Time-Dependent Variational Principle for Predicting the Expectation Value of an Observable

Roger Balian

Service de Physique Théorique, Commissariat à l'Energie Atomique, Centre de Saclay,
F-91191 Gif-sur-Yvette, France

and

Marcel Vénéroni

Division de Physique Théorique (Laboratoire associé au Centre National de la Recherche Scientifique),
Institut de Physique Nucléaire, F-91406 Orsay, France

For a given statistical state at time t_0, the expectation value of some observable at a later time t_1 is expressed in a variational form. Different trial choices for the quantities to be varied (state and observable) generate different approximations, in which the evolution of the state is optimally fitted to the measured quantity. Examples are given in the context of mean-field theories.

Let us consider the following general problem: Knowing the state of a system at time t_0, we wish to obtain in the framework of some approximation a best estimate for the average value at time t_1 of a given observable. In the case of quantum mechanics, the inputs are the initial state at time t_0, characterized by a density operator D, and the observable to be measured, represented by a Hermitean operator A. The output to be determined is the average $\langle A \rangle$ at time t_1. The connection between t_0 and t_1 is controlled by the given Hamiltonian H. The sought-for average,

$$\langle A \rangle = \mathrm{Tr} \exp[-iH(t_1 - t_0)]D$$
$$\times \exp[iH(t_1 - t_0)]A, \qquad (1)$$

is often difficult to evaluate. In the following, we write a variational expression I, which admits $\langle A \rangle$ as its stationary value, and which by restriction of the trial space lends itself to various approximations, some well known and some not.

The independent variational degrees of freedom are the matrix elements of two time-dependent matrices $D(t)$ and $\underline{A}(t)$, and the quantity to be rendered stationary is

$$I = - \int_{t_0}^{t_1} dt [\mathrm{Tr}\underline{A}\, d\underline{D}/dt - h(\underline{D},\underline{A})]$$
$$+ \mathrm{Tr}\underline{D}(t_1)\underline{A}(t_1) \qquad (2)$$

with

$$h(\underline{D},\underline{A}) \equiv i\, \mathrm{Tr}\underline{D}(t)[H,\underline{A}(t)]. \qquad (3)$$

The variation δI associated with variations $\delta\underline{D}(t)$ and $\delta\underline{A}(t)$ involves two end-point terms $\mathrm{Tr}\underline{D}(t_1)$ $\times \delta\underline{A}(t_1) + \mathrm{Tr}\delta\underline{D}(t_0)\underline{A}(t_0)$ which vanish if $\underline{D}(t)$ and $\underline{A}(t)$ obey the boundary conditions

$$\underline{D}(t_0) = D, \qquad \underline{A}(t_1) = A. \qquad (4)$$

Equations of motion for $\underline{D}(t)$ and $\underline{A}(t)$ are then obtained by requiring that

$$\mathrm{Tr}\delta\underline{A}(d\underline{D}/dt + i[H,\underline{D}]) = 0, \qquad (5)$$

$$\mathrm{Tr}\delta\underline{D}(d\underline{A}/dt + i[H,\underline{A}]) = 0, \qquad (6)$$

for any variation $\delta\underline{A}$ and $\delta\underline{D}$. With the boundary conditions (4), one gets

$$\underline{D}(t) = \exp[-iH(t - t_0)]D \exp[iH(t - t_0)], \qquad (7)$$

$$\underline{A}(t) = \exp[iH(t_1 - t)]A \exp[-iH(t_1 - t)]. \qquad (8)$$

As stated, we find that the stationary value of I is the expression (1) of the average value of the observable A at time t_1, for an initial state D at time t_0.

Thus, the particulars of the problem enter through the boundary conditions (4): The initial condition on $\underline{D}(t)$ determines the information on the state, whereas the final condition on $\underline{A}(t)$ tells which quantity is to be measured. Starting from the value D, $\underline{D}$ evolves from t_0 to t according to the Liouville–von Neumann equation (7), while $\underline{A}$ proceeds backwards in time from t_1 to t according to the Heisenberg representation (8) [the unusual plus sign in (6) reflects this backward evolution]. The quantity $\mathrm{Tr}\underline{D}(t)\underline{A}(t)$ does not depend on the intermediate time t, and is equal to the stationary value of I, that is to the average $\langle A \rangle$ at time t_1.

