Spin-charge decoupling and orthofermi quantum statistics

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(Received 26 July 2000; published 12 March 2001)

Currently Gutzwiller projection technique and nested Bethe ansatz are two main methods used to handle electronic systems in the U infinity limit. We demonstrate that these two approaches describe two distinct physical systems. In the nested Bethe ansatz solutions, there is a decoupling between the spin and charge degrees of freedom. Such a decoupling is absent in the Gutzwiller projection technique. Whereas in the Gutzwiller approach, the usual antisymmetry of space and spin coordinates is maintained, we show that the Bethe ansatz wave function is compatible with a form of quantum statistics, viz., orthofermi statistics. In these statistics, the wave function is antisymmetric in spatial coordinates alone. This feature ultimately leads to spin-charge decoupling.

DOI: 10.1103/PhysRevB.63.132405 PACS number(s): 75.10.Jm, 05.30.Pr

We had earlier envisaged a quantum system of spin-half particles obeying a new exclusion principle, viz., an orbital state should not contain more than one particle, whether spin up or spin down.[1] This modified exclusion principle is more restrictive than Pauli's principle, which allows two electrons having opposite spin to occupy the same orbital state. When the Coulomb interaction U between two such electrons tends to infinity, the resulting system naturally satisfies the new exclusion principle (NEP).

In the present paper, we consider the physical consequences of such a singular potential on a system of electrons. In particular, we show that in the limit of $U\rightarrow\infty$, there exists a possibility that the antisymmetry under the simultaneous exchange of spatial and spin coordinates in an electronic wave function may be violated. Instead, the antisymmetry is valid only with respect to the spatial coordinates, whereas no symmetry is *a priori* imposed on the spin component of a multiparticle wave function. Next we elucidate how this new symmetry of the wave function ultimately leads to (i) a form of quantum statistics, namely, orthofermi statistics,[1–3] and (ii) a concept of spin-charge decoupling proposed in the context of high-temperature superconductivity.[4–7] We also provide a critical comparison of our results with the existing algebraic approaches to the U infinity problem.

Both Pauli's exclusion principle and the NEP can be formulated in terms of particle creation operator $c^{\dagger}$. Given an orbital index i, and spin indices σ, $\overline{\sigma}$, the former is expressed as

$$c^{\dagger}_{i\alpha}c^{\dagger}_{i\alpha}=0, \quad (\alpha=\sigma \text{ or } \overline{\sigma}). \tag{1}$$

The more exclusive NEP satisfies

$$c^{\dagger}_{i\alpha}c^{\dagger}_{i\beta}=0, \quad (\alpha,\beta=\sigma \text{ or } \overline{\sigma}). \tag{2}$$

The relation (2) completely takes into account the local effect of the intraorbital infinite Coulomb potential, and leads to an alteration in the conventional fermionic Fock or state space.

It is pertinent here to ask whether (i) the U infinity constraint has any possible nonlocal manifestation, and (ii) it is possible to describe such a system consistently through appropriate commutation relations involving particle creation and annihilation operators. Concerning the first query, we note that the earlier-mentioned modified symmetry property of the wave function reflects the nonlocal consequence of the U infinity limit. The answer to the second question is also in the affirmative. In fact consistent with the NEP, two independent sets of commutation relations, valid for any spatial dimension, can be constructed.[1]

The first set of the commutation relations (CRI) is

$$c_{i\alpha}c_{j\beta}+(1-\delta_{ij})c_{j\beta}c_{i\alpha}=0, \tag{3}$$

$$c_{i\alpha}c^{\dagger}_{j\beta}+(1-\delta_{ij})c^{\dagger}_{j\beta}c_{i\alpha}=\delta_{ij}\delta_{\alpha\beta}\left(1-\sum_{\gamma} c^{\dagger}_{i\gamma}c_{i\gamma}\right). \tag{4}$$

The second set of commutation relations (CRII) is

$$c_{i\alpha}c_{j\beta}+c_{j\alpha}c_{i\beta}=0, \tag{5}$$

$$c_{i\alpha}c^{\dagger}_{j\beta}=\delta_{\alpha\beta}\left(\delta_{ij}-\sum_{\gamma} c^{\dagger}_{j\gamma}c_{i\gamma}\right). \tag{6}$$

