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Unified pair-coupling theory of fermion systems

D. J. Rowe, T. Song, and H. Chen
Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7
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A coherent-state theory of many-fermion systems is presented and shown to have some novel and useful properties. It leads naturally to variational equations for wave functions of the number-projected Hartree-Bogolyubov type. It is designed with the objective of describing finite nuclei in which both short-range pairing and long-range collective correlations are important.

We present a coherent-state representation of many-fermion quantum mechanics, suitable for describing finite nuclei in which both short-range pairing and long-range collective correlations are important.

The problem for a long-range quadrupole-quadrupole Hamiltonian in a spherical harmonic-oscillator shell with degenerate single-particle energies is solved with Elliott's SU(3) algebra [1]. Similarly, the pairing problem for a valence space with degenerate single-particle energies is resolved with Kerman's quasispin algebra [2]. However, except for simple cases where numerical diagonalizations are possible, no exact solutions are known for a Hamiltonian with nondegenerate single-particle energies and both pairing and long-range interactions. Approximate solutions are given by variational and mean-field theories and by their extensions to admit quasiparticles and deformed and/or time-dependent fields. The progression of variational solutions from one symmetry type to another with change of parameters in the Hamiltonian yields insight into the competition between independent-particle degrees of freedom, long-range shape-deformation correlations, and short-range pairing correlations. Unfortunately, spurious phase transitions can result from unrealistic variational constraints [3]. Furthermore, number nonconserving quasiparticle constraints are known to be unsatisfactory in finite nuclei.

Our formalism has much in common with the so-called "coherent correlated pair" method of Vary and co-workers [4] and the "collective pair" approximation of Maglione and co-workers [5]. Unlike independent-particle and quasiparticle based formalisms, the pair-coupled approaches utilize the fermion pair algebra; i.e., an SO(2d) Lie algebra spanned by operators

$$a_i^\dagger a_j^\dagger,\ \tfrac{1}{2}(a_i^\dagger a^j - a^j a_i^\dagger),\ a^i a^j,\ i,j=1,\ldots,d\,, \qquad (1)$$

where $a_i^\dagger$ and a^i are fermion operators satisfying anticommutation relations

$$\{a^i,a_j^\dagger\}=\delta_{ij},\ \{a^i,a^j\}=\{a_i^\dagger,a_j^\dagger\}=0\,. \qquad (2)$$

In addition, the formalism we propose exploits some elegant and useful properties of a coherent-state representation of the fermion pair algebra [6,7].

The set of all even fermion states span an irreducible representation of the SO(2d) algebra and the set of all states of odd fermion number span another irreducible representation. We consider here the former. Let $|0\rangle$ denote the fermion vacuum state. The coherent-state representation of an even fermion state $|\psi\rangle$ is then defined

$$\psi(\beta)=\langle\beta|\psi\rangle=\langle 0|e^{X(\beta)}|\psi\rangle\,, \qquad (3)$$

where

$$X(\beta)=\tfrac{1}{2}\sum_{ij}\beta_{ij}a^j a^i\,. \qquad (4)$$

A linear operator $\hat{W}$ on the fermion states has representation $\Gamma(W)$ defined by

$$\Gamma(W)\psi(\beta)=\langle\beta|\hat{W}|\psi\rangle=\langle 0|\{\hat{W}+[X,\hat{W}]+\tfrac{1}{2}[X,[X,\hat{W}]]+\cdots\}e^{X(\beta)}|\psi\rangle\,. \qquad (5)$$

It follows that

$$\begin{aligned}\Gamma(a^j a^i)&=\partial/\partial\beta_{ij}\,,\\ \Gamma(a_i^\dagger a_j^\dagger)&=\beta_{ij}+\sum_{kl}\beta_{il}\beta_{jk}\partial/\partial\beta_{kl}\,,\\ \Gamma(a_i^\dagger a^j)&=\sum_l\beta_{il}\partial/\partial\beta_{jl}\,,\end{aligned} \qquad (6)$$

as given in Refs. [7] and [8]. Thus, the Hamiltonian

$$H=\sum_i\epsilon_i a_i^\dagger a^i+\tfrac{1}{4}\sum_{ijkl}V_{ijkl}a_i^\dagger a_j^\dagger a^l a^k \qquad (7)$$

has coherent-state representation

$$\Gamma(H)=\sum_{il}\epsilon_i\beta_{il}\frac{\partial}{\partial\beta_{il}}+\tfrac{1}{4}\sum_{ijkl}V_{ijkl}\left[\beta_{ij}\frac{\partial}{\partial\beta_{kl}}+\sum_{st}\beta_{is}\beta_{jt}\frac{\partial^2}{\partial\beta_{ts}\partial\beta_{kl}}\right]. \qquad (8)$$

The advantages of this apparently more complicated expression of the Hamiltonian (7) are realized when one works with pair coupled as opposed to independent-particle states.

