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Variational Coupling Between q-Number and c-Number Dynamics

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Abstract We generalize the time dependent quantum variatlonal princlple for Hamiltonian operators, which contain real parameters and Its time derivatives. The consequent variational system is formed by a Schrödinger equation coupled to Lagrangian equations, where the Lagrangian is the spectation mean value of the parametrized Hamiltonian operator. This dynamlcs describes the interaction between a q–number sub-dynarnics and a c-nurnber one. In the zero order W.K.B. approximation, the variational system is reduced to a Hamilton-Jacobi like equation, coupled to a family of Lagrangian equations. The formal structure of the parametrized varlational principie postulated in this paper, may be convenient as a startlng point for the formal treatment of generaiized semi-classical models.

1. INTRODUCTION

Dynamics which involve c-number and q–number variables are called semi-classical dynamics. The study of semi-classical models is of great importance for the understanding of the transition from a purely quantum behavior to a classical one. Many interesting papers dealing with semi-classlcal dynamics have appeared recently[1,2,3]. Sudarshan and Gordov start from a quantum dynamical model which, later, Is reduced to a semi-classical description. In his paper, Sudarshan imposes super-selection rules, while Gordov formulates his model in an extended Hilbert space. Liran[4], Schütte[5], and Griffin[7], which are Interested in the non-adiabatic nuclear behaviour consider, In their models, the existence of a collective dynamics, represented by time dependent real parameters, coupled to a microscopic quantum dynamics. In all papers listed above, the proposed dynamical equations are not of varlatlonal origin.

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The purpose of thls paper is to establish the variational equations describing the coupllng between the q-number and the c-number (parametric) behavlour of the same global dynamics. For this purpose, we start from a generallzed quantum, time-dependent, variational principle with a Hamiltonian operator depending on real parameters and its time derivatives.

The resultant set of variational equations is formed by a Schrödinger equation (whose time evolution operator is the parametrized Hamilton operator) coupled to a family of Lagrangian equations. The Lagranglan is the spectation mean value of the parametrized Hamilton operator. The W.K.B. approxlmation is evaluated and we show that in the zero order, the system of equatlons is consistent with the expected classical limit.

2. CLASSICAL ACTION FOR PARAMETRIZED HAMILTONIAN

Let us consider the classlcal parametrized Hamiltonian

$$H(x^j,p_j;x^J,\dot{x}^J) = \sum_{j=1}^{n} \dot{x}^j p_j - L(x^j,\dot{x}^j;x^J,\dot{x}^J) \tag{2.1}$$

where $\{x^j,p_j\}$, $j = 1,\ldots,n$, are n pairs of canonical variables and $\{x^J,\dot{x}^J\}$, $J = 1,\ldots,R$, are R pairs of real parameters and its time derivatives. The n coordinates $\{x^j\}$ are cartesian and orthogonal. The R parameters $\{x^J\}$ are carteslan orthogonal coordinates in the configuration manifold, V_R, of an external dynamlcal system in interaction with the internal canonical one. The presence of the parameters in eq. (2.1), will allow the formulation of a variational classical principle for the interaction between the internal and the parametric dynamics. In the simplest cases discussed in the literature[7], the parametric dynamics acts on the internal system, without the corresponding reaction, which means that the quantitles $X^J(t)$ are prescribed.

By convenience we postulate the determinantal regularity condltlons

$$\left|\frac{\partial^2 L}{\partial \dot{x}^j\,\partial \dot{x}^k}\right| \neq 0 \quad , \quad j,k = 1,\ldots,n \tag{2.2}$$

Let us consider, then, the classlcal action

$$A = \int_{t_1}^{t_2} \{ \sum_{j=1}^{n} \dot{x}^j p_j - H(x^j, p_j; x^J, \dot{x}^J) \} dt \tag{2.3}$$

