# COMMENTS

*Comments are short papers which criticize or correct papers of other authors previously published in* **Physical Review B.** *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

## Comment on ''Lagrange-multiplier method in correlated-electron systems: Exact diagonalization study''

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We discuss the Lagrange-multiplier method in a many-body system, and how to apply the Lagrange multiplier correctly to realize quantum constraint in a Hamiltonian for a quantum system. It is pointed out that the discussion in Yanagisawa's paper [Phys. Rev. B **57**, 6208 (1998)] lacks a basic knowledge of mathematics, and that his conclusion is generally wrong. [S0163-1829(99)02720-4]

The Lagrange-multiplier method is often used to minimize a function with a condition. In quantum many-body physics it is also applied to realize some quantum constraint when we treat the Schrödinger equation or the Hamiltonian of a quantum system. A famous example is the use of the chemical potential in a Hamiltonian of a many-body quantum system to adjust the number of particles in grand canonical ensembles. Although the method is well established, there still exists some misunderstanding of its application. In his recent paper, Yanagisawa investigated the Lagrange-multiplier method in quantum systems by an exact diagonalization study[1] (referred to as Ref. 1 in this Comment). His discussion is based on a misunderstanding of the method, and lacks a rigorous mathematics basis. His work also contains some responses to my recent comment on his previous work.[2] In this Comment, I clarify several problems and make a response to his comment on how to introduce Lagrange multipliers into a Hamiltonian correctly.

To compare with Yanagisawa's work, I use the same notations in this Comment as in Ref. 1. A Schrödinger equation with quantum constraint(s) is written as

$$H|\Psi\rangle = E|\Psi\rangle, \tag{1}$$

$$Q_i|\Psi\rangle = 0, \quad (i=1,\ldots,M), \tag{2}$$

where $H$ is the Hamiltonian, $E$ is the eigenvalue, $|\Psi\rangle$ is the wave function, and $Q_i$ is the operator for the constraints. In order to solve Eqs. (1) and (2), we can introduce the Lagrange multipliers to form a generalized Hamiltonian to realize the quantum constraints in Eq. (2).

(1) *The Lagrange multiplier* $\lambda_i Q_i$: One way to introduce the Lagrange multiplier is to generalize the Hamiltonian in Eq. (1) to

$$H_{L1} = H + \sum_{i=1}^{M} \lambda_i Q_i \tag{3}$$

to replace the $M$ constraints [Eq. (2)]. It is expected that the constraint could be realized by minimizing the expectation energy with respect to the Lagrange multipliers $\lambda_i$:

$$\frac{\delta}{\delta \lambda_i}\langle\Psi|H_{L1}|\Psi\rangle = 0. \tag{4}$$

The resulting equations are

$$\left(H + \sum_i \lambda_i Q_i\right)|\Psi\rangle = E|\Psi\rangle, \tag{5}$$

$$\langle\Psi|Q_i|\Psi\rangle = 0, \quad (j=1,\ldots,M). \tag{6}$$

From the notations, we should note the differences between Eqs. (2) and (6): the averages of $Q_i$ in the state $|\Psi\rangle$ replace the original equations. Generally speaking, Eqs. (6) are weaker than Eqs. (2). They are not equivalent except for some special cases. For example, if $Q_i$ is semipositive definite, the Lagrange multipliers can realize the constraints because, in this case, Eqs. (6) are equivalent to Eqs. (2). Another available case is that if we consider only the ground-state properties and know that the ground state is nondegenerate, Equations. (2) and (6) are also equivalent. However, we cannot use this if we want to prove the nondegeneracy of the ground state of a system.

