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Hamiltonian semigroups associated with boson systems: a probabilistic approach

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Abstract. In a previous paper we introduced a path integral technique based on birth and death processes. The method provides an analogue of the Feynman-Kac formula which is associated to the Hamiltonian semigroups of some boson systems. In the present work we briefly demonstrate this technique in a general form. Furthermore, we study a simple spin-boson model for which we obtain some estimates on ground-state energy and spin-flip rate.

1. Introduction

The motivation of this paper is to demonstrate a probabilistic technique which is useful for studying systems described by Hamiltonians of the following form

$$H = \omega a^+ a + \lambda(a + a^+) + f(a^+ a) \tag{1}$$

where a^+ and a are the ordinary creation and annihilation operators and f is a function of the product a^+a. One sees immediately that it is not possible to associate an ordinary Feynnan-Kac formula to the Hamiltonian semigroup $\psi_0 \to e^{-tH}\psi_0$. The reason is that the Hamiltonian (1) contains, in general, powers of the momentum $p \equiv (i/\sqrt{2})(a^+ - a)$ higher than two and, therefore, the Schrödinger equation in configuration-space does not have a heat-like structure. Nevertheless it is possible to have a very natural probabilistic formula associated to the Hamiltonian semigroup which uses birth and death processes.

In the first part of this paper we derive the formula and we show some general properties of it. In the second we demonstrate our technique with an application to a simple spin-boson model for which we obtain some estimates on ground-state energy and spin-flip rate.

2. The formula

Consider the Hamiltonian (1); the associated imaginary time Schrödinger equation in occupation number representation is (we assume in this paper, without loss of generality, $\omega = 1$ and λ real)

$$\frac{d}{dt}\psi_t(n) = -H\psi_t(n) = -n\psi_t(n) - \lambda\sqrt{n+1}\,\psi_t(n+1) - \lambda\sqrt{n}\,\psi_t(n-1) - f(n)\psi_t(n) \tag{2}$$

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where n is the integer which represents the occupation number. Perform now the transformation $\psi_t(n) \to \phi_t(n) = \psi_t(n)/\Omega(n)$ with $\Omega(n) \equiv (-\lambda)^n/\sqrt{n!}$ Note that $\Omega(n)$ is the ground-state wavefunction of the Schrödinger equation where $f(n) = 0$. The new function satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi_t(n) = -(\lambda^2 + n)\phi_t(n) + \lambda^2\phi_t(n+1) + n\phi_t(n-1) - (f(n) - \lambda^2)\phi_t(n)$$

$$\equiv L\phi_t(n) - (f(n) - \lambda^2)\phi_t(n). \tag{3}$$

It is easy to realise that L is the generator of a birth and death process N_t with death rate equal to N_t and birth rate equal to λ^2, while $(f(n) - \lambda^2)$ plays the role of a potential. We remark that this process has been extensively studied (see for example [31]) and the associated transition probability is known.

As a consequence of the Trotter product formula one has

$$\phi_t(n) = \mathbb{E}_{n,0}\left[\phi_0(N_t)\exp\left\{\int_0^t [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right] \tag{4}$$

where the expectation is taken with respect to the process which starts in n at time 0. This is our analogue of the Feynman–Kac formula [1, 2] (see the appendix for a heuristic derivation).

Furthermore, taking into account the definition of $\phi_t(n)$ one sees that

$$\psi_t(n) \equiv \mathbb{E}_{n,0}\left[\psi_0(N_t)\frac{\Omega(n)}{\Omega(N_t)}\exp\left\{\int_0^t [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right] \tag{5}$$

which is the simple probabilistic solution of equation (2).