We now construct two independent first order variations, δ_I and δ_{II} for eq.(2.3), such that $\delta_I x^j$ and $\delta_I p_j$ are independent and arbitrary, but with

$$\delta_I x^J = 0$$

and later we take $\delta_{II} x^J$ arbitrary, but with

$$\delta_{II} x^j = \delta_{II} p_j = 0$$

In both variations, the time is not varied. As a consequence, we obtain the following variational equations

$$\dot{x}^j = \frac{\partial H}{\partial p_j} \ ; \quad \dot{p}_j = - \frac{\partial H}{\partial x^j} \tag{2.4}$$

$$\frac{d}{dt} \frac{\partial (-H)}{\partial \dot{x}^J} - \frac{\partial (-H)}{\partial x^J} = 0 \tag{2.4'}$$

The system formed by eqs. (2.4) and (2.4') specifies the interaction between an internal, Hamiltonian, dynamics and an external, parametric, Lagrangian, dynamics.

Let us take a new variation Δ, defined as

$$\Delta = \delta + \Delta t \frac{d}{dt}$$

which varies also t_1 and t_2 in eq. (2.3). Now, the Δx^j are free, but we impose the constraint

$$\Delta x^J = 0 \quad , \quad J = 1, \ldots, R \tag{2.5}$$

As eqs. (2.4) and (2.4') are considered valid between the extrema t_1 and t_2, we have

$$\begin{aligned} \Delta A(\Delta x^J = 0) &= (\delta + \Delta t \frac{d}{dt}) \int_{t_1}^{t_2} \{ \dot{x}^j p_j - H \} dt = \\ &= \left[p_j \delta x^j + \Delta t \dot{x}^j p_j - \Delta t H \right]_{t_1}^{t_2} = \left[p_j \Delta x^j - H \Delta t \right]_{t_1}^{t_2} \end{aligned} \tag{2.6}$$

Developing the left hsnd side of eq. (2.6) in terms of Δx^j and Δt, which are independent, we have In place of eqs. (2.4) arid (2.4'), the new võriatlonai system of dynamlcal equations

$$\frac{\partial A}{\partial x^j} = p_j \quad ; \quad \frac{\partial A}{\partial t} = - H \tag{2.7}$$

$$\frac{d}{dt}\left(\frac{\partial H}{\partial \dot{x}^J}\right) - \frac{\partial H}{\partial x^J} = 0 \tag{2.4'}$$

wlth the constraint

$$\Delta x^J = 0 \quad , \quad J = 1,\ldots,R \tag{2.5}$$

where

$$A = A(x^j;x^J,\dot{x}^J,t) \tag{2.5'}$$

$$H = H(x^j, \frac{\partial A}{\partial x^j};x^J,\dot{x}^J) \tag{2.5''}$$

The system formed by eqs. (2.4) and (2.4') is a Routhian System[6], equivalent to the standard Lagrangian or Hamiltonian formulations of dynamics. But the dynamics description contained in eqs. (2.7), (2.4') ls of a different nature. This ls a direct consequence of the boundary condltion, eq. (2.5), which destroys the symmetry of the global dynamics. The constraint, eq. (2.5), makes it possible to vary arbitrarlly only the internal coordinates, i.e., take as arbitrary only the quantltles h'. This allow us to interpret the Lagranglan behavior represented in eq. (2.4') as a boundary dynamics which influences the internal motlon, described In eq. (2.7), which is a Hamilton-Jacobi-like parametrized equation. The system of eqs. (2.4'), *(2.7)* represents a Lagrangian picture whose conflguration space is the carteslan product of the parametric and internal configuration spaces.