Using either set of commutation relations independently, it can be shown that the only permissible states associated with an orbital index i are $|0\rangle$, $|1_{i\sigma}\rangle$, and $|1_{i\overline{\sigma}}\rangle$. The states $\{|1_{i\alpha}1_{i\beta}\rangle\}$ are always null states. Thus both sets of commutation relations are compatible with the NEP. Now a system of electrons subject to the $U\rightarrow\infty$ constraint cannot be described through two distinct types of commutation relations. But before taking up this important aspect of the problem, we consider salient features as well as the critical differences between the two algebras. This step would also help us in determining the correct set of commutation relations.

The CRI is not invariant under the unitary transformation

$$d_{i\alpha}=\sum_{j} U_{ij}c_{j\alpha}; \quad UU^{\dagger}=U^{\dagger}U=1. \tag{7}$$

As a consequence, it is not preserved under a change in representation. This contrasts with the usual fermionic anticommutation relations which are representation invariant.

The CRI is invariant under the phase transformation

$$e_{i\alpha}=e^{i\phi_{i\alpha}}c_{i\alpha}. \tag{8}$$

Therefore, the particle number operator $N_{i\alpha}$ exists. Next, the commutation relation (3) signifies the antisymmetry when both spatial and spin coordinates are simultaneously exchanged. We note that both these features are valid for the usual fermions too.

The overall antisymmetry prevents the spin-charge decoupling when the number of particles N exceeds 2. This is true for the particles obeying CRI as well as for canonical fermions. In fact for an N particle system having M down spins, the spatial and spin part of the wave function, respectively, satisfy conjugate symmetries $[2^K 1^{N-2K}]$ and $[N-K,K]$, $0 \leqslant K \leqslant M$.[8] In this case, the associated wave function cannot be represented as a product of the Slater determinant corresponding to spinless fermions multiplied by a spin-wave function, or a superposition of such states, unless $N \leqslant 2$ or $K=0$.

The CRII is invariant under the unitary transformation (7), and hence it is representation invariant. But the relations in CRII are not invariant under the phase transformation (8) involving both indices i and α. These are invariant only with respect to the following phase transformations:

$$h_{i\alpha}=e^{i\phi_i}c_{i\alpha}; \quad l_{i\alpha}=e^{i\phi_\alpha}c_{i\alpha}. \tag{9}$$

Consequently only number operators N_i and N_α exist, but not the number operator $N_{i\alpha}$. We note here that it is the relation (5) in CRII that decouples the spatial and spin coordinates. It is this decoupling that prevents us from mapping i and α to a single index—a mapping that is possible for usual fermions and in CRI. Therefore, we cannot define $N_{i\alpha}$ with composite index $i\alpha$. Only the number operators N_i and N_α are allowed.

The commutation relation (5) implies that a state vector is antisymmetric only when the spatial indices i and j are exchanged, whereas states having different permutations of σ and $\overline{\sigma}$ are independent, orthonormal states. It may be noted here that as far as the spin variables are concerned, a similar situation arises in Greenberg's infinite statistics.[9,10] The only difference is that in infinite statistics, the range of index α is unrestricted, whereas in the present context, α can take only two values, viz., σ and $\overline{\sigma}$.

To summarize, the quanta characterized by CRII satisfy Fermi-Dirac statistics with respect to spatial coordinates, and infinite statistics with regard to the spin variable. Even though no *a priori* symmetry restriction is imposed on the spin variables, it is always possible to construct states that are an eigenfunction of a given spin Hamiltonian. To achieve this, one has to take an appropriate superposition of states constructed through strings of creation operators acting on the unique vacuum state $|0\rangle$.

We have termed the statistics associated with the CRII as orthofermi statistics. This represents an instance wherein quanta having composite statistical character (viz., indices belonging to different classes exhibit uncorrelated permutation properties) is proposed.

The above discussion makes it clear that the CRI and CRII describe two fundamentally distinct physical systems.

Algebraic relations similar to the CRI have been reported earlier in the context of Gutzwiller projection[11] and Hubbard operators.[12–14] But problems exist with these earlier constructions. The algebra satisfied by the Gutzwiller projection operator is not closed, as shown in Ref. 1. On the other hand, Hubbard operators are local in nature,[14] and additional postulates are needed to obtain their multisite relations.[1] These problems do not arise in the CRI.

