Holstein-Primakoff theory for many-body systems

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We discuss the relationship between generalized coherent states and suitable extensions of the Holstein-Primakoff theory of quantum spin systems, illustrating the common origin of a variety of semiclassical approximation schemes encountered in many-body theory.

A diversity of apparently disconnected approximation schemes [the semiclassical $1/s$ expansion for magnetic systems, the Bogoliubov theory of the Bose gas, the generalized random-phase approximation (RPA) for Fermi systems, mean-field approaches of the BCS type, the $1/N$ expansion in quantum mechanics and field theory] may all be based on the theory of generalized coherent states. While the details of an overcomplete set of coherent states denoted by $|z\rangle$ depend on the particular system under consideration, the associated dynamics is governed by a Lagrangian of the general form

$$L=\left\langle z\left|\left(\frac{i}{2}\frac{\overleftrightarrow{d}}{dt}-H\right)\right|z\right\rangle \ , \tag{1}$$

where H is the Hamiltonian. Lagrangian (1) has been the starting point for the derivation of the time-dependent Hartree-Fock approximation (TDHF), recently reviewed by Kramer and Saraceno,[1] which is but the Gaussian approximation based on Eq. (1). On the other hand, the same Lagrangian occurs in a phase-space path integral in the sense of Klauder[2] suggesting that Eq. (1) is an essentially exact statement. In fact, an exact operator formalism may be abstracted from Eq. (1) which is a generalization of the Holstein-Primakoff (HP) theory[3] developed some 40 years ago for the study of spin systems.

The HP theory has already received considerable attention in its original context as well as in the study of nuclear models in terms of pseudospin algebras.[4,5] Applications have also included the $1/N$ expansion in quantum mechanics and field theory.[6-8] Although the relevance of generalized coherent states is implicit in the above work, the precise relationship is often obscured or ignored in the literature. The purpose of this Brief Report is to shed light on the precise connection in the context of many-body theory.

Thus we consider systems whose Hamiltonian $H=H(A)$ may be expressed entirely in terms of the bilinear operators

$$A_{ij}=a_i^{\sigma *}a_j^{\sigma},\quad \{a_i^{\rho},a_j^{\sigma *}\}=\delta_{ij}\delta_{\sigma\rho}\ ,$$
$$\rho,\sigma=1,2,\ldots,n,\quad n=2s+1\ , \tag{2}$$

where enclosure by the curly brackets denotes the usual anticommutator and summation over the repeated spin index σ is assumed. The spin s of the particles involved is taken to be arbitrary, whereas $n=2s+1$ stands for the spin multiplicity. For convenience we assume that the indices $i,j,\ldots$ take over discrete values the total number of which may be infinite. It is a simple exercise to show that the operators A_{ij} close the unitary pseudospin algebra

$$[A_{ij},A_{kl}]=\delta_{jk}A_{il}-\delta_{il}A_{kj}\ , \tag{3}$$

which is formally identical to the pseudospin algebra occurring in the description of the Bose gas. However, the representations of the pseudospin algebra that are relevant for Fermi systems are different.

Strictly speaking, an infinite number of irreducible representations of (3) are relevant for the description of Fermi systems, in analogy with the ordinary Schrödinger equation where an infinite number of angular-momentum sectors is necessary for the description of an atom. To make the analogy more complete, we note that the symmetry group of a Hamiltonian of the form $H=H(A)$ defined in terms of operators (2) is the unitary group $U(n)\sim U(1)\times SU(n)$, with $n=2s+1$, which should be clearly distinguished from the "pseudosymmetry" (3). The U(1) component is the usual number symmetry, whereas the non-Abelian component $SU(n)$ pertains to the spin degeneracy. It should be noted that the $SU(n)$ "flavor" group is larger than the normally expected SU(2) group associated with spin rotations, except for the special case of spin-$\frac{1}{2}$ particles. This situation is somewhat analogous to the n-dimensional harmonic oscillator whose symmetry group is $U(n)$ that contains the group of $O(n)$ rotations as a subgroup.

