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Theory of Resonating Quantum Fluctuations in a Fermion System

—— *Resonating Hartree-Fock Approximation* ——

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We develop a new general theory for large quantum fluctuations in a Fermion many-body system that cannot be described by fluctuations around the Hartree-Fock ground state but arises from resonance of different correlation structures. We start with an exact coherent state representation of a Fermion system on a unitary group. We show that the Hamiltonian in the coherent state representation has a close connection with the Hartree-Fock energy functional. From this, we can derive a new approximation called the resonating Hartree-Fock approximation in which a state is approximated by a superposition of non-orthogonal Slater determinants with different correlation structures. We derive the variation equations to determine a resonating Hartree-Fock wavefunction. We show that the resonance between degenerate broken symmetry Slater determinants may partially recover the symmetry. We discuss how to choose trial Slater determinants in a resonating Hartree-Fock wavefunction. We suggest that resonance of Slater determinants representing localized defects, such as solitons, polarons and breathers, produced in the long range order of the HF ground state may be the most important content of large quantum fluctuations in condensed matter systems.

§ 1. Introduction

A Fermion system with small quantum fluctuations can be described by a standard method of Fermion many-body theory. The ground state is approximated by a single determinantal Hartree-Fock (HF) wavefunction and collective excitations due to quantum fluctuations around the HF ground state are described by the random phase approximation (RPA). There are Fermion systems with large quantum fluctuations that cannot be described by the HF-RPA method. Nuclei in the transition region between spherical and highly deformed shapes, magnetic substances with narrow d bands and low dimensional electronic systems are typical examples of such Fermion systems.

If quantum fluctuations around the HF ground state become large, nonlinear couplings between RPA excitation modes, so called mode-mode couplings, become important. If quantum fluctuations grow further, what happens has not been understood. There has been no satisfactory general theory to describe large quantum fluctuations in Fermion systems. The quantum Monte Carlo method[1] provides a general technique to inspect numerically such systems but it does not disclose analytical structures of correlations involved in them.

To approach large amplitude collective excitations in transition region nuclei, theories based on Boson representations of Fermion pair operators were proposed[2] but satisfactory understanding has not yet been achieved suggesting that quantum fluctuations in those nuclei are perhaps too large to be described by mode-mode couplings and quite a new concept may be necessary. For the problem of magnetism, a selfconsistent mode-mode coupling theory for weak itinerant magnetism and a

functional integral theory interpolating the extreme regimes of weak itinerant magnetism and localized spin moments have been developed.[3]

In a one dimensional system where no real long range order can exist, quantum fluctuations are intrinsically large unless a large gap is produced by a Peierls' lattice distortion. A theory called the bosonization[4] has been developed for one dimensional systems. It was successful in describing charge density waves (CDW) in quasi-one dimensional systems.[5] It, however, is a theory valid only in the weak coupling limit where the band gap is much smaller than the band width. The case of large quantum fluctuations, where nonlinear effects of the Boson becomes important, has not yet been treated. A two dimensional system with an enough large interaction may have large quantum fluctuations. The nature of electron correlation in a two dimensional system has become an important problem in connection with high T_c superconductivity. It, however, is a new and hot unsolved problem.

The purpose of this paper is to develop a general theory of large quantum fluctuations in Fermion systems. To do this we use an exact coherent state representation of a Fermion system on a unitary group[6)~9)] that is derived from the fact that Fermion pair operators satisfy the Lie commutation relation of a unitary group.[10] In § 2, we give a brief explanation of the unitary group coherent state representation of a Fermion system. In § 3, we clarify the structure of the Schrödinger equation in the coherent state representation. We introduce a new density matrix that depends on two non-orthogonal Slater determinants and is called the interstate density matrix. We show that the Hamiltonian can be expressed by the interstate density matrix in a form similar to the HF energy functional. From this, we derive in § 4 a new approximation called the resonating HF approximation in which a low energy state is approximated by a superposition of non-orthogonal Slater determinants with different correlation structures. We derive the variation equations to determine a resonating HF wavefunction. We show in § 5 that resonance of degenerate broken symmetry Slater determinants may partially recover the symmetry. We discuss in § 6 how to choose trial Slater determinants in a resonating HF wavefunction, that is equivalent to the most important physical problem to know what are the natures of resonating correlation structures, and other problems.

§ 2. Unitary group coherent state representation of a Fermion system

We describe here an exact representation of a Fermion system on a unitary group, that is the basis of our theory, according to Refs. 8) and 9). We consider a Fermion system with N single particle states. Let a_i and $a_i^\dagger$, $i=1, 2\cdots N$, be the annihilation and creation operators of the Fermion. Owing to the anticommutation relation of a_i and $a_i^\dagger$, the pair operators $a_i^\dagger a_j$ satisfy the Lie commutation relation of the unitary group of N dimension[10] (U(N))

$$[a_i^\dagger a_j, a_k^\dagger a_l]=\delta_{jk}a_i^\dagger a_l-\delta_{il}a_k^\dagger a_j\,. \tag{2·1}$$

With an $N\times N$ antihermitian matrix $\gamma=(\gamma_{ij})$, $\gamma^\dagger=-\gamma$, we define a unitary operator

$$U(u)=e^{\gamma_{ij}a_i^\dagger a_j}\,. \tag{2·2}$$

We use the dummy index convention to sum up repeated indices and u is a U(N) matrix given by $u=e^{r}$, $u^{\dagger}u=uu^{\dagger}=1$. Owing to the Lie commutation relation (2·1), the operator $U(u)$ satisfies the group properties

$$U(u)U(v)=U(uv),\ U(u^{-1})=U^{-1}(u)=U^{\dagger}(u),\ U(1)=1\,. \tag{2·3}$$

Therefore, the set $\{U(u);\ u\in\mathrm{U(N)}\}$ makes a unitary representation of U(N).

