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Contribution to the Theory of Collective Motion of Particles in Quantum Mechanical Systems

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A method for separating the collective motions in a system of interacting particles is presented. The connection between this method and Refs. 1-4 is established. An attempt is made to give a basis to the generalized heavy nucleus model.

1. MOST quantum mechanical systems that are dealt with in the various fields of physics consist of a large number of particles. The problems of finding the energy spectrum of such a system presents great mathematical difficulties. From among the quantum mechanical systems with large number of particles, we can separate out that class of systems in which collective motion, reminiscent of the motion of a continuous system, takes place. Among such systems are, for instance, heavy atomic nuclei, the electrons and ions of a metal, and others.

The problem of the approximate methods for describing such systems reduces to finding those terms in the Hamiltonian which correspond to collective motion. In the case of central forces, the problem of separating out the collective motions was solved by Zubarev [1], and for the case of Coulomb forces by Bohm and Pines [2] using a different method. An interesting method for describing collective motion, well set forth and of great generality, has been developed by Tomonaga [3,4]. The present article describes a method for separating out collective motions is systems, which is very simple in the sense that it does not require the complex apparatus of second quantization and unitary transformations. At the same time this method is quite general.

2. At the basis of the method lies the transformation of the Hamiltonian with the aid of auxiliary variables introduced into the wave function of the system, as has been described by Zubarev [1].

We consider the wave function $\Psi(r_1 \ldots r_N; t)$ describing a system whose Hamiltonian is

$$H = \sum_j \mathbf{p}_j^2/2M + {}^1/_2 \sum_{ij} G(\mathbf{r}_i, \mathbf{r}_j), \qquad (1)$$

and introduce the auxiliary ("superfluous") variable functions $\varphi_j(r_j)$ (where $j=1, 2, \ldots, N$), which for the time being are arbitrary, and instead of Ψ we shall consider the new wave function (a functional of the φ_j)

$$\Phi(r_1 \ldots r_N;\ \varphi_1(r_1) \ldots \varphi_N(r_N); t). \qquad (2)$$

since Φ depends on r_j explicitly as well as through the φ_j, the operator $\mathbf{p}_j$ must be replaced by

$$-i\hbar[\nabla_j + (\nabla_j \varphi_j)\partial/\partial\varphi_j]. \qquad (3)$$

As will be shown below, part of the potential energy can also be described in terms of the $\varphi_j(r_j)$.

Let us now make some comments about the $\varphi_j(r_j)$. We assume that $\varphi_j(r_j)$ is the wave function of the stationary state of the j-th particle in the zeroth

approximation. As will be shown later, the coordinates of the collective motion can be described in terms of the φ_j. When the φ_j are given this interpretation, the description of the collective motion in the system will be most accurate if the single-particle functions φ_j are chosen accurately. We shall consider below several special choices of the φ_j. This interpretation of the φ_j makes it possible on the one hand to obtain the Hamiltonians derived in previous works [1,2,4], and on the other hand indicates the possible paths that may be taken in solving a boundary value problem. Let us now conconsider certain special choices of the $\varphi_j(r_j)$.

3. Let us make the choice

$$\varphi_j(r_j) = N^{-1/2} \exp\{-i\mathbf{k}\mathbf{r}_j\}. \tag{4}$$

This wave function describes the stationary states of a free particle with momentum $\mathbf{p}=\hbar\mathbf{k}$. The kinetic energy operator for this choice of the φ_j can be written

$$T = -(\hbar^2/2M)\sum_j [\nabla_j + (\nabla_j \rho_k)\partial/\partial\rho_k]^2, \tag{5}$$

if we bear in mind the obvious relation

$$\sum_j \varphi_j = N^{-1/2}\sum_j \exp\{-i\mathbf{k}\mathbf{r}_j\} = \rho_k . \tag{6}$$

In order to account for states with various k in Eq. (5), we must sum over all values of k. From physical considerations $|\mathbf{k}|$ may not be infinite, and we shall therefore introduce a certain maximum wave number k_0. Thus in Eq. (5) and those that follow, whenever the index k occurs twice we are to sum over k from zero to k_0.

In the case of a central interaction the potential energy can be written

$$\frac{1}{2}\sum_{i,j} G(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{N}{2} G(k)\rho_k\rho_k^* + \frac{1}{2}\sum_{j,j,k>k_0} G(k)\, e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} + \text{const}, \tag{7}$$

$$\text{const} = -N\sum_{k<k_0} G(k),$$

where $G(k)$ is the Fourier transform of the interaction kernel, the constant is the self-energy of the particles, and N is the number of particles per unit volume.