The fact that both the algebra of the symmetry group and the pseudospin algebra (3) are unitary is merely an accident. Nevertheless, an important link between the above algebras exists, in general, when the question of specific representations is addressed, because the generators of the pseudospin algebra are invariant under transformations of the symmetry group. The Fock states associated with the original Fermi operators may be classified according to their $U(n)$ quantum numbers that reflect the underlying symmetry, in particular, according to the total particle number N and the total spin, which should be distinguished from the spin multiplicity. The essence of pseudospin algebra (3) is that it allows classification of states with definite $U(n)$ transformation properties but varying "radial" quantum numbers within the same irreducible representation.

Our intention here is certainly not to provide a complete reduction of the Fock space according to the irreducible representations of the pseudospin algebra, but to concretely implement the above general discussion in specific examples of low-lying sectors (with small total spin) which are the most relevant for physical applications. In fact, explicit results are derived only for the singlet sector that encompasses N-particale states with vanishing total spin. We further restrict ourselves to systems with a total number of particles N that is an integer multiple of the spin multiplicity:

$$N = nN_0 = (2s+1)N_0 \ , \tag{4}$$

where N_0 is an integer. [For an electron system $(s=\frac{1}{2})N$ is taken to be even.] Hence the filled Fermi sea described by the N-particle state,

$$|\Omega_0\rangle = \prod_{j=1}^{N_0} \prod_{\sigma=1}^{n} a_j^{\sigma *}|\text{vac}\rangle \ , \tag{5}$$

carries vanishing total spin (singlet state).

A complete set of N-particle singlet states may be obtained by repeated application of the operators $A_{ij}, A_{kl}, \dots$ defined from (2) on the state $|\Omega_0\rangle$. However, we shall prefer to describe the singlet sector through the covercomplete set of generalized coherent states

$$|z\rangle = \text{const}\exp\left[\sum_{i=N_0+1}^{\infty} \sum_{j=1}^{N_0} z_{ij}A_{ij}\right]|\Omega_0\rangle \ , \tag{6}$$

which are essentially the coherent states introduced by Thouless,[9] except for the ramifications concerning the spin multiplicity discussed above. The same author pointed out the relevance of the states (6) for the derivation of the RPA as a time-dependent Hartree-Fock approximation. Those and related results on quasiboson representations will be strengthened here to obtain a complete HP theory that may be used for the derivation of systematic corrections to the RPA by means of ordinary perturbation theory in inverse powers of the spin multiplicity.

To motivate the HP theory a more detailed study of the coherent states is required than that given by Thouless. Fortunately, coherent states analogous to (6) have been studied by Perelomov in his work on pair creation of Fermi particles in an external field,[10] which applies to the current problem with suitable adaptations. Indices taking values outside the Fermi sea will now be denoted by $\mu, \nu, \dots \geq N_0+1$, whereas indices inside the sea will be taken to be $\alpha, \beta, \dots \leq N_0$.

The (normalized) coherent states (6) read

$$|z\rangle = [\det(\underline{I}+\underline{z}^\dagger \underline{z})]^{-n/2}\exp\left[\sum_{\mu,\alpha} z_{\mu\alpha}A_{\mu\alpha}\right]|\Omega_0\rangle \ ,$$
$$\langle z|z\rangle = 1, \quad n = 2\underline{s}+1 \ . \tag{7}$$

The matrix $\underline{z}^\dagger\underline{z}$ is the $N_0 \times N_0$ matrix defined from

$$(\underline{z}^\dagger\underline{z})_{\alpha\beta} = \sum_\mu z^*_{\mu\alpha}z_{\mu\beta} \ , \tag{8}$$

where the asterisk denotes ordinary complex conjugation whereas the dagger also implies transposition of indices $[(\underline{z}^\dagger)_{\alpha\mu} \equiv (\underline{z}^*)_{\mu\alpha}]$.

The time-dependent dynamics associated with the overcomplete set of states (7) is governed by the Lagrangian (1) written as

$$L = \left\langle z\left|\left(\frac{i}{2}\frac{\overleftrightarrow{d}}{dt} - H\right)\right|z\right\rangle = L_0 - \langle z|H|z\rangle \ ,$$
$$L_0 = \frac{i}{2}\sum_{\mu,\alpha}\dot{z}_{\mu\alpha}\langle z|A_{\mu\alpha}|z\rangle + \text{H.c.} \ . \tag{9}$$

