Quantization of a General Dynamical System by Feynman's Path Integration Formulation*

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The Schrödinger equation is obtained by Feynman's path integration method of quantization for a general dynamical system. The meaning of the results is discussed.

I. INTRODUCTION

We present a derivation of the "Schrödinger equation" for a general dynamical system using Feynman's path integral[1] method of quantization. The result differs from the "usual Schrödinger equation" in that there is an additional term proportional to the total curvature R of the coordinate space defined with a geometry given by the kinetic energy. This result had been given before by DeWitt.[2] In a curved space or in cases of constraints where $R \neq$ numerical constant, the presence of this additional term would change the energy spectrum of the whole system. In Sec. III we discuss the meaning of this additional term.

II. DERIVATION OF THE SCHRÖDINGER EQUATION

We will give a detailed derivation of the Schrödinger equation for a general mechanical system by using the path-integral method of Feynman. For a given mechanical system described by a set of coordinates $q\ (q^1, q^2, \cdots q^N)$, let the Lagrangian be

$$L(\dot{q}(t), q(t)) = \tfrac{1}{2} g_{ij}(q(t))\, \dot{q}^i \dot{q}^j. \tag{1}$$

Following Ref. 1, we can generalize Eqs. (1)–(18) to the above system, that is,

$$\psi(q(t+\epsilon), t+\epsilon) = (1/A) \int \exp[(i/\hbar) S(q(t+\epsilon), q(t))] \times \psi(q(t), t) \sqrt{g(q(t))}\, dq(t), \tag{2}$$

where $\psi(q(t+\epsilon), t+\epsilon)$ and $\psi(q(t), t)$ are, respectively, wavefunctions at time $t+\epsilon$ and t, $S(q(t+\epsilon), q(t))$ is the classical action, that is,

$$S(q(t+\epsilon), q(t)) = \text{minimum of } \int_t^{t+\epsilon} L(\dot{q}(t'), q(t'))\, dt' \tag{3}$$

with the boundary conditions

$$q(t')|_{t'=t} = q(t), \qquad q(t')|_{t'=t+\epsilon} = q(t+\epsilon). \tag{4}$$

A is a normalization factor to be determined later and g is the determinant of (g_{ij}). Taking the limit of Eq. (2) when $\epsilon \to 0$, we can derive the Schrödinger equation. Now as $\epsilon \to 0$, the factor $\exp[(i/\hbar) S(q(t+\epsilon), q(t))]$ oscillates very rapidly. Only the vicinity of the stationary point of $S(q(t+\epsilon), q(t))$ contributes to the integral in Eq. (2). The stationary point is

$$q(t) = q(t+\epsilon). \tag{5}$$

As we shall see the region which contributes to the integral in Eq. (2) is $|\Delta q| = |q(t) - q(t+\epsilon)| \lesssim \epsilon^{1/2}$. Thus we can expand $S(q(t+\epsilon), q(t))$ as a power series of Δq. This is done in Appendix A and gives

$$S(q(t+\epsilon), q(t)) = \frac{1}{2\epsilon} g_{ij}(q(t+\epsilon)) \times \Big[\Delta q^i \Delta q^j - \left\{ {i \atop mn} \right\} \Delta q^j \Delta q^m \Delta q^n + \frac{1}{4} \left\{ {i \atop mn} \right\} \left\{ {j \atop \alpha\beta} \right\} \Delta q^m \Delta q^n \Delta q^\alpha \Delta q^\beta + \frac{1}{3} \left(\frac{\partial}{\partial q^l} \left\{ {i \atop mn} \right\} + \left\{ {i \atop \alpha l} \right\} \left\{ {\alpha \atop mn} \right\} \right) \Delta q^j \Delta q^m \Delta q^n \Delta q^l + \cdots \Big]. \tag{6}$$

We also need the following expansions:

$$\sqrt{g(q(t))} = \sqrt{g(q(t+\epsilon))} - \Delta q^i \frac{\partial \sqrt{g}}{\partial q^i} + \tfrac{1}{2} \Delta q^i \Delta q^j \frac{\partial^2 \sqrt{g}}{\partial q^i \partial q^j} + \cdots, \tag{7}$$

$$\psi(q(t), t) = \psi(q(t+\epsilon), t) - \Delta q^i \frac{\partial \psi}{\partial q^i} + \tfrac{1}{2} \Delta q^i \Delta^j \frac{\partial^2 \psi}{\partial q^i \partial q^j} + \cdots. \tag{8}$$

