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Nuclear Physics 58 (1964) 678—686; © *North-Holland Publishing Co., Amsterdam*

THE COLLECTIVE VIBRATIONS OF A MANY-FERMION SYSTEM

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Received 21 February 1964

Abstract: The energy levels of a many-fermion system are investigated through an extension of the generator coordinate method of Peierls-Yoccoz and Wheeler-Griffin. A trial wave function Ψ for the system is taken as a superposition $\Psi = \int F(z)\Phi(z)\mathrm{d}z$ of all possible independent particle wave functions Φ in the neighbourhood of the Hartree-Fock ground-state wave function Φ_0; the functions Φ depend on many parameters z. An integral equation is established for the generator function $F(z)$ Through appropriate approximations, this integral equation is transformed into the Schrödinger equation for a set of coupled harmonic oscillators, which can be solved. The energies and wave functions are obtained for the ground state and the low excited states of the system. The present approach is equivalent to the random phase approximation.

1. Introduction

The present paper contains few new results; it provides mainly one more presentation of an approximation method already known, under various names and forms, as the random phase approximation [1]), the quasi-boson approximation [2-4]) and the time-dependent Hartree-Fock approximation [5]). The present approach, however, provides a link with the simpler generator coordinate method [6-7]); and also, in our opinion, it may cast some additional light on the physical meaning of the theory.

One of the simplest descriptions, at least in principle, of a many-fermion system, is through the Hartree-Fock approximation. The ground-state wave function Φ_0 then is the one among all independent-particle wave functions, which minimizes the energy; Φ_0 is built from the one-particle eigenstates in some fixed potential.

The generator coordinate method††† was devised to describe the collective motions of the system, by allowing the potential well to undergo displacements or deformations specified by one or a few parameters α. From the one-particle eigenstates of the modified well, an independent-particle wave function $\Phi(\alpha)$ can be made, which depends on the parameters α. The generator coordinate method takes as a trial wave function a superposition

$$\Psi = \int F(\alpha)\Phi(\alpha)\mathrm{d}\alpha, \tag{1}$$

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†† Work supported in part by the United States Air Force through the European Office, Office of Aerospace Research.

††† Ref. [6]) is very illuminating in its description of the physical meaning of the generator coordinate method.

where $F(\alpha)$ is a "generator function" which is to be determined by the requirement that the energy be stationary; an integral equation is obtained in this way, with $F(\alpha)$ as its eigenfunction and the corresponding energy as its eigenvalue. This method has very nice features, the collective coordinates α appear only as integration "generator" variables in eq. (1) and therefore there are no redundant variables. Furthermore, a formulation with a trial wave function like eq. (1) is conceptually simple. Unfortunately, the method in its primitive version, failed to reproduce properly the right energy of the centre-of-mass motion, in the case of a uniform translation; this defect probably hindered further developments very much. More recently, however, it was shown that the defect could be eliminated by including more independent-particle wave functions $\Phi(\alpha)$ in eq. (1) (cf. ref. [8])). Therefore, it seems that the time has now come to reinvestigate what can be done with wave functions like eq. (1) for the description of collective vibrations. This is the subject of the present paper.

The trial wave function form will be discussed in sect. 2. An integral equation for determining this wave function and the corresponding energy will be derived in sect. 3. The equation will be solved in sect. 4.

2. The Trial Wave Function

In accordance with the ideas underlining the generator coordinate method, the trial wave function for N particles will be chosen as a superposition of independent-particle wave functions Φ, the class of which will be taken here as large as possible. It has been shown [9]) that Φ can be constructed in the following way.