The operator $U(u)$ induces a canonical transformation, the Thouless transformation,[11] which transforms the $a_i^{\dagger}$'s and a_i's to their unitary linear combinations

$$\left.\begin{aligned} U(u)a_i^{\dagger}U^{\dagger}(u)&=(a^{\dagger}u)_i\,,\\ U(u)a_iU^{\dagger}(u)&=(au^{*})_i\,,\end{aligned}\right\} \tag{2·4}$$

where $a^{\dagger}$ and a are the row vectors $(a_i^{\dagger})$ and (a_i), respectively, and * denotes the complex conjugation. Let $|\phi\rangle=a_1^{\dagger}\cdots a_n^{\dagger}|0\rangle$ be an n particle Slater determinant (S det) where $|0\rangle$ is the vacuum. From Eq. (2·4) and $U(u)|0\rangle=|0\rangle$, we see that $U(u)$ transforms $|\phi\rangle$ to another S det

$$U(u)|\phi\rangle=(a^{\dagger}u)_1\cdots(a^{\dagger}u)_n|0\rangle\equiv|u\rangle\,. \tag{2·5}$$

Any n particle S det can be obtained by a Thouless transformation of a reference S det $|\phi\rangle$ (the Thouless theorem) and labeled with a U(N) matrix u.

Let $\boldsymbol{H}_n$ be the Hilbert space of n particles. Equation (2·5) shows that $\boldsymbol{H}_n$ is the space of a totally antisymmetric representation of U(N). $\boldsymbol{H}_n$ is irreducible because its dimension ${}_NC_n$ is identical to that of a totally antisymmetric irreducible representation.[12] Let $|\Phi\rangle$ and $|\Psi\rangle$ be state vectors in $\boldsymbol{H}_n$, then $\langle\Psi|U(u)|\Phi\rangle$ is a matrix element of an irreducible representation (irrep) on $\boldsymbol{H}_n$. By the orthonormality of matrix elements of an irrep[12] we obtain

$${}_NC_n\int\langle\Psi'|U(u)|\Phi'\rangle\langle\Phi|U^{\dagger}(u)|\Psi\rangle du=\langle\Psi'|\Psi\rangle\langle\Phi|\Phi'\rangle\,, \tag{2·6}$$

where the integration is the normalized group integration on U(N). Putting $|\Phi\rangle=|\Phi'\rangle=|\phi\rangle$, we obtain from Eq. (2·6) the following relation because $|\Psi'\rangle$ can be an arbitrary state vector in $\boldsymbol{H}_n$:

$$|\Psi\rangle={}_NC_n\int U(u)|\phi\rangle\langle\phi|U^{\dagger}(u)|\Psi\rangle du={}_NC_n\int|u\rangle\langle u|\Psi\rangle du\,. \tag{2·7}$$

This is a coherent state representation (CS rep) of Fermion state vectors on U(N) in the sense of Perlemov.[13] In the U(N) CS rep, a state vector $|\Psi\rangle$ is represented by a function $\Psi(u)=\langle u|\Psi\rangle$ on U(N). Equation (2·6) gives also

$${}_NC_n\int|u\rangle\langle u|du=1\,. \tag{2·8}$$

Since arbitrarily chosen two S dets are usually not orthogonal, Eq. (2·8) shows that the set of all S dets, $\{|u\rangle;\ u\in\mathrm{U(N)}\}$, is overcomplete, which is a common property of CS reps.

From Eq. (2·6), the overlap integral $\langle u|v\rangle=\langle\phi|U(u^{\dagger}v)|\phi\rangle$ of S dets satisfies

$$\left.\begin{aligned}\Psi(u)&={}_NC_n\int\langle u|v\rangle\Psi(v)dv\,,\\ \langle u|v\rangle&={}_NC_n\int\langle u|w\rangle\langle w|v\rangle dw\,.\end{aligned}\right\}\tag{2·9}$$

This shows that ${}_NC_n\langle u|v\rangle$ has the character of a δ function in the space of totally antisymmetric functions $\Psi(u)$ on U(N) though it is not a singular function.

The Schrödinger equation $(H-E)|\Psi\rangle=0$ can be converted to an integral equation on U(N) by using Eq. (2·7):

$$\left.\begin{aligned}&\int\{\langle u|H|v\rangle-E\langle u|v\rangle\}\Psi(v)dv=0\,,\\ &\langle u|H|v\rangle=\langle\phi|U^\dagger(u)HU(v)|\phi\rangle\,.\end{aligned}\right\}\tag{2·10}$$

The Schrödinger equation on U(N) is given in terms of the matrix element of the Hamiltonian and the overlap integral between S dets which are usually non-orthogonal.

We note that an S det $|u\rangle$ is dependent only on the $N\times n$ submatrix $\tilde{u}=(u_{ia})$ of u. We use $a, b\cdots$ as the indices to run only on the n single particle states $1\cdots n$ while $i, j\cdots$ as those running all the single particle states $1\cdots N$. Furthermore, $|u\rangle$ is invariant to transformations from the right side of $\tilde{u}$, $\tilde{u}\to\tilde{u}\tilde{v}$, by a U(n) matrix $\tilde{v}=(\tilde{v}_{ab})$. Therefore, the U(N) CS rep of n particle states is a representation on the right coset U(N)/U(n). In the following, we use the notation to write $\tilde{u}$ as u, i.e., $u=(u_{ia})$ is an $N\times n$ submatrix of a U(N) matrix.

§ 3. Interstate density matrix and the Schrödinger equation on U(N)

To obtain the explicit form of the Schrödinger equation on U(N), it is necessary to calculate the overlap integral and the matrix element of the Hamiltonian between non-orthogonal S dets. Their expressions were first obtained by Löwdin.[14] We give here another derivation based on the second quantization formalism.

By using Eq. (2·5), the overlap integral between two S dets is calculated as

$$\begin{aligned}\langle u|v\rangle&=\langle\phi|z\rangle=\langle 0|a_n\cdots a_1(a^\dagger z)_1\cdots(a^\dagger z)_n|0\rangle\\ &=\det z\,,\qquad z=u^\dagger v=((u^\dagger v)_{ab})\,,\end{aligned}\tag{3·1}$$

where z is an $n\times n$ matrix and $\det z$ is the determinant of z.

