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The Markov Master Equations and the Fermi Golden Rule

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Abstract

We give a proof that for a large class of systems weakly coupled to heat baths the transition probabilities per unit time obtained from the Markov approximation are equal to those that are calculated using the Fermi golden rule.

1. *Introduction*

There is a well-known formula in the quantum mechanics, the so-called Fermi golden rule (Messiah, 1962), which describes the probability of transition per unit time P_{fi} from the initial state $|i\rangle$ to the final one $|f\rangle$:

$$P_{fi} = 2\pi |\langle f | V | i \rangle|^2 \delta(\epsilon_i - \epsilon_f) \tag{1.1}$$

where the total Hamiltonian of the system has the form

$$H = H_0 + V \tag{1.2}$$

and

$$H_0 | i \rangle = \epsilon_i | i \rangle, \qquad H_0 | f \rangle = \epsilon_f | f \rangle \tag{1.3}$$

The formula (1.1) is often successfully used for the study of relaxation processes (Isihara, 1971). Its derivation based on the perturbation method, however, is unsatisfactory from the mathematical point of view.

A more rigorous derivation of (1.1) is given by Fonda et al. (1975), where the quantum theory of measurements is applied.

On the other hand, the latest rigorous studies (Davies, 1975, 1974, 1976) give us a method of derivation of the Markovian master equations for physical systems weakly coupled to heat baths. In this paper we show that for a large class of such systems the notion of the transition probability per unit time from $|i\rangle$ to $|f\rangle$ has clear meaning and such probabilities are equal to those calculated using formula (1.1).

2. *Physical System Weakly Coupled to a Heat Bath*

We consider a quantum physical system with free Hamiltonian H_S that has pure point spectrum interacting with an infinite system whose Hamiltonian has a continuous spectrum. The total Hamiltonian has the form:

$$H^\lambda = H_S + H_R + \lambda V \tag{2.1}$$

where the interaction term is

$$\lambda V = \lambda S \otimes R \tag{2.2}$$

Here S and R are bounded and self-adjoint operators on the Hilbert spaces of the system and the bath, respectively.

The rigorous derivation of the Markovian master equations is based on the weak coupling limit method developed recently by Davies (1974, 1975, 1976). In that method we examine the convergence of the reduced dynamics in the interaction picture when $\lambda \to 0$ and the rescaled time $\tau = \lambda^2 t$ is introduced:

$$\lim_{\lambda \to 0} \operatorname{tr}_R [e^{iH_0\tau/\lambda^2} e^{-iH^\lambda \tau/\lambda^2} \rho \otimes \sigma_0 e^{iH^\lambda \tau/\lambda^2} \times e^{-iH_0\tau/\lambda^2}] = \Lambda(\tau)\rho, \qquad H_0 = H_S + H_R \tag{2.3}$$

Here, ρ is an arbitrary state of the system, σ_0 is a fixed state of the bath invariant under the free evolution, and tr_R is a partial trace over the bath variables.

The conditions for the existence of the limit dynamics are given in Davies' works (Davies, 1974, Theorems 2.1, 2.2, 2.3). A wide class of models is considered from this point of view and the limit dynamics derived (Davies, 1974; Davies and Eckmann, 1975; Alicki, 1977).

If we assume that $\Lambda(\tau)$ exists, then we have the following equations of motion (Davies, 1974, Theorem 2.1):

$$\frac{d\rho(\tau)}{d\tau} = K^0 \rho(\tau) \tag{2.4}$$

where

$$\rho(\tau) = \Lambda(\tau)\rho, \qquad \rho \in D(K^0) \tag{2.5}$$

$$K^0 = \lim_{t \to \infty} \frac{1}{2t} \int_{-t}^{t} e^{-i\hat{H}_S x} K e^{i\hat{H}_S x}\, dx, \qquad \hat{H}_S = [H_S, \cdot\,] \tag{2.6}$$

$$K\rho = \int_0^\infty dt\, \{-\operatorname{tr}(R_t R \sigma_0) S_t S \rho + \operatorname{tr}(R_t R \sigma_0) S \rho S_t + \operatorname{tr}(R R_t \sigma_0) S_t \rho S - \operatorname{tr}(R R_t \sigma_0) \rho S S_t\} \tag{2.7}$$

and

$$S_t = e^{iH_S t} S e^{-iH_S t}, \qquad R_t = e^{iH_S t} R e^{-iH_S t} \tag{2.8}$$