In these equations

$$\Delta q = q(t+\epsilon) - q(t) \tag{9}$$

and $\left\{ {i \atop mn} \right\}$ is the Christoffel symbol,

$$\left\{ {i \atop mn} \right\} = g^{ik} [mn, k], \tag{10}$$

$$[mn, k] = \frac{1}{2} \left(\frac{\partial g_{mk}}{\partial q^n} + \frac{\partial g_{nk}}{\partial q^m} - \frac{\partial g_{mn}}{\partial q^k} \right), \tag{11}$$

and (g^{ik}) is the inverse matrix of (g_{ik}). Keeping the zero-order term $(1/2\epsilon) g_{ij} \Delta q^i \Delta q^j$ in the exponential and expanding higher-order terms into power series, we get from Eq. (2)

$$\begin{aligned}
\psi(q(t+\epsilon), t+\epsilon) = \frac{1}{A} \int \exp\left(\frac{i}{2\hbar\epsilon} g_{ij} \Delta q^i \Delta q^j\right)
&\times \Big[1 - \frac{i}{2\hbar\epsilon} g_{ij} \left\{ {i \atop mn} \right\} \Delta q^j \Delta q^m \Delta q^n \\
&+ \frac{i}{8\hbar\epsilon} g_{ij} \left\{ {i \atop mn} \right\} \left\{ {j \atop \alpha\beta} \right\} \Delta q^m \Delta q^n \Delta q^\alpha \Delta q^\beta \\
&+ \frac{i}{6\hbar\epsilon} g_{ij} \left(\frac{\partial}{\partial q^l} \left\{ {i \atop mn} \right\} + \left\{ {i \atop \alpha l} \right\} \left\{ {\alpha \atop mn} \right\} \right) \Delta q^j \Delta q^m \Delta q^n \Delta q^l \\
&- \frac{g_{ij} g_{st}}{8\hbar^2 \epsilon^2} \left\{ {i \atop mn} \right\} \left\{ {s \atop \alpha\beta} \right\} \Delta q^j \Delta q^t \Delta q^m \Delta q^n \Delta q^\alpha \Delta q^\beta + \cdots \Big] \\
&\times \left(\sqrt{g(q(t+\epsilon))} - \Delta q^i \frac{\partial \sqrt{g}}{\partial q^i} + \tfrac{1}{2} \Delta q^i \Delta q^j \frac{\partial^2 \sqrt{g}}{\partial q^i \partial q^j} \right) \\
&\times \Big(\psi(q(t+\epsilon), t) - \Delta q^i \frac{\partial \psi}{\partial q^i} + \tfrac{1}{2} \Delta q^i \Delta q^j \frac{\partial^2 \psi}{\partial q^i \partial q^j} + \cdots \Big) d(\Delta q^1) \cdots d(\Delta q^N).
\end{aligned} \tag{12}$$

The following are two useful identities:

$$\iint_{-\infty}^{\infty} \cdots \int \exp\left(\frac{i}{2\hbar\epsilon} g_{ij} \Delta q^i \Delta q^j\right) d(\Delta q) = (i\pi\hbar\epsilon)^{N/2} g^{-1/2} \tag{13}$$

$$\iint_{-\infty}^{\infty} \cdots \int \exp\left(\frac{i}{2\hbar\epsilon} g_{ij} \Delta q^i \Delta q^j\right) \times \Delta q^{\alpha_1} \Delta q^{\alpha_2} \cdots \Delta q^{\alpha_{2m}} d(\Delta q) = (i\pi\hbar\epsilon)^{N/2} g^{-1/2} (i\hbar\epsilon)^m \{ g^{\alpha_1\alpha_2} g^{\alpha_3\alpha_4} \cdots g^{\alpha_{2m-1}\alpha_{2m}}$$

+ terms with other possible permutations of

$$\alpha_1, \alpha_2, \cdots, \alpha_{2m}. \tag{14}$$

There are altogether $(2m-1)(2m-3)\cdots 5\cdot 3\cdot 1$ terms.

Using the two identities, we can easily find out the coefficients of $\psi(q(t+\epsilon),t), \partial\psi/\partial q^m, \partial^2\psi/\partial q^m\partial q^n$. The calculations are in Appendix B.