We consider a matrix element of a pair operator between two non-orthogonal S dets

$$Q_{ij}(u, v)=\langle u|a_j^\dagger a_i|v\rangle\,.\tag{3·2}$$

By using Eq. (2·4), it is calculated as

$$\begin{aligned}Q_{ij}(u, v)&=\langle\phi|(a^\dagger u^\dagger)_j U(z)(av^T)_i|\phi\rangle\\ &=v_{ia}u^*_{jb}\langle\phi_b|U(z)|\phi_a\rangle\\ &=v_{ia}u^*_{jb}(-1)^{a+b}\langle 0|a_n\cdots a_{b+1}a_{b-1}\cdots a_1\end{aligned}$$

$$\times(a^\dagger z)_1\cdots(a^\dagger z)_{a-1}(a^\dagger z)_{a+1}\cdots(a^\dagger z)_n|0\rangle$$
$$=v_{ia}u^*_{jb}D_{ba}\,, \tag{3·3}$$

where $|\phi_a\rangle=a_a|\phi\rangle$, T denotes the transpose and D_{ba} is the b-a cofactor of det z. By using the relation

$$D_{ba}=\frac{\partial}{\partial z_{ba}}\det z=(z^{-1})_{ab}\det z\,, \tag{3·4}$$

Eq. (3·3) becomes

$$Q_{ij}(u,v)=W_{ij}(u,v)\det z\,, \tag{3·5}$$
$$W_{ij}(u,v)=v_{ia}(z^{-1})_{ab}u^*_{jb}=(vz^{-1}u^\dagger)_{ij}\,. \tag{3·6}$$

The $N\times N$ matrix $W(u,v)=vz^{-1}u^\dagger$ satisfies the idempotency condition and is not hermitian as an $N\times N$ matrix but hermitian as an integral operator on U(N)

$$W^2(u,v)=W(u,v)\,,\qquad W^\dagger(u,v)=W(v,u)\neq W(u,v)\,. \tag{3·7}$$

We call $W(u,v)$ the interstate density matrix. It was first introduced by Löwdin and called the fundamental invariant.[14]

The matrix element of a two-body normal product of pair operators between non-orthogonal S dets is calculated as follows:

$$\langle u|a_k{}^\dagger a_l{}^\dagger a_j a_i|v\rangle$$
$$=\langle\phi|(a^\dagger u^\dagger)_k(a^\dagger u^\dagger)_l U(z)(av^T)_j(av^T)_i|\phi\rangle$$
$$=\frac{1}{4}(v_{ia}v_{jb}-v_{ib}v_{ja})(u^*_{kc}u^*_{ld}-u^*_{kd}u^*_{lc})\langle\phi_{cd}|U(z)|\phi_{ab}\rangle\,, \tag{3·8}$$

where $|\phi_{ab}\rangle=a_b a_a|\phi\rangle$ and

$$\langle\phi_{cd}|U(z)|\phi_{ab}\rangle$$
$$=(-1)^{a+b+c+d}\langle 0|a_n\cdots a_{d+1}a_{d-1}\cdots a_{c+1}a_{c-1}\cdots a_1$$
$$\times(a^\dagger z)_1\cdots(a^\dagger z)_{a-1}(a^\dagger z)_{a+1}\cdots(a^\dagger z)_{b-1}(a^\dagger z)_{b+1}\cdots(a^\dagger z)_n|0\rangle$$
$$=D_{cd,ab} \tag{3·9}$$

is the cd-ab cofactor of det z. Using the relations

$$\frac{\partial}{\partial z_{cd}}(z^{-1})_{ba}=-(z^{-1})_{da}(z^{-1})_{bc}\,, \tag{3·10}$$

$$D_{cd,ab}=\frac{\partial^2(\det z)}{\partial z_{ca}\partial z_{db}}=\{(z^{-1})_{ac}(z^{-1})_{bd}-(z^{-1})_{ad}(z^{-1})_{bc}\}\det z \tag{3·11}$$

and Eq. (3·6), we obtain

$$\langle u|a_k{}^\dagger a_l{}^\dagger a_j a_i|v\rangle=(W_{ik}W_{jl}-W_{il}W_{jk})\det z\,. \tag{3·12}$$

Thus, a matrix element of a two-body operator between non-orthogonal S dets can be

expressed in terms of the interstate density matrix and the overlap integral. In the limit of $u=v$, $z=1$ and $W=uu^\dagger$ so that Eqs. (3·5) and (3·12) reduce to the well known results for the expectation values by an S det.

Let the Hamiltonian of the system be

$$H=h_{ji}a_j^\dagger a_i+\frac{1}{2}\langle ki|lj\rangle a_k^\dagger a_l^\dagger a_j a_i\,. \tag{3·13}$$

Then, from Eqs. (3·5) and (3·12)

$$\left.\begin{aligned}&\langle u|H|v\rangle=H[W(u,v)]\det(u^\dagger v)\,,\\&H[W]=h_{ji}W_{ij}+\frac{1}{2}[ki|lj]W_{ik}W_{jl}\,,\\&[ki|lj]=\langle ki|lj\rangle-\langle kj|li\rangle\,.\end{aligned}\right\} \tag{3·14}$$

Therefore, from Eqs. (3·14) and (3·1), an explicit form of the Schrödinger equation (2·10) is

$$\int\{H[W(u,v)]-E\}\det(u^\dagger v)\Psi(v)dv=0\,. \tag{3·15}$$

We note that $H[W]$ has the same form as the Hartree-Fock energy functional except for the difference that $W(u,v)$ is the interstate density matrix (3·6) dependent on two S dets $|u\rangle$ and $|v\rangle$.

From Eqs. (2·7), (3·5) and (3·12), the expectation values of one- and two-body pair operators by a state $|\Psi\rangle$ are given by

$$\langle\Psi|a_j^\dagger a_i|\Psi\rangle={}_NC_n{}^2\iint\Psi^*(u)W_{ij}(u,v)\det(u^\dagger v)\Psi(v)dudv\,, \tag{3·16}$$

$$\begin{aligned}\langle\Psi|a_k^\dagger a_l^\dagger a_j a_i|\Psi\rangle={}_NC_n{}^2\iint\Psi^*(u)\{&W_{ik}(u,v)W_{jl}(u,v)\\&-W_{il}(u,v)W_{jk}(u,v)\}\det(u^\dagger v)\Psi(v)dudv\,.\end{aligned} \tag{3·17}$$

From these equations, we can obtain expressions of densities and correlation functions of physical quantities in the U(N) CS rep.

