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くり込まれた指数積公式と量子解析

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1．はじめに

統計物理学およびその他の理論科学においては系統的に近似をあげることが現象の本質を理解するのに極めて重要である。例えば、臨界現象の研究においては、系統的な平均場近似を作ることにより、真の臨界現象に迫ることが可能である。（筆者のコヒーレント異常法[1-3]を参照。）

この講演の目的は時間に依存する指数演算子[4-11]に対する指数積公式の新しい利用法と拡張を説明することである。一般論は文献６を参照してほしい。

2．量子解析と指数積公式

指数演算子の関数を演算子で微分する量子解析（岩波の現代物理学叢書「統計力学」の補章参照）を用いると、高次指数積公式[12-19] を一般的に構築することが容易となる。詳しくは、岩波の現代物理学叢書「経路積分の方法」の第６章を参照して頂きたい。（高次指数積公式の応用に関しては文献[22-26] を参照。）

3．くり込まれた指数積公式に関しては、D.P. Landau et al., の本(Computer Simulation Studies in Condensed Matter Physics, Springer-Verlag, (2002) の原稿の第３節をそのまま利用することに致します。

New Schemes for Self-Consistent Calculations with Applications to the Kohn-Sham Hamiltonian

In order to study the time-dependent behaviour of electrons, we have to solve the following Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(t) = \mathcal{H}(t)\,\psi(t)\;. \tag{3.1}$$

Even for a time-independent Hamiltonian $\mathcal{H} = K + V$ (where K denotes a kinetic energy, and V a potential energy), the Kohn-Sham theory gives an effective time-dependent Hamiltonian

$$\mathcal{H}_{\mathrm{KS}}(t) = K + V_{\mathrm{KS}}(\rho(t)) , \tag{3.2}$$

and

$$\rho(t) = |\psi(t)|^2 , \tag{3.3}$$

and $\psi(t)$ is the solution of the equation

$$i\hbar \frac{\partial}{\partial t} \psi(t) = \mathcal{H}_{\mathrm{KS}}(t)\, \psi(t) . \tag{3.4}$$

Thus, this is a self-consistent equation on the wave function $\psi(t)$ through the equations (3.2) and (3.3).

A sophisticated scheme to sovle this nonlinear Schrödinger equation was proposed by Sugino and Miyamoto[8] using the higher-order Suzuki-Trotter type split method. For details, see their original paper.

In the present paper, we propose a simple systematic higher-order scheme to solve this problem. As was explained in the previous section, the formal solution of Eq. (3.4) is expressed by the time-ordered exponential

$$\begin{aligned} \psi(t) &= \exp_+ \int_{t_0}^{t} \mathcal{H}_{\mathrm{KS}}(s)\, ds \cdot \psi(t_0) \\ &= \exp_+ \int_{t_0}^{t} (K + V(\rho(s)))\, ds \cdot \psi(t_0). \end{aligned} \tag{3.5}$$

This can be approximated by the following product formula

$$\lim_{n\to\infty} u_2(t, t-\Delta t)\, u_2(t-\Delta t, t-2\Delta t) \cdots u_2(t_0+\Delta t, t_0) \cdot \psi(t_0) \tag{3.6}$$

with $\Delta t = (t - t_0)/n$ and

$$u_2(t, t-\Delta t) = \mathrm{e}^{\frac{\Delta t}{2}K} \mathrm{e}^{\Delta t\, V(\rho(t-\Delta t/2))} \mathrm{e}^{\frac{\Delta t}{2}K} \tag{3.7}$$

As was discussed by Sugino and Miyamoto[8], the complication appears here in that the potential V in Eq. (3.7) contains the electron density $\rho(t-\Delta t/2)$ at the time $t-\Delta t/2$. However, we remark here that we do not have to solve this nonlinear equation self-consistently, but that we can solve this equation as follows. The keypoint here for this problem is to note that it is sufficient upto the second order of Δt to calculate $\rho(t-\Delta t/2)$ in Eq. (3.7) upto the *first – order* of Δt, namely

$$\rho(t-\Delta t/2) = |\,U_1(t,t-\Delta t/2)\,\psi(t-\Delta t)|^2 \,. \tag{3.8}$$

Here, $\psi(t-\Delta t)$ should be calculated, at least, upto the first-order of Δt and

$$U_1(t-\Delta t/2) = \mathrm{e}^{\frac{\Delta t}{2}K}\mathrm{e}^{\frac{\Delta t}{2}V(\rho(t-\Delta t))}. \tag{3.9}$$

This procedure can be repeated step by step from the time t_0 to the time t. Thus, this is a new second-order scheme to solve the Kohn-Sham theory. Similarly, the n-th order scheme is constructed using the $(n-1)$-th order density matrix, which can be calculated using the $(n-2)$-th order split formula and so on.

There is another scheme to solve the nonlinear problem by interpreting $\mathcal{H}_{\mathrm{KS}}(\rho(t))$ as a nonlinear maping of $\rho(t)$ with $\rho(t) = |\psi(t)|^2$, as in solving nonlinear dynamics of classical Hamiltonian systems[25,26].

Explicit applications of these new schemes will be published elsewhere.

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