hbar S_0' \int \left[ \tilde{\chi}_K^* \frac{\partial}{\partial a} \tilde{\chi}_K + c.c. \right] d\phi = 0$$

(30)

in agreement with our general result eq. (15). As before the result is a consequence of the presence of back-reaction terms $\langle \hat{H}^M \rangle$ and $\frac{h^2}{2m^2} \langle \xbar{\chi} \frac{\partial}{\partial a} \xbar{\chi} \rangle$, indeed as can be seen from eq. (28) such terms are subtracted from the corresponding operators acting on $\tilde{\chi}_K$, thus leading to zero on integrating over all matter configurations. The presence of back-reaction terms also modifies the definitions of $N_K$ and $\sigma_2$ with respect to those employed elsewhere [4], indeed from eq. (22) and (23) one sees that these quantities are not associated with pure gravity, but include the mean effect of matter (see eq. (19)).

One may alternatively attempt to use instead of $N_K$ a prefactor $N_G$ satisfying eq. (22) for $\langle \hat{H}^M \rangle_0 = 0$ (pure gravity) and introduce simultaneously an adiabatic phase factor in eq. (18), that is using instead of $\tilde{\psi}_K$:

$$\psi_K = e^{-i \int^a \bar{A} \bar{a}' \tilde{\psi}_K}$$

(31)

which will modify eq. (22) leading to [5, 13]:

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\(- \hbar i S_0' \left( \frac{N'_G}{N_G} - \langle \frac{\partial}{\partial a} \rangle_0 \right) + \frac{\hbar i S_0''}{2} + \langle \hat{H}^M \rangle_0 = i \hbar S_0'(\frac{\partial}{\partial a})_0 + \langle \hat{H}^M \rangle_0 = 0 \) (32)

which however is in disagreement with the distinction between the adiabatic and dynamical phases [14, 16]. Indeed as a consequence of reparametrization invariance the dynamical phases of gravity and matter wave-functions cancel (Einstein equation). Similarly it is known that the light and heavy systems have equal and opposite adiabatic phases [1, 14]. Further the presence of the adiabatic phase and the fluctuations on the right hand sides of eqs. (6) and (10) are associated with corrections to the adiabatic approximation, that is they are related to transitions between different states and are expected to be small [15] (if such were not the case one would not have the usual evolution equations).

Let us now compare our result with yet another approach [6]. Our equation (6) was obtained by substituting the BO decomposition into the WDW equation and contracting with \( |\chi\rangle \). One may also expand \( |\chi\rangle \) on a suitable orthonormal basis \( |l\rangle \):

\[ |\chi\rangle = \sum_l c_l(\eta) |l\rangle \] (33)

and contract with respect to \( \langle n| \). One obtains [6] instead of eq. (6):

\[ \frac{\hbar^2}{2m^2} D_n^2 \psi + m^2 V + \frac{\langle n| \hat{H}^M |\chi\rangle}{\langle n| \chi\rangle} = - \frac{\hbar^2}{2m^2} \frac{\langle n| D_n^2 |\chi\rangle}{\langle n| \chi\rangle} \psi \] (34)

where:

\[ D_n \equiv \frac{\partial}{\partial a} + iA_n \quad \bar{D}_n \equiv \frac{\partial}{\partial a} - iA_n \] (35)

with:

\[ A_n \equiv -i \frac{\langle n| \frac{\partial}{\partial n} |\chi\rangle}{\langle n| \chi\rangle} \] (36)

Of course if one multiplies eq. (34) by \( c^*_n \) and sums over \( n \) eq. (6) is again obtained.