(2) *The Lagrange multiplier* $\lambda_i Q_i^\dagger Q_i$: If $Q_i$ are not semipositive definite, or we have to consider the complete set of solutions, the introduction of the Lagrange multipliers in Eq. (3) usually enlarges the Hilbert space. $H_{L1}$ are usually no longer equivalent to the original problem. Some unexpected solutions may exist in Eqs. (5) and (6). Hence the Lagrange multipliers cannot realize the constraints as expected. To this end one of the correct ways to introduce the Lagrange multiplier to realize the quantum constraint is to use $\lambda_i Q_i^\dagger Q_i$ instead of $\lambda_i Q_i$ in Eq. (3):

 

$$H_{L2}=H+\sum_i \lambda_i Q_i^\dagger Q_i, \tag{7}$$

which was, to my best knowledge, first proposed in my paper.[2] (Reference 1 did not mention any reference, while the method was commented upon.) The resulting conditions are

$$\langle\Psi|Q_i^\dagger Q_i|\Psi\rangle=0 \tag{8}$$

instead of Eqs. (6). Due to the semipositive definiteness of $Q_i^\dagger Q_i$, the conditions are reduced to Eqs. (2). This proves that the problem of $H_{L2}$ is equivalent to the original problem. Mathematically, it also proves the validity of the method in Eq. (7). Generally speaking, any mathematical transformation should guarantee that the transformed problem is equivalent to the original problem. However, it is anticipated that the transformed problem could be treated in a simpler way. If the transformed problem is not equivalent to the original one, it is hard to justify the transformation.

Reference 1 proposed that square terms cannot be used in a real analysis. This is not true. Consider the same problem in Ref. 1; i.e., minimizing $x^2+y^2$ under the condition $x+y=1$, the function with a Lagrange multiplier is

$$f(x,y,\lambda)=x^2+y^2-\lambda(x+y-1)^2. \tag{9}$$

Based on the variational principle we have $x=y=\frac{1}{2}$ and $\lambda=+\infty$ with $\lambda(x+y-1)=\frac{1}{2}$. It is apparent that Ref. 1 neglected this set of solutions. The same minimum of $x^2+y^2$ is obtained as in the usual way. $\lambda$ is determined by the Euler equations. If we assume that $\lambda$ is purely imaginary here, we cannot find a solution no matter which way we introduce the Lagrange multiplier.[3] It is worth emphasizing that whether $\lambda_i$ are complex or imaginary is a pseudoscientific problem. From the principle of mathematics, $\lambda_i$ must be determined by solving the resulting equations simultaneously. In the quantum system we discussed, the expectation value of $H$ is energy, which should be real. The author of Ref. 1 performed an exact diagonalization for a finite system by setting $\lambda_i$ imaginary. It should be noted how to compare a real eigenvalue with a complex one. We cannot say simply that the state with the lowest real part of the eigenvalue is the ground state. Thus the data listed in Tables I and II in Ref. 1 do not make sense.

(3) *A two-site example*: To compare the results of the two ways to introduce the Lagrange multiplier, let us re-examine the two-site $S=\frac{1}{2}$ Heisenberg model,

$$H_1=\mathbf{S}_1\cdot\mathbf{S}_2. \tag{10}$$

There are four eigenstates of $H_1$: one is the spin singlet state with $E=-\frac{3}{4}$, and others are the spin triplet with $E=\frac{1}{4}$. In order to justify the different Lagrange-multiplier methods, we solve the problem in the fermion representation, where the single occupancy of a fermion on a site is expected to be realized by the Lagrange multiplier. The spin operator can be expressed in terms of the fermion operator c,

$$\mathbf{S}_i^+=c_{i,\uparrow}^\dagger c_{i,\downarrow}, \tag{11}$$

$$\mathbf{S}_i^-=c_{i,\downarrow}^\dagger c_{i,\uparrow}, \tag{12}$$

$$\mathbf{S}_i^z=\tfrac{1}{2}(n_{i,\uparrow}-n_{i,\downarrow}), \tag{13}$$

with the constraints of single occupancy,

$$(n_{i,\uparrow}+n_{i,\downarrow}-1)|\Psi\rangle=0. \tag{14}$$

$n_{i,\sigma}=c_{i,\sigma}^\dagger c_{i,\sigma}$ $(\sigma=\uparrow,\downarrow)$. Usually the quantum constraint is very difficult to realize. If we introduce the Lagrange multiplier as in Ref. 1,