We consider pair-coupled states of the form

$$|n(\alpha)\rangle=[X^\dagger(\alpha)]^n|0\rangle \qquad (9)$$

with $X(\alpha)$ given by Eq. (4). Such states are known to provide remarkably accurate approximations to pairing force problems [3,9,10]. With suitably chosen $\{\alpha_{ij}\}$ coefficients, both ($J=0$) pair-coupled states and independent-particle Slater determinants are of this form as are the components of a BCS or Hartree-Bogolyubov wave function of fermion number equal to 2n. They play a central role in the so-called "broken pair approximation" (cf.

Ref. [11] and references quoted therein). With the additional step of angular momentum projection, they can also generate exact SU(3) states for leading representations (i.e., ones having determinantal intrinsic wave functions). Finally, any $2n$-fermion state can be expressed as a linear combination of states of the type (9).

The coherent-state wave functions

$$\psi_n(\beta,\alpha)=\langle\beta|n(\alpha)\rangle,\quad n=0,1,2,\ldots \tag{10}$$

for $n=0$ and $n=1$ are given by $\psi_0(\beta,\alpha)=1$ and $\psi_1(\beta,\alpha)=\frac{1}{2}\sum_i z_i^i$, where

$$z_i^j=(\beta\alpha)_i^j=\sum_k\beta_{ik}\alpha^{jk} \tag{11}$$

and $\alpha^{ij}=\alpha_{ij}^*$. For $n\geq 1$, they satisfy the recursion relation

$$\psi_n(\alpha,\beta)=\langle 0|e^{X(\beta)}X^\dagger(\alpha)|n-1\rangle$$
$$=\frac{1}{2}\sum_{ij}\alpha^{ij}\left[\beta_{ij}+\sum_{kl}\beta_{il}\beta_{jk}\frac{\partial}{\partial\beta_{kl}}\right]\psi_{n-1}(\alpha,\beta)\,. \tag{12}$$

Now, one easily shows that the polynomials

$$\phi_n(z)=\frac{1}{2}\operatorname{Tr}(z^n)=\frac{1}{2}\sum_i z_{i_1}^{i_2}z_{i_2}^{i_3}\ldots z_{i_n}^{i_1}\,, \tag{13}$$

satisfy the equation

$$\frac{1}{2}\sum_{ij}\alpha_{ij}\sum_{kl}\beta_{il}\beta_{jk}\frac{\partial}{\partial\beta_{kl}}\phi_n=-n\phi_{n+1}\,. \tag{14}$$

It follows that

$$\sum_{ij}\alpha_{ij}\sum_{kl}\beta_{il}\beta_{jk}\frac{\partial}{\partial\beta_{kl}}=-\sum_m m\phi_{m+1}\nabla_m,\quad \nabla_m=\partial/\partial\phi_m \tag{15}$$

and that the solutions of Eq. (12) are given by

$$\psi_n(\beta,\alpha)=\varphi_n(\beta\alpha)=\varphi_n(z)\,, \tag{16}$$

where φ_n satisfies the recursion relation

$$\varphi_n=\left[\phi_1-\sum_m m\phi_{m+1}\nabla_m\right]\varphi_{n-1}\,. \tag{17}$$

This recursion relation is easily solved by use of the following theorem.

Theorem 1:

$$\nabla_m\varphi_n=(-1)^{m+1}\frac{1}{m}\frac{n!}{(n-m)!}\varphi_{n-m}\,. \tag{18}$$

Proof: Suppose $\nabla_1\varphi_n=n\varphi_{n-1}$, for some n. It then follows that

$$\nabla_1\varphi_{n+1}=\nabla_1\left[\phi_1\varphi_n-\sum m\phi_{m+1}\nabla_m\varphi_n\right]=(n+1)\varphi_n\,. \tag{19}$$

Therefore, since $\nabla_1\varphi_1=\varphi_0$, the theorem holds for $m=1$ and all n. Next, suppose the theorem holds for all m and some φ_n. We similarly show that it then holds for all m and φ_{n+1} and, since it does hold for all m and $n=1$, it is proved generally.