The sum of expressions (5) and (7) gives the Hamiltonian of the system, which agrees with the Hamiltonian as obtained by Zubarev. [1] The dynamical variables ρ_k describe the collective motion of the system and can be written in terms of the stationary state free particle wave functions of Eq. (4). Following Zubarev, the ρ_k can be treated as the Fourier transform of the particle density operator

$$\rho(\mathbf{r}) = \sum_j \delta(\mathbf{r} - \mathbf{r}_j) . \tag{7a}$$

If we perform the substitution

$$-i\hbar\partial/\partial\rho_k = (4\pi e^2 N^2/k^2)^{1/2} q_k, \qquad \rho_k = -i(k^2/4\pi e N^2)^{1/2} p_{-k}, \tag{7b}$$

in the Hamiltonian we have obtained, we arrive at that of Bohm and Pines, [2] which is equivalent to that of Tomonaga, as has been shown [4].

The separation of the collective motion of the system is related to maintaining a term proportional to $[\nabla_j \rho_k\, \partial/\partial\rho_k]^2$ in the Hamiltonian. For the case of the electromagnetic and Coulomb interactions, this term is proportional to the square of the vector potential of the transverse and longitudinal fields, respectively.

4. As an example of a solution of a boundary value problem, let us consider a system of particles enclosed within a surface described by the equation

$$R = R_0\Big[1 + \sum_{m,l<l_0} \alpha_{lm} Y_{lm}(\vartheta, \varphi)\Big], \tag{8}$$

where Y_{lm} is a spherical function, and R_0 is the radius of the unperturbed sphere. From physical considerations, the summation in (8) is taken over all $l<l_0$. Since the surface bounding the system is defined by the set of particles on the boundary, surface oscillations of the order of the mean distance between particles have no physical meaning; this leads to the inequality $l<l_0$.

Our problem consists of choosing the $\varphi_j(r_j)$, in terms of which we can express the collective coordinates. In the approximation of a constant particle density in the system (neglecting compressibility) we may choose the $\varphi_j(r_j)$ in the form

$$\varphi_j(r_j) = \exp\{iS_j(r_j)/\hbar\}, \tag{9}$$

where the S_j give the velocity potential of the j-th

particle up to a factor of $1/M$. In the constant-density approximation the stationary particle states are given by the functions of Eq. (9) with

$$S_j(r_j) = \beta_{lm} Y_{lm}(\vartheta_j, \varphi_j) r_j^l. \tag{10}$$

The function S_j is a solution of the Laplace equation satisfying the boundary condition

$$(\partial S_j/\partial r_j)_{r_j=R} = \partial R/\partial t, \tag{11}$$

which makes it possible to express the β_{lm} coefficients in terms of the normal coordinates of the surface α_{lm}. For small oscillations we have

$$\beta_{lm} = l^{-1} R_0^{2-l} \dot{\alpha}_{lm}. \tag{12}$$

Let us consider the kinetic energy operator

$$T = -(\hbar^2/2M) \sum_j [\nabla_j + (\nabla_j S_j)\, \partial/\partial S_j]^2 \tag{13}$$

and transform from the variables S_j to α_{lm}:

$$T = -(\hbar^2/2M) \sum_j [\nabla_j + (\nabla_j \alpha_{lm})\, \partial/\partial \alpha_{lm}]. \tag{14}$$

Here, as in the previous problem, we sum from zero to l_0 over all indices m and l which occur twice, so as to take account of all possible stationary single-particle states.

In order to interpret the expression $(\nabla_j \alpha_{lm})$, we must write α_{lm} in terms of the particle coordinates $\mathbf{r}_j$. For this purpose, let us introduce the function $S = \Sigma_j S_j$. It is clear that

$$\nabla_j S_j \frac{\partial}{\partial S_j} = \nabla_j S \frac{\partial}{\partial S} = \beta_{lm} \nabla_j \times \left[\sum_j r_j^l Y_{lm}(\vartheta_j \psi_j)\right] \frac{\partial \beta_{lm}}{\partial S} \frac{\partial}{\partial \beta_{lm}}.$$

But it follows from the definition of S that

$$\frac{\partial \beta_{lm}}{\partial S} = \frac{\partial}{\partial S}(l^{-1} R^{-l+2} \dot{\alpha}_{lm}) = \left[\sum_j r_j^l Y_{lm}(\vartheta_j \varphi_j)\right]^{-1};$$

or

$$\nabla_j S_j \frac{\partial}{\partial S_j} = \frac{\beta_{lm} \nabla_j [\sum_j r_j^l Y_{lm}(\vartheta_j \varphi_j)]}{\sum_j r_j^l Y_{lm}(\vartheta_j \varphi_j)} \frac{\partial}{\partial \beta_{lm}}. \tag{15}$$

Expressing the β_{lm} in Eq. (15) in terms of the α_{lm}, after multiplication and division by $4\pi/3N$ we obtain

$$\nabla_j S_j \frac{\partial}{\partial S_j} = \frac{(4\pi/3N)}{(4\pi/3N)} \frac{\alpha_{lm} \nabla_j [\sum_j (r_j/R_0)^l Y_{lm}(\vartheta_j \varphi_j)]}{\sum_j (r_j/R_0)^l Y_{lm}(\vartheta_j \varphi_j)} \frac{\partial}{\partial \alpha_{lm}}. \tag{16}$$