In case the state D and the operator A reduce to projectors $|\psi\rangle\langle\psi|$ and $|\varphi\rangle\langle\varphi|$, the "action" (2) takes the special form

$$I = -2\,\mathrm{Im}\int_{t_0}^{t_1} dt \langle\psi|\varphi\rangle\langle\varphi|(id/dt - H)|\psi\rangle$$
$$+ |\langle\psi(t_1)|\varphi(t_1)\rangle|^2. \qquad (9)$$

This is reminiscent of various types of variation-

al principles aimed at evaluating probability amplitudes. The present principle, however, deals directly with the measured quantity $\mathrm{Tr}\underline{D}\,\underline{A}$ which is the *square* of an amplitude. Notice also that the extension to quantum statistical mechanics has led us to treat the density matrix and observable, rather than the usual bra and ket, as conjugate dynamical variables.[1]

The quantum structure of the theory is embedded in the form (3). To treat problems in classical statistical mechanics, it would be sufficient to replace in (3) the commutator by a Poisson bracket.

We now list briefly a few examples of application. As usual for variational principles, approximations are derived by restricting $\underline{D}$ and $\underline{A}$ (as well as their boundary values D and $\bar{A}$) to subspaces simple enough for making the evaluation of I feasible. The approximate equations of motion which replace (7) and (8) are obtained by requiring Eqs. (5) and (6) to hold for any *allowed* $\delta\underline{A}$ and $\delta\underline{D}$. The corresponding value of I is $\mathrm{Tr}\underline{D}(t_1)\underline{A}(t_1)$ provided the variation $\delta\underline{A}\propto\underline{A}$ is permitted. If moreover $\delta\underline{D}\propto\underline{D}$ is permitted, $\mathrm{Tr}\underline{D}(t)\times\underline{A}(t)$ remains constant in time.[2] We shall focus on many-body fermion systems (having for instance in mind collisions between atoms or heavy nuclei) and we shall choose trial forms of $\underline{D}$ and $\underline{A}$ which allow the use of some form of Wick's theorem. We shall denote by γ_m either a creation or an annihilation operator in Fock space, by $\{Q\}$ the class of operators which are quadratic in γ, and by $\{Y\}$ the class of operators of the form $\exp Q$.

(1) $\underline{D}\in\{Y\},\underline{A}\in\{Q\}$.—With these special choices for $\underline{D}$ and $\underline{A}$, Eq. (5) yields immediately the time-dependent Hartree-Fock-Bogoliubov evolution equation for $\underline{D}$. Within the class of independent (quasi)particle states, this equation appears therefore as the best choice (in the sense of our variational principle) for predicting the average of a single-particle observable (and more generally of any observable Q). In the present framework, it should be supplemented by the equation of evolution of $\underline{A}$, derived from (6) by restricting the variation $\delta\underline{D}$ to the class $\delta\underline{D}=\underline{D}\delta Q$ (δQ arbitrary) which is associated with $\underline{D}\in\{Y\}$. The resulting equation for $\underline{A}$ is complicated and is *coupled* with that for $\underline{D}$. It should be considered as an approximation for the Heisenberg evolution (8), adapted to the initial state D. It needs not to be solved however, because the approximate $\langle A\rangle$ can be evaluated at time t_1 by solving only for $\underline{D}(t)$. In contrast, the evolution of $\underline{D}$ does not de-

pend on the particular choice of the observable A nor on the time t_1, provided A belongs to the class $\{Q\}$. This feature of the time-dependent Hartree-Fock (TDHF) equation, which will be absent from the forthcoming examples, appears here somewhat as a happy accident.

The usual "cold" TDHF approximation is obtained from the variational principle by further restricting D to be a projector on a Slater determinant. Another special case is the Vlasov equation, associated with the replacement of h by its classical counterpart.