We remark that it is possible to rewrite the solution (4) (as well as (5)) in the form

$$\begin{aligned}\phi_t(n) = \mathbb{E}_{n,0}\Bigg[\!\!\Bigg[& \phi_0(N'_t)\exp\left\{\int_0^t [\lambda^2 - f(N'_s)]\,\mathrm{d}s\right\} \\ & \times\exp\left\{-\int_0^t [\lambda^2 + N'_s]\,\mathrm{d}s + \int_0^t\left[\frac{\lambda^2}{A(N'_s+1)} + N'_s A(N'_s)\right]\mathrm{d}s\right\} \\ & \times\left[\left(\prod_{i=1}^{N'_t} A(i)\right)\left(\prod_{i=1}^{n} A(i)\right)^{-1}\right]\Bigg]\!\!\Bigg]\end{aligned} \tag{6}$$

where $A(i)$ is any strictly positive function of positive integers, and N'_s is a new process for which $\lambda^2/[A(N'_s+1)]$ is the death rate and $N'_s A(N'_s)$ the birth rate. The reason why it is possible to rewrite (4) in this form is a consequence of the fact that the expression in the second line of (6) is the Radon–Nikodym derivative of the measure of the process N with respect to the process N' (see the appendix). Formula (6) is a useful starting point for approximate calculations of many physical quantities.

We also remark that the ground-state energy E_0 of Hamiltonian (1) is given by

$$E_0 = \lim_{t\to\infty} -\frac{1}{t}\log p_n(t) \tag{7}$$

where

$$\begin{aligned} p_n(t) &\equiv \mathbb{E}_{n,0}\left[\delta(N_t - n)\exp\left\{\int_0^t \frac{[\lambda^2 - f(N_s)]\,\mathrm{d}s}{\mathbb{E}[\delta(N_t - n)]}\right\}\right] \\ &\equiv \left\langle \exp\left\{\int_0^t [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right\rangle_n \end{aligned} \tag{8}$$

which is easy to verify. The expectation in the numerator of (8) is, in fact, the imaginary time transition probability amplitude from n to n (it can be obtained from (5) by considering an initial function $\psi_0(m) = \delta(m-n)$). It is well known that this amplitude can be written as $\Sigma_{i=0}^{\infty} |\psi_i(n)|^2 \exp\{-E_i t\}$ where the ψ_i are the eigenfunctions of the Hamiltonian (1) and the E_i are the relative energies. Therefore, since the expression in the denominator tends to a constant (the equilibrium probability of finding the process in n) when t is large, the equality (7) is verified.

In a probabilistic language $p_n(t)$ is simply the expectation of the exponential function with the condition $N_0 = N_t = n$; this is the meaning of the notation in the second line of (8).

Combining the above definition with the statement (8) we also obtain

$$p_n(t) \equiv \left\langle \exp\left\{ -\int_0^t [f(N'_s) + N'_s]\,\mathrm{d}s + \int_0^t \left[\frac{\lambda^2}{A(N'_s+1)} + N'_s A(N'_s) \right] \mathrm{d}s \right\} \right\rangle_n \tag{9}$$

where the expectation is also conditioned by $N'_0 = N'_t = n$. Note that the rate of products which is contained in formula (6) has disappeared since it is, by definition, equal to 1 over trajectories which start and end in the same point.

3. An application

We discuss now the possible applications of the formulae which we have introduced by means of a simple (but non-trivial) example. Consider the Hamiltonian

$$H = a^+a + \lambda\sigma_z(a + a^+) + |\varepsilon|\sigma_x \tag{10}$$

which describes a single spin interacting with a vibration mode. There is a vast literature on this subject; we just mention [4] where it has been studied in connection with a highly simplified description of an elastic magnetic crystal. Furthermore, related models (with, in general, many vibrational modes) have been considered in many other physical contexts, for example in solid state physics in order to model the Kondo problem (see for example [5]) and for the Dicke model of the maser (see for example [6]), or even to describe quantum tunnelling in presence of an interaction with the surrounding (see for example [7]). The method of this paper can be easily adapted to these more complicated situations but in this paper we simply consider the 'toy' Hamiltonian (10) since it captures the most important physical features of this class of models.

Looking at (10), we remark that $|\varepsilon|$ is a positive parameter which represents the bare spin-flip (tunnelling) rate of the two-state system. We also remark that there is a conserved quantity; the operator $\sigma \equiv (-1)^{a^+a}\sigma_x$ commutes, in fact, with the Hamiltonian.