The evaluation of useful matrix elements in the basis of coherent states is facilitated by various identities derived by Perelomov[10] (currently adapted to account for the spin multiplicity):

$$\begin{aligned}
A_{\mu\nu}(z,z^*) &= n\{\underline{z}(\underline{I}+\underline{z}^\dagger\underline{z})^{-1}\underline{z}^\dagger\}_{\nu\mu} \ ,\\
A_{\alpha\beta}(z,z^*) &= n\{(\underline{I}+\underline{z}^\dagger\underline{z})^{-1}\}_{\beta\alpha} \ ,\\
A_{\mu\alpha}(z,z^*) &= n\{(\underline{I}+\underline{z}^\dagger\underline{z})^{-1}\underline{z}^\dagger\}_{\alpha\mu} \ ,\\
A_{\alpha\mu}(z,z^*) &= n\{\underline{z}(\underline{I}+\underline{z}^\dagger\underline{z})^{-1}\}_{\mu\alpha} \ .
\end{aligned} \tag{10}$$

We are now able to derive an explicit form for the Lagrangian L_0 of Eq. (9), namely,

$$L_0 = \frac{i}{2}n\,\text{tr}\{\dot{\underline{z}}(\underline{I}+\underline{z}^\dagger\underline{z})^{-1}\underline{z}^\dagger\} + \text{H.c.} \ , \tag{11}$$

where tr stands for the usual trace of matrices and involves summation over all particle states, including the summation over hole states implied by the matrix multiplication in (11).

The information summarized in Eqs. (10) and (11) will be sufficient for the derivation of the HP theory. As expected, the phase space implied by (11) is nonlinear; namely, the canonical momenta associated with the dynamical variables $z_{\mu\alpha}$ are nonlinear functions of the latter. We thus seek a stereographic projection that linearizes the phase space:

$$\underline{\xi} = \underline{z}[n^{1/2}(\underline{I}+\underline{z}^\dagger\underline{z})^{-1/2}] \ . \tag{12}$$

It is a simple exercise to show that

$$L_0 = \tfrac{1}{2}\text{tr}(\dot{\underline{\xi}}\underline{\xi}^\dagger - \underline{\xi}\dot{\underline{\xi}}^\dagger) = \tfrac{1}{2}i\sum_{\mu,\alpha}(\dot{\xi}_{\mu\alpha}\xi^*_{\mu\alpha} - \xi_{\mu\alpha}\dot{\xi}^*_{\mu\alpha}) \ , \tag{13}$$

whereas the diagonal matrix elements (10) transform into

$$A_{\mu\nu}=\sum_{\alpha}\xi^{*}_{\mu\alpha}\xi_{\nu\alpha}\ ,$$
$$A_{\alpha\beta}=n\delta_{\alpha\beta}-\sum_{\mu}\xi^{*}_{\mu\beta}\xi_{\mu\alpha}\ ,$$
$$A_{\mu\alpha}=\sum_{\beta}\xi^{*}_{\mu\beta}R_{\alpha\beta}\ ,\qquad (14a)$$
$$A_{\alpha\mu}=\sum_{\beta}R_{\beta\alpha}\xi_{\mu\beta}\ ,$$

where $\underline{R}=(R_{\alpha\beta})$ is the $N_0\times N_0$ matrix

$$\underline{R}=(n\underline{I}-\underline{\xi}^{\dagger}\underline{\xi})^{1/2}\ . \qquad (14b)$$

Furthermore, the Lagrangian (13) implies the (Bose) commutation relations

$$[\xi_{\mu\alpha},\xi^{*}_{\nu\beta}]=\delta_{\mu\nu}\delta_{\alpha\beta}\ . \qquad (14c)$$

Equations (14a), (14b), and (14c) provide the HP representation suitable for the description of the singlet sector of a Fermi system interacting through a spin-independent potential.

However, the preceding derivation hides an important fact associated with the ordering of operators in (14a). In view of nonlinear coordinate transformation such as (12) one would normally expect that ordering difficulties beset the validity of (14). While the expressions (14a) close to the unitary algebra at the level of Poisson brackets essentially by construction, the transition to operators implied by (14c) may not preserve the correct commutation relations. Nevertheless, the ordering of operators judiciously chosen in (14a) can be shown to provide the correct HP representation, whose validity must be established by an independent proof.