(2) $\underline{D}\in\{Y\},\underline{A}\in\{Y\}$.—This example generalizes a problem which has recently attracted attention,[3-5] namely the evaluation of transition amplitudes in the framework of mean-field approximations. It has been shown that the usual TDHF approximation, which is then inadequate, should be replaced by coupled equations for two sets of orbitals. To treat this problem in the present language, one should take for the state D and the channel operator A, as well as for the trial operators $\underline{D}$ and $\underline{A}$, (unnormalized) projectors on the Slater determinants generated by the unknown orbitals. By using the form (9) for I, we recover the coupled equations of Refs. 3–5. Actually, our formalism extends to operators $\underline{D}$ and $\underline{A}$ belonging to the class $\{Y\}$, which includes the projectors on Slater determinants as limiting cases. The equations of motion then result from (5) and (6) by letting $\delta\underline{A}=\underline{A}\delta Q$ and $\delta\underline{D}=\delta Q'\underline{D}$ (δQ and $\delta Q'$ arbitrary). Their explicit form may be written by a straightforward use of the group properties of $\{Y\}$ and of a generalization of Wick's theorem.[6] Since they couple $\underline{D}$ and $\underline{A}$, their solution is made complicated by the mixed boundary conditions (4). A simplification occurs for the combination $\mathrm{Tr}\underline{D}\,A\gamma_m\gamma_n/\mathrm{Tr}\underline{D}\,A$, which evolves according to a TDHF equation (with a non-Hermitean mean field).

Being less specific and better suited to generalization than the previous derivations, the present approach to the problem of transition amplitudes has the main interest of setting this example into a wider perspective, as illustrated by the next example.

(3) $\underline{D}\in\{Y\},\underline{A}\in\{Q^2\}$.— This choice is fitted to the prediction of quantities such as the statistical fluctuation of some single-particle operator, for instance the width of the mass distribution of final fragments in a heavy-ion reaction. Here again, the approximate equations of motion result from (5) and (6) by letting $\delta\underline{A}=Q\,\delta Q+\delta Q\,Q$ and $\delta\underline{D}=\underline{D}\delta Q'$. We do not write them here, since their

explicit form is rather lengthy but easily obtained by means of Wick's theorem. Their main feature is an intricate coupling between $\underline{D}$ and $\underline{A}$: Because the observable A is *not quadratic* in γ, the evolution of $\underline{D}$ does *not* follow the TDHF equation. This may explain why the latter equation, which has been so successful for evaluating averages of operators Q, seems unadapted for reproducing fluctuations such as the experimental mass dispersions. Actually, one should not consider TDHF as an approximation for the *full* density matrix (7), but rather as a tool for evaluating averages of operators Q only.

A common feature of these examples is the *coupling* between $\underline{D}$ and $\underline{A}$. Its origin lies in the boundary conditions (4), which force us to start from both end points of the time interval (t_0, t_1), as well as in the reduction of the trial space implied by the approximation scheme. Of course, the usefulness of the variational principle will be limited by the intricacy of the approximate evolution equations. Should these equations prove to be untractable, a compromise might be found through a further reduction in the number of variational degrees of freedom parametrizing $\underline{D}$ and $\underline{A}$.

As a price paid for this unavoidable contraction of the description, *the best choice for $\underline{D}(t)$ does not depend in general on the observable A to be measured at time t_1*. In other words, *one is not entitled to use $\underline{D}(t)$ as a genuine density operator, i.e., for predicting the average value of any other observable.*[7] In particular, it is not required that $\mathrm{Tr}\underline{D}(t_1)$, the average at time t_1 of the unit operator, be unity [indeed, in examples (2) and (3) it is not]. Neither is it required that $\underline{D}(t)$ be Hermitean ($\mathrm{Tr}\underline{D}B$ need not be real for *any* observable B), a freedom which may be helpful for problems of a tunneling type (the time t may then become complex). Also, nothing prevents an initially pure state ($D^2 = D$) from evolving into a mixture [indeed, in example (3) above, the property $\underline{D}^2 = \underline{D}$ is not preserved]. The contraction of the trial space is again responsible for such violations of evolution properties which are fulfilled by the exact density operator (7). Their occurrence does not necessarily mean that the approximation is unphysical. Actually, the situation may be compared with symmetry breaking in static mean-field approximations. In this case, satisfactory values may be produced for symmetry-invariant observables, even though a finite unphysical value is then assigned to a quantity known to vanish in the exact state for symmetry reasons (e.g., pairing assigns a nonzero value to the aver-

age of a pair of creation operators in the ground state of a nucleus).