As a starting point, a complete orthonormal set of one-particle wave functions ϕ_i is defined. A Slater determinant Φ_0 is built with the first N wave functions ϕ_i. Then, any N-independent particle wave function which is not orthogonal to Φ_0 can be written as a Slater determinant Φ built with the N one-particle wave functions

$$\chi_i = \phi_i + \sum_{m=N+1}^{\infty} z_{mi}^* \phi_m, \qquad (1 \leqq i \leqq N), \tag{2}$$

where the complex coefficients z_{mi} define Φ in a unique way †. In terms of the annihilation and creation operators a_i and $a_m^\dagger$ in the states ϕ_i and ϕ_m, respectively, Φ can be written as

$$\Phi(z) = \prod_{i=1}^{N} \prod_{m=N+1}^{\infty} (1 + z_{mi}^* a_m^\dagger a_i)\Phi_0 = \exp\Big(\sum_{i=1}^{N} \sum_{m=N+1}^{\infty} z_{mi}^* a_m^\dagger a_i\Big)\Phi_0 . \tag{3}$$

It may be noted that $\langle \Phi_0 | \Phi \rangle$ is unity, but that $\langle \Phi | \Phi \rangle$ is not; this non-unity norm for Φ and the appearance of Φ_0 in eq. (3) as a reference state make this formulation especially useful for the description of states Φ which do not differ too much from Φ_0, in which case the coefficients z_{mi} are small; Φ_0 will be taken as the ground-state wave function in the Hartree-Fock approximation.

† The choice of the complex conjugates z_{mi}^* in eq. (2) will later prove convenient.

The coefficients z_{mi} will now be used as a generalization of the generator coordinates α. The trial wave function Ψ is chosen as a superposition

$$\Psi = \int F(z)\Phi(z)\mathrm{d}z, \tag{4}$$

where z denotes the ensemble of all variables z_{mi}.

The generator function F, to be determined, is a function of all the variables z_{mi} (that is to say a function of their real and imaginary parts x_{mi} and y_{mi}). The integration is to be taken on the whole complex plane of each variable z_{mi} (that is to say on all the variables x_{mi} and y_{mi} separately).

3. An Equation for the Generator Function

The generator function F which appears in eq. (4) is now to be determined through the requirement that Ψ makes the energy stationary. With the energy E appearing as a Lagrange multiplier, the quantity to be stationary is

$$\langle\Psi|H|\Psi\rangle - E\langle\Psi|\Psi\rangle = \iint F^*(z)[\langle\Phi(z)|H|\Phi(z')\rangle - E\langle\Phi(z)|\Phi(z')\rangle]F(z')\mathrm{d}z\mathrm{d}z', \tag{5}$$

where H is the total Hamiltonian of the system. The stationary character of this expression (5) with respect to F^* leads to the integral equation

$$\int [\langle\Phi(z)|H|\Phi(z')\rangle - E\langle\Phi(z)|\Phi(z')\rangle]F(z')\mathrm{d}z' = 0. \tag{6}$$

This equation should give the energy E as its eigenvalue and the generator function F as its eigenfunction.

In order to solve eq. (6) it is necessary to evaluate the overlap kernel $\langle\Phi(z)|\Phi(z')\rangle$ and the Hamiltonian kernel $\langle\Phi(z)|H|\Phi(z')\rangle$. Since $\Phi(z)$ is the Slater determinant built with the one-particle-wave-function χ_i defined by eq. (2), the overlap kernel is easily shown to be the $N \times N$ determinant

$$\langle\Phi(z)|\Phi(z')\rangle = \det|\langle\chi_i(z)|\chi_j(z')\rangle| = \det|\delta_{ij} + A_{ij}|, \tag{7}$$

$$A_{ij} = \sum_{m=N+1}^{\infty} z_{mi} z'^*_{mj}.$$

Expression (7) is exact. In order, however, that eq. (6) be a tractable equation, approximations will be made on the kernels. Although the matrix A in general is not hermitian, it can be put at least in a triangular form [10], the diagonal elements of which are the characteristic values A_i, and eq. (7) can be written as

$$\langle\Phi(z)|\Phi(z')\rangle = \prod_{i=1}^{N} (1 + A_i). \tag{8}$$

The approximation will consist in replacing the exact expression (8) by

$$\langle\Phi(z)|\Phi(z')\rangle \approx \exp\Big(\sum_{i=1}^{N} A_i\Big) = \mathrm{e}^{\mathrm{Tr}\,A} = \exp\Big(\sum_{i=1}^{N} \sum_{m=N+1}^{\infty} z_{mi} z'^*_{mi}\Big). \tag{9}$$