As before, one may now multiply eq. (34) by \( \psi \) and subtract it from eq. (4) obtaining:

\[ \psi \left( \hat{H}^M - \frac{\langle n| \hat{H}^M |\chi\rangle}{\langle n| \chi\rangle} \right) \chi + \frac{\hbar^2}{m^2} (D_n \psi) \bar{D}_n \chi = - \frac{\hbar^2}{m^2} \psi \left( D_n^2 - \frac{\langle n| D_n^2 |\chi\rangle}{\langle n| \chi\rangle} \right) \chi \] (37)

and on multiplying the above by \( c^*_n \) and summing over \( n \) the usual result eq. (10) is obtained. Thus, again, we have separated the gravitational and matter equations of motion and equations (19) and (20) now become:
\[
\left( \frac{\hbar^2}{2m^2} \frac{\partial^2}{\partial a^2} + m^2 V + \frac{\langle n| \hat{H}^M| \chi \rangle}{\langle n| \chi \rangle} \right) \tilde{\psi}_n = - \frac{\hbar^2}{2m^2} \frac{\langle n| \hat{D}_n^2| \chi \rangle}{\langle n| \chi \rangle} \tilde{\psi}_n
\]

and:

\[
\left( \hat{H}^M - \frac{\langle n| \hat{H}^M| \chi \rangle}{\langle n| \chi \rangle} \right) \tilde{\chi}_n + \frac{\hbar^2}{m^2} \frac{\partial \ln \tilde{\psi}_n}{\partial a} \frac{\partial \tilde{\chi}_n}{\partial a} = - \frac{\hbar^2}{2m^2} \left( \frac{\partial^2}{\partial a^2} - \frac{\langle n| \hat{D}_n^2| \chi \rangle}{\langle n| \chi \rangle} \right) \tilde{\chi}_n
\]

where we have defined:

\[
\tilde{\psi}_n \equiv e^{i \int^a A_{nn} da'} \psi \equiv e^{i \int^a (A_{nn} - A_{nn}) da'} \tilde{\psi}
\]

\[
\tilde{\chi}_n \equiv e^{-i \int^a A_{nn} da'} \chi \equiv e^{-i \int^a (A_{nn} - A_{nn}) da'} \tilde{\chi}
\]

The above expressions simplify considerably if \(|\chi\rangle = |n\rangle\) with \(\chi_n = \langle \phi | n \rangle\), in which case one has:

\[
\left( \frac{\hbar^2}{2m^2} \frac{\partial^2}{\partial a^2} + m^2 V + \langle n| \hat{H}^M| n \rangle \right) \tilde{\psi}_{nn} = - \frac{\hbar^2}{2m^2} \langle n| \hat{D}_n^2| n \rangle \tilde{\psi}_{nn}
\]

and:

\[
\left( \hat{H}^M - \langle n| \hat{H}^M| n \rangle \right) \tilde{\chi}_{nn} + \frac{\hbar^2}{m^2} \frac{\partial \ln \tilde{\psi}_{nn}}{\partial a} \frac{\partial \tilde{\chi}_{nn}}{\partial a} = - \frac{\hbar^2}{2m^2} \left( \frac{\partial^2}{\partial a^2} - \langle n| \hat{D}_n^2| n \rangle \right) \tilde{\chi}_{nn}
\]

where we have correspondingly defined:

\[
D_{nn} \equiv \frac{\partial}{\partial a} + iA_{nn} ; \quad \bar{D}_{nn} \equiv \frac{\partial}{\partial a} - iA_{nn}
\]

with:

\[
A_{nn} \equiv -i\langle n| \frac{\partial}{\partial a} | n \rangle = i\langle n| \frac{\partial}{\partial a} | n \rangle
\]

and:

\[
\tilde{\psi}_{nn} = e^{i \int^a A_{nn} da'} \psi_n
\]

\[
\tilde{\chi}_{nn} = e^{-i \int^a A_{nn} da'} \chi_n
\]
Similarly, instead of eq. (14) one obtains:

$$\chi_{ns} \equiv e^{-\frac{i}{\hbar} \int^{\eta(n)} \tilde{H}^M |n\rangle d\eta' - i \int^{a_n(\eta)} dA_{nn} \chi_n}$$

(48)

where in this case $a_n(\eta)$ is the trajectory obtained in the semiclassical limit for $\tilde{\psi}_{nn}$.