Here we just write down the results. Equation (12) becomes

$$\psi(q(t+\epsilon),t) + \epsilon\frac{\partial\psi}{\partial t} + \cdots = \frac{(i\pi\hbar\epsilon)^{N/2}}{A}\left\{\psi(q(t+\epsilon),t) + i\hbar\epsilon\left[\frac{1}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^m}\left(\sqrt{g}\,g^{mn}\frac{\partial\psi}{\partial q^n}\right) - \frac{R}{6}\psi\right]\right\}, \tag{15}$$

where

$$R = g^{ij}R_{ij}, \tag{16}$$

$$R_{ij} = R^{\alpha}_{ij\alpha}, \tag{17}$$

and

$$R^l_{ijk} = \frac{\partial}{\partial q^k}\begin{Bmatrix} l \\ ij \end{Bmatrix} - \frac{\partial}{\partial q^j}\begin{Bmatrix} l \\ ik \end{Bmatrix} + \begin{Bmatrix} \alpha \\ ij \end{Bmatrix}\begin{Bmatrix} l \\ \alpha k \end{Bmatrix} - \begin{Bmatrix} \alpha \\ ik \end{Bmatrix}\begin{Bmatrix} l \\ \alpha j \end{Bmatrix}. \tag{18}$$

Compare the coefficient up to order ϵ in Eq. (15). We get

$$A = (i\pi\hbar\epsilon)^{N/2} \tag{19}$$

and

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^m}\left(\sqrt{g}\,g^{mn}\frac{\partial\psi}{\partial q^n}\right) + \frac{\hbar^2 R}{6}\psi. \tag{20}$$

Equation (20) is the "Schrödinger equation" using Feynman's path integration formulation of quantum mechanics.

III. DISCUSSION

(a) Equation (20) above is different from the "usual Schrödinger equation" in which the term $\hbar^2R/6$ is absent. Notice that *both* equations are convariant under any coordinate transformation $q^1\cdots q^N \to Q^1\cdots Q^N$.

(b) In case the curvature R vanishes, one does not have to discuss which of the two equations is to be preferred, since they are the same. Such is the case when the kinetic energy is that of a collection of nonrelativistic particles in Euclidean space where $N=(3$ times the number of particles).

(c) If $R \neq 0$, it may seem at first sight that canonical quantization rules will yield the "usual Schrödinger equation." That is incorrect! In fact, only in the case $g_{ij}=$ constants are the canonical quantization rules

$$[P_i, q^j] = -i\hbar\delta_i^{\ j}$$

unambiguous and independent of coordinate transformations (if they maintain $g_{ij}=$ const). If $R\neq 0$, "canonical quantization rules" are ambiguous.

(d) The limit $\hbar \to 0$ of both equations give[2] the same results as classical mechanics, since the term $-\hbar^2R/6$ is an equivalent potential energy and approaches 0 as $\hbar$ approaches 0.

(e) If $R\neq 0$, one can always embed the coordinate space $q^1\cdots q^N$ as a curved subspace in a Euclidean space S of larger dimension. Does canonical quantization in the larger space S lead to a unique Schrödinger equation in the subspace? The answer to this question is no. To analyze this question, one would have to investigate first the constraint to be applied to the system in S so as to restrict the motion to the subspace. This constraint is to confine motion to a thin layer of "thickness" $\Delta(q^1\cdots q^N)$ around the subspace and then to approach the limit $\Delta\to 0$. In classical mechanics *any* nondissipative constraint would yield the same result in the limit $\Delta \to 0$. The limiting trajectories would satisfy the Lagrangian equations for the q's, and one need not concern oneself with the larger space S. In particular the thickness Δ can depend on $q^1\cdots q^N$. E.g., one could have

$$\Delta = A(q^1\cdots q^N)\epsilon + O(\epsilon^2), \tag{21}$$

and take the limit $\epsilon\to 0$.

In quantum mechanics, however, the constraint produces a zero point energy. The limit for the Schrödinger equation would then depend on precisely how the limit $\Delta\to 0$ is taken. If one takes (21), and the fact that $A\neq$ const, the Schrödinger equation would acquire an infinite term $\alpha(A\epsilon)^{-2}$ which varies wildly over the q's. Consequently, the Schrödinger equation approaches no definite limit. If, on the other hand, one takes $A=$ const, then everything depends on the higher order terms in $O(\epsilon^2)$ in (21).

(f) To summarize, for a case $R\neq 0$, canonical quantization does not produce a unique Schrödinger equation, and embedding the system in a higher-dimensional Euclidean space would not help to produce a unique Schrödinger equation. The correspondence limit also does not uniquely determine a Schrödinger equation. Feynman's path integration formulation of quantization, however, does produce a unique equation, which is Eq. (20) above. The "usual Schrödinger equation" appears to be foundationless.