This approximation is valid if every characteristic value A_i is small compared to unity, although N may be large. Since we are interested in small vibrations around Φ_0, we assume that the main contribution to Ψ comes from determinants Φ which are close to Φ_0, in the sense that each one-particle wave function χ_i is close to the corresponding function ϕ_i. More precisely, this means that all the matrix elements A_{ij} are small compared to unity. This does not ensure the smallness of all the *characteristic* values of A in general. In most cases, however, the characteristic values will be of the order of the matrix elements, and we therefore assume that the characteristic values are actually small, and therefore that the approximation (9) is valid †.

An alternative justification of (9) can be given through the usual quasi-boson picture [2]). If Φ is written as the last expression in eq. (3) and if the operator product $a_m^\dagger a_i$ is approximated by a boson creation operator, eq. (9) follows without further approximation.

We now proceed to the evaluation of the Hamiltonian kernel. The Hamiltonian is

$$H = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij} a_i^\dagger a_j + \tfrac{1}{2}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\sum_{l=1}^{\infty} V_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k; \tag{10}$$

the first term describes the kinetic energy and possibly the interactions with external fields, the second term is the usual interaction between the particles. Since H acts at most on two particles at a time, the Hamiltonian kernel will behave much like the overlap kernel. We shall expand the ratio of these kernels in powers of the z_{mi} and z'^*_{mi} up to the second order only. One finds

$$\begin{aligned}\frac{\langle\Phi(z)|H|\Phi(z')\rangle}{\langle\Phi(z)|\Phi(z')\rangle} \approx E_0 &+ \sum_{i=1}^{N}\sum_{m=N+1}^{\infty}(\varepsilon_m-\varepsilon_i) z_{mi} z'^*_{mi} \\ &+ \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{m=N+1}^{\infty}\sum_{n=N+1}^{\infty}[(V_{in,mj}-V_{in,jm}) z_{nj} z'^*_{mi} + \tfrac{1}{2}(V_{ij,mn}-V_{ij,nm}) z'^*_{mi} z'^*_{nj} \\ &+ \tfrac{1}{2}(V_{mn,ij}-V_{nm,ij}) z_{mi} z_{nj}],\end{aligned} \tag{11}$$

where E_0 is the Hartree-Fock ground-state total energy, and ε_i the Hartree-Fock energy of the one-particle state ϕ_i:

$$\varepsilon_i = T_{ii} + \sum_{m=1}^{N}(V_{im,im}-V_{im,mi}). \tag{12}$$

There are no first order terms, because Φ_0 is the Hartree-Fock ground state. In order to have a more compact notation, we shall replace by one Greek index like α each pair of indices like i and m ($i \leqq N, m > N$) which appear together; eq. (11) for instance is then written as

$$\frac{\langle\Phi(z)|H|\Phi(z')\rangle}{\langle\Phi(z)|\Phi(z')\rangle} = E_0 + \sum_{\alpha\beta}(K_{\alpha\beta} z_\alpha z'^*_\beta + \tfrac{1}{2} W^*_{\alpha\beta} z'^*_\alpha z'^*_\beta + \tfrac{1}{2} W_{\alpha\beta} z_\alpha z_\beta), \tag{13}$$

† The present approximation is analogous to the gaussian approximation which has been previously used [6, 7]) in which the overlap kernel $\langle\Phi(\alpha)|\Phi(\alpha')\rangle$ for normalized functions $\Phi(\alpha)$ and $\Phi(\alpha')$ was replaced by a gaussian $\exp(-s(\alpha-\alpha')^2)$.

where the numerical coefficients $K_{\alpha\beta}$ and $W_{\alpha\beta}$ are obvious combinations of the parameters T_{ij} and $V_{ij,kl}$ which appear in eq. (10). The matrix K is Hermitian and W is a symmetrical matrix.