3. QUANTUM ACTION FOR PARAMETRIZED DYNAMICS

As it is well known[8,9], the non-relativistic quantum fundamental equation, may be obtained from a time dependent quantum variational principle

$$\delta A = 0 \tag{3.1}$$

$$A = \int_{t_1}^{t_2} L(\psi,\bar{\psi})dt \tag{3.2}$$

with

$$L(\psi,\bar{\psi}) = \langle\psi(t)|i\hbar \frac{\partial}{\partial t} - \hat{H}|\psi(t)\rangle \tag{3.3}$$

and where the bracket <| |> means an integration in the configuration space $\{x^j\}$ of the quantum system. In this paper, we extend the quantum variational principle given by eqs. (3.1), (3.2), (3.3), for the case in which the Hamiltonian operator, $\hat{H}$, has the pararnetric dependance

$$\hat{H} = \hat{H}^{+} = \hat{H}(\hat{x}^j, \hat{p}_j; x^J, \dot{x}^J) \tag{3.3'}$$

As we will see, in this situation, the resultant Euler-Lagrange equations describe a quantum Hamiltonian dynamics embedded in a Lagrangian bath $\{x^J, \dot{x}^J\}$, with whom it interacts. In this bath, the quantum system is supposed to be pointlike, in the of first order variations Δx^J.

Then, inserting eqs. (3.3) and (3.3') into eq. (3.2), we obtain

$$A = \int_{t_1}^{t_2} dt \, \underline{d^3x^j} \, \bar{\psi}(x^j; x^J, \dot{x}^J, t) \, | i\hbar \frac{\partial}{\partial t} - \hat{H}(\hat{x}^j, \hat{p}_j; x^J, \dot{x}^J) \, |\psi \tag{3.4}$$

with

$$\hat{p}_j = -i\hbar \frac{\partial}{\partial x^j} \tag{3.4'}$$

where $\bar{\psi}$ is the adjoint of ψ, and $\underline{d^3x^j}$ is the volume element in the configuration space $\{x^j\}$. Now, as in the classical action, eq. (2.3) we consider two independent types of variations, δ_a and δ_b, for eq. (3.4)

a) $\delta_a\psi = 0$; $\delta_a x^J = \delta_a \hat{H} = 0$, with $\delta_a\bar{\psi}$ arbitrary and also $\delta_a t = 0$. With this and imposing the condition $\delta_a A = 0$, in eq. (3.4), we obtain

$$(i\hbar \frac{\partial}{\partial t} - \hat{H}(x^j, i\hbar \frac{\partial}{\partial x^j}; x^J, \dot{x}^J)\psi(x^j, x^J, \dot{x}^J, t) = 0 \tag{3.5}$$

the corresponding equations for $\bar{\psi}$ are easily obtained.

b) $\delta_b\bar{\psi} = \delta_b\psi = \delta_b x^J = \delta_b t$, with $\delta_b x^J$ arbitrary, but $\delta_b x^J(t_1) = \delta_b x^J(t_2) = 0$. Here, we corisider $\delta_b \hat{H} \neq 0$, induced by the variations $\delta_b x^J$.

With these variational conditions we obtain from the variations $\delta_b A = 0$ that

$$\int_{t_1}^{t_2} dt \; \underline{d^3x^j} \; \bar{\psi}(\delta_b \hat{H})\psi = 0 \tag{3.6}$$

As

$$\delta_b \hat{H} = \sum_J \frac{\partial \hat{H}}{\partial x^J} \delta_b x^J + \sum_J \frac{\partial \hat{H}}{\partial \dot{x}^J} \delta_b \dot{x}^J \tag{3.7}$$

we obtain

$$0 = \int_{t_1}^{t_2} dt \; \underline{d^3x^j} \; \psi [\sum_J \{\frac{\partial \hat{H}}{\partial x^J} - \frac{d}{dt} (\frac{\partial \hat{H}}{\partial \dot{x}^J})\}] \psi \; \delta_b x^J$$

$$+ [\sum_J \delta_b x^J \int \underline{d^3x^j} \; \bar{\psi} \; \frac{\partial \hat{H}}{\partial \dot{x}^J} \psi]_{t_1}^{t_2} \tag{3.8}$$