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APPENDIX A

In this appendix, we want to expand $S(q(t+\epsilon), q(t))$ as a power series of Δq. The equations of motion are

$$g_{mj}\ddot{q}^j = -\frac{1}{2}\left(\frac{\partial g_{mj}}{\partial q^\alpha} + \frac{\partial g_{m\alpha}}{\partial q^j} - \frac{\partial g_{\alpha j}}{\partial q^m}\right)\dot{q}^\alpha\dot{q}^j \tag{A1}$$

or

$$\ddot{q}^k = -\begin{Bmatrix} k \\ \alpha\beta \end{Bmatrix}\dot{q}^\alpha\dot{q}^\beta. \tag{A2}$$

Via Eq. (A2) it is not very difficult to prove

$$\frac{d}{dt}\left(\tfrac{1}{2}g_{ij}\dot{q}^i\dot{q}^j\right) = 0. \tag{A3}$$

That is,

$$S(q(t+\epsilon), q(t)) = \int_t^{t+\epsilon} L\,dt = \left[\tfrac{1}{2}g_{ij}(q(t+\epsilon))\,\dot{q}^i(t+\epsilon)\,\dot{q}^j(t+\epsilon)\right]\epsilon. \tag{A4}$$

Now if we know $\dot{q}^i(t+\epsilon)$ as a series of Δq, we know $S(q(t+\epsilon), q(t))$. In order to find out $\dot{q}^i(t+\epsilon)$, we need $\dddot{q}^k$. From Eq. (A2), we find

$$\dddot{q}^{k} = -\left(\frac{\partial}{\partial q^{\gamma}}\begin{Bmatrix}k\\ \alpha\beta\end{Bmatrix} - 2\begin{Bmatrix}k\\ m\beta\end{Bmatrix}\begin{Bmatrix}m\\ \alpha\gamma\end{Bmatrix}\right)\dot{q}^{\alpha}\dot{q}^{\beta}\dot{q}^{\gamma}. \qquad \text{(A5)}$$

Now for small ϵ and $|\Delta q| \lesssim \epsilon^{1/2}$, we can write

$$q^{i}(t) = q^{i}(t+\epsilon) - \epsilon\dot{q}^{i}(t+\epsilon) + (\epsilon^{2}/2!)\ddot{q}^{i}(t+\epsilon) - (\epsilon^{3}/3!)\dddot{q}^{i}(t+\epsilon) + \cdots \qquad \text{(A6)}$$

or

$$q^{i}(t) = q^{i}(t+\epsilon) - \epsilon\dot{q}^{i}(t+\epsilon) - \frac{\epsilon^{2}}{2!}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\dot{q}^{\alpha}\dot{q}^{\beta} + \frac{\epsilon^{3}}{3!}\left(\frac{\partial}{\partial q^{\gamma}}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix} - 2\begin{Bmatrix}i\\ m\beta\end{Bmatrix}\begin{Bmatrix}m\\ \alpha\gamma\end{Bmatrix}\right)\dot{q}^{\alpha}\dot{q}^{\beta}\dot{q}^{\gamma} + \cdots. \qquad \text{(A7)}$$

From Eq. (A7) we get

$$\dot{q}^{i}(t+\epsilon) = \frac{\Delta q^{i}}{\epsilon} - \frac{1}{2\epsilon}\begin{Bmatrix}i\\ mn\end{Bmatrix}\Delta q^{m}\Delta q^{n} + \frac{1}{6\epsilon}\left(\frac{\partial}{\partial q^{l}}\begin{Bmatrix}i\\ mn\end{Bmatrix} + \begin{Bmatrix}i\\ \alpha l\end{Bmatrix}\begin{Bmatrix}\alpha\\ mn\end{Bmatrix}\right)\Delta q^{m}\Delta q^{n}\Delta q^{l} + \cdots. \qquad \text{(A8)}$$

Substituting Eq. (A8) into Eq. (A4), we get

$$S(q(t+\epsilon), q(t)) = \frac{1}{2\epsilon}g_{ij}\left[\Delta q^{i}\Delta q^{j} - \begin{Bmatrix}i\\ mn\end{Bmatrix}\Delta q^{j}\Delta q^{m}\Delta q^{n} + \frac{1}{4}\begin{Bmatrix}i\\ mn\end{Bmatrix}\begin{Bmatrix}j\\ \alpha\beta\end{Bmatrix}\Delta q^{m}\Delta q^{n}\Delta q^{\alpha}\Delta q^{\beta} + \frac{1}{3}\left(\frac{\partial}{\partial q^{l}}\begin{Bmatrix}i\\ mn\end{Bmatrix} + \begin{Bmatrix}i\\ \alpha l\end{Bmatrix}\begin{Bmatrix}\alpha\\ mn\end{Bmatrix}\right)\Delta q^{j}\Delta q^{m}\Delta q^{n}\Delta q^{l} + \cdots\right]. \qquad \text{(A9)}$$

This is Eq. (6).