With the appropriate forms of eqs. (9) and (13) for the kernels, the integral equation (6) becomes

$$\int [\sum_{\alpha\beta}(K_{\alpha\beta} z_\alpha z'^*_\beta + \tfrac{1}{2} W^*_{\alpha\beta} z'^*_\alpha z'^*_\beta + \tfrac{1}{2} W_{\alpha\beta} z_\alpha z_\beta) - (E - E_0)] \exp(\sum_\alpha z_\alpha z'^*_\alpha) F(z') \mathrm{d}z' = 0. \quad (14)$$

In order to avoid convergence problems, we shall cut off the number of variables z_α to some finite value M. This amounts to cutting off the set of states ϕ_m at some irrelevant high energy.

4. Resolution of the Integral Equation

It will now be shown that eq. (14) can be transformed into the well-known equation for coupled harmonic oscillators. A transformed function G can be defined as

$$G(z) = \int \exp(\sum_\alpha z_\alpha z'^*_\alpha) F(z') \mathrm{d}z'; \quad (15)$$

$G(z)$ is an analytical function of z whenever the integral converges.

Since

$$\frac{\partial G(z)}{\partial z_\alpha} = \int z'^*_\alpha \exp(\sum_\alpha z_\alpha z'^*_\alpha) F(z') \mathrm{d}z', \quad (16)$$

eq. (14) is transformed into a partial differential equation for G

$$\left[\sum_{\alpha\beta}\left(K_{\alpha\beta} z_\alpha \frac{\partial}{\partial z_\beta} + \tfrac{1}{2} W^*_{\alpha\beta} \frac{\partial^2}{\partial z_\alpha \partial z_\beta} + \tfrac{1}{2} W_{\alpha\beta} z_\alpha z_\beta\right) - (E - E_0)\right] G(z) = 0. \quad (17)$$

This is actually the Schrödinger equation for M coupled harmonic oscillators in an unusual but known [11]) representation, which is surveyed in the appendix. The operators z_α and $\partial/\partial z_\alpha$ behave like creation and annihilation operators respectively. In eq. (17), G is acted upon by an operator which is fully equivalent to the quadratic form of boson operators which appears in the quasi-boson method [3,4]), and therefore our approximation is equivalent to the quasi-boson method.

The search for the eigenvalues of eq. (17) amounts to a well known diagonalization problem [4,12]). Let us assume for the time being that Φ_0 is a non-degenerate solution of the Hartree-Fock problem and that the corresponding extremum of the energy is actually a minimum. It is then possible to find M new operators

$$B_\mu = \sum_\alpha u_{\mu\alpha} \frac{\partial}{\partial z_\alpha} + v_{\mu\alpha} z_\alpha \quad (18)$$

such that eq. (17) has the diagonal form

$$[\sum_{\mu} \nu_{\mu}(B_{\mu}^{\dagger}B_{\mu}+\tfrac{1}{2})-\tfrac{1}{2}\sum_{\alpha} K_{\alpha\alpha}-(E-E_0)]G(z) = 0. \tag{19}$$

The coefficients $u_{\mu\alpha}$, $v_{\mu\alpha}$ and the eigenfrequencies ν_{μ} are given by a system of linear equations

$$\begin{aligned} \sum_{\beta}(K_{\beta\alpha}u_{\mu\beta}-W_{\beta\alpha}^{*}v_{\mu\beta}) &= \nu_{\mu}u_{\mu\alpha} \\ \sum_{\beta}(W_{\beta\alpha}u_{\mu\beta}-K_{\beta\alpha}^{*}v_{\mu\beta}) &= \nu_{\mu}v_{\mu\alpha}. \end{aligned} \tag{20}$$

The normalization can be chosen in such a way that the operators B_{μ} obey the commutation relations

$$[B_{\mu}, B_{\rho}] = 0, \qquad [B_{\mu}, B_{\rho}^{\dagger}] = \delta_{\mu\rho}. \tag{21}$$

The eigenvalue problem (20) has $2M$ solutions; M eigenvalues ν_{μ} are real positive numbers, and only these appear in eq. (19). Eq. (19) is now the Schrödinger equation for M independent harmonic oscillators.