After having performed a unitary transformation of the Hamiltonian which also transforms the commuting operator σ in a 'c' number we have

$$H = a^+a + \lambda(a + a^+) + \sigma|\varepsilon|(-1)^{a^+a} \tag{11}$$

where σ can be ± 1. Now the Hamiltonian has the form (1) and, having defined $\varepsilon \equiv \sigma|\varepsilon|$, we can write

$$E_0 = E_0(\varepsilon, \lambda) = \lim_{t\to\infty} -\frac{1}{t} \log\left\langle \exp\left\{ -\varepsilon \int_0^t (-1)^{N_s}\,\mathrm{d}s + \lambda^2 t \right\} \right\rangle_n . \tag{12}$$

For any choice of the parameters λ and $|\varepsilon|$ we must consider both energies $E^{\pm}=E_0(\pm|\varepsilon|,\lambda)$ since they are the lowest energies corresponding to the two values ± 1 of σ. E^- is the ground-state energy of (10) since it is lower than E^+ [4] and $J=E^+-E^-$ is the effective spin-flip rate.

Expression (12) is the starting point of many estimates of physically relevant quantities. Let us start with the obvious remark that the spin-flip rate J is smaller than the bare one ε. From (12), taking into account that $-1\leqslant(-1)^{N_s}\leqslant 1$, one has in fact the bounds

$$-\lambda^2-|\varepsilon|\leqslant E^-\leqslant E^+\leqslant -\lambda^2+|\varepsilon|. \tag{13}$$

Another bound can be obtained by (12) through the Jensen inequality

$$E_0\leqslant -\lambda^2+\varepsilon \lim_{t\to\infty}\left\langle \frac{1}{t}\int_0^t (-1)\,\mathrm{d}s\right\rangle_n = -\lambda^2+\varepsilon\,\mathrm{e}^{-2\lambda^2}. \tag{14}$$

The above expectation is easily calculated because the transition probability of the process is known.

One can improve (14) by using the Jensen inequality together with (9); one has in this case

$$E_0\leqslant -\lim_{t\to\infty}\left\langle \frac{1}{t}\int_0^t\left(-\varepsilon(-1)^{N'_s}+\frac{\lambda^2}{A(N'_s+1)}+N'_s[A(N'_s)-1]\right)\mathrm{d}s\right\rangle_n \tag{15}$$

where N' is the process defined in (6). The inequality holds for any choice of the positive trial function $A(m)$; for example, $A(m)=A=\text{constant}$ produces

$$E_0\leqslant \min_A\left\{\varepsilon\,\mathrm{e}^{-2\lambda^2/A^2}+\frac{\lambda^2}{A^2}-\frac{2\lambda^2}{A}\right\} \tag{16}$$

which is a more accurate bound than (13). Other trial functions $A(m)$ could be considered together with the Jensen inequality, but this is beyond the scope of this paper which essentially illustrates the possible uses of the proposed probabilistic method.

Formula (9) is useful in other contexts than the Jensen inequality, as may be seen through an example. For any even m define $A(m)=1$ and $A(m+1)$ solution of

$$-\varepsilon+\frac{\lambda^2}{A(m+1)}=\varepsilon+\lambda^2+(m+1)(A(m+1)-1). \tag{17}$$

From (9) it turns out that

$$p_n(t)=\left\langle \exp\left\{-\int_0^t [R(N_s)]\,\mathrm{d}s\right\}\right\rangle_n$$
$$\min_m R(m)\leqslant E_0\leqslant \max_m R(m) \tag{18}$$

with $R(m)=G(m+1)$ when m even, $R(m)=G(m)$ when m odd and $G(m+1)$ defined as

$$G(m+1)=\frac{m+1-\lambda^2}{2}-\left[\left(\frac{\lambda^2+m+1}{2}\right)^2+\varepsilon^2-\varepsilon(m+1-\lambda^2)\right]^{1/2}. \tag{19}$$