APPENDIX B

In this appendix, we calculate the coefficients of ψ, $\partial\psi/\partial q$, $\partial^{2}\psi/\partial q\partial q$ by using Eqs. (12)–(14).

(a) $$\frac{\partial^{2}\psi}{\partial q^{m}\partial q^{n}} : \frac{1}{2A}\int \exp\left(\frac{i}{2\hbar\epsilon}g_{ij}\Delta q^{i}\Delta q^{j}\right)\Delta q^{m}\Delta q^{n}\sqrt{g}\,d(\Delta q) = \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(i\hbar\epsilon)\frac{g^{mn}}{2} \qquad \text{(B1)}$$

(b) $$\frac{\partial\psi}{\partial q^{n}} : \frac{1}{A}\int \exp\left(\frac{1}{2\hbar\epsilon}g_{ij}\Delta q^{i}\Delta q^{j}\right)\sqrt{g}\left(\frac{i}{2\hbar\epsilon}\right) \times g_{ij}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\Delta q^{n}\Delta q^{j}\Delta q^{\alpha}\Delta q^{\beta}\,d(\Delta q) + \frac{1}{A}\int \exp\left(\frac{i}{2\hbar\epsilon}g_{ij}\Delta q^{i}\Delta q^{j}\right)\frac{\partial\sqrt{g}}{\partial q^{i}}\Delta q^{i}\Delta q^{n}$$
$$= \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(-i\hbar\epsilon)\frac{1}{2}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}g_{ij}\{g^{nj}g^{\alpha\beta} + g^{n\alpha}g^{j\beta} + g^{n\beta}g^{j\alpha}\} + \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(i\hbar\epsilon)g^{n\alpha}\begin{Bmatrix}\beta\\ \alpha\beta\end{Bmatrix}$$
$$= \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(-i\hbar\epsilon)\left(\tfrac{1}{2}g^{\alpha\beta}\begin{Bmatrix}n\\ \alpha\beta\end{Bmatrix} + g^{n\alpha}\begin{Bmatrix}\beta\\ \alpha\beta\end{Bmatrix}\right) + \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(i\hbar\epsilon)g^{n\alpha}\begin{Bmatrix}\beta\\ \alpha\beta\end{Bmatrix}$$
$$= \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(-i\hbar\epsilon)\tfrac{1}{2}g^{\alpha\beta}\begin{Bmatrix}n\\ \alpha\beta\end{Bmatrix}$$
$$= \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(i\hbar\epsilon)\frac{1}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^{m}}(\sqrt{g}\,g^{mn}). \qquad \text{(B2)}$$

In obtaining Eq. (B2) we use the identities

$$\frac{1}{\sqrt{g}}\frac{\partial\sqrt{g}}{\partial q^{i}} = \begin{Bmatrix}\beta\\ i\beta\end{Bmatrix} \qquad \text{(B3)}$$

and

$$\frac{\partial g^{mn}}{\partial q^{k}} = -g^{m\alpha}g^{n\beta}\frac{\partial g_{\alpha\beta}}{\partial q^{k}}. \qquad \text{(B4)}$$

Equation (B4) can be derived from

$$\frac{\partial}{\partial q^{k}}(g_{m\alpha}g^{n\alpha}) = \frac{\partial}{\partial q^{k}}(\delta^{n}_{m}) = 0. \qquad \text{(B5)}$$

(c) ψ ·

(1) $$\frac{1}{A}\int \exp\left(\frac{i}{2\hbar\epsilon}g_{ij}\Delta q^{i}\Delta q^{j}\right)\sqrt{g}\,d(\Delta q) = \frac{(i\pi\hbar\epsilon)^{N/2}}{A} \qquad \text{(B6)}$$