The ground energy is

$$E = E_0+\tfrac{1}{2}\sum_{\mu}\nu_{\mu}-\tfrac{1}{2}\sum_{\alpha}K_{\alpha\alpha}; \tag{22}$$

it is smaller than the Hartree-Fock energy E_0, because of the use of a better trial function (expression (4)), which allows for zero-point oscillations around Φ_0. To each eigenfrequency ν_{μ} is associated a vibration type excitation spectrum † with the level spacing $\hbar\nu_{\mu}$.

An explicit form can be obtained for the wave functions. The function $G(z)$ which corresponds to the ground state is the solution of the usual equations involving the lowering operators

$$B_{\mu}G(z) = 0. \tag{23}$$

The solution is of the form

$$G(z) = \exp(-\tfrac{1}{2}\sum_{\alpha\beta} c_{\alpha\beta}z_{\alpha}z_{\beta}), \tag{24}$$

where the symmetrical coefficients $c_{\alpha\beta}$ are determined through the system of linear equations

$$\sum_{\alpha} u_{\mu\alpha}c_{\alpha\beta} = v_{\mu\beta}. \tag{25}$$

It can be shown that the solution of eq. (25) actually provides symmetrical coefficients $c_{\alpha\beta}$.

The excited states can be reached through the application of elevation operators $B_{\mu}^{\dagger}$ to the ground state G function.

† Approximations (9) and (11) which lead to eq. (19) will actually break down if too highly excited states are considered.

After G has been found, the generator function F is not uniquely determined by eq. (15), because $F(z)$ is separately a function of the real and imaginary parts of z. This indetermination can be traced back to the choice of the form of the trial function (4). The independent-particle wave functions $\Phi(z)$ form an overcomplete set, since they include almost all the independent particle wave functions (almost refers to the slight restriction of non-orthogonality to Φ_0). Therefore it is natural that the coefficients $F(z)$ of the expansion cannot be uniquely determined for a given Ψ, and this is not a serious drawback. On the contrary, it is possible to use this freedom for choosing F in a convenient way. The identity

$$G(z) = \left(\frac{1}{\pi}\right)^M \int \exp\left(\sum_\alpha z_\alpha z'^*_\alpha - \sum_\alpha |z'_\alpha|^2\right) G(z')\mathrm{d}z' \tag{26}$$

is easily proved by verifying it on every term of a series expansion of G. Therefore, a possible solution to eq. (15) is

$$F(z) = \left(\frac{1}{\pi}\right)^M \exp\left(-\sum_\alpha |z_\alpha|^2\right) G(z). \tag{27}$$

If the number N of particles is large, the exponential in eq. (27) will make $F(z)$ small as soon as $\sum_m |z_{mi}|^2$ is significantly larger than $1/N$. The approximation (9) is therefore valid. Using eqs. (27) and (3) in the expression (4), and again the identity (26), one finds

$$\Psi = G(a_m^\dagger a_i)\Phi_0; \tag{28}$$

$G(a_m^\dagger a_i)$ is the operator obtained through the replacement in eq. (24) of each z_{mi} by the operator $a_m^\dagger a_i$.

It can be easily verified that in the limiting case of no interaction between the particles, G is identically unity and Ψ is the exact solution Φ_0: the independent particle wave function in the external fields.