In the context of CRII, the quantum-mechanical problem associated with a system of electrons in one dimension, mutually interacting with delta-function potential having weight U, can be mentioned. This problem has been exactly solved using the nested Bethe ansatz (NBA) by Yang.[15] The NBA uses Bethe ansatz twice—once for the charge (or spatial) degree of freedom, and thereafter for the spin component. The solution for the discrete version of this problem, namely the one-dimensional (1D) Hubbard Hamiltonian has been given by Lieb and Wu.[16] The $U\to\infty$ limit of the 1D Hubbard Hamiltonian has been considered by Ogata and Shiba.[4,5] In their work, the U is taken to be infinity while calculating the spatial component of the wave function. The ensuing wave function is a Slater determinant describing noninteracting spinless fermions. As for the spin part, U is not exactly infinity in the sense that terms up to the order of t^2/U are retained. This is equivalent to effectively replacing the Hubbard Hamiltonian by the t-J Hamiltonian where $J=4t^2/U$.[4–6] The complete wave function is a product of a Slater determinant involving only the spatial variables multiplied by a spin wave function, which is the exact solution of the 1D Heisenberg Hamiltonian. It may be mentioned here that if U is put exactly as infinity in the sense that $J=0$, all possible 2^N spin configurations become degenerate. Retaining a J as $4t^2/U$ removes this degeneracy.[6] However, the symmetry properties of the spin degree of freedom remains the same whether $J=0$ or is finite.

It has been also mentioned in the literature that instead of using complicated NBA, this wave function can be obtained directly through simple physical arguments.[5,6] The three main characteristics of the wave function are as follows.

(1) Decoupling occurs between space and spin components.

(2) The spatial part of the wave function is antisymmetric when two spatial coordinates are exchanged. It vanishes when any two coordinates coincide.

(3) Because of the factorization or decoupling between the space and spin parts, it is no longer possible to specify whether a particle with a given spatial coordinate also has a definite spin σ or $\overline{\sigma}$, and vice versa. As a result, the number operator $N_{i\alpha}$ with composite index $i\alpha$ cannot be defined.

These features of the wave function are valid both for the half-filled and less than half-filled cases. That the factorization of the wave function constitutes a remarkable result has been earlier highlighted by Fulde.[6]

We have shown earlier[1] that the orthofermions characterized by CRII possess all of the above three characteristics.

We may also clarify why in the $U\to\infty$ limit, the symmetry property of the wave function gets altered only in the NBA, and not in the Gutzwiller projection technique. In the conventional approach, the symmetry property of the wave function (and hence the statistics of the system) is *a priori* postulated. Starting with a given eigenfunction, the corresponding wave function having a particular symmetry is obtained through appropriate usage of permutation operators. For example, for a three-particle boson system, we can start with the state $\psi(1,2,3)$, and get the symmetric state using the following symmetrizer:

$$\psi_s(1,2,3)=\{I+P(12)+P(13)+P(23)+P(123)+P(132)\}\psi(1,2,3). \tag{10}$$

We note that in this process of generating the wave function of a particular symmetry type, permutation operators are never scaled by any dynamical variable.

In the NBA, one starts with the wave function in a particular ordered configuration.[4,15,16] Next, in order to generate the wave function (of a required symmetry type) over the entire configuration space, we use permutation operators and suitable boundary conditions. In this process, the permutation operators get scaled by the dynamical variables t and U. And this is quite a nontrivial feature. We note that this scaling is absent when $U=0$, and the corresponding situation is similar to the one depicted in Eq. (10). On the other hand, when we take the U infinity limit, the permutation operators linking the one sector to another (or exchanging the particles residing in the adjacent sectors), according to the desired symmetry requirement, become redundant. To make these points more explicit, we consider the wave function given in Refs. 4 and 16. The amplitude in the wave function, when down spins are located at the sites $x_1,\ldots,x_M$ and up spins at $x_{M+1},\ldots,x_N$, is given as

$$f(x_1,\ldots,x_N)=\sum_P [Q,P]\exp\left(i\sum_{j=1}^{N} k_{Pj}x_{Qj}\right), \tag{11}$$