(2) $$\frac{1}{A}\int \exp\left(\frac{i}{2\hbar\epsilon}g_{ij}\Delta q^{i}\Delta q^{j}\right)\times\sqrt{g} \times\left[\frac{i}{2\hbar\epsilon}g_{i\gamma}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}m\\ \delta m\end{Bmatrix}\Delta q^{\alpha}\Delta q^{\beta}\Delta q^{\gamma}\Delta q^{\delta} + \frac{1}{2}\left(\begin{Bmatrix}\beta\\ m\beta\end{Bmatrix}\begin{Bmatrix}\alpha\\ n\alpha\end{Bmatrix} + \frac{\partial}{\partial q^{n}}\begin{Bmatrix}\beta\\ m\beta\end{Bmatrix}\right)\Delta q^{m}\Delta q^{n} + \left(\frac{i}{8\hbar\epsilon}g_{ij}\begin{Bmatrix}j\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ \gamma\delta\end{Bmatrix} + \frac{i}{6\hbar\epsilon}g_{i\delta} \times\left(\frac{\partial}{\partial q^{\gamma}}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix} + \begin{Bmatrix}i\\ m\alpha\end{Bmatrix}\begin{Bmatrix}m\\ \beta\gamma\end{Bmatrix}\right)\right)\Delta q^{\alpha}\Delta q^{\beta}\Delta q^{\gamma}\Delta q^{\delta} - \frac{1}{8\hbar^{2}\epsilon^{2}}g_{i\gamma}g_{j\delta}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ mn\end{Bmatrix} \times \Delta q^{\alpha}\Delta q^{\beta}\Delta q^{\gamma}\Delta q^{\delta}\Delta q^{m}\Delta q^{n}\right]d(\Delta q)$$
$$= \frac{(i\pi\hbar\epsilon)^{N/2}}{A}(i\hbar\epsilon)\times\left\{-\tfrac{1}{2}g_{i\gamma}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}m\\ \delta m\end{Bmatrix}(\alpha\beta\gamma\delta) + \frac{1}{2}\left(\begin{Bmatrix}\beta\\ m\beta\end{Bmatrix}\begin{Bmatrix}\alpha\\ n\alpha\end{Bmatrix} + \frac{\partial}{\partial q^{n}}\begin{Bmatrix}\beta\\ m\beta\end{Bmatrix}\right)(mn) - \left[\frac{1}{8}g_{ij}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ \partial\delta\end{Bmatrix} + \frac{1}{6}g_{i\delta}\left(\frac{\partial}{\partial q^{\gamma}}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix} + \begin{Bmatrix}i\\ m\alpha\end{Bmatrix}\begin{Bmatrix}m\\ \beta\gamma\end{Bmatrix}\right)\right](\alpha\beta\gamma\delta) + \frac{1}{8}g_{i\gamma}g_{j\delta}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ mn\end{Bmatrix}(\alpha\beta\gamma\delta mn)\right\}. \qquad \text{(B7)}$$

In these equations, $(\alpha_{1}, \alpha_{2}\cdots\alpha_{2m})$ stands for $(g^{\alpha_1\alpha_2}\cdots g^{\alpha_{2m-1}\alpha_{2m}})$ + terms with other possible permutation of $(\alpha_{1}\alpha_{2}\cdots\alpha_{2m})$.

The term

$$\tfrac{1}{8}g_{i\gamma}g_{j\delta}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ mn\end{Bmatrix}(\alpha\beta\gamma\delta mn)$$
$$= \tfrac{1}{8}g_{i\gamma}g_{j\delta}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ mn\end{Bmatrix}[g^{m\delta}(\alpha\beta\gamma n) + g^{n\delta}(\beta\gamma\delta m) + g^{\alpha\delta}(mn\gamma\beta) + g^{\beta\delta}(mn\alpha\gamma) + g^{\gamma\delta}(mn\alpha\beta)]$$
$$= \tfrac{1}{8}g_{i\gamma}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}m\\ m\delta\end{Bmatrix}(\alpha\beta\gamma\delta) + \tfrac{1}{8}g_{i\gamma}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}m\\ m\delta\end{Bmatrix}(\alpha\beta\gamma\delta) + \tfrac{1}{8}g_{i\gamma}\begin{Bmatrix}i\\ m\beta\end{Bmatrix}\begin{Bmatrix}m\\ \alpha\delta\end{Bmatrix}(\alpha\beta\gamma\delta) + \tfrac{1}{8}g_{i\gamma}\begin{Bmatrix}i\\ m\beta\end{Bmatrix}\begin{Bmatrix}m\\ \alpha\delta\end{Bmatrix}(\alpha\beta\gamma\delta) + \tfrac{1}{8}g_{ij}\begin{Bmatrix}i\\ \alpha\beta\end{Bmatrix}\begin{Bmatrix}j\\ \gamma\delta\end{Bmatrix}(\alpha\beta\gamma\delta).$$