It is easy to check that $R(m)$ is a decreasing function of m when $\varepsilon \leqslant 0$ and it is an increasing function when $0 \leqslant \varepsilon$; therefore (see (18)) we obtain

$$E^- \leqslant \frac{1-\lambda^2}{2} - \left[\left(\frac{\lambda^2+1}{2}\right)^2 + |\varepsilon|^2 + |\varepsilon|(1-\lambda^2)\right]^{1/2}$$

$$E^+ \geqslant \frac{1-\lambda^2}{2} - \left[\left(\frac{\lambda^2+1}{2}\right)^2 + |\varepsilon|^2 - |\varepsilon|(1-\lambda^2)\right]^{1/2} \tag{20}$$

where the equalities hold for every $|\varepsilon|$. An obvious consequence is

$$J \geqslant \left[\left(\frac{\lambda^2+1}{2}\right)^2 + |\varepsilon|^2 + |\varepsilon|(1-\lambda^2)\right]^{1/2} - \left[\left(\frac{\lambda^2+1}{2}\right)^2 + |\varepsilon|^2 - |\varepsilon|(1-\lambda^2)\right]^{1/2} \tag{21}$$

which gives a realistic estimate of spin-flip rate for small coupling λ.

4. Some more estimates

Simple probabilistic reasoning generates other bounds. Consider again (12) and take $n=0$; since the function in the expectation is positive one has that $p_0(t)$ is larger than the value obtained considering only a smaller number of realisations. For example, the probability that a trajectory which starts in 0 always remains in 0 during the time interval t is equal to $\exp(-\lambda^2 t)$ (the rate of exit from 0 is λ^2) while the function in the expectation takes the value $\exp(-\varepsilon t + \lambda^2 t)$ for this trajectory. One has therefore

$$p_0(t) \geqslant \exp(-\lambda^2 t)\exp(-\varepsilon t + \lambda^2 t) \rightarrow E_0 \leqslant \varepsilon. \tag{22}$$

If we repeat the reasoning for $p_1(t)$ and we consider the trajectories which start in 1 and which remain there during the time interval t we obtain

$$p_1(t) \geqslant \exp(-\lambda^2 t + t)\exp(\varepsilon t + \lambda^2 t) \rightarrow E_0 \leqslant -\varepsilon + 1 \tag{23}$$

where we have used the fact that the rate of exit from 1 is $\lambda^2 + 1$. Inequalities (16) and (17) together lead to

$$E^- \leqslant -|\varepsilon| \qquad E^+ \leqslant \tfrac{1}{2} - ||\varepsilon| - \tfrac{1}{2}|. \tag{24}$$

We remark that the above upper bounds are the ground-state energies of Hamiltonian (9) when $\lambda = 0$ and therefore we conclude that the coupling has always the effect of lowering the ground-state energies.

Similar probabilistic arguments can be also applied to the expression (15). The probability that a trajectory which starts and ends in n always remains in the sites n and $n+1$ is larger than $\exp[-\lambda^2 t/A(n+2) - nA(n)t]$. To be convinced of this fact it is sufficient to remember that $nA(n)$ is the rate for $n \rightarrow 1$ and $\lambda^2/A(n+2)$ is the rate for $n+1 \rightarrow n+2$. Furthermore, choosing $A(n+1)$ solution of

$$-(-1)^n\varepsilon + \frac{\lambda^2}{A(n+1)} - m = (-1)^n\varepsilon + (n+1)(A(n+1)-1) \tag{25}$$

it turns out that the function in the expectation of (15), for these trajectories which always remain in n and $n+1$, is larger than

$$\exp\{-T(n)\} = \exp\{-(n+\tfrac{1}{2}) + [((-1)^n\varepsilon - \tfrac{1}{2})^2 + \lambda^2(n+1)]^{1/2}\} \tag{26}$$

and therefore following the same reasoning as before we have

$$P_n(t) \geq \exp\{-\lambda^2 t/A(n+2) - nA(n)t\} \exp\{-T(n)\}. \tag{27}$$

Since we can make $A(n)$ as small as we want and $A(n+2)$ as large as we want, we obtain

$$E_0 \leq \min_n T(n). \tag{28}$$

For the positive ε and small values of λ, the above upper bound combined with the lower bound (20) implies $E_0(\varepsilon, \lambda) - E_0(\varepsilon, 0) \sim \lambda^2$ when $\varepsilon \neq \frac{1}{2}$ and $E_0(\varepsilon, \lambda) - E_0(\varepsilon, 0) \sim \lambda$ when $\varepsilon = \frac{1}{2}$. On the other hand, from (20) and (24), also it turns out that the derivative of $E_0(\varepsilon, \lambda)$ with respect to ε is discontinuous in $\varepsilon = \frac{1}{2}$ when $\lambda = 0$. In conclusion, the derivatives of the ground-state energy $E_0(\varepsilon, \lambda)$ (which can be interpreted as the free energy of a statistical model for a one-dimensional spin system with continuous index) are both discontinuous in $\varepsilon = \frac{1}{2}$ when $\lambda = 0$.