Using Eq. (2·8), we obtain an expression of the partition function in the U(N) CS rep as

$$\mathrm{tr}(e^{-\beta H})={}_NC_n\int\langle u|e^{-\beta H}|u\rangle du\,, \tag{3·18}$$

where tr means trace and $\beta=1/k_BT$. By a canonical transformation

$$d_a(u)=(a^\dagger u)_a\,,\qquad d_p(u)=(a\bar{u}^*)_p\,, \tag{3·19}$$

that makes $|u\rangle$ a quasiparticle vacuum satisfying $d_i(u)|u\rangle=0$, where $\bar{u}$ is the $N\times(N-n)$ matrix (u_{ip}), $p=n+1\cdots N$, consisting of the unoccupied orbitals in $|u\rangle$, the Hamiltonian is transformed to

$$H=\langle u|H|u\rangle+H(u)\,. \tag{3·20}$$

From Eq. (3·14), $\langle u|H|u\rangle$ is just identical to the HF energy functional and $H(u)$ is the quasiparticle Hamiltonian depending only on normal products of $d_i^\dagger(u)$ and $d_i(u)$. Then, the partition function (3·18) becomes

$$\mathrm{tr}(e^{-\beta H})={}_NC_n\int e^{-\beta\langle u|H|u\rangle}\,\langle u|e^{-\beta H(u)}|u\rangle du\,. \tag{3·21}$$

This shows that if the HF energy functional has multiple low energy local minima then they give a large contribution to the partition function.

§ 4. Resonating Hartree-Fock approximation

The theory developed above is exact. We now try to solve approximately the Schrödinger equation (3·15). This new expression of the Schrödinger equation suggests us a new approach to Fermion correlation problems. The key to the new approach is the fact that the diagonal element $\langle u|H|u\rangle$ of the Hamiltonian matrix in the U(N) CS rep is just identical with the HF energy functional. In the HF aproximation, the ground state is approximated by an S det that makes $\langle u|H|u\rangle$ minimal. The HF equation, however, has many solutions owing to its nonlinear character. Since an eigenstate $|\Psi\rangle$ of H is a continuous superposition of all S dets as seen from Eq. (2·7), it contains all the solutions of the HF equation. If the HF energy $\langle u|H|u\rangle$ has multiple low energy local minima, then a low energy $|\Psi\rangle$ will contain S dets in neighbourhoods of those local minima with a large probability as suggested by Eq. (3·21). $|\Psi\rangle$ may also have a large mixing of other S dets which are not near those local minima but have large off-diagonal matrix elements of H with them and consequently give a substantial stabilization of $|\Psi\rangle$.

We now try to approximate a low energy eigenstate $|\Psi\rangle$ of H by a discrete superposition of S dets which are in neighbourhoods of low energy local minima of the HF energy $\langle u|H|u\rangle$ and those having large off-diagonal matrix elements $\langle u|H|v\rangle$ with them. We denote these sampling S dets by $|u_f\rangle, |u_g\rangle\cdots$. We do not use the dummy index convention for the summation over the sampling indices $f, g\cdots$. Then, we approximate $|\Psi\rangle$ as

$$|\Psi\rangle=\sum_f|u_f\rangle c_f\,. \tag{4·1}$$

The S dets $|u_f\rangle$'s are usually not orthogonal and the mixing coefficients c_f are normalized by

$$\langle\Psi|\Psi\rangle=\sum_{fg}\langle u_f|u_g\rangle c_f^*c_g=\sum_{fg}\det(z_{fg})c_f^*c_g=1\,, \tag{4·2}$$

where $z_{fg}=u_f^\dagger u_g$ is an $n\times n$ matrix. The U(N) CS wavefunction $\Phi_f(u)$ corresponding to an S det $|u_f\rangle$ is given from Eqs. (2·7) and (3·1) by

$$\left.\begin{aligned}|u_f\rangle&={}_NC_n\int|u\rangle\Phi_f(u)du\,,\\ \Phi_f(u)&=\langle u|u_f\rangle=\det(u^\dagger u_f)\,,\end{aligned}\right\} \tag{4·3}$$

so that $|\Psi\rangle$ in Eq. (4·1) corresponds to the function

$$\Psi(u)=\sum_f \langle u|u_f\rangle c_f=\sum_f \det(u^\dagger u_f)c_f\,. \tag{4·4}$$

The energy expectation value of $|\Psi\rangle$ is given from Eq. (3·14) by

$$\langle\Psi|H|\Psi\rangle=\sum_{fg}\langle u_f|H|u_g\rangle c_f^* c_g=\sum_{fg}H(W_{fg})\det(z_{fg})c_f^* c_g\,, \tag{4·5}$$

where $W_{fg}=u_g z_{fg}^{-1}u_f^\dagger$ is the interstate density matrix of $|u_f\rangle$ and $|u_g\rangle$.

We determine the $|u_f\rangle$'s and c_f's by variation of the Lagrangian

$$L=\langle\Psi|H|\Psi\rangle-E\langle\Psi|\Psi\rangle=\sum_{fg}\{H(W_{fg})-E\}\det(z_{fg})c_f^* c_g\,, \tag{4·6}$$

where E is the Lagrange multiplier to secure the normalization condition (4·2) and has the meaning of the energy of the state $|\Psi\rangle$. We shall discuss in § 6 how to choose trial $|u_f\rangle$'s. The approximation is called the resonating Hartree-Fock approximation and abbreviated as Res HF to distinguish from RHF that usually means the restricted Hartree-Fock which is the Hartree-Fock approximation with symmetry adapted orbitals. The most important feature of a Res HF wavefunction (4·1) is that it is constructed as a superposition of S dets with different correlation structures. Namely, the $|u_f\rangle$'s are unrestricted Hartree-Fock (UHF) type S dets with different broken symmetries. Some of them may have broken symmetries connected with some order parameters and others may have stronger broken symmetries representing defects in those order parameters. We shall discuss important physical aspects of the Res HF approximation in § 6.

From the variation of L with respect to c_f^* we get the equation to determine the mixing coefficients c_f

$$\sum_g\{H(W_{fg})-E\}\det(z_{fg})c_g=0\,. \tag{4·7}$$

This equation is called the Res HF CI (configuration interaction) equation.