Using the theorem, we can express the recursion relation (17)

$$\varphi_n=\sum_{m=1}^n(-1)^{m+1}\frac{(n-1)!}{(n-m)!}\varphi_{n-m}\phi_m \tag{20}$$

implying that φ_n is a determinant of the form

$$\varphi_n=\begin{vmatrix}\phi_1 & 1 & 0 & 0 & \cdots & 0\\ \phi_2 & \phi_1 & 2 & 0 & \cdots & 0\\ \phi_3 & \phi_2 & \phi_1 & 3 & \cdots & 0\\ & & \cdots & & & \\ \phi_n & \phi_{n-1} & \phi_{n-2} & \phi_{n-3} & \cdots & \phi_1\end{vmatrix}. \tag{21}$$

Functions of this type are known in character theory as antisymmetric Schur functions.

The states $|n(\alpha)\rangle$ span the space of $2n$-particle states and have overlaps

$$\langle n(\beta)|n(\alpha)\rangle=n!\langle\beta|n(\alpha)\rangle=n!\varphi_n(\beta\alpha)\,. \tag{22}$$

Thus, by diagonalizing the overlap matrix (22) for a linearly independent set of $\{|n(\alpha)\rangle\}$, one can construct an orthonormal basis of states that are not substantially more difficult to use than the Slater determinants of an independent-particle approximation. Matrix elements of the Hamiltonian, for example, are obtained from the identity

$$\langle n(\beta)|H|n(\alpha)\rangle=n!\Gamma(H)\varphi_n(\beta\alpha)\,, \tag{23}$$

with $\Gamma(H)$ given by Eq. (8) and derivatives of φ_n evaluated as follows.

From theorem 1, partial derivatives of φ_n are given by

$$\frac{\partial}{\partial\beta_{kl}}\varphi_n=\sum_q\frac{\partial\phi_q}{\partial\beta_{kl}}\nabla_q\varphi_n$$
$$=\sum_q(-1)^{q+1}\frac{(n-1)!}{(n-q)!}\varphi_{n-q}\Phi_{kl}^q\,, \tag{24}$$

where

$$\Phi_{kl}^q=\frac{n}{q}\frac{\partial\phi_q}{\partial\beta_{kl}}\,. \tag{25}$$

Thus, the function $\partial\varphi_n/\partial\beta_{kl}$ is the determinant

$$\frac{\partial}{\partial\beta_{kl}}\varphi_n=\begin{vmatrix}\phi_1 & 1 & 0 & 0 & \cdots & 0\\ \phi_2 & \phi_1 & 2 & 0 & \cdots & 0\\ \phi_3 & \phi_2 & \phi_1 & 3 & \cdots & 0\\ & & \cdots & & & \\ \Phi_{kl}^n & \Phi_{kl}^{n-1} & \Phi_{kl}^{n-2} & \Phi_{kl}^{n-3} & \cdots & \Phi_{kl}^1\end{vmatrix}. \tag{25a}$$

Second derivatives of φ_n are obtained by means of the following theorem.

Theorem 2: If $\chi(\beta,\alpha)$ is any determinantal function of the form

$$\chi(\beta,\alpha)=\sum_{q=1}^n(-1)^{q+1}\frac{(n-1)!}{(n-q)!}\varphi_{n-q}(\beta\alpha)F_q(\beta,\alpha)\,, \tag{26}$$

then $\partial\chi/\partial x$ is the determinantal function

$$\frac{\partial\chi}{\partial x}=\sum_{q=1}^n(-1)^{q+1}\frac{(n-1)!}{(n-q)!}\varphi_{n-q}\frac{DF_q}{Dx}\,, \tag{27}$$

where

$$\frac{DF_q}{Dx}=\frac{\partial F_q}{\partial x}-\sum_{p=1}^{q-1}\frac{1}{p}\frac{\partial\phi_p}{\partial x}F_{q-p}\,, \tag{28}$$

and x is any of α_{ij}, β_{ij}, or z_{ij}.

Proof: We have

$$\frac{\partial \chi}{\partial x}=\sum_{q=1}^{n}(-1)^{q+1}\frac{(n-1)!}{(n-q)!}\left[\varphi_{n-q}\frac{\partial F_q}{\partial x}+\frac{\partial \varphi_{n-q}}{\partial x}F_q\right] \tag{29}$$

and

$$\frac{\partial \varphi_{n-q}}{\partial x}=\sum_p \nabla_p \varphi_{n-q}\frac{\partial \phi_p}{\partial x}=\sum_p (-1)^{p+1}\frac{1}{p}\frac{(n-q)!}{p(n-q-p)!}\varphi_{n-q-p}\frac{\partial \phi_p}{\partial x}. \tag{30}$$

Therefore

$$\sum_{q=1}^{n}(-1)^{q+1}\frac{(n-1)!}{(n-q)!}\frac{\partial \varphi_{n-q}}{\partial x}F_q=\sum_{m=1}^{n}(-1)^{m}\frac{(n-1)!}{(n-m)!}\varphi_{n-m}\sum_{p=1}^{m-1}\frac{1}{p}\frac{\partial \phi_p}{\partial x}F_{m-p}, \tag{31}$$

which leads to the desired result.

