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Reduced System Dynamics from the N-Body Schrödinger Equation

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We derive the time-dependent wave function for one particle in the company of $N - 1$ other particles using the method of iterated projection. Using this approach, we confirm the general philosophy of describing a quantum system by a flow component and another component which may be given various descriptions as stochastic, heat bath, or quantum jump processes. The possible equivalence of the Breuer-Petruccione reduced system dynamics [Phys. Rev. Lett. **74**, 3788 (1995)] and ours is explored.

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In a recent Letter, Breuer and Petruccione [1] derived a differential Chapman-Kolmogorov equation for the probability distribution of a reduced system. It has the form of a Liouville master equation defining a flow-jump process in projective Hilbert space. The simplifying conditions used are the Markov and weak-coupling assumptions. We call this result the main qualified conclusion of Ref. [1], to which we refer the reader to for the definitions used in that derivation. In this Letter, we adopt a reduced system dynamic approach as well, but use a different strategy: We formally find the reduced wave function for k particles from the N-body Schrödinger equation using the method of iterated projection [2,3], without using the above simplifying assumptions. We then approximate the resulting exact series solution, not a differential equation.

We start with the Schrödinger equation

$$i\hbar \frac{\partial \psi_N}{\partial t} = H\psi_N , \tag{1}$$

where $\psi_N = \psi_N(r^N, t)$ and $r^N = (r_1, r_2, \ldots, r_N)$, the coordinates of the N particles making up the system. Instead of using the reduced probability distribution, we define the reduced wave function

$$\psi_k = P_k \psi_N = (1/\Omega^{N-k}) \int dr^{N-k}\, \psi_N \tag{2}$$

to represent the wave function of k particles in the company of $N - k$ other particles. Ω is the volume of the system. We may drop the subscript k and simply call ψ_k, P_k as ψ, P. Using Refs. [2,3], we may write the formal solution for this k-particle reduced wave function ψ as

$$\psi = g + h, \qquad g = \sum_{m=0}^{\infty,\mathrm{even}} g_m, \qquad h = \sum_{n=1}^{\infty,\mathrm{odd}} h_n , \tag{3}$$

where

$$g_m = -(1/\hbar)^2 \int_0^t ds_1 \int_0^{s_1} ds_2\, F(t, s_1) \times PHQHG(s_1, s_2) g_{m-2}(s_2) , \tag{4}$$

$$g_0 = \exp(-itH/\hbar)\psi(0) , \tag{5}$$

$$h_n = -(1/\hbar)^2 \int_0^t ds_1 \int_0^{s_1} ds_2\, F(t, s_1) \times PHQHG(s_1, s_2) h_{n-2}(s_2) , \tag{6}$$

$$h_1 = -(i/\hbar) \int_0^t ds_1\, F(t, s_1) PHG(s_1, 0)\,(1 - P)\psi_N(0) , \tag{7}$$

$$F(t, t_1) = \exp\left[-\frac{i}{\hbar}(t - t_1)PH\right], \tag{8}$$

$$G(t, t_1) = \exp\left[-\frac{i}{\hbar}(t - t_1)QH\right], \tag{9}$$

and

$$Q = 1 - P . \tag{10}$$

We have dropped all subscripts k for the moment.

Let us differentiate Eqs. (4) and (6) twice with respect to time:

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$$g_m' + (i/\hbar)PHg_m + (1/\hbar)^2PHQH\int_0^t ds_2\, G(t,s_2)g_{m-2}(s_2) = 0\,, \tag{11}$$

$$g_m'' + (i/\hbar)PHg_m' + (1/\hbar)^2PHQHg_{m-2} - i(1/\hbar)^3PHQHQH\int_0^t ds_2\, G(t,s_2)g_{m-2}(s_2) = 0\,, \tag{12}$$

$$h_n' + (i/\hbar)PHh_n + (1/\hbar)^2PHQH\int_0^t ds_2\, G(t,s_2)h_{n-2}(s_2) = 0\,, \tag{13}$$

$$h_n'' + (i/\hbar)PHg_n' + (1/\hbar)^2PHQHg_{n-2} - i(1/\hbar)^3PHQHQH\int_0^t ds_2\, G(t,s_2)h_{n-2}(s_2) = 0\,. \tag{14}$$