where $P=(P1,P2,...,PN)$ and $Q=(Q1,Q2,...,QN)$ are two permutations of $(1,2,...,N)$ and f is given in the sector $x_{Q1}<x_{O2}<\ldots<x_{QN}$. The $[Q,P]$ are determined by the relation

$$[Q,P]=Y_{nm}^{i,i+1}[Q,P'], \tag{12}$$

where $P=(P1,P2,...,Pi=m,P(i+1)=n,\ldots,PN)$ and $P'=(P1,P2,...,n,m,\ldots,PN)$,

$$Y_{mn}^{i,i+1}=\frac{P_{i,i+1}-x_{nm}}{1+x_{nm}}, \tag{13}$$

$$x_{nm}=i(U/2)/(t\sin k_n-t\sin k_m). \tag{14}$$

$P_{i,i+1}$ is a permutation operator for the interchange between Qi and $Q(i+1)$ and for an N particle system, it admits an appropriate $N\times N$ matrix representation of the symmetry group S_N.[8,15] It may be noted here that the amplitude in the wave function is in fact the wave function in coordinate representation.[15]

In Eq. (13), if we take antisymmetric representation for $P_{i,i+1}$, then $P_{i,i+1}[Q,P']=-[Q,P']$ and hence $[Q,P]=-[Q,P']$ follows from Eq. (12). Note that this result is not valid for any other representation for $P_{i,i+1}$ when U is either zero or finite. But in case U is taken to be infinity in Eq. (13), $[Q,P]=-[Q,P']$ always holds true, irrespective of the representation of $P_{i,i+1}$. It is this peculiar limiting behavior of the operator Y that is responsible for the spin-charge decoupling in the U infinity limit, and subsequently gives rise to spinless fermions.

In the Gutzwiller projection technique, on the other hand, we start with antisymmetric wave functions. These wave functions are constructed analogous to Eq. (10), but they use an antisymmetrizer in place of a symmetrizer operator. In fact the wave function is a Slater determinant built from the Bloch states of electrons on a lattice, and the U infinity constraint is then implemented through the projection operator $\Pi_i(1-n_{i\sigma}n_{i\bar{\sigma}})$.[6] Note that in this process of constructing the wave function, the permutation operators never get scaled by U or t. Also the original fermionic antisymmetry now remains intact.

It would be instructive here to consider the particular case of NBA when the U infinity limit is taken for both spatial and spin components. It has been often argued that in this situation, electrons cannot exchange their positions within the 1D chain.[5,6] But a closer examination reveals that the antisymmetry associated with the spatial part of the wave function allows us to exchange the spatial coordinates of the electrons. Similarly, a finite J term implies that spin coordinates can also be permuted. However when $J=0$ $(U=\infty)$, it may appear that the spin sequence gets frozen to its initial order. If this is true, then the decoupled spin component of the system would satisfy the ''null statistics.''[17] Also the earlier statement that the electrons cannot exchange their positions within the chain has to be modified to read, ''the spatial coordinates can be exchanged in the 1D chain, but not the spin coordinates.''

Irrespective of the above discussion, we ought to demand that even when $J=0$, the wave function is still an eigenfunction of the total S^2 and S_z operators. Consequently, for a given set of spatial coordinates and with S_z being $(N-2M)/2$, all the spin configurations, classified according to $\{[N-K,K],\ 0\leqslant K\leqslant M\}$ symmetries, are accessible. On the other hand, in the case of frozen spin order, only one spin configuration is allowed for a given set of spatial coordinates and a given value of S_z.

We have already highlighted the important distinction between CRI and CRII. Next, the $U=\infty$ case of the Hubbard Hamiltonian, i.e.,

$$H=t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma} \tag{15}$$

can be taken as a typical example to show how these commutation relations lead to different types of dynamical evolution. We consider the time evolution equation for $c_{i\sigma}$, which is needed to evaluate single-particle Green's function or correlation function. In the case where $c^{\dagger}$, c satisfy CRII,

$$i\dot{c}s_{i\sigma}=t\sum_j c_{j\sigma}, \tag{16}$$

where $\dot{c}_{i\sigma}$ is the time derivative of $c_{i\sigma}$. The presence of single annihilation operators on the right-hand side implies that the system remains in the original operator space $\{c_{i\sigma}\}$

and its dual $\{c^{\dagger}_{i\sigma}\}$. Consequently, the Hamiltonian is exactly solvable, a feature compatible with the NBA case.