Note that the expression (2) for I has the *formal* structure of a classical action in phase space; the matrix elements of $\underline{D}$ and $\underline{A}$ play the role of coordinates q and momenta p, respectively, and the corresponding Hamiltonian h is bilinear in q and p. The end-point term $\mathrm{Tr}\underline{D}(t_1)\underline{A}(t_1)$ is associated with a Legendre transform, needed to replace the usual conditions on q at times t_0 and t_1 by the mixed conditions (4). With this analogy, restricting the spaces for $\underline{D}$ and $\underline{A}$ amounts to setting constraints on the q's and p's; the approximate equations of motion thus enter the framework of the constrained Hamiltonian dynamics,[8] which should serve as a guide to ensure the consistency of one or another approximation.

In view of its flexibility, the present variational principle for state and observable seems a good starting point for a microscopic introduction of collective coordinates. Indeed, if $\underline{D}$ and $\underline{A}$ are parametrized by a few variables λ_i and μ_j, respectively, the variational equations (5) and (6), where $\delta\underline{A}$ and $\delta\underline{D}$ are replaced by $\partial\underline{A}/\partial\mu_j$ and $\partial\underline{D}/\partial\lambda_i$ for each j and i, would provide equations of motion for $\lambda_i(t)$ and $\mu_j(t)$. In addition, the built-in asymmetry between the states, which enter at the initial time, and the observables, which enter at the final time, might prove helpful to deal with irreversible behavior. Finally, the variational principle seems suited to build time-dependent approximations that would go beyond mean-field theory.

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[1]The duality between density operators and observables underlies the definition of a density operator as a linear mapping from the observables to their average values. See, for instance, the introductory review by U. Fano, Rev. Mod. Phys. $\underline{29}$, 74 (1957). At a more mathematical and general level, algebraic quantum statistics defines a state as an element of the dual space of the algebra of observables. Here, density operators and observables remind us in addition of canonically conjugate variables in classical dynamics.

[2]The constancy of $\mathrm{Tr}\underline{D}(t)\underline{A}(t)$ may be used to build an alternative variational principle, in which the integrand of (2) would be divided by this quantity. The corresponding expression (9) would be akin to the effective action of J. P. Blaizot and G. Ripka, to be published, which has been an incentive for the present work.

[3]S. Levit, Phys. Rev. C **21**, 1594 (1980).

[4]J. J. Griffin, P. C. Lichtner, and M. Dworzecka, Phys. Rev. C **21**, 1351 (1980); Y. Alhassid and S. E. Koonin, Phys. Rev. C **23**, 1590 (1981); K. R. Sandhya Devi and S. E. Koonin, Phys. Rev. Lett. **47**, 27 (1981); J. P. Blaizot and H. Orland, Phys. Rev. C **24**, 1740 (1981).

[5]Blaizot and Ripka, Ref. 2.

[6]R. Balian and E. Brézin, Nuovo Cimento B **64**, 37 (1969).

[7]This idea of adapting the evolution of the state to the observation underlies Refs. 3–5. It was already stated in the context of mean-field theories by J. W. Negele, S. Levit, and Z. Patiel, in *Time-Dependent Hartree-Fock Theory*, edited by P. Bonche and B. Giraud (Editions de Physique, Orsay, France, 1979), p. 138. Similarly, as is well known, the Rayleigh-Ritz principle is not necessarily suited to the evaluation of observables other than the energy.

[8]P. A. M. Dirac, *Lectures on Quantum Mechanics* (Belfer Graduate School of Science, Yeshiva University, New York, 1964).