Summing Eqs. (11) and (12) from $m = 2$ to ∞, and likewise for Eqs. (13) and (14) from $n = 3$ to ∞,

$$g' + (i/\hbar)PHg + (1/\hbar)^2PHQH\int_0^t ds_2\, G(t,s_2)g(s_2) = g_0' + (i/\hbar)PHg_0 = 0 \tag{15}$$

using Eq. (5),

$$g'' + (i/\hbar)PHg' + (1/\hbar)^2PHQHg - i(1/\hbar)^3PHQHQH\int_0^t ds_2\, G(t,s_2)g(s_2) = 0\,, \tag{16}$$

$$\begin{aligned} h' + (i/\hbar)PHh + (1/\hbar)^2PHQH\int_0^t ds_2\, G(t,s_2)h(s_2) &= h_1' + (i/\hbar)PHh_1 \\ &= -(i/\hbar)PHG(t,0)\,(1 - P)\psi_N(0) \end{aligned} \tag{17}$$

using Eq. (7), and

$$\begin{aligned} h'' + (i/\hbar)PHh' + (1/\hbar)^2PHQHh - i(1/\hbar)^3PHQHQH\int_0^t ds_2\, G(t,s_2)h(s_2) \\ = -(1/\hbar)^2PHQHG(t,0)\,(1 - P)\psi_N(0)\,. \end{aligned} \tag{18}$$

From Eqs. (15) and (17),

$$\begin{aligned} (1/\hbar)^2QH\int_0^t ds_2\, G(t,s_2)g(s_2) \\ = -(PH)^{-1}g' - (i/\hbar)g\,, \end{aligned} \tag{19}$$

$$\begin{aligned} (1/\hbar)^2QH\int_0^t ds_2\, G(t,s_2)h(s_2) \\ = -\,(PH)^{-1}h' - (i/\hbar)h \\ -\,(i/\hbar)G(t,0)\,(1 - P)\psi_N(0)\,, \end{aligned} \tag{20}$$

which we can substitute into Eqs. (16) and (18) to give

$$g'' + (i/\hbar)[PH + PHQH(PH)^{-1}]g' = 0\,, \tag{21}$$

$$h'' + (i/\hbar)[PH + PHQH(PH)^{-1}]h' = 0\,, \tag{22}$$

identical except for the boundary conditions, which are obtained from Eqs. (5), (7), (15), and (17):

$$g(0) = \psi(0), \qquad g'(0) = -(i/\hbar)PH\psi(0)\,, \tag{23}$$

$$h(0) = 0, \qquad h'(0) = -(i/\hbar)PHG(t,0)\,(1 - P)\psi_N(0)\,. \tag{24}$$

The only assumption made so far is that the inverse operator $(PH)^{-1}$ exists. Where necessary, it is possible to use the Feynman definition: $(PH)^{-1} = \int_0^\infty d\omega\, \exp(-\omega PH)$. Similar inverse operators were used with the partitioning technique [4–6] to calculate the energy spectra of simple molecules.