Because of the matrix stucture associated with (14) such a proof is not straightforward. Since nontrivial examples have already been worked out in a related context,[6-8] we shall restrict ourselves to the description of some important checks of consistency of (14). Thus the matrix in (14b) may be approximated by a series expansion in inverse powers of the spin multiplicity:

$$R_{\alpha\beta}\simeq\sqrt{n}\left[\delta_{\alpha\beta}-\frac{1}{2n}\sum_{\mu}\xi^{*}_{\mu\alpha}\xi_{\mu\beta}+\cdots\right]\ . \qquad (15)$$

Substitution of (15) in (14a) allows for an explicit (albeit tedious) verification of the commutation relations (3) to any desired accuracy, for the various partitions of indices shown in Eq. (14a). In fact, Eqs. (14) become useful for practical purposes through an expansion of the form (15).

Other checks of consistency involve calculating the Casimir invariants from (14) and showing that they are identically equal to their eigenvalues characterizing the N-body singlet subspace. Thus the first two invariants of the pseudospin algebra (3) read

$$C_1=\sum_{i}A_{ii}\ ,\quad C_2=\sum_{i,j}A_{ij}A_{ji}\ . \qquad (16)$$

It is not difficult to rearrange the above definitions to obtain

$$C_1=\sum_{\sigma}Q^{\sigma\sigma}\ ,$$
$$C_2=-\sum_{\sigma,\rho}Q^{\sigma\rho}Q^{\rho\sigma}+(n+N_0+\Lambda)\sum_{\sigma}Q^{\sigma\sigma}\ , \qquad (17)$$

where $N_0+\Lambda$ is the total number of available levels (which may be infinite) and $Q^{\sigma\rho}$ are the generators of the U(n) symmetry:

$$Q^{\sigma\rho}=\sum_{i}a_i^{\sigma *}a_i^{\rho}\ . \qquad (18)$$

We thus find that the Casimir invariants of the pseudospin algebra may be expressed in terms of the Casimir invariants of the underlying symmetry. Furthermore, the eigenvalues of C_1 and C_2 that characterize the N-body singlet subspace may be identified from

$$C_1|\Omega_0\rangle=N|\Omega_0\rangle,\quad C_2|\Omega_0\rangle=(n+\Lambda)N|\Omega_0\rangle\ , \qquad (19)$$

which may be established by a simple calculation.

Equations (16)–(18) were derived using properties of the original Fermi operators alone. On the other hand, one may write

$$C_1=\sum_{i}A_{ii}=\sum_{\mu}A_{\mu\mu}+\sum_{\alpha}A_{\alpha\alpha}\ ,\quad C_2=\sum_{i,j}A_{ij}A_{ji}=\sum_{\mu,\nu}A_{\mu\nu}A_{\nu\mu}+\sum_{\alpha,\beta}A_{\alpha\beta}A_{\beta\alpha}+\sum_{\mu,\alpha}(A_{\alpha\mu}A_{\mu\alpha}+A_{\mu\alpha}A_{\alpha\mu})\ , \qquad (20)$$

and substitute the HP representation (14) for $A_{\mu\nu}$, $A_{\alpha\beta}$, $A_{\mu\alpha}$, and $A_{\alpha\mu}$. A relatively simple calculation employing only the commutation relations (14c) shows that C_1 and C_2 are *identically* equal to the c-numbers

$$C_1=N,\quad C_2=(n+\Lambda)N\ , \qquad (21)$$

which coincide with the eigenvalues of the Casimir invariants found in Eq. (19). The preceding calculation confirms our earlier assertion that the HP representation (14) is a restriction of the pseudospin algebra to the N-body singlet subspace.

The appearance of the parameter Λ ($\rightarrow\infty$) in (21) is an artifact associated with the definition of the Casimir invariants of the pseudospin algebra which bear no direct physical significance. The parameter Λ never appears explicitly in calculations involving the HP representation (14). Furthermore, it was noted earlier [cf. Eq. (17)] that $C_1, C_2, \ldots$ are related to the Casimir invariants of the underlying symmetry group which do possess direct physical significance. Thus the total number operator is equal to $C_1(=N)$, whereas C_2 contains information about the total spin. We illustrate this situation for the simplest spin-$\frac{1}{2}$