We next derive the variation equation to determine the $|u_f\rangle$'s. To make this, we first consider the variation of an interstate density matrix $W=vz^{-1}u^\dagger$, $z=u^\dagger v$. We note that W is invariant to a general linear transformation, $u\to ux$ and $v\to vx$ where x is an arbitrary $n\times n$ matrix with $\det(x)\neq 0$. Hence u and v can be regarded as arbitrary $N\times n$ matrices with $\det(u^\dagger v)\neq 0$, so that we can make constraintless variation of u and v, $u\to u+\delta u$ and $v\to v+\delta v$. Using the relation

$$\delta z^{-1}=-z^{-1}\delta z z^{-1}=-z^{-1}(\delta u^\dagger v+u^\dagger\delta v)z^{-1} \tag{4·8}$$

in $\delta W=\delta v z^{-1}u^\dagger+vz^{-1}\delta u^\dagger+v\delta z^{-1}u^\dagger$, we obtain

$$\left.\begin{aligned}&\delta W=D(1-W)+(1-W)\tilde{D}\,,\\ &D=vz^{-1}\delta u^\dagger\,,\qquad \tilde{D}=\delta v z^{-1}u^\dagger\,.\end{aligned}\right\} \tag{4·9}$$

From Eq. (3·4), the variation of the overlap integral (3·1) is given by

$$\delta(\det z)=\mathrm{tr}(z^{-1}\delta z)\det z=\mathrm{tr}(D+\tilde{D})\det z\,. \tag{4·10}$$

We obtain also

$$\left.\begin{aligned}&\delta H(W)=F_{ij}(W)\delta W_{ji}=\mathrm{tr}(F\delta W)\,,\\&F_{ij}(W)=\delta H(W)/\delta W_{ji}=h_{ij}+[ij|kl]\,W_{lk}\,.\end{aligned}\right\}\tag{4·11}$$

The $N\times N$ matrix $F(W)$ is called the interstate Fock operator since it has the same form as the Fock operator in the HF approximation with only one difference to have the interstate density matrix instead of the usual HF density matrix.

Let $L=\{H(W)-E\}\det z$, then from Eqs. (4·9)~(4·11) we have

$$\delta L=\mathrm{tr}[\{(1-W)F+H-E\}D+\tilde{D}\{F(1-W)+H-E\}]\det z\,.\tag{4·12}$$

From Eqs. (4·6), (4·12) and (4·9), the variation equation $\delta L/\delta u^{*}_{ia}=0$ is given as

$$\sum_{g}[\{(1-W_{fg})F(W_{fg})+H(W_{fg})-E\}u_{g}z^{-1}_{fg}]_{ia}\det(z_{fg})c_{f}{}^{*}c_{g}=0\,.\tag{4·13}$$

By multiplying $u_{f}{}^{\dagger}$ from right, Eq. (4·13) becomes

$$\left.\begin{aligned}&\sum_{g}K_{fg}\,c_{f}{}^{*}c_{g}=0\,,\\&K_{fg}=\{(1-W_{fg})F(W_{fg})+H(W_{fg})-E\}\,W_{fg}\,\det z_{fg}\,.\end{aligned}\right\}\tag{4·14}$$

We call Eq. (4·14) the Res HF equation. The Res HF CI equation (4·7) can be derived from Eq. (4·14), by multiplying $u_{f}{}^{\dagger}$ from left and u_{f} from right and using the relation

$$u_{f}{}^{\dagger}W_{fg}=u_{f}{}^{\dagger}\,.\tag{4·15}$$

Therefore, Eq. (4·14) only is enough to determine both u_{f}'s and c_{f}'s.

The matrices u_{f} satisfy the unitarity condition $u_{f}{}^{\dagger}u_{f}=1$. We can obtain the variation equation for the u_{f}'s under the unitarity constraint. The Lagrangian to take it explicitly into account is

$$L^{c}=\sum_{f}[\{H(W_{ff})-E\}|c_{f}|^{2}-\sum_{a}\tilde{\varepsilon}_{fa}(u_{f}{}^{\dagger}u_{f})_{aa}]+\sum_{fg}{}'L_{fg}c_{f}{}^{*}c_{g}\,,\tag{4·16}$$

where $z_{ff}=1$, $W_{ff}=u_{f}u_{f}{}^{\dagger}$, $L_{fg}=\{H(W_{fg})-E\}\det z_{fg}$, the primed summation is made under the restriction $g\neq f$ and the $\tilde{\varepsilon}_{fa}$'s are the Lagrange multipliers to secure the unitarity of the u_{f}'s. Using Eq. (4·12), we obtain from variation of L^{c} the equation

$$[\{F(W_{ff})|c_{f}|^{2}+\sum_{g}{}'K_{fg}c_{f}{}^{*}c_{g}\}u_{f}]_{ia}=\tilde{\varepsilon}_{fa}u_{fia}\,.\tag{4·17}$$

By using the following relations obtained from Eqs. (4·15) and (4·7)

$$\left.\begin{aligned}&K^{\dagger}_{fg}u_{f}=\{H(W_{gf})-E\}\det z_{gf}u_{f}\,,\\&\sum_{g}{}'\{H(W_{gf})-E\}\det(z_{gf})c_{g}{}^{*}c_{f}=-\{H(W_{ff})-E\}|c_{f}|^{2}\,,\end{aligned}\right\}\tag{4·18}$$

Eq. (4·17) can be written as

$$\left.\begin{aligned}&[F_{f}u_{f}]_{ia}=\varepsilon_{fa}u_{fia}\,,\\&F_{f}=F(W_{ff})|c_{f}|^{2}+\sum_{g}{}'\{K_{fg}c_{f}{}^{*}c_{g}+K^{\dagger}_{fg}c_{f}c_{g}{}^{*}\}\,,\\&\varepsilon_{fa}=\tilde{\varepsilon}_{fa}-\{H(W_{ff})-E\}|c_{f}|^{2}\,.\end{aligned}\right\}\tag{4·19}$$

This is a set of coupled nonlinear eigenvalue equations for the u_{f}'s and is called the

Res HF eigenvalue equation. It includes as a special case the well known HF eigenvalue equation. The hermitian $N\times N$ matrices F_f are called the Res Fock operators. Equation (4·19) shows that every S det $|u_f\rangle$ in a Res HF state has its own orbital energies ε_{fa}, $a=1\cdots n$. Therefore, the orbital concept is still surviving in the Res HF approximation. Different orbital motions are in resonance in a Res HF state. A particle in one of those orbital motions, that corresponds to an S det $|u_f\rangle$, moves in a mean field given by the Res Fock operator F_f.