The bracketed operator in Eqs. (21) and (22) may be simplified to give

$$\begin{aligned} PH + PHQH(PH)^{-1} &= PH + PH^2(PH)^{-1} \\ &\quad - PHPH(PH)^{-1} \\ &= PH^2(PH)^{-1} = K\,, \end{aligned} \tag{25}$$

and the solutions of Eqs. (21) and (22) are

$$g = \psi(0) + [\exp(-itK/\hbar) - 1]K^{-1}PH\psi(0)\,, \tag{26}$$

$$h = [\exp(-itK/\hbar) - 1]K^{-1}PH(1 - P)\psi_N(0)\,. \tag{27}$$

From Eq. (2)

$$\psi(t) = \psi(0) + [\exp(-itK/\hbar) - 1]K^{-1}PH\psi_N(0) \tag{28}$$

or

$$\psi(t) = \psi(0) + \sum_{j=1}^{\infty} \frac{(-it)^j}{j!} K^{j-1}PH\psi_N(0)\,. \tag{29}$$

Equation (29) formally expresses the time evolution of the reduced k-particle wave function in terms of its initial value and the additional effect of the entire N-particle wave function of all particles at initial time. Equation (29) is deceptively simple, but expressed in a form ideal for symbolic computation. Also Eq. (29) has the feature that approximations may be introduced after the formal solution is written down, not before, as in Ref. [1] and many other formulations [7,8]. The richness, complexity, or statistics of the system in consideration are all defined with the initial condition, including bound states. At this point, we remark that while the early projection techniques used to derive generalization master equations use the same operator ($k = 0$), the method of iterated projection substantially differs in approach because it focuses on the formal, reduced solution of the exact differential equation (1), instead of deriving differential equations which can be solved only for special cases.

We first put

$$H = H_0 + H_i = \sum_{j=1}^{N} H_0(j) + \sum_{i,j}^{i,j} V(r_i - r_j) \tag{30}$$

and assume that $H_0 P_k = P_k H_0$; this is true for a large class of Hamiltonians summed over one-particle labels.

For the purpose of this Letter, we put $k = 1$ and evaluate the operators in Eq. (29) one by one. For $j = 1$:

$$\frac{(-it)}{1!} PH\psi_N(0) = \frac{(-it)}{1!} [H_0(1)\psi_1(0) + PH_i\psi_N(0)] . \tag{31}$$

Suppressing details, we find for $j = 2$:

$$\frac{(-it)^2}{2!} KPH\psi_N(0) = \frac{(-it)^2}{2!} H_0^2(1)\psi_1(0) + \frac{(-it)^2}{2!} PM\psi_N(0) , \tag{32}$$

where

$$M\psi(0) = (H_0 H_i + H_i H_0 + H_i^2)\psi_N(0) .$$

For $j = 3$:

$$\begin{aligned}\frac{(-it)^3}{3!} K^2 PH\psi_N(0) = \frac{(-it)^3}{3!} \{&[H_0^2(1) + PM][H_0(1) + b]^{-1} H_0^2(1)\psi_1(0) \\ &+ [H_0^2(1) + PM][H_0(1) + b]^{-1} PM\psi_N(0)\} .\end{aligned} \tag{33}$$

In arriving at Eq. (32), we have used the property of projection operators $P^2 = P$, and

$$\begin{aligned}(PH)^{-1}P &= \int_0^\infty d\omega \exp(-\omega PH)P = \sum_{J=0}^{\infty} \frac{(-\omega)^j}{j!} [P(H_0 + H_i)]^j P \\ &= \sum_{j=0}^{\infty} \frac{(-\omega)^j}{j!} [H_0(1) + a]^j P = \int d\omega \exp\{-\omega[H_0(1) + b]\}P = (H_0 + b)^{-1}P ,\end{aligned} \tag{34}$$

where

$$b = PH , \tag{35}$$

which is simply a scalar for pair potentials. $H_0(1)$ is the single-particle Hamiltonian for particle 1 alone, like a free particle, or an electron in a Landau state, for example. Later we may simply write it as H_0 where there is no confusion. For $j = 4$:

$$\begin{aligned}\frac{(-it)^4}{4} \{&[H_0^2(1) + PM][H_0(1) + b]^{-1}[H_0^2(1) + PM][H_0(1) + b]^{-1} H_0^2(1)\psi_1(0) \\ &+ [H_0^2(1) + PM][H_0(1) + b]^{-1}[H_0^2(1) + PM][H_0(1) + b]^{-1} PM\psi_N(0)\}\end{aligned} \tag{36}$$

using the simplifications used earlier.