Application of theorem 2 gives

$$\frac{\partial^2}{\partial \beta_{ts}\partial \beta_{kl}}\varphi_n=\sum_q (-1)^{q+1}\frac{(n-1)!}{(n-q)!}\varphi_{n-q}\left[\frac{\partial}{\partial \beta_{ts}}\Phi^q_{kl}-\frac{1}{n}\sum_p \Phi^p_{ts}\Phi^{q-p}_{kl}\right]. \tag{32}$$

Thus, we obtain

$$\langle \beta|H|n(\alpha)\rangle=\sum_{q=1}^{n}(-1)^{q+1}\frac{n!}{(n-q)!}\varphi_{n-q}(\beta\alpha)H_q(\beta,\alpha), \tag{33}$$

where

$$H_q(\beta,\alpha)=\frac{1}{n}\left\{\sum_{il}\epsilon_i\beta_{il}\Phi^q_{jl}+\tfrac{1}{4}\sum_{ijkl}V_{ijkl}\left[\beta_{ij}\Phi^q_{kl}(\beta,\alpha)+\sum_{st}\beta_{is}\beta_{jt}\left(\frac{\partial \Phi^q_{kl}(\beta,\alpha)}{\partial \beta_{ts}}-\frac{1}{n}\sum_p \Phi^p_{ts}(\beta,\alpha)\right)\right]\right\}. \tag{34}$$

Besides solving the eigenvalue equations exactly, one can seek the value of α for which the energy expectation $\langle n(\alpha)|H|n(\alpha)\rangle$ is a minimum subject to the normalization constraint $\langle n(\alpha)|n(\alpha)\rangle=1$. Thus, one solves the variational equation

$$\delta[\langle \alpha|H|n(\alpha)\rangle-\lambda\varphi_n(\alpha\alpha)]=0. \tag{35}$$

Solutions of this variational equation for the ground state can be found iteratively as we shall demonstrate in a forthcoming paper.

Once it has been solved, one can also seek excited states of the form

$$O^\dagger_\gamma|(n-1)(\alpha)\rangle=\sum_{ij}\gamma_{ij}a^\dagger_i a^\dagger_j|(n-1)(\alpha)\rangle. \tag{36}$$

One easily shows that the excitation operators for these states are given by solution of the eigenvalue equation

$$\sum_{kl}(\mathcal{H}_{ij,kl}-\lambda\mathcal{N}_{ij,kl})\gamma_{kl}=0, \tag{37}$$

where

$$\mathcal{H}_{ij,kl}=\left[\frac{\partial^2\langle \beta|H|n(\alpha)\rangle}{\partial \beta_{ij}\partial \alpha_{kl}}\right]_{\beta=\alpha}=\sum_q (-1)^{q+1}\frac{n!}{(n-q)!}\varphi_{n-q}\frac{D^2H_q}{D\beta_{ij}D\alpha_{kl}},$$
$$\mathcal{N}_{ij,kl}=\left[\frac{\partial^2\varphi_n(\beta\alpha)}{\partial \beta_{ij}\partial \alpha_{kl}}\right]_{\beta=\alpha}=\sum_q (-1)^{q+1}\frac{n!}{(n-q)!}\varphi_{n-q}\frac{D^2\phi_q}{D\beta_{ij}D\alpha_{kl}}. \tag{38}$$

This equation has the desirable property that one of its solutions, with $\gamma=\alpha$, is precisely the pair-creation operator for the variational ground state $|n(\alpha)\rangle$.

Although we shall not pursue it here, one can also project states of good angular momentum from a variational state of the form (9). Moreover, the projection can be performed before or after energy minimization.

In a forthcoming paper, we shall illustrate the utility of the formalism by calculation of the eigenstates of a pairing Hamiltonian with nondegenerate single-particle energies. We shall show that one can calculate exact solutions of the multilevel pairing problem and that the approximate variational equations provide solutions of the broken pair model equations [8]. We shall further discuss the more general circumstances for which our variational equations can be solved, e.g., for pairing plus quadrupole Hamiltonians.

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