$$H_2=\tfrac{1}{2}(c_{1,\uparrow}^\dagger c_{1,\downarrow}c_{2,\downarrow}^\dagger c_{2,\uparrow}+c_{1,\downarrow}^\dagger c_{1,\uparrow}c_{2,\uparrow}^\dagger c_{2,\downarrow})+\frac{1}{4}(n_{1,\uparrow}-n_{1,\downarrow})\times(n_{2,\uparrow}-n_{2,\downarrow})+\sum_{i=1,2}\lambda_i(n_{i,\uparrow}+n_{i,\downarrow}-1), \tag{15}$$

the physical space has been enlarged so that the condition of single occupancy is replaced by

$$\langle\Psi|(n_{i,\uparrow}+n_{i,\downarrow}-1)|\Psi\rangle=0. \tag{16}$$

In the case the number of particle per site is no longer always equal to 1, and will be determined by the Schrödinger equation of $H_2$ and the condition of Eq. (16). The condition cannot guarantee single occupancy. For example, a local state

$$|\phi_i\rangle=\frac{1}{\sqrt{2}}(1-c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger)|0\rangle,$$

consisting of empty and double occupancies, satisfies the condition

$$\langle\phi_i|(n_{i,\uparrow}+n_{i,\downarrow})|\phi_i\rangle=1,$$

where $|0\rangle$ is the vacuum state.

If we focus on a fixed number of particle, say 2, and the $z$ component of total spin 0, the wave function is

$$\Psi=(ac_{1,\uparrow}^\dagger c_{2,\downarrow}^\dagger+cc_{2,\uparrow}^\dagger c_{1,\downarrow}^\dagger+bc_{1,\uparrow}^\dagger c_{1,\downarrow}^\dagger+dc_{2,\uparrow}^\dagger c_{2,\downarrow}^\dagger)|0\rangle. \tag{17}$$

From Eq. (16), we have $|b|=|d|$. There are two sets of solutions: (1) $E=-\frac{3}{4}$ with $a=c\neq 0$ and $b=d=0$, and $E=\frac{1}{4}$ with $a=-c\neq 0$ and $b=d=0$. The two $\lambda_i$'s can be any finite values. These two solutions correspond to the two states with total spin 0 and 1. (2) $E=0$ with $a=c=0$, $b=\pm d$, and $\lambda_1=\lambda_2$. Solutions (2) satisfy the condition [Eq. (16)], but do not satisfy the condition of the single occupancy. These two states do not exist in the original Heisenberg model. This illustrates that the Lagrange multipliers in Eq. (15) do not realize the single occupancy, as expected. It enlarges the physical space, and some unphysical states are included.

If we introduce the Lagrange multipliers $\lambda_i(n_{i,\uparrow}+n_{i,\downarrow}-1)^2$ in Eq. (15) instead of $\lambda_i(n_{i,\uparrow}+n_{i,\downarrow}-1)$,

$$H_3=\frac{1}{2}(c_{1,\uparrow}^\dagger c_{1,\downarrow}c_{2,\downarrow}^\dagger c_{2,\uparrow}+c_{1,\downarrow}^\dagger c_{1,\uparrow}c_{2,\uparrow}^\dagger c_{2,\downarrow})+\frac{1}{4}(n_{1,\uparrow}-n_{1,\downarrow})\times(n_{2,\uparrow}-n_{2,\downarrow})+\sum_{i=1,2}\lambda_i(n_{i,\uparrow}+n_{i,\downarrow}-1)^2, \tag{18}$$

we have the solutions $E=-\frac{3}{4}$ with $a=c\neq 0$ and $b=d=0$, and $E=\frac{1}{4}$ with $a=-c\neq 0$ and $b=d=0$. The two $\lambda_i$'s can be

any finite values. These are the two physical states. The other two unphysical states are excluded spontaneously.