Making the simple calculations we obtain

$$K^0\rho = \tfrac{1}{2}\sum_{\alpha} D_\alpha\{[A_\alpha, \rho A_\alpha^+] + [A_\alpha\rho, A_\alpha^+]\} + \sum_{\alpha} ih_\alpha[A_\alpha^+A_\alpha, \rho] \quad (2.9)$$

where

$$S_t = \sum_{\alpha} A_\alpha e^{-i\omega_\alpha t}, \qquad \omega_\alpha = \epsilon_n - \epsilon_m \quad (2.10)$$

and

$$\{\epsilon_n\} \text{ are the eigenvalues of } H_S; \quad (2.11)$$

$$D_\alpha = \hat{h}(\omega_\alpha) \equiv \int_{-\infty}^{+\infty} e^{i\omega_\alpha t} h(t)\, dt \quad (2.12)$$

$$h(t) = \mathrm{tr}\,[R_t R \sigma_0] \quad (2.13)$$

$$h_\alpha = Im \int_0^\infty h(t)\, e^{i\omega_\alpha t} dt \quad (2.14)$$

We have also the very useful property

$$K^0 U_t = U_t K^0 \quad (2.15)$$

where

$$U_t = e^{-i\hat{H}_S t} \quad (2.16)$$

The dynamical semigroups generated by (2.9) were studied in detail by Alicki (1976a) for the systems with the finite-dimensional Hilbert spaces and for the special case of N-level atom interacting with the fermion heat bath by Davies (1974).

3. *Pauli Master Equations*

From the property (2.15) it follows that the time evolution given by the generator (2.9) leaves invariant the subset of all density matrices commuting with the Hamiltonian H_S. We can choose an orthonormal base in the Hilbert space of the system to obtain a classical Markov process for the diagonal density matrices. In contrast to Davies' (1974) and Alicki's (1976) work, we do not assume that H_S has nondegenerate eigenvalues. We prove in the Appendix the following theorem.

Theorem 3.1. There exists an orthonormal base $\{|n\rangle\}$ in the Hilbert space $\mathscr{H}_S$ such that

$$H_S|n\rangle = \epsilon_n|n\rangle \quad (3.1)$$

and the set of diagonal density matrices

$$\mathscr{P}_d = \left\{\rho_d \,|\, \rho_d = \sum_n |n\rangle p_n \langle n|; p_n \geqslant 0, \sum_n p_n = 1\right\} \quad (3.2)$$

is invariant under the semigroup $\Lambda(\tau)$.

Moreover, we obtain the classical Markov process of the following form:

$$\frac{dp_n(\tau)}{d\tau} = \sum_m a_{nm}p_m(\tau) - a_{nm}p_n(\tau) \tag{3.3}$$

where

$$a_{nm} = |\langle n\,|S|\,m\rangle|^2\,\hat{h}(\epsilon_m - \epsilon_m) \tag{3.4}$$

The equation (3.3) is the so-called Pauli master equation and the coefficients a_{nm} are the probabilities of transition from the state $|m\rangle$ to the state $|n\rangle$ per unit time in the Markov approximation.

Now we derive the same transition probabilities using the Fermi golden rule. We make formal calculations only, but it can be done in a mathematically rigorous way.

Suppose that the initial state of the composite system has the form

$$|m\rangle \otimes |E,\gamma\rangle \tag{3.5}$$

and the final one

$$|n\rangle \otimes |E',\gamma'\rangle \tag{3.6}$$

where $\{|E,\gamma\rangle\}$ is an orthonormal and complete set of eigenvectors for the Hamiltonian H_R. Then using (1.1) we obtain the transition probability

$$\begin{aligned} P_{m,E,\gamma;n,E',\gamma'} &= 2\pi\lambda^2|\langle m\,|S\,|n\rangle|^2|\langle E,\gamma\,|R\,|\gamma',E'\rangle|^2 \\ &\times \delta(\epsilon_m + E - \epsilon_n - E') \end{aligned} \tag{3.7}$$

We integrate over all final states $|E',\gamma'\rangle$ of the bath and we assume that its initial state is described by the density matrix σ_0, where $\langle E,\gamma\,|\,\sigma_0\,|E',\gamma'\rangle = \sigma_0(E,\gamma) \times \delta(E-E')\delta_{\gamma\gamma'}$.