The boundary term in eq. (3.8) vanishes, and from the restrlctions whlch define the δ_b variations, we have

$$\int_{t_1}^{t_2} dt \; \sum_J \delta_b x^J \; [\frac{\partial}{\partial x^J} - \frac{d}{dt}(\frac{\partial}{\partial \dot{x}^J})] \int \bar{\psi}(\hat{H})\psi \; \underline{d^3x^j} = 0 \tag{3.9}$$

SInce the variations $6_b x^J$ are arbitrary in the open interval (t_2, t_1) it follows that

$$[\frac{\partial}{\partial x^J} - \frac{d}{dt} (\frac{\partial}{\partial \dot{x}^J})] \; \langle\psi|\hat{H}|\psi\rangle = 0 \tag{3.10}$$

with

$$\langle\psi|\hat{H}|\psi\rangle = \int \underline{d^3x^j} \; \bar{\psi} \; \hat{H} \; \psi \tag{3.11}$$

The coupled variational equations, deduced from the generalized quantum action In eq. (3.4) with the aid of δ_a and 6_b variations, are

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi$$

$$[\frac{\partial}{\partial x^J} - \frac{d}{dt} (\frac{\partial}{\partial \dot{x}^J})] \; \langle\psi|\hat{H}|\psi\rangle = 0 \tag{3.12}$$

where

$$\hat{H} = \hat{H}(\hat{x}^j, \hat{p}_j; x^J, \dot{x}^J)$$

and

$$\psi = \psi(x^j; x^J, \dot{x}^j; t)$$

As a consequence of the δ_b variations properties, the boundary term in of (3.8) may be written In the form

$$\Big[\sum_J \delta_b x^J \langle\psi|\frac{\partial \hat{H}}{\partial \dot{x}^J}|\psi\rangle\Big]_{t_1}^{t_2} = \Big[\sum_J \delta_b x^J \frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle\Big]_{t_1}^{t_2} \qquad (3.13)$$

From the form of eq. (3.13), we define the canonical momentum conjugate to x^J, as

$$p_J = \frac{\partial}{\partial \dot{x}^J} \langle\psi\mid\hat{H}\mid\psi\rangle \qquad (3.14)$$

It is ímportant to remark that eq. (3.10) is a Lagrangian equations in which $\langle\psi|\hat{H}|\psi\rangle$ plays the role of the classical Lagrangian. This aspect is unusual in the literature of the semi-classical model. Liran[4] in the treatment of nuclear collective processes by the Cranking non-adiabatic model[10], arbitrarilly postulates an additional Lagrangian system of equations which allows to calculate the coupling between the classical, collective dynamics with the interna1 quantum dynamics. But Liran takes $\langle\psi|\hat{H}|\psi\rangle$ as the classical Hamiltonian and from it he constructs, in the usual way, the classical Lagrangian.

4. THE *c*-NUMBER HAMILTONIAN

In this section we obtain the classical Hamiltonian, which is assoclated with $\langle\psi|H|\psi\rangle$ by a Legendre transformation. For this purpose, we multiplyeq. (3.10) and summing over J, we obtain

$$\sum_J \Big\{\ddot{x}^J \frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle + \dot{x}^J \frac{\partial}{\partial x^J} \langle\psi|\hat{H}|\psi\rangle - \frac{d}{dt}\Big(\dot{x}^J \frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle\Big)\Big\} = 0 \qquad (4.1)$$

but

$$\frac{d}{dt} \langle\psi|\hat{H}|\psi\rangle = \sum_J \Big\{\ddot{x}^J \frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle + \dot{x}^J \frac{\partial}{\partial x^J} \langle\psi|\hat{H}|\psi\rangle\Big\} \qquad (4.2)$$

Hence, from eqs. (4.1) and (4.2) we have

$$\frac{d}{dt}\{\sum_J \dot{x}^J \frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle\} = 0 = \frac{d}{dt}\{\sum_J \dot{x}^J p_J - \langle\psi|\hat{H}|\psi\rangle\} \qquad (4.3)$$