We now note that the r.h.s. of eq. (13) (similarly for eq. (43)) always consists of an operator acting on a state minus its expectation value with respect to that state, that is it is associated with fluctuations. Let us then denote by $|\nu\rangle (\chi_\nu)$ the eigenstates obtained instead of $|n\rangle (\chi_n)$ on omitting fluctuations in eq. (43). Correspondingly one will have a solution $\chi_\nu s$ to the Schrödinger equation:

$$\left(\tilde{H}^M - \frac{\hbar}{\partial \eta}\right) e^{-\frac{i}{\hbar} \int^{\eta(\nu)} \tilde{H}^M |\nu\rangle d\eta' - i \int^{a_\nu(\eta)} dA_{\nu\nu} \chi_\nu} = 0$$

(49)

From eq. (49) one can obtain some information about the orthonormal basis $|\nu\rangle$, indeed on contracting the above equation with $\chi^*_\lambda (\langle \lambda \rangle)$ one sees that it is identically satisfied for $\langle \lambda \rangle = \langle \nu \rangle$ but for $\langle \lambda \rangle \neq \langle \nu \rangle$ one has:

$$\langle \lambda | \left(\tilde{H}^M - \frac{\hbar}{\partial \eta}\right) | \nu \rangle = 0$$

(50)

The above equations (49) and (50) allow us to identify the $|\lambda\rangle$ with the eigenstates of the time-dependent invariants [17] associated with our time dependent matter hamiltonian $\tilde{H}^M$.

On using eq. (14), in analogy with eq. (33), one may express $\chi_s$ in our new basis:

$$\chi_s = e^{-\frac{i}{\hbar} \int^{\eta} (\tilde{H}^M) d\eta' - i \int^{a(\eta)} dA'} \sum_\lambda c_\lambda(\eta) \chi_{\lambda s}$$

$$e^{-\frac{i}{\hbar} \int^\eta (\tilde{H}^M) d\eta' - i \int^{a(\eta)} dA'} \sum_\lambda c_\lambda(\eta) e^{\frac{i}{\hbar} \int^\eta (\lambda | \tilde{H}^M | \lambda) d\eta' + i \int^{a(\lambda)} dA_{\lambda\lambda} ^{\lambda s} \chi_{\lambda s}$$

(51)

which on substituing in eq. (13) leads to:

$$\sum_\lambda \left( -\langle \tilde{H}^M \rangle - \hbar \dot{A} + \langle \lambda | \tilde{H}^M | \lambda \rangle + \hbar \dot{A}_\lambda(\eta) A_{\lambda\lambda} - i \frac{\dot{c}_\lambda}{c_\lambda} \right) \chi_{\lambda s} \propto \text{fluctuations}$$

(52)

and on neglecting fluctuations (and denoting the quantities then obtained by the additional superscript 0) one has:

9
\[ c_0^\lambda(\eta) = c_0^\lambda(0)e^{\frac{i}{\hbar} \int_0^\eta \langle \hat{H}^M | \hat{A}' \rangle d\eta' + i \int_{\eta(0)}^{\eta} da' A^0 - \frac{i}{\hbar} \int_0^\eta \langle \lambda | \hat{H}^M | \lambda \rangle d\eta' - i \int_{\lambda}^{\eta} da' A_{\lambda \lambda} } \]  

(53)

From the above one then obtains:

\[ \chi_0^s = \sum_\lambda c_0^\lambda(0)e^{\int_0^\eta \langle \lambda | \hat{H}^M | \lambda \rangle d\eta' - i \int_{\lambda}^{\eta} da' A_{\lambda \lambda}} \chi_\lambda \]  

(54)

which is the form for the general solution of the Schrödinger equation for a time dependent Hamiltonian in terms of the eigenfunctions of the time-dependent invariants [17].

If we do not neglect the fluctuations we may write:

\[ \chi_s = \sum_\lambda \left( c_0^\lambda(0) + \delta_\lambda(\eta) \right) e^{-\frac{i}{\hbar} \int_0^\eta \langle \lambda | \hat{H}^M | \lambda \rangle d\eta' - i \int_{\lambda}^{\eta} da' A_{\lambda \lambda}} \chi_\lambda = \sum_\lambda c_0^\lambda(0) \chi_\lambda \]  