case for which $n=2s+1=2$, and the spin generators are defined from

$$S^a=\frac{1}{2}\sum_{i,\lambda,\rho} a_i^{\lambda *}\sigma^a{}_{\lambda\rho}a_i^\rho, \quad a=1,2,3 \ , \tag{22}$$

where $\underline{\sigma}^a=(\sigma^a{}_{\lambda\rho})$ are the familiar Pauli matrices. A simple calculation shows that the total spin S^aS^a may be expressed in terms of C_1 and C_2 according to

$$S^aS^a=\frac{1}{2}(2+N_0+\Lambda)C_1-\frac{1}{4}C_1^2-\frac{1}{2}C_2 \ , \tag{23}$$

a relation that is valid for all sectors. On the other hand, if the eigenvalues (21) with $n=2$ and $N=2N_0$ are inserted in (23), one finds that $S^aS^a=0$, which is characteristic of the singlet sector.

The HP representation (14) is the main result of this Brief Report. Given a Hamiltonian $H=H(A)$, its restriction to the N-body subspace with vanishing total spin is obtained by the simple substitution $A\rightarrow A(\xi,\xi^*)$ from Eq. (14). This results in an exact effective Hamiltonian for the description of the singlet sector. The ensuing method of calculation is briefly illustrated here in the case of the interacting Bose gas for which the HP theory may be obtained as a special case of (14). Hence a Bose system may be viewed as a degenerate Fermi system with a number of flavors n that is equal to the particle number N. Then $N=nN_0=n \rightarrow N_0=1$, and the $N_0\times N_0$ matrix $\xi^\dagger\xi$ in Eq. (14) becomes a scalar. Using an obvious change in notation Eqs. (14) reduce to

$$A_{00}=N-\xi^*\xi, \quad A_{pq}=\xi_p^*\xi_q \text{ for } pq\neq 0 \ ,$$
$$A_{op}=(N-\xi^*\xi)^{1/2}\xi_p, \quad A_{po}=\xi_p^*(N-\xi^*\xi)^{1/2} \text{ for } p\neq 0 \ . \tag{24}$$

The operators ξ_p and ξ_p^* are defined only for nonvanishing momenta and satisfy the usual Bose commutation relations

$$[\xi_p,\xi_q^*]=\delta_{pq} \ . \tag{25}$$

We have also used the abbreviation $\xi^*\xi=\sum_{p\neq 0}\xi_p^*\xi_p$. Roughly speaking, the operator ξ_p^* excites a particle with momentum $p\neq 0$ from the N-body condensate. The HP representation (24) coincides with that derived earlier by Okubo[11] for the symmetric representation of the unitary algebra.

The effective N-body Hamiltonian for the interacting Bose gas may then be written as

$$H=\frac{N^2}{V}V_0-\frac{N}{V}\sum_k V_k+\sum_{k\neq 0}\left[k^2\xi_k^*\xi_k+\frac{V_k}{V}\rho_k\rho_{-k}\right],$$
$$\rho_k=(N-\xi^*\xi)^{1/2}\xi_k+\xi_{-k}^*(N-\xi^*\xi)^{1/2}+\sum_{\substack{p\neq 0\\ p+k\neq 0}}\xi_p^*\xi_{p+k} \ , \tag{26}$$

where V_k is the Fourier transform of the potential and V is the volume of the system. A systematic formal expansion in inverse powers of N and ordinary perturbation theory yield a method of successive approximations in complete analogy with the $1/N$ expansion studied in Refs. 6–8. The leading approximation coincides with the familiar Bogoliubov theory, whereas higher-order corrections are free of ordering difficulties that have been known to occur in the closely related hydrodynamical approach of Bogoliubov and Zubarev.[12,13] We have checked the current procedure with a detailed calculation of the ground-state energy in the Lieb-Liniger model[14] for which an exact solution was obtained through the Bethe ansatz. Taking $V_k=g^2$ and restricting (26) to one dimension yields, after a long calculation,

$$E_{\text{g.s.}}=N\rho^2\left[\gamma-\frac{4}{3\pi}\gamma^{3/2}+\left(\frac{1}{6}-\frac{1}{\pi^2}\right)\gamma^2+\cdots\right] \ , \tag{27}$$

where $\rho=N/V$ is the density of the system and γ is the dimensionless coupling constant $\gamma=g^2/\rho$. The result (27) agrees with the numerical solution of the Lieb-Liniger equations.[12]

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