We can then write

$$\begin{aligned}\psi(t) = \psi(0) &+ \frac{(-it)}{1!} H_0(1)\psi(0) + \frac{(-it)}{1!} PH_i\psi_N(0) \\ &+ \sum_{j=2}^{\infty} \frac{(-it)^j}{j!} \{(PH_0^2 + PM)[PH_0 + b]^{-1}\}^{j-2}(PH_0^2 + PM)\psi_N(0) ,\end{aligned} \tag{37}$$

where

$$M = H_0 H_i + H_i H_0 + H_i^2 . \tag{38}$$

Now there is a class of potentials for which $b = 0$, such as the universal van der Waals potential introduced by Lu and Marlow [9]—that this is so has not been observed before. We will treat the most general case ($b \neq 0$) later [10], but for this class of potentials, and for illustrative purposes, Eq. (29) may be expanded, then regrouped, to include in a series expression, the Taylor expansion of $\exp[(-it/\hbar)H_0(1)]$. Skipping all the details, we can write for $b = 0$ the exact equation

$$\psi(t) = e^{-itH_0/\hbar}\psi(0) + \sum_{j=1}^{\infty} \frac{(-it)^j}{j!} B_j \psi(0) + \sum_{j=1}^{\infty} \frac{(-it)^j}{j!} C_j \psi_N(0), \tag{39}$$

where

$$\begin{aligned} B_1 &= B_2 = 0, \qquad B_3 = PMH_0, \\ B_4 &= PMH_0^2 + H_0PMH_0 + PMH_0^{-1}PMH_0, \\ B_5 &= H_0PMH_0^2 + H_0^2PMH_0 + H_0PMH_0^{-1}PMH_0 \\ &\quad + PMH_0^3 + PMPMH_0 + PMH_0^{-1}PMH_0^2 \\ &\quad + PMH_0^{-1}PMH_0^{-1}PMH_0, \end{aligned} \tag{40}$$

and

$$\begin{aligned} C_1 &= PH_i, \qquad C_2 = PM, \\ C_3 &= PMH_0^{-1}PM, \\ C_4 &= (H_0^2 + PM + H_0PMH_0^{-1} + PMH_0^{-1}PMH_0^{-1})PM \\ C_5 &= (H_0^3 + H_0^2PMH_0^{-1} + H_0PM \\ &\quad + H_0PMH_0^{-1}PMH_0^{-1} + PMH_0 \\ &\quad + PMPMH_0^{-1} + PMH_0^{-1}PM)PM. \end{aligned} \tag{41}$$

The combinatorial rules for writing the other B_j, C_j may be deduced.

Before we continue, we stress that one can invent interaction Hamiltonians H_i where $b = 0$, such as a properly defined potential that includes attraction at large distance and repulsion at short distance.

For the case $b = 0$, it is easy to verify by a term-by-term integration over the coordinate r_1 in Eq. (39) that normalization is preserved and, therefore, guarantees the validity of the usual probabilistic interpretation. The general case is more subtle, for which we cannot make the same statement so quickly [10]. We associate this difficulty with the possibility of bound states.

But even when $b \neq 0$, it could still be assumed to be zero for the purpose of approximating the exact equation (37). We will show in Ref. [10] that this is equivalent to a generalized form of a weak-coupling approximation.