We remark, as a final comment, that it is straightforward to extend the technique which we have proposed here to Hamiltonians of many oscillators. In this more general case a different process will be associated with any oscillator.

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Appendix

In this appendix we give an heuristic proof of formulae (4) and (6).

We first prove formula (4) showing that it is a solution of the equation (3) with initial conditions $\phi_0(n)$. We start by rewriting the formula (4) for a larger time $t+\mathrm{d}t$:

$$\begin{aligned}\phi_{t+\mathrm{d}t}(n) &= \mathbb{E}_{n,0}\left[\phi_0(N_{t+\mathrm{d}t}) \exp\left\{\int_0^{t+\mathrm{d}t} [\lambda^2 - f(N_s)])\,\mathrm{d}s\right\}\right] \\ &= \mathbb{E}_{n,0}\left[\mathbb{E}_{N_{\mathrm{d}t},\mathrm{d}t}\left[\phi_0(N_{t+\mathrm{d}t}) \exp\left\{\int_{\mathrm{d}t}^{t+\mathrm{d}t} [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right]\right. \\ &\qquad \left.\times \exp\left\{\int_0^{\mathrm{d}t} [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right].\end{aligned} \tag{A1}$$

In writing the second equality we have used a decomposition of the trajectories in two parts; one goes from time 0 to time $\mathrm{d}t$, the other from $\mathrm{d}t$ to $t+\mathrm{d}t$. The first expectation in the second line concerns the process N_s when $0 \leq s \leq \mathrm{d}t$ while the second is the conditional expectation with respect to N_s when $\mathrm{d}t \leq s \leq t+\mathrm{d}t$ and when $N_{\mathrm{d}t}$ is fixed at time $\mathrm{d}t$. We are now able to compute the first expectation up to the first order in $\mathrm{d}t$ and we obtain

$$\begin{aligned}\phi_{t+\mathrm{d}t}(n) &= (\lambda^2\,\mathrm{d}t)\mathbb{E}_{n+1,\mathrm{d}t}\left[\phi_0(N_{t+\mathrm{d}t}) \exp\left\{\int_{\mathrm{d}t}^{t+\mathrm{d}t} [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right] \\ &\quad + (n\,\mathrm{d}t)\mathbb{E}_{n-1,\mathrm{d}t}\left[\phi_0(N_{t+\mathrm{d}t}) \exp\left\{\int_{\mathrm{d}t}^{t+\mathrm{d}t} [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right] \\ &\quad + (1 - \lambda^2\,\mathrm{d}t - n\,\mathrm{d}t)\mathbb{E}_{n,\mathrm{d}t}\left[\phi_0(N_{t+\mathrm{d}t}) \exp\left\{\int_{\mathrm{d}t}^{t+\mathrm{d}t} [\lambda^2 - f(N_s)]\,\mathrm{d}s\right\}\right] \\ &\quad \times (1 + (\lambda^2 - f(n))\,\mathrm{d}t)\end{aligned} \tag{A2}$$

where we have used the fact that N_{dt} equals $n+1$ with probability $\lambda^2\,dt$ and equals $n-1$ with probability $1-\lambda^2\,dt-n\,dt$. Since the process is homogeneous in time we can rewrite this equality as

$$\begin{aligned}\phi_{t+dt}(n)=(\lambda^2\,dt)\mathbb{E}_{n+1,0}\left[\phi_0(N_t)\exp\left\{\int_0^t[\lambda^2-f(N_s)]\,ds\right\}\right]\\ +(n\,dt)\mathbb{E}_{n-1,0}\left[\phi_0(N_t)\exp\left\{\int_0^t[\lambda^2-f(N_s)]\,ds\right\}\right]\\ +(1-\lambda^2\,dt-n\,dt)\mathbb{E}_{n,0}\left[\phi_0(N_t)\exp\left\{\int_0^t[\lambda^2-f(N_s)]\,ds\right\}\right]\\ \times(1+(\lambda^2-f(n))\,dt)\end{aligned}\tag{A3}$$

from which equation (3) immediately follows.

