Lagrange Method in Reflection Positivity in the Spin Space

In their Letter [1], Yanagisawa and Shimoi (YS) attempted to apply spin-reflection positivity, which was first used in the Hubbard model by Lieb [2], to the Kondo-Hubbard model at half filling by using the so-called "Lagrangian multiplier method." YS introduced the Lagrange multipliers in the Hamiltonian to realize constraints of single occupancy of fermion for localized spin. Unfortunately, the method of YS is incorrect, and does not form a proof as it is. In this Comment I describe the problems, and how they can be dealt with by modifying their proof.

YS wrote spin $1/2$ operator in the fermion representation and introduced the Lagrange multipliers in the Hamiltonian to realize the constraints of the single occupancy of fermions,

$$H_\lambda = H_0 + \sum_i \lambda_i \mathbf{Q}_i \,, \tag{1}$$

where $\mathbf{Q}_i = n_{i\uparrow} + n_{i\downarrow} - 1$ and $n_{i,\sigma}$ is the number operator for fermion at site i with spin σ $(= \uparrow, \downarrow)$. H_0 is the Hamiltonian for the Hubbard-Kondo lattice model in Ref. [1]. Let $|\Psi\rangle$ be the variational ground state, which is λ_i dependent as in Eq. (1). YS expected that the resulting conditions in the variational principle are $\mathbf{Q}_i|\Psi\rangle = 0$ for all i. The Lagrange multipliers break the spin up-down symmetry under the partial particle-hole transformation [3]: $\mathbf{Q}_i \rightarrow \tilde{\mathbf{Q}}_i = n_{i\uparrow} - n_{i\downarrow}$, although they do not break the symmetry in Eq. (1). This symmetry containing in the transformed Hamiltonian (not the original one) plays an essential role in reflection positivity in the spin space when we investigate the half-filled system. Without this symmetry, we cannot naively assume that the coefficient matrix C for the ground state is Hermitian [2]. YS obviously overlooked this fact and assumed C (for any λ_i) to be Hermitian "because of the up-down symmetry of the spin" [1]. This is only true if we set λ_i to be the (unique) solution of the variational problem. Thus the uniqueness proof of YS must be restricted to the special values of λ_i. Their "proof" for any λ_i, which does not make use of any calculus of variation, is not justified.

By following the procedure in the Lagrange multiplier method correctly, we get

$$\langle\Psi|\mathbf{Q}_i|\Psi\rangle = 0 \,, \tag{2}$$

as the resulting variational condition (or Euler equation), rather than $\mathbf{Q}_i|\Psi\rangle = 0$ as YS expected [1]. The condition [Eq. (2)] is weaker than the desired condition $\mathbf{Q}_i|\Psi\rangle = 0$. Hence the Lagrange multiplier in Eq. (1) does not guarantee the single occupancy condition in general. Fortunately, we can get rid of this problem by the following (somewhat unnatural) argument. Fix λ_i to the solution of the variational problem. Since the ground state of Eq. (1) is proven to be unique and $\mathbf{Q}_i$ commutes with the Hamiltonian, the condition [Eq. (2)] implies the desired one.

I note that YS later presented a "proof" of the equivalence between $\langle\Psi|\mathbf{Q}_i|\Psi\rangle = 0$ and $\mathbf{Q}_i|\Psi\rangle = 0$ in the limit $|\lambda_i| \rightarrow \infty$ [4]. This "proof" is based on an obvious misunderstanding of the Lagrange method, and is incorrect. YS treat λ_i as free parameter that one can choose as one wishes, ignoring the fact that they must be determined by solving the Euler equation simultaneously in the calculus of variations [5].

A correct way to introduce the Lagrange multipliers is to use $\sum_i \lambda_i \mathbf{Q}_i^\dagger \mathbf{Q}_i$ instead of $\sum_i \lambda_i \mathbf{Q}_i$ in Eq. (1). These terms keep the spin up-down symmetry under the partial particle-hole transformation and can realize the desired condition. A more transparent method for proving the uniqueness and positive definiteness of the coefficient matrix C is to choose a suitable set of basis to realize the desired condition as I have done previously [6].

In conclusion, the Lagrange multipliers introduced by YS break the spin up-down symmetry after the partial particle-hole transformation, and cannot realize the physical constraints as YS expected. Their so-called "Lagrangian multipliers method" is incorrect, and must be modified considerably to be a complete proof.

This work was supported by the Alexander von Humboldt foundation of Germany.

Shun-Qing Shen*
Max Planck Institute for Physics of Complex Systems
Bayreuther Str. 40, Haus 16, 01187 Dresden, Germany

Received 26 December 1996 [S0031-9007(97)03886-6]
PACS numbers: 75.30.Mb, 75.20.Hr

*Present address: Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152, Japan.

[1] T. Yanagisawa and Y. Shimoi, Phys. Rev. Lett. **74**, 4939 (1995).
[2] E. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).
[3] H. Shiba, Prog. Theor. Phys. **48**, 217 (1972); V.J. Emery, Phys. Rev. B **14**, 2989 (1976); F.-C. Pu and S.-Q. Shen, Phys. Rev. B **50**, 16 086 (1994).
[4] T. Yanagisawa and Y. Shimoi, Int. J. Mod. Phys. B **10**, 3383 (1996); T. Yanagisawa, J. Phys. Soc. Jpn. **65**, 1930 (1996).
[5] For instance, see I.B. Vapnyarskii, in *Encyclopedia of Mathematics*, p. 336 (Kluwer Academic Publishers, Dordrecht, 1990).
[6] S.-Q. Shen, Phys. Rev. B **53**, 14 252 (1996); **54**, 4397 (1996).