The case when Φ_0 is a degenerate solution of the Hartree-Fock problem is important in practice, because it occurs whenever Φ_0 has less symmetry than the total Hamiltonian H. For instance, in the absence of external fields, H is invariant under translations and rotations; Φ_0 is usually not invariant under translations and sometimes not invariant under rotations. It has been shown [12]) that in such cases, eqs. (20) provide zero frequency solutions; they are associated with B operators which are Hermitian and cannot be normalized by eq. (21). Such a B_ρ actually is no longer a lowering operator associated with a vibration mode, but a displacement operator associated with a possible translation or rotation, for instance, of Φ_0. Strictly speaking, these types of motion cannot be correctly described without a modification of the prsent approximations (9) and (11), because for collective displacements no return force prevents the parameters z from becoming large. If, however, the diagonalization of eq. (17) is nevertheless attempted, one finds [13]) instead of eq. (19)

$$\left[\sum_\mu \nu_\mu (B_\mu^\dagger B_\mu + \tfrac{1}{2}) + \sum_\rho \alpha_\rho B_\rho^2 - \tfrac{1}{2}\sum_\alpha K_{\alpha\alpha} - (E - E_0)\right] G(z) = 0, \tag{29}$$

where the first sum runs over the non-zero frequency modes, and the second sum over the zero-frequency modes; to the latter are associated inertial parameters α_ρ, depending on the normalization which has been chosen for the operators B_ρ. The ground state energy is still given by eq. (22) where of course only the non-zero frequencies enter. The ground state G function is still given by the whole set of equations (23) involving both the lowering and the displacement operators, and the following calculations proceed as previously. In addition to the vibrational spectrum, there is now a continuous spectrum associated with the displacement modes. But the different types of motion are decoupled, at least within the present approximations, and the study of the vibrational modes can be carried on without worrying any longer about the displacement modes which must be separately studied.

The authors had valuable discussions with many of their colleagues, especially B. Bremond, K. Chadan, G. Flamand, D. Kastler, J. Lascoux and F. Lurçat.

Appendix

The state of a system depending on M position coordinates q_α is usually represented by a wave function $\psi(q)$, which is a complex function of the real variables q_α. An alternative representation is to use an analytic entire function $G(z)$ of M complex variables $z_\alpha = x_\alpha + iy_\alpha$. The scalar product is defined as

$$\langle G|H\rangle = \frac{1}{\pi^M}\int G^*(z)\exp\left(-\sum_\alpha |z_\alpha|^2\right)H(z)\prod_\alpha \mathrm{d}x_\alpha \mathrm{d}y_\alpha . \tag{A.1}$$

The Hilbert space is the space of functions the norm of which, defined by eq. (A.1), is finite. The operators $\partial/\partial z_\alpha$ and z_α are adjoint in the sense that

$$\langle z_\alpha G|H\rangle = \left\langle G\middle|\frac{\partial H}{\partial z_\alpha}\right\rangle , \tag{A.2}$$

and since they obey the commutation relations

$$\left[\frac{\partial}{\partial z_\alpha}, z_\beta\right] = \delta_{\alpha\beta} , \tag{A.3}$$

they represent the annihilation and creation operators; in other words, if p_α is the momentum conjugate to q_α, $\partial/\partial z_\alpha$ and z_α represent $(1/\sqrt{2})(q_\alpha + ip_\alpha)$ and $(1/\sqrt{2})(q_\alpha - ip_\alpha)$, respectively.

This representation is especially well adapted to the study of the M dimensional harmonic oscillator, the Hamiltonian of which,

$$\tfrac{1}{2}\sum_\alpha (p_\alpha^2 + q_\alpha^2), \tag{A.4}$$

leads to the very simple Schrödinger equation

$$\left[\sum_\alpha \left(z_\alpha \frac{\partial}{\partial z_\alpha} + \tfrac{1}{2}\right) - E\right] G(z) = 0. \tag{A.5}$$

The solution which corresponds to the energy

$$E = \sum_\alpha (n_\alpha + \tfrac{1}{2}) \tag{A.6}$$

is the monomial

$$G(z) = \prod_\alpha \frac{1}{\sqrt{n_\alpha!}} z_\alpha^{n_\alpha}, \tag{A.7}$$

instead of the more familiar Hermite function product which occurs in the usual representation.

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