The two forms of the Res HF equation, Eqs. (4·19) and (4·14) are equivalent. From Eq. (4·19), we have

$$F_f W_{ff}=W_{ff}F_f\,. \tag{4·20}$$

This equation showing the commutability of the two hermitian matrices F_f and W_{ff} implies that they have common eigenvectors to diagonalize them so that it leads to Eq.(4·19). Therefore, Eqs.(4·19) and (4·20) are equivalent. Because of the idempotency of W_{ff}, $W_{ff}^2=W_{ff}$, Eq. (4·20) is equivalent to

$$F_f W_{ff}-W_{ff}F_f W_{ff}=0\,. \tag{4·21}$$

Using the relations

$$W_{ff}W_{fg}=W_{ff}\,,\qquad W_{fg}W_{ff}=W_{fg}\,,\qquad W_{gf}W_{ff}=W_{ff}\,, \tag{4·22}$$

and Eq. (4·7), we can show

$$F_f W_{ff}-W_{ff}F_f W_{ff}=\sum_g K_{fg}c_f{}^*c_g\,. \tag{4·23}$$

Hence, the equivalence of Eqs. (4·19) and (4·14) has been proved.

Once the S dets $|u_f\rangle$ in the Res HF ground state are determined, then the Res HF CI equation (4·7) gives a series of excited states. We call these excited states the Res HF excited states. The Hilbert subspace spanned by the Res HF ground and excited states is called the Res HF subspace. Since the Res HF subspace is spanned by the S dets $|u_f\rangle$'s the projection operator to it is given by

$$P=\sum_{fg}|u_f\rangle(S^{-1})_{fg}\langle u_g|\,, \tag{4·24}$$

where $S=(S_{fg})$ is the matrix composed of the overlap integrals $S_{fg}=\langle u_f|u_g\rangle$. The partition function in the Res HF subspace is given by

$$\mathrm{tr}(Pe^{-\beta H})=\sum_{fg}\langle u_f|e^{-\beta H}|u_g\rangle(S^{-1})_{gf}\,. \tag{4·25}$$

We will discuss elsewhere how to calculate the partition function.

§ 5. Resonance of degenerate broken symmetry Slater determinants
—— *the generalized Peierls-Yoccoz projection* ——

We now consider a system with a symmetry group G. G is a subgroup of U(N) since an element s in G induces a linear transformation of the creation and annihilation operators in a manner of Eq. (2·4) and there is a unitary operator $U(s)$ that is a

special case of $U(u)$ and makes a representation of G. Let $|u\rangle$ be a broken symmetry S det. All the elements s of G that leave $|u\rangle$ invariant, $|su\rangle=|u\rangle$, make a subgroup G_u of G. For an $s\neq 1$ in the right coset G/G_u, $|su\rangle\neq|u\rangle$ but they are degenerate in energy. We call the set $\{|su\rangle;\ s\in G/G_u\}$ of degenerate broken symmetry S dets the Goldstone set of $|u\rangle$. Degenerate S dets in a Goldstone set are in just resonance. We consider in the following this special kind of resonance.

Let $|QK\rangle$ be a state belonging to an irrep Q of G. It transforms for operation of G as

$$U(s)|QK\rangle=\sum_M|QM\rangle D^Q_{MK}(s)\,, \tag{5·1}$$

where the $D^Q_{MK}(s)$'s are matrix elements of an irrep Q of G satisfying

$$\left.\begin{aligned} &D^Q_{MK}(ss')=\sum_{M'}D^Q_{MM'}(s)D^Q_{M'K}(s')\,,\\ &D^Q_{MK}(s^{-1})=D^{Q*}_{KM}(s)\,,\qquad D^Q_{MK}(1)=\delta_{MK}\end{aligned}\right\} \tag{5·2}$$

and the quantum numbers M and K denote orthogonal bases of the irrep. We do not write in $|QK\rangle$ the other quantum numbers unrelated to G. From Eq. (2·7) and $U(s)|u\rangle=|su\rangle$ we obtain

$$U(s)|QK\rangle={}_NC_n\int|su\rangle\langle u|QK\rangle du\,. \tag{5·3}$$

Matrix elements of irreps of G satisfy the orthonormal relation

$$\int D^{Q*}_{MK}(s)D^{Q'}_{M'K'}(s)ds=d_Q{}^{-1}\delta_{QQ'}\delta_{MM'}\delta_{KK'}\,, \tag{5·4}$$

where d_Q is the dimension of the irrep Q and the integration is the normalized group integration on G. If G is a discrete group, the integration is the normalized summation on G. From Eqs. (5·1)~(5·4), we obtain a U(N) CS rep of a symmetry adapted wavefunction

$$\left.\begin{aligned} &|QM\rangle=d_Q\cdot{}_NC_n\int|\Phi^Q_{MK}(u)\rangle\Psi_K{}^Q(u)du\,,\\ &\Psi_K{}^Q(u)=\langle u|QK\rangle\,,\end{aligned}\right\} \tag{5·5}$$

$$|\Phi^Q_{MK}(u)\rangle=\int D^{Q*}_{MK}(s)|su\rangle ds\,. \tag{5·6}$$

The wavefunction defined by Eq. (5·6) is called the projected Slater determinant (PS det) because a broken symmetry S det $|u\rangle$ is projected to an irrep Q as shown below. This method of projection to make the group integration with an irrep matrix was first introduced by Peierls and Yoccoz in description of rigid rotational motion of a deformed nucleus[15] and is called the Peierls-Yoccoz projection. The universal significance of the Peierls-Yoccoz projection in exact CS reps were noted in Refs. 8) and 16).