The c-number Hamiltonian H is

$$H = \sum_J \dot{x}^J p_J - \langle\psi|\hat{H}|\psi\rangle \qquad (4.4)$$

It is now easy, to obtain the Hamilton equations defined by H, namely

$$\dot{p}_J = -\frac{\partial H}{\partial x^J}$$
$$\dot{x}^J = \frac{\partial H}{\partial p_j} \qquad (4.5)$$

5. THE CLASSICAL APPROXIMATION TO EQ: (3.12)

Let us represented ψ given in eq. (3.4), as

$$\psi(x^j;x^J,\dot{x}^J,t) = e^{\frac{i}{\hbar}S} = e^{\frac{i}{\hbar}(S_0 + \frac{\hbar}{i}S_1 + \frac{\hbar^2}{i^2}S_2 + \dots)} \qquad (5.1)$$

where

$$S = S(x^j;x^J,\dot{x}^J,t)$$

S_0 is supposed to be real and is an scalar by regular coordinate transformations of the $\{x^j\}$. Generalizing Pauli[11] and Stachel[12], we may rewrite eq.(5.1) as

$$\psi(x^j;x^J,\dot{x}^J,t) = e^{\frac{i}{\hbar}S_0}[R_0 + \frac{\hbar}{i}R_1 + \frac{\hbar^2}{i^2}R_2 + \dots] \qquad (5.2)$$

where R_0 is necessarilly not real. If we substitute eq.(5.1) into (3.4), in the approximation where R coincides with R_0, we obtain

$$A(R=R_0) = A_0 = \int_{t_1}^{t_2} d^3x^j\, e^{-\frac{i}{\hbar}S_0} R_0^*[i\hbar\frac{\partial}{\partial t} - \hat{H}]R\, e^{\frac{i}{\hbar}S_0} \qquad (5.3)$$

If we consider variations δ_1, restricted by the conditions

$$\delta_1 R_0 = \delta_1 S_0 = \delta_1 x^J = \delta_1 \hat{H} = \delta_1 x^j = 0$$

$\delta_1 t = 0$, but $\delta_1 R_0^*$ arbitrary, we obtain with $\delta_1 A_0 = 0$

$$\int_{t_1}^{t_2} \underline{d^3x^j}\, dt\ \delta_1 R_0^*\ e^{-\frac{i}{\hbar}S_0} \left[\frac{\partial S_0}{\partial t} - \hat{H}\right] R_0\ e^{\frac{i}{\hbar}S_0} = 0 \qquad (5.4)$$

The term $i\hbar \frac{\partial R_0}{\partial t}$ has been neglected because it is of order h.

Developing $\hat{H}$ as a power series in $(-i\hbar \frac{\partial}{\partial x^j})$; with normal orderlng, we obtain for the zero order term

$$\hat{H}(x^j, -i\hbar \frac{\partial}{\partial x^j}; x^J, \dot{x}^J) R_0\ e^{\frac{i}{\hbar}S_0} = e^{\frac{i}{\hbar}S_0} H(x^j, \frac{\partial S_0}{\partial x^j}; x^J, \dot{x}^J) R_0 \qquad (5.5)$$

Inserting eq.(5.5) Into (5.4), we have

$$\int_{t_1}^{t_2} \underline{d^3x^j}\, dt\ \delta_1 R_0^* \left[\frac{\partial S_0}{\partial t} + H(x^j, \frac{\partial S_0}{\partial x^j}, x^J, \dot{x}^J)\right] R_0 = 0 \qquad (5.6)$$

Keeplng $R_0 \neq 0$ and $\delta_1 R_0^*$ arbitrary, we obtain the zero order variational equation

$$\frac{\partial S_0}{\partial t} + H(x^j; \frac{\partial S_0}{\partial x^j}; x^J, \dot{x}^J) = 0 \qquad (5.7)$$

This is a Hamilton-Jacobi like equation for dynamics endowed with an action S_0, parametrized with x^J and $\dot{x}^J$.