Then we have

$$\begin{aligned} P_{nm} &= 2\pi\lambda^2|\langle n\,|S\,|m\rangle|^2 \int dE d\gamma \int dE' d\gamma' \sigma_0(E,\gamma) \\ &\times \langle E,\gamma\,|R\,|E',\gamma'\rangle\langle E',\gamma'\,|R\,|E,\gamma\rangle\,\delta(\epsilon_m + E - \epsilon_n - E') \end{aligned} \tag{3.8}$$

Using the following representation of $\delta(x)$

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{itx}\,dt \tag{3.9}$$

we obtain

$$\begin{aligned} P_{nm} &= \lambda^2|\langle n\,|S\,|m\rangle|^2 \int_{-\infty}^{+\infty} dt\, e^{i(\epsilon_m - \epsilon_n)t}\,\mathrm{tr}(\sigma_0 R_t R) \\ &= \lambda^2|\langle n\,|S\,|m\rangle|^2\,\hat{h}(\epsilon_m - \epsilon_n) \end{aligned} \tag{3.10}$$

Introducing the rescaled time $\tau = \lambda^2 t$ we have new transition probabilities per unit time

$$\tilde{P}_{nm} = P_{nm}/\lambda^2 = a_{nm} \tag{3.11}$$

This result can be extended to certain cases where the interaction Hamiltonians have more complicated forms and the operators involved are unbounded.

Appendix: Proof of Theorem 3.1.

We consider the master equation

$$\frac{d\rho}{d\tau} = \frac{1}{2} \sum_{\alpha} D_\alpha \{[A_\alpha, \rho A_\alpha^+] + [A_\alpha \rho, A_\alpha^+]\} \tag{A.1}$$

Let

$$A_\alpha = \sum_{n,k} A_{nk}^\alpha E_{nk} \tag{A.2}$$

where

$$E_{nk} = |n\rangle\langle k| \tag{A.3}$$

and $\{|n\rangle\}$ is an arbitrary base of eigenvectors of H_S. W have also $\rho(\tau) = \Sigma_{r,s}\, \rho_{rs}(\tau) E_{rs}$. Introducing the probability distribution $\{P_j\}$;

$$p_j = \operatorname{tr}[E_{jj}\rho(\tau)] \tag{A.4}$$

we obtain, using (A.1),

$$\frac{dp_j}{d\tau} = \sum_{\alpha,r,s} D_\alpha A_{jr}^\alpha \bar{A}_{js}^\alpha \rho_{rs} - \frac{1}{2} \sum_{\alpha,k,s} D_\alpha A_{kj}^\alpha \bar{A}_{ks}^\alpha \rho_{js} - \frac{1}{2} \sum_{\alpha,k,r} D_\alpha A_{kr}^\alpha \bar{A}_{kj}^\alpha \rho_{kj} \tag{A.5}$$

For every j, α we have a matrix

$$\mathscr{K}^{\alpha,j} = [A_{jr}^\alpha \bar{A}_{js}^\alpha] \tag{A.6}$$

The matrix elements of $\mathscr{K}^{\alpha,j}$ are different from 0 if $\epsilon_r = \epsilon_s$ and $\epsilon_r - \epsilon_j = \epsilon_s - \epsilon_j = \omega_\alpha$ [see (2.10)]. Now, we can introduce the new base $\{|n'\rangle\}$ of eigenvectors which diagonalizes the matrices $\mathscr{K}^{\alpha,j}$. Then we obtain

$$\frac{dp_{j'}}{d\tau} = \sum_{\alpha,j',r'} D_\alpha A_{j'r'}^\alpha \bar{A}_{j'r'}^\alpha p_{r'} - D_\alpha A_{r'j'}^\alpha \bar{A}_{r'j'}^\alpha p_{j'} \tag{A.7}$$

From (2.10) we have $\Sigma_\alpha D_\alpha |A_{j'r'}^\alpha|^2 = |\langle j'|S|r'\rangle|^2\, \hat{h}(\epsilon_{j'} - \epsilon_{r'})$ and this finishes the proof.

References

Alicki, R. (1976). *Reports on Mathematical Physics*, **10**, 249.
Alicki, R. (1977). *Reports on Mathematical Physics*, **11**, 1.
Davies, E. B. (1974). *Communications in Mathematical Physics*, **39**, 91.
Davies, E. B. (1975). *Annales de l'Institut Henri Poincaré*, **BXI**, 265.
Davies, E. B. (1976). *Mathematische Annalen*, **219**, 147.
Davies, E. B., and Eckmann, J. P. (1975). *Helvetica Physica Acta*, **48**, 731.
Fonda, L., Ghirardi, G. C., and Rimini, A. (1975). *Nuovo Cimento*, **25A**, 573.
Isihara, A. (1971). *Statistical Physics*, Academic Press, New York, London.
Messiah, A. (1962). *Quantum Mechanics*, Vol. II, North Holland, Amsterdam.