From Eq. (39), it is already possible to confirm the suggestion from Ref. [1] that the behavior of the system consists of a "flow" component from the first two terms and some form of interaction with the large system. However, we stress that up to this point we assume a Hermitian Hamiltonian, and therefore we limit ourselves to reversible systems. A detailed discussion of reversibility and irreversibility, applicable to the present work, may be obtained from Refs. [11,12], where projection operator techniques are also used. In brief, to arrive at irreversible behavior, it is necessary to introduce one or more of some common assumptions used to introduce irreversibility, like an explicitly non-Hermitian Hamiltonian that includes dissipative terms, weak coupling, a "heat bath," or the neglect of "memory effects." For this reason, we cannot immediately compare the last term of Eq. (39) with the corresponding terms in Ref. [1] which describe a "jump process in Hilbert space." What else we need to do to reproduce the exact form of the "discontinuous quantum jumps" of Ref. [1] from the third term is an open question. But it is already possible to approximate the third term of Eq. (39) with stochastic terms, depending on the system under study.

Furthermore, our development in this Letter cannot apply to any nonlinear Schrödinger equation because of the explicit form of the projection operator used in our work, in contrast to other abstract and more general projection operators used by many authors [13]. However, it is the simple character of our projection operator that allows further reductions of the formal solution. In our formulation, any semblance of nonlinearity can only arise from the last terms of Eq. (37) or (39), perhaps providing an insight on how nonlinear behavior could arise out of a linear Schrödinger equation. Nontrivial assumptions must be introduced with the initial conditions, such as the initial presence of bound or metastable states.

Hermitian or not, evaluating only a few terms of Eqs. (37) and (39) eventually results in the violation of conservation of probability, as we have verified in previous work that uses essentially the same method [2]. This is the analog, but not the equivalent, of secular behavior in classical perturbation theory and means only that the approximate solutions so obtained—and the differential equations that such solutions satisfy—are valid only for limited times. We have found that evaluating more terms "postpones" divergent behavior for later times, just as the corresponding differential equations become valid for longer times. But when for analogous simple models it becomes possible to evaluate all terms and sum the analogous infinite series of Eq. (37), the exact solutions are fully convergent [3,10].

We emphasize that Eqs. (37) and (39) are solutions contracted from the many-body Schrödinger equation, instead of an exact or approximate solution of an approximate differential master equation with identifiable "flow-jump" components. Nevertheless, we reiterate that at no point in the derivation did we have to invoke a Markov assumption, nor assume weak coupling. So, in addition to the clarification of conceptual modifications needed to arrive at irreversible behavior, this Letter serves as an independent confirmation of the qualified conclusions of Ref. [1], using a straightforward reduced wave-function approach, instead of a reduced probability distribution formulation, and therefore, indirectly, an independent, perhaps stronger, indication of the validity of different realizations of stochastic methods [14].

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[1] H. Breuer and F. Petruccione, Phys. Rev. Lett. **74**, 3788 (1995).

[2] A. Muriel and M. Dresden, Physica (Amsterdam) **81D**, 221 (1995).

[3] A. Muriel, Phys. Rev. A **50**, 4286 (1994).

[4] E. J. Brandas and R. J. Bartlett, Chem. Phys. Lett. **8**, 153 (1971).

[5] Th. Hoffman-Ostenhoff and F. Mark, Chem. Phys. Lett. **23**, 302 (1973).

[6] P. O. Lowdin, Int. J. Quantum Chem. **29**, 1651 (1986).

[7] See, for example, R. Zwanzig, *Statistical Mechanics of Irreversibility,* Lectures in Theoretical Physics Vol. III (Interscience, New York, 1961).

[8] M. Dresden, in *Twentieth Century Physics* (Institute of Physics Publishing, Bristol, 1995).

[9] J. X. Lu and W. H. Marlow, Phys. Rev. Lett. **74**, 1724 (1995).

[10] A. Muriel (to be published).

[11] E. Brandas, Physica (Amsterdam) **82A**, 97 (1976).

[12] E. J. Brandas and P. Froelich, Int. J. Quantum Chem. **S9**, 457 (1976).

[13] See, for example, N. Gisin, Phys. Rev. Lett. **52**, 1657 (1984).

[14] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1992).