A PS det transforms for a symmetry operation as

$$U(s)|\Phi^{Q}_{MK}(u)\rangle=\int D^{Q*}_{MK}(s')|ss'u\rangle ds'$$
$$=\int D^{Q*}_{MK}(s^{-1}s')|s'u\rangle ds'=\sum_{M'}|\Phi^{Q}_{M'K}(u)\rangle D^{Q}_{M'M}(s)\,, \tag{5·7}$$

where we have used Eq. (5·2). This shows that $|\Phi^{Q}_{MK}(u)\rangle$ belongs to the irrep Q and the index M responds to usual symmetry operations from outside. We can see in a similar way that the index K responds to transformations of the argument u:

$$|\Phi^{Q}_{MK}(su)\rangle=\sum_{K'}D^{Q}_{KK'}(s)|\Phi^{Q}_{MK'}(u)\rangle\,. \tag{5·8}$$

By using Eqs. (5·2) and (5·4), the inner product and the matrix element of the Hamiltonian between PS dets are calculated to be

$$\left.\begin{aligned}&\langle\Phi^{Q}_{MK}(u)|\Phi^{Q'}_{M'K'}(v)\rangle=d_Q^{-1}\delta_{QQ'}\delta_{MM'}S^{Q}_{KK'}(u,v)\,,\\&S^{Q}_{KK'}(u,v)=\langle u|\Phi^{Q}_{KK'}(v)\rangle=\int D^{Q*}_{KK'}(s)\langle u|sv\rangle ds\,,\end{aligned}\right\} \tag{5·9}$$

$$\left.\begin{aligned}&\langle\Phi^{Q}_{MK}(u)|H|\Phi^{Q'}_{M'K'}(v)\rangle=d_Q^{-1}\delta_{QQ'}\delta_{MM'}H^{Q}_{KK'}(u,v)\,,\\&H^{Q}_{KK'}(u,v)=\langle u|H|\Phi^{Q}_{KK'}(v)\rangle=\int D^{Q*}_{KK'}(s)\langle u|H|sv\rangle ds\,.\end{aligned}\right\} \tag{5·10}$$

From Eqs. (5·5), (5·9) and (5·10), the Schrödinger equation $(H-E)|QM\rangle=0$ can be brought into the projected U(N) CS rep as

$$\sum_{K'}\int\{H^{Q}_{KK'}(u,v)-ES^{Q}_{KK'}(u,v)\}\Psi^{Q}_{K'}(v)dv=0\,. \tag{5·11}$$

The above results are exact. However, we have to note here that the Peierls-Yoccoz projection is always meaningful in a finite system but it may become meaningless in a large system with a very large particle number n. In a large system, all S dets in a Goldstone set may become asymptotically orthogonal, i.e., $\langle u|su\rangle$ may approach 0 for all $s\neq 1$ in G/G_u in the limit $n\to\infty$, because all the eigenvalues ρ_a, $a=1\cdots n$, of the matrix $u^{\dagger}su$ have absolute values smaller than 1 and $\langle u|su\rangle=\det(u^{\dagger}su)=\rho_1\cdots\rho_n$. Such a situation arises, for instance, in simultaneous rotation of spins in a spin density wave state. Then, the Peierls-Yoccoz projection has no sense and the system has a real broken symmetry. This is an explanation for the well known possibility of real broken symmetry in a large system from the U(N) CS rep theory. In the following, we consider only a symmetry group having Goldstone sets with non-orthogonal S dets.

We now consider a Res HF wavefunction composed of various Goldstone sets. S dets in a Goldstone set are degenerate so that they are in just resonance. The above theory shows that their mixing coefficients are determined only by the symmetry group and the symmetry is recovered in a Res HF wavefunction with resonance in every Goldstone set. It is given in the form

$$|QM\rangle=d_Q^{1/2}\sum_{fK}|\Phi^{Q}_{MK}(u_f)\rangle c^{Q}_{fK}\,, \tag{5·12}$$

where the S dets $|u_f\rangle$'s belong to different Goldstone sets. It is called the projected Res HF (P Res HF) wavefunction. The Lagrangian for a P Res HF wavefunction is

$$L^Q=\langle QM|(H-E)|QM\rangle$$
$$=\sum_{fgKK'}\{H^Q_{KK'}(u_f,u_g)-ES^Q_{KK'}(u_f,u_g)\}c^{Q*}_{fK}c^Q_{gK'}$$
$$=\sum_{fgKK'}c^{Q*}_{fK}c^Q_{gK'}\int D^{Q*}_{KK'}(s)\{H[W_{fg}(s)]-E\}\det z_{fg}(s)ds\,, \tag{5·13}$$

where $z_{fg}(s)=u_f{}^\dagger s u_g$ and $W_{fg}(s)=su_g z^{-1}_{fg}(s)u_f{}^\dagger$. The variation equations for c^Q_{fK} and u_f are given by

$$\sum_{gK'}\{H^Q_{KK'}(u_f,u_g)-ES^Q_{KK'}(u_f,u_g)\}c^Q_{gK'}=0\,, \tag{5·14}$$

$$\sum_{gKK'}c^{Q*}_{fK}c^Q_{gK'}\int D^{Q*}_{KK'}(s)K_{fg}(s)ds=0\,,$$

$$K_{fg}(s)=\{(1-W_{fg}(s))F(W_{fg}(s))+H(W_{fg}(s))-E\}W_{fg}(s)\det z_{fg}(s)\,. \tag{5·15}$$

In Eqs. (5·12) and (5·15), the number of independent S dets are reduced compared to Eqs. (4·1) and (4·14) where no consideration of broken symmetries of resonating S dets is made. The mixing coefficients c^Q_{fK} are already partially diagonalized with respect to the symmetry recovered by the resonance within Goldstone sets and the energy eigenvalues have a dispersion with respect to the irrep index Q, $E=E^Q$.

§ 6. Discussion

In order to apply the Res HF approximation to a concrete system, it is necessary to have a guiding principle how to choose a trial of sampling S dets. This technical problem is just equivalent to the most important physical problem, what are the correlation structures which are most effectively resonating in a given Fermion system. A clue for this problem in condensed matter systems is obtained from consideration of low energy solutions of the HF equation in a one dimensional electronic system.