Comparison of the results of this simple example clearly illustrates that the two ways to introduce the Lagrange multipliers will lead to different results. $H_2$ in Eq. (15) contains two unphysical states that $H_1$ in Eq. (10) does not. Hence we cannot say that the Lagrange multiplier in Eq. (15) is correct. Although some other conditions can be used to exclude the unphysical states for a few-body system, those conditions are neither attached to the method itself nor have a solid mathematical foundation. They have gone beyond the method itself. It is common sense that a conclusion drawn from a concrete example cannot be naively extended to a general case without a solid mathematical foundation, especially when we discuss a general method.

(4) *Compatible* $H$ and $Q_i$: When $Q_i$ are not semipositive definite, but all $Q_i$ and $H$ are compatible, i.e., $[H,Q_i]=0$ and $[Q_i,Q_j]=0$, are Eqs. (1) and (2) equivalent to Eqs. (5) and (6)? The two-site problem we just discussed has given a negative answer. It is well known that two compatible operators can be diagonalized simultaneously, but this does not mean that eigenstates of $H$ are always the eigenstates of $Q_i$. Assume $|\psi_1\rangle$ and $|\psi_2\rangle$, two eigenstates of $H$ with energy eigenvalues $E_1$ and $E_2$. From the commutators of $H$ and $Q_i$, we obtain

$$\langle\psi_1|[H,Q_i]|\psi_2\rangle=(E_1-E_2)\langle\psi_1|Q_i|\psi_2\rangle=0. \qquad (19)$$

If $E_1\neq E_2$, $\langle\psi_1|Q_i|\psi_2\rangle$ must be zero. But if $E_1=E_2$, $\langle\psi_1|Q_i|\psi_2\rangle$ can be nonzero. Therefore, if all eigenstates of $H$ are nondegenerate, the eigenstates of $H$ are automatically the eigenstates of $Q_i$. In this case the Lagrange multipliers in Eq. (3) can realize the constraints in Eq. (2). However, if part of the eigenstates of $H$ are degenerate, the eigenstates of $H$ are no longer always the eigenstates of $Q_i$. Thus Eqs. (1) and (2) are not equivalent to Eqs. (4) and (5). The latter can contain more solutions that do not appear in Eqs. (1) and (2). In the example of a two-site problem, the Hamiltonian in Eq. (7) has two unphysical states which are degenerate. That is why we have two unphysical solutions in the example. Therefore, the compatible properties of $H$ and $Q_i$ do not guarantee that the Lagrange multipliers in Eq. (3) can realize the constraints.

Although we can justify very easily whether the $Q_i$ operators are semipositive definite, it is extremely difficult to determine whether the eigenstates of $H$ for a many-body system are nondegenerate or not. Especially when we want to prove the nondegeneracy of the ground state of a Hamiltonian (see references in Ref. 2), $\lambda_i Q_i$ is not a correct way to realize the quantum constraints. In many-body physics, there are many examples to introduce the Lagrange multipliers. One of the most famous examples in a many-body systems is the chemical potential to adjust the number of particles. In a grand canonical ensemble the dispersion of the particle numbers

$$\langle(\Delta N)^2\rangle=\langle N^2\rangle-(\langle N\rangle)^2\propto\langle N\rangle.$$

This is acceptable, or reasonable, since the relative dispersion $\sqrt{\langle(\Delta N)^2\rangle}/\langle N\rangle$ approaches zero in the thermodynamic limit. In a quantum many-body system, for example, the spin-$\frac{1}{2}$ Heisenberg model in the fermion representation, it is quite difficult to realize the condition of single occupancy of a fermion at each lattice site. On the Lagrange multipliers $\lambda_i Q_i^\dagger Q_i$ we have taken into account the strong correlations between particles. How to make approximation to treat the multipliers goes beyond the scope of this Comment. When we introduce one type of Lagrange multiplier, at least we should guarantee that the method is correct for a solvable case before we make other approximations such as a mean-field approximation.

## ACKNOWLEDGMENT

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[1] T. Yanagisawa, Phys. Rev. B **57**, 6208 (1998).
[2] S. Q. Shen, Phys. Rev. Lett. **79**, 1781 (1997).
[3] Since the condition $x+y-1=0$ is absolutely equal to the condition $(x+y-1)^2=0$, it is not strange that we obtain the same result in two different ways.