Inserting (16) into (13), and comparing the result with (14), we obtain an expression for the α_{lm} which occurs in A. Bohr's phenomenological theory of the nucleus:

$$\alpha_{lm} = (4\pi/3N) \sum_j (r_j/R_0)^l Y_{lm}(\vartheta_j \varphi_j). \tag{17}$$

Let us use the α_{lm} to write part of the potential energy. We shall assume that the potential energy is the sum of interactions between pairs of particles, so that

$$V = \tfrac{1}{2} \sum_{ij} G(\mathbf{r}_i, \mathbf{r}_j) = \tfrac{1}{2} \sum G_{lm}^{l'm'} r_j^l Y_{lm}(\vartheta_j \varphi_j) r_i^{l'} Y_{l'm'}(\vartheta_i \varphi_i) \tag{18}$$

(the summation is taken over all indices). Bearing in mind Eq. (17) and the fact that $l < l_0$, we can write (18) in the form

$$V = \left(\frac{3N}{16\pi}\right)^2 R_0^{-l-l'} G_{lm}^{l'm'} \alpha_{lm} \alpha_{l'm'} + \left(\frac{3N}{4\pi}\right) \sum_{m',\, l' > l_0;\, j} G_{lm}^{l'm'} \alpha_{lm} Y_{l'm'}(\vartheta_j \varphi_j) r_j^l + \frac{1}{2} \sum_{ij} G_{l_0}(\mathbf{r}_i, \mathbf{r}_j),$$

$$\frac{1}{2} \sum_{ij} G_{l_0}(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum G_{lm}^{l'm'} r_i^l r_j^{l'} Y_{lm}(\vartheta_i \varphi_i)\, Y_{l'm'}(\vartheta_j \varphi_j), \tag{19}$$

$$m', l', m, l > l_0.$$

When the indices m and l occur twice, we sum from zero to l_0.

The first term in Eq. (19) describes the potential energy of collective motion, the second term the interaction energy between the individual particles and the collective oscillations, and the final term the interaction between particles screened by the surface oscillations.

The final expression for the Hamiltonian describing a system undergoing small surface oscillations in the constant density approximation is given by

the sum of (14) and (19). This Hamiltonian agrees with that of the phenomonological theory of the generalized nuclear model.

The introduction of auxiliary ("superfluous") variables leads to the necessity of applying subsidiary conditions to the wave function, and these can be written

$$\left(\varrho_k - N^{-1/2}\sum_j \exp\{-i\,\mathbf{k}\mathbf{r}_j\}\right)\Phi = 0 \qquad (20)$$

for the first of the problems considered here (Sec. 3), and

$$\left[\alpha_{lm} - (4\pi/3N)\sum_j (r_j/R_0)^l Y_{lm}(\vartheta_j\varphi_j)\right]\Phi = 0 \qquad (21)$$

for the case of surface oscillations.

5. The special choices of the $\varphi_j(r_j)$ considered above can be generalized for other problems. The generalization consists of indicating a method for finding the $\varphi_j(r_j)$.

In solving boundary value problems the Schrödinger equation can be written in the hydrodynamic form

$$-E_j + \frac{1}{2M}(\nabla S_j)^2 - \frac{\hbar^2}{4M}\left[\frac{\Delta p_j}{p_j} - \frac{1}{2}\left(\frac{\Delta p_j}{p_j}\right)^2\right] = 0;$$

$$\frac{1}{M}\nabla(p_j\nabla S_j) = 0,\quad \varphi_j(r_j) = \sqrt{p_j}\exp(i/\hbar S_j).$$

This representation of the Schrödinger equation is convenient in that it is simple to formulate boundary conditions for it in analogy with hydrodynamics.

In the constant density case the S_j satisfy Laplace's equation. However this is not the only generalization. The $\varphi_j(r_j)$ can, for instance, be found from self-consistent field equations.

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Electrical, Optical and Elastic Properties of Diamond Type Crystals. I

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The energy of a homopolar crystal is expressed as a function of the displacements and of the dipole moments of the atoms. By means of a variational method, the relation between the displacements and the deformation of the electronic shells of the atoms is established and equations of motion are presented in which the displacements and dipole moment of the atoms play the role of generalized coordinates.

As was shown in a paper by one of the authors[1], Born's atomic theory[2] can be improved by taking into consideration the deformability of the atoms. In the foundation of a theory of the lattice one must assume an expression for the energy U in the form of a quadratic function of the displacements $\mathbf{u}_s^l$ and of the dipole moments $\mathbf{P}_s^l$ of all the atoms (l is the cell number and s the number of the atom in the cell). In the calculation of delay of interaction, one can consider optical, electrical and elastic properties of crystals from a single point of view. The explicit introduction of the quantities $\mathbf{P}_s^l$ is necessary also in the microscopic theory of localized electron states in a crystal[4].

While in ionic crystals the consideration of the deformability of the ions improves the quantitative agreement of theory with experiment[1], in homopolar crystals, where the dipole moments of the displacements $\mathbf{p}_s^l = e_s\mathbf{u}_s^l$ are absent ($e_s = 0$), such considerations lead to a series of qualitatively new conse-