Thus Eq. (B7) becomes

$$(\mathrm{B7}) = \frac{(i\pi\hbar\epsilon)^{N/2}}{A} (i\hbar\epsilon) \times \Big[\Big(-\frac{1}{4} g_{i\gamma} \begin{Bmatrix} i \\ \alpha\beta \end{Bmatrix}\begin{Bmatrix} m \\ \delta m \end{Bmatrix} - \tfrac{1}{6} g_{i\delta} \frac{\partial}{\partial q^\gamma}\begin{Bmatrix} i \\ \alpha\beta \end{Bmatrix} + \frac{1}{12} g_{i\delta}\begin{Bmatrix} i \\ m\alpha \end{Bmatrix}\begin{Bmatrix} m \\ \beta\gamma \end{Bmatrix}\Big) \times (\alpha\beta\gamma\delta) + \frac{1}{2}\Big(\begin{Bmatrix} \beta \\ m\beta \end{Bmatrix}\begin{Bmatrix} \alpha \\ n\alpha \end{Bmatrix} + \frac{\partial}{\partial q^n}\begin{Bmatrix} \beta \\ m\beta \end{Bmatrix}\Big)(mn)\Big]$$

$$= \frac{(i\pi\hbar\epsilon)^{N/2}}{A}\Big(\frac{-ih\epsilon}{6}\Big)\Big(\frac{\partial}{\partial q^m}\begin{Bmatrix} m \\ \alpha\beta \end{Bmatrix} - \frac{\partial}{\partial q^\alpha}\begin{Bmatrix} m \\ \beta m \end{Bmatrix} + \begin{Bmatrix} m \\ mn \end{Bmatrix}\begin{Bmatrix} n \\ \alpha\beta \end{Bmatrix} - \begin{Bmatrix} m \\ m\alpha \end{Bmatrix}\begin{Bmatrix} n \\ n\beta \end{Bmatrix}\Big) g^{\alpha\beta}. \qquad (\mathrm{B8})$$

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An "H-Theorem" for Multiplicative Stochastic Processes

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In a recent paper the author showed how multiplicative stochastic processes lead to a potentially comprehensive theory for nonequilibrium phenomena. In this paper an "*H* theorem" is proved from results obtained using multiplicative stochastic processes.

INTRODUCTION

In another paper,[1] the theory of multiplicative stochastic processes was explained, and it was shown how such a mathematical theory leads to a formalism for nonequilibrium thermodynamics: In this paper the thermodynamical "*H* function" will be introduced, and a proof of an "*H* theorem" will be presented.

RECAPITULATION

The Schrödinger equation for nonrelativistic quantum mechanics may be written in matrix form as

$$i\frac{d}{dt}C_\alpha(t) = \sum_{\alpha'} M_{\alpha\alpha'}C_{\alpha'}(t), \qquad (1)$$

where $M_{\alpha\alpha'} = M^*_{\alpha'\alpha}$, which is the condition of Hermiticity, and $\sum_\alpha C^*_\alpha(t)C_\alpha(t) = 1$, which is the condition of conservation of total probability. The Hermiticity of $M_{\alpha\alpha'}$ in (1) is necessary and sufficient for the conservation of total probability. Suppose that a fluctuating contribution to the Hamiltonian is considered. Then (1) becomes

$$i\frac{d}{dt}C_\alpha(t) = \sum_{\alpha'} M_{\alpha\alpha'}C_{\alpha'}(t) + \sum_{\alpha'} \tilde{M}_{\alpha\alpha'}(t)C_{\alpha'}(t), \qquad (2)$$

where $\tilde{M}_{\alpha\alpha'}(t) = \tilde{M}^*_{\alpha'\alpha}(t)$, and the following properties hold for the averaged moments of $\tilde{M}_{\alpha\alpha'}(t)$[1]:

$$\langle \tilde{M}_{\alpha\alpha'}(t)\rangle = 0, \qquad (3)$$

$$\langle \tilde{M}_{\alpha\alpha'}(t)\tilde{M}_{\beta\beta'}(s)\rangle = 2Q_{\alpha\alpha'\beta\beta'}\delta(t-s), \qquad (4)$$