(55)

where the \( \delta_\lambda(\eta) \) will be determined by the fluctuations and, on substituting into our general probability conservation constraint eq. (15), we obtain:

\[ i\hbar \frac{\partial}{\partial \eta} \int \chi_s^* \chi_s d\phi = i\hbar \frac{\partial}{\partial \eta} \sum_\lambda \left| c_0^\lambda(0) + \delta_\lambda(\eta) \right|^2 = i\hbar \sum_\lambda \left[ \delta_\lambda^*(\eta) \delta_\lambda(\eta) + \delta_\lambda^*(\eta) c_0^\lambda(0) + \delta_\lambda^*(\eta) \delta_\lambda(\eta) + \delta_\lambda^*(\eta) \delta_\lambda(\eta) \right] = 0 \]  

(56)

which just reflects the fact that an increase of the weight \( \delta_\lambda(\eta) \) of one state is compensated by the decrease of another. Thus there is no overall violation of unitarity, it is only on considering a single state that the evolution appears to be non unitary [16], and the result is obtained without having to resort to the limit \( m^2 \to \infty \). [6].

Let us conclude: the approach we have illustrated consists of writing the total matter-gravity wave function \( \Psi \) in a factorized form \( \psi \chi \) (Born-Oppenheimer) satisfying coupled equations, where \( \psi \) describes gravitation with the back-reaction of matter and \( \chi \) describes matter on a curved background with both equations including fluctuations. It can be seen, on neglecting fluctuations and considering a semiclassical approximation for gravity, that the two wave functions \( \psi \) and \( \chi \) can be interpreted as describing gravitation with a back-reaction due to the mean energy of matter and matter satisfying a Schwinger-Tomonaga equation and following gravitation adiabatically. The initial coupled equations themselves are a consequence of the factorization ansatz and do not involve any approximation.
Other approaches in general also write a factorized wave function which is substituted in the WDW equation, however they do not proceed to obtain coupled equations for matter and gravitation, but the diverse terms in their resulting single equation are identified by equating powers of $m^2$ and subsequently a non-unitary evolution for matter is obtained.

We have seen in one case [4] that if such an expansion is performed in our coupled equations which include the effects of all backreaction no difficulty arises with unitary evolution and in the other case [6] that there is no need to neglect lower powers of $m^2$ in order to obtain unitary evolution.

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[9] The diverse expressions may be written in a more symmetric fashion by considering normalized states $|\chi\rangle_N = \frac{|\chi\rangle}{\langle\chi|\chi\rangle^{1/2}}$ in which case $A = -\frac{i}{2} \left[ N \langle\chi|\frac{\partial}{\partial a}\chi\rangle_N - N \langle\chi|\frac{\partial^2}{\partial a^2}\chi\rangle_N \right] = -\frac{i}{2N} \langle\chi|\frac{\partial^2}{\partial a^2}\chi\rangle_N$ which is explicitly Hermitian.
Of course we assume that a classical limit exists which implies that $|\psi|^2$ is strongly peaked on the classical trajectory $a(\eta)$. For a molecule this will correspond to considering the motion of the nuclei to be quasi-classical while that of the electrons is quantum-mechanical. Clearly the semiclassical limit is an addition to the Born-Oppenheimer factorization and is necessary for time to emerge. In the semiclassical limit, in a path integral representation for the wave function, neighbouring paths will tend to yield cancelling contributions on account of the rapid variation of the phase associated the exponential of the (effective) action. An exception to this rule occurs at stationary points of the exponent and the associated paths are related to classical trajectories. It is clear that for this limit to exist the fluctuations about the solutions to the classical equations of motions must be small and the integral over them finite. In general this leads to a constraint on the effective potential associated with the fluctuations, should this not be satisfied one could have for example fluctuations which increase exponentially in time which, of course, signal an instability.

Let us note the distinction in the wave function between the adiabatically induced phase (related to $A$) and the dynamical phase (related to $\langle \hat{H}^M \rangle$).

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That is eigenstates of explicitly time dependent non-trivial Hermitian operators $\hat{I}(\eta)$ satisfying $\frac{d\hat{I}}{d\eta} \equiv \frac{\partial \hat{I}}{\partial \eta} - i \left[ \hat{I}, \hat{H} \right] = 0$. See H. R. Lewis jr. and W. B. Riesenfeld, *Journal of Math. Phys.* 10, 1458 (1969)