We prove now formula (6) showing that the expression

$$\exp\left\{-\int_0^t[\lambda^2+N'_s]\,ds+\int_0^t\left(\frac{\lambda^2}{A(N'_s+1)}+N'_sA(N'_s)\right)ds\right\}\left[\left(\prod_{i=1}^{N'_t}A(i)\right)\left(\prod_{i=1}^{n}A(i)\right)^{-1}\right]\tag{A4}$$

is the Radon-Nikodym derivative of the measure of the process N with respect to the process N' (where N and N' are the processes previously defined). It will be sufficient to show that

$$\begin{aligned}p_t(n,m)=\mathbb{E}_{n,0}\left[\!\!\left[\delta(m-N'_t)\exp\left\{-\int_0^t[\lambda^2+N'_s]\,ds+\int_0^t\left(\frac{\lambda^2}{A(N'_s+1)}+N'_sA(N'_s)\right)ds\right\}\right.\right.\\ \left.\left.\times\left[\left(\prod_{i=1}^{N'_t}A(i)\right)\left(\prod_{i=1}^{n}A(i)\right)^{-1}\right]\right]\!\!\right]\end{aligned}\tag{A5}$$

is equal to the transition probability from n to m associated with the process N. The function $\delta(m-n)$ is the usual Kronecker delta. For $t=0$ this is trivially verified; therefore it will be sufficient to show that the expression above satisfies the equation $(d/dt)p_t=Lp_t$, where L is the generator associated with the process N.

The proof is similar to the previous one; we start again by decomposing the trajectories in two parts and we obtain

$$\begin{aligned}p_{t+dt}(n,m)=\mathbb{E}_{n,0}\left(\mathbb{E}_{N'_{dt},dt}\left[\!\!\left[\delta(m-N'_t)\right.\right.\right.\\ \times\exp\left\{-\int_{dt}^{t+dt}[\lambda^2+N'_s]\,ds+\int_{dt}^{t+dt}\left(\frac{\lambda^2}{A(N'_s+1)}+N'_sA(N'_s)\right)ds\right\}\\ \left.\left.\times\left[\left(\prod_{i=1}^{N'_t+dt}A(i)\right)\left(\prod_{i=1}^{N'_{dt}}A(i)\right)^{-1}\right]\right]\!\!\right]\\ \times\exp\left\{-\int_0^{dt}[\lambda^2+N'_s]\,ds+\int_0^{dt}\left(\frac{\lambda^2}{A(N'_s+1)}+N'_sA(N'_s)\right)ds\right\}\\ \left.\times\left[\left(\prod_{i=1}^{N'_{dt}}A(i)\right)\left(\prod_{i=1}^{n}A(i)\right)^{-1}\right]\right).\end{aligned}\tag{A6}$$

In order to compute the first expectation up to the first order in dt we must remember that N'_{dt} equals $n+1$ with probability $\lambda^2\,dt/[A(n+1)]$, equals $n-1$ with probability

$nA(n)\,\mathrm{d}t$ and equals $n+1$ with probability $1-\lambda^2\,\mathrm{d}t/A(n+1)-nA(n)\,\mathrm{d}t$. We easily obtain

$$
\begin{aligned}
p_{t+\mathrm{d}t}(n,m)=&\frac{\lambda^2\,\mathrm{d}t}{A(n+1)}\,p_t(n+1,m)A(n+1)+nA(n)\,\mathrm{d}t\,p_t(n-1,m)/A(n)\\
&+\left(1-\frac{\lambda^2\,\mathrm{d}t}{A(n+1)}-nA(n)\,\mathrm{d}t\right)p_t(n,m)\\
&\times\left(1-\lambda^2\,\mathrm{d}t-n\,\mathrm{d}t+\frac{\lambda^2\,\mathrm{d}t}{A(n+1)}+nA(n)\,\mathrm{d}t\right)
\end{aligned}
\qquad \text{(A7)}
$$

from which the equation $(\mathrm{d}/\mathrm{d}t)p_t=Lp_t$ immediately follows.

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