If $c^{\dagger},c$ obey the CRI,

$$i\dot{c}_{i\sigma}=t\sum_{j}\{c_{j\sigma}-c^{\dagger}_{i\bar{\sigma}}c_{i\bar{\sigma}}c_{j\sigma}+c^{\dagger}_{i\bar{\sigma}}c_{i\sigma}c_{j\bar{\sigma}}\}. \tag{17}$$

The presence of a triple operator product in the above equation implies no closure in the equation of the motion chain. Thus an exact solution cannot be obtained in this case; appropriate truncations or projections are needed to arrive at approximate solutions.[14]

By seeking the mutual consistency between (i) the conjugate permutation symmetries associated with the spatial and spin components of the wave function of usual fermions, and (ii) the U infinity constraint, it is possible to provide a more transparent physical argument for the validity of orthofermi statistics and Bethe ansatz solutions and the ensuing spin-charge decoupling. For definiteness we consider the continuum case and take $N>2$. The U infinity constraint demands that all multiparticle wave functions must vanish when the spatial coordinates of any two particles coincide.

$$\psi(x_1,x_2\ldots,x_i\ldots x_j\ldots x_N,\alpha_1,\alpha_2\ldots,\alpha_N)\rightarrow 0 \quad \text{as } x_i\rightarrow x_j \text{ for any } \{i,j\}, \tag{18}$$

otherwise the energy of the system diverges. This is true for any number of dimensions. As noted earlier, for a N electron system having M down spins, the respective permutation symmetries for spatial and spin parts of the wave function are[8,15] $[2^K1^{N-2K}]$ and $[N-K,K]$; $0\leqslant K\leqslant M$. Now to be consistent with the U infinity case, we should retain only those wave functions that have a node when any two position coordinates coincide, and remove all others that do not have such nodes. Accordingly, the only permissible spatial wave function corresponds to $[1^N]$ symmetry, i.e., the $K=0$ case. All other wave functions corresponding to finite K and $N>2$ do not possess required nodes. Also the spatial and spin coordinates are not decoupled for the wave functions characterized by mixed-symmetry representations. If we demand total antisymmetry including the spatial and spin parts, only allowed spin configuration corresponds to the conjugate symmetry $[N]$. Though one is able to achieve spin-charge decoupling in this case, the dimension of the state space stands greatly reduced. Now only symmetric spin configuration is permissible. If we stipulate that all eigenfunctions of S^2 and S_z are permissible, then every 2^N spin configuration, classified according to $\{[N-K,K]\}$ symmetries, is allowed. But all these spin configurations are coupled with the same spatial configuration $[1^N]$, and not with the conjugate spatial configuration $[2^K1^{N-2K}]$. It is this $[1^N][N-K,K]$ symmetry of the permissible wave function that leads to the spin-charge decoupling. The CRII for the orthofermions obviously reflects this property of the wave function at kinematic level.

To conclude, we have considered two sets of commutation relations (CRI and CRII) compatible with the ‘‘no double occupancy in a single orbital’’ constraint for spin-half particles. The subsequent analysis brings out the distinctive features of CRI and CRII, both at the level of kinematics and dynamics, and highlights the possibility of a violation of fermionic antisymmetry in the present context. Since Gutzwiller projection technique is closer to CRI, and the nested Bethe ansatz to CRII, we conclude that these two widely used approaches to model the U infinity constraint lead to quite different physical consequences. In fact, they describe two distinct physical systems. We have finally provided the reasons why electrons in U infinity limit may behave like orthofermions described by the CRII leading to a spin-charge decoupling, and have supported our analysis through a comparison with the exact NBA solutions.

I am grateful to Professor P. Fulde for a critical reading of the manuscript and for suggesting improvements. I am also indebted to him for providing valuable insights and many enlightening discussions during my visit to MPI-PKS. I thank Professors G. Rajasekarn and G. Baskaran for discussions and various comments.

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