Now, let us consider δ_{11} variations, subject to the following conditions

$$\delta_{11} R_0^* = \delta_{11} R_0 = \delta_{11} S_0 = \delta_{11} t = 0$$

$\delta_{11} x^J$ arbitrary, except in the boundarles:

$$\delta_{11} x^J(t_1) = \delta_{11} x^J(t_2) = 0$$

Hence, if $\delta_{11}\hat{H} \neq 0$, then $\delta_{11} A_0 = 0$, implies in that

$$\delta_{11} A_0 = 0 = \int_{t_1}^{t_2} dt\ \underline{d^3x^j}\ R_0^*\ e^{-\frac{i}{\hbar}S_0} [-\delta_{11}\hat{H}] R_0 e^{\frac{i}{\hbar}S_0} \qquad (5.8)$$

If we admit that δ_{11}-like variations commute with R_0, R_0^*, S_0 and x^J, we can wrlte

$$0 = \int_{t_1}^{t_2} dt \sum_J \delta_{\shortparallel} x^J \left\{ \frac{\partial}{\partial x^J} \langle\psi|\hat{H}|\psi\rangle - \frac{d}{dt}\frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle \right\}$$

$$+ \left[\sum_J \delta_{\shortparallel} x^J \frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle \right]_{t_1}^{t_2} \qquad (5.9)$$

where

$$|\psi\rangle = R_0 e^{\frac{i}{\hbar} S_0}$$

The boundary term in eq. (5.9) vanishes, but from it, we can derive the canonical momentum p_J. The arbitrariness of the variations $\delta_{\shortparallel} x^J$, in eq. (5.9) generate variational equations, which are of the Euler-Lagrange tipe

$$\frac{\partial}{\partial x^J} \langle\psi|\hat{H}|\psi\rangle - \frac{d}{dt}\frac{\partial}{\partial \dot{x}^J} \langle\psi|\hat{H}|\psi\rangle = 0 \qquad (5.10)$$

Eqs. (5.10) and (5.7), show that In the zero order approximation, $(\hbar)^0$, the system in eq. (3.12) is equivalent to the equations obtalned from a classical action prIncIple, where S_0 is the action and the Lagrangian is $\langle\psi|\hat{H}|\psi\rangle$, with

$$|\psi\rangle = R_0 \, e^{\frac{i}{\hbar} S_0}$$

With this correspondence, eqs. (5.10) and (5.7) are equivalent to the system formed by eqs. (2.4') and (2.7).

6. CONCLUSIONS

The dynamics generated by Hamiltonian operators, which depend on c-number parameters and its time derivative, describe, necessarily, a c-number dynamics interactlng with a q-number one. The equatlons (3.12), have a dynamical structure which exhibits clearly this aspect, and its variational orlgin suggests that they may provlde a natural candltate to representation for this semi-classicai coupling. A very Interestlng and open problem to be studied is the semi-classical system wlth Incomplete quantum information. This will lead, naturally, to the coupling between an statlstical quantum dynamics and a c-number dynamics. Work in this issue Is In progress.

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Resumo

Generaliza-se o princípio variacional quântico, dependente do tempo, para o caso de operadores Hamiltonianos contendo parâmetros reais e suas derivadas temporais. O sistema variacional obtido é constituído de uma equação de Schrödinger acoplada a um sistema de equaçoes de Lagrange, onde a Lagrangeana é o valor médio do operador Hamiltoniano parametrizado. A dinâmica consequente do princípio variacional, descreve a interação entre uma sub-dinâmica q-number com uma subdinâmica c-number. Na aproximação W.K.B. de ordem ($\hbar$), o sístema variacional reduz-se a uma equação do tipo Hamilton-Jacobi, acoplada a uma família de equações de Lagrange. As características formais do sistema variacional obtido são apropriadas para a descrição de interações q-number - c-number, adiabáticas e não adiabáticas, dependentes do tempo.