$$\langle \tilde{M}_{\mu_1\nu_1}(t_1)\cdots\tilde{M}_{\mu_{2n-1}\nu_{2n-1}}(t_{2n-1})\rangle = 0 \quad \text{for } n = 1, 2, \ldots, \qquad (5)$$

$$\begin{aligned}\langle \tilde{M}_{\mu_1\nu_1}(t_1)\cdots\tilde{M}_{\mu_{2n}\nu_{2n}}(t_{2n})\rangle &= \frac{1}{2^n n!}\sum_{\rho\in S_{2n}}\prod_{j=1}^{n}\langle \tilde{M}_{\mu_{\rho(2j-1)}\nu_{\rho(2j-1)}} \times (t_{\rho(2j-1)})\tilde{M}_{\mu_{\rho(2j)}\nu_{\rho(2j)}}(t_{\rho(2j)})\rangle \\ &= \frac{1}{2^n n!}\sum_{\rho\in S_{2n}}\prod_{j=1}^{n} 2Q_{\mu_{\rho(2j-1)}\nu_{\rho(2j-1)}\mu_{\rho(2j)}\nu_{\rho(2j)}} \times \delta(t_{\rho(2j-1)} - t_{\rho(2j)}),\end{aligned} \qquad (6)$$

where S_{2n} is the symmetric group of order $(2n)!$ The properties given by (3)–(6) are those appropriate for a purely random, Gaussian, stochastic matrix.

A density matrix representation for the Schrödinger equation is obtained in terms of the density matrix $\rho_{\alpha\beta}$, which is defined by

$$\rho_{\alpha\beta}(t) \equiv C^*_\alpha(t)C_\beta(t). \qquad (7)$$

If $L_{\alpha\beta\alpha'\beta'}$ and $\tilde{L}_{\alpha\beta\alpha'\beta'}(t)$ are defined by

$$\begin{aligned} L_{\alpha\beta\alpha'\beta'} &\equiv \delta_{\alpha\alpha'}M_{\beta\beta'} - \delta_{\beta\beta'}M^*_{\alpha\alpha'}, \\ \tilde{L}_{\alpha\beta\alpha'\beta'}(t) &\equiv \delta_{\alpha\alpha'}\tilde{M}_{\beta\beta'}(t) - \delta_{\beta\beta'}\tilde{M}^*_{\alpha\alpha'}(t), \end{aligned} \qquad (8)$$

then Eq. (2) may be used to directly verify

$$i\frac{d}{dt}\rho_{\alpha\beta}(t) = \sum_{\alpha'}\sum_{\beta'}[L_{\alpha\beta\alpha'\beta'} + \tilde{L}_{\alpha\beta\alpha'\beta'}(t)]\rho_{\alpha'\beta'}(t). \qquad (9)$$

This is the density matrix equation. By averaging over the stochastic contribution by means of properties (3)–(6), an equation for the averaged density matrix, $\langle\rho_{\alpha\beta}(t)\rangle$, may be obtained, although only after significant computation[1]:

$$\frac{d}{dt}\langle\rho_{\alpha\beta}(t)\rangle = -i\sum_{\alpha'}\sum_{\beta'}L_{\alpha\beta\alpha'\beta'}\langle\rho_{\alpha'\beta'}(t)\rangle - \sum_{\alpha'}\sum_{\beta'}R_{\alpha\beta\alpha'\beta'}\langle\rho_{\alpha'\beta'}(t)\rangle. \qquad (10)$$

The matrix $R_{\alpha\beta\alpha'\beta'}$ which appears in (10) is defined by[1]

$$R_{\alpha\beta\alpha'\beta'} \equiv \delta_{\alpha\alpha'}\sum_\theta Q_{\beta\theta\theta\beta'} + \delta_{\beta\beta'}\sum_\theta Q_{\theta\alpha\alpha'\theta} - Q_{\beta\beta'\alpha'\alpha} - Q_{\alpha'\alpha\beta\beta'}. \qquad (11)$$

It is also provable that for arbitrary complex matrices $X_{\alpha\beta}$,

$$\sum_\alpha\sum_\beta\sum_{\alpha'}\sum_{\beta'} X^*_{\alpha\beta}R_{\alpha\beta\alpha'\beta'}X_{\alpha'\beta'} \geq 0 \qquad (12)$$

and

$$\sum_\alpha R_{\alpha\alpha\mu\nu} = 0. \qquad (13)$$

Conditions (12) and (13) lead to irreversible behavior in (10) with the equilibrium state being proportional