The HF ground state in a commensurate, e.g., half filled, one dimensional system is a state with a long range order such as a spin density wave (SDW) or a charge density wave (CDW). It is a very important fact that the HF equation has low energy solutions representing localized defects in the long range order, such as solitons and polarons.[17)~19)] We use the words solitons and polarons in a sense to represent purely electronic defects that do not involve lattice distortions. The HF ground state with a long range order usually has several degenerate inequivalent phases due to its broken symmetry. A soliton is a localized defect connecting a ground state phase to another and a polaron is a defect with a localized change of the long range order but does not convert the ground state phases.

Static soliton and polaron solutions break the translational symmetry. There are degenerate soliton (polaron) solutions $|S_n\rangle(|P_n\rangle)$ which are different only in the position n of their centers. Two soliton solutions $|S_n\rangle$ and $|S_{n+m}\rangle$ are non-orthogonal if they are separated by a finite distance and their regions of varying order parameter have an overlap. They are not asymptotically orthogonal unless their separation is infinite because their wavefunctions are different only in a finite region. Therefore, the set $\{|S_n\rangle\}$ is a Goldstone set with non-orthogonal S dets. Similar situation holds

also in polaron solutions $|P_n\rangle$. The theory developed in § 5 can be applied to soliton and polaron solutions. An irrep of the Abelian translational group is always one dimensional and characterized by a dimensionless wave number q. The resonance in the Goldstone set $\{|S_n\rangle\}$ just corresponds to make moving soliton wavefunctions

$$|S_q\rangle = A\sum_n e^{iqn}|S_n\rangle\,, \tag{6·1}$$

where A is a normalization constant. Thus, the resonance of degenerate soliton (polaron) solutions give a soliton (polaron) band.

The HF equation has not only the solutions representing a soliton or polaron but also solutions representing many solitons and polarons. Let us consider solutions $|S_{n-m}, \bar{S}_{n+m}\rangle$ representing a soliton-antisoliton pair. Such static solutions exist if the distance between the soliton and antisoliton is large enough to make their wavefunctions having no overlap. If the wavefunctions of a soliton and an antisoliton have an overlap, then no stable static solution of the pair may exist but a time dependent solution corresponding to a dynamical bound state of a soliton-antisoliton pair, a breather, may exist. Resonating wavefunctions in the form

$$|S\bar{S}_q\rangle = A\sum_n e^{iqn}\sum_m |S_{n-m}, \bar{S}_{n+m}\rangle c_m\,, \tag{6·2}$$

may represent bands of a breather and an unbound soliton-antisoliton pair. Thus, the Res HF approximation may provide a method of quantizing a breather.

If the total charge and spin of a soliton-antisoliton pair are zero, then the wavefunction $|S\bar{S}_0\rangle$ can be mixed with the HF ground state $|u_0\rangle$ because the wavefunction $|S_{n-m}, \bar{S}_{n+m}\rangle$ differs from $|u_0\rangle$ only in a finite region so that $|S\bar{S}_0\rangle$ is not asymptotically orthogonal to $|u_0\rangle$. More generally, the Res HF ground state may have mixing of any number of soliton-antisoliton pairs and polaron-antipolaron pairs

$$|\text{Res HF}_0\rangle = c_0|u_0\rangle + c_1|S\bar{S}_0\rangle + \cdots\,. \tag{6·3}$$

The resonance of this kind will stabilize the ground state because a soliton-antisoliton pair and a polaron-antipolaron pair are separated from the HF ground state by finite and usually small energies and their wavefunctions have finite overlaps to each other giving finite off-diagonal matrix elements of H. We note that dynamical bound states breathers may have an important contribution in the ground state resonance because a soliton and antisoliton pair in them has smaller separation than a stable static separated pair so that it has a larger overlap to $|u_0\rangle$.

In two and three dimensional systems, solitons usually have one or two dimensional extensions and really localized solitons are exceptional. Polarons, on the other hand, can be really localized and may be the most important defects in Res HF states in a two or three dimensional system. Bound states of polarons and antipolarons, which are equivalent to drops of bound particle-hole pairs, may also be conceivable as localized defects. However, no systematic study has been made about HF solutions representing localized defects in two and three dimensional systems. It is an important problem to be studied.

Summarizing the above discussion, we can suggest that S dets involved in low energy solutions of the HF equation, both static and dynamical, which represent

localized defects in the long range order of the HF ground state will be the physically most resonable trial for a Res HF wavefunction.

In a large system, resonance between S dets with different long range orders or belonging to different phases of a long range order cannot take place because they are asymptotically orthogonal. In a finite system, such resonance is possible. The ground state of Res HF type can exist even in small molecular systems. We found that the ground state of a diatomic molecule, carbon mono-oxide, at large interatomic distances has resonance of at least two S dets with different broken symmetries.[8),20)] Transition region nuclei may have the possibility of resonance between a superconductive state with a small deformation and a HF state with a large deformation. Direct application of the present theory cannot be made because a superconductive state is involved. However, it is possible to make generalization of the present theory to include superconductive system. We derived another exact CS rep on SO (2N) (special orthogonal group of 2N dimension) which represents a Fermion wavefunction by superposing Hartree-Bogoliubov wavefunctions and can treat superconductive systems.[9)] We shall derive elsewhere a resonating Hartree-Bogoliubov theory that may be useful to study nuclear collective motions and high T_c superconductivity.

If we have a reasonable trial, there is a problem of how to calculate a Res HF wavefunction. It may be possible to solve iteratively the Res HF eigenvalue equation (4·19) as usually done for the HF equation. However, in a system where resonance is important, the HF energy $\langle u|H|u\rangle$ and perhaps the off-diagonal matrix element $\langle u|H|v\rangle$ too have rather complicated structures with many minima, suddle points and maxima. Therefore, it is very likely to meet difficulties in convergence if we try to solve Eq. (4·19) iteratively as we have often experienced in the HF equation. We can develop a direct optimization algorism to avoid difficulties in convergence. It will be described elsewhere.

The Res HF approximation can treat large quantum fluctuations which cannot be described by RPA and mode-mode coupling theories. It also is able to take into account small quantum fluctuations which are describable by RPA. We can derive a generalized RPA for small quantum fluctuations of S dets involved in a Res HF state. It is derived from the time dependent Res HF theory in a similar manner to the time dependent HF derivation of RPA. However, algebraic manipulations involved are complicated. So, it will be described elsewhere.

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