Density of a Many-Fermion System in a Harmonic-Oscillator Potential.

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(ricevuto il 17 Dicembre 1982)

PACS. 21.10. – General and average properties of nuclei; properties of nuclear energy levels.

Summary. – The ground-state density of a system of noninteracting fermions in a harmonic-oscillator potential well can be given in terms of the wave functions of a few single-particle states around the Fermi level.

We are going to demonstrate that the derivative of the density of a system of fermions occupying the lowest levels in a three-dimensional harmonic-oscillator well can be written in terms of a few radial wave functions. If N major oscillator shells are occupied, the derivative implies only the last occupied shell and the first nonoccupied one.

In the one-dimensional case, the relation is very simple. If F is the quantum number of the last occupied shell (Fermi level), and if the φ_i's are the normalized wave functions, one has

$$a_0 \frac{\mathrm{d}\varrho(z)}{\mathrm{d}z} = -\sqrt{2(F+1)}\,\varphi_F \varphi_{F+1}\,. \tag{1}$$

In this relation, ϱ is the density and a_0 is the harmonic-oscillator length

$$a_0 = \sqrt{\frac{\hbar}{m\omega}}\,, \tag{2}$$

ω being the oscillator frequency. The proof of relation (1) is given in ref. [1] and is based on recurrence relations fulfilled by the harmonic-oscillator wave functions. The method cannot be extended to the three-dimensional case easily. We therefore prefer to start

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[1] J. CUGNON and O. HAROUNA: *Z. Phys. A*, **301**, 59 (1981).

with the following sum rule [2]:

$$\sum_n (E_n - E_0)\langle 0|\varrho(\boldsymbol{r})|n\rangle\langle n|z|0\rangle = \langle 0|\tfrac{1}{2}[\varrho(\boldsymbol{r}), [H, z]]|0\rangle \,. \tag{3}$$

In this relation, $|0\rangle$ is the ground state for the many-fermion Hamiltonian H, and $\varrho(\boldsymbol{r})$ is the density operator

$$\varrho(\boldsymbol{r}) = \sum_{i=1}^{A} \delta^3(\boldsymbol{r} - \boldsymbol{r}_i) \,. \tag{4}$$

Relation (3) is easily verified by expanding the double commutator. For the harmonic-oscillator Hamiltonian

$$H = \sum_i \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 r_i^2 \right), \tag{5}$$

the r.h.s. is readily evaluated. One has

$$\sum_n (E_n - E_0)\langle 0|(\boldsymbol{r})|n\rangle\langle n|z|0\rangle = -\frac{\hbar^2}{2m}\frac{\mathrm{d}\varrho}{\mathrm{d}z} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}\varrho}{\mathrm{d}r}\frac{1}{\cos\theta} \,. \tag{6}$$

In the last relation, the spherical symmetry of the ground-state density has been used. The dependence upon the polar angle θ is eliminated by multiplying by $\cos\theta$ and integrating over the solid angles. One has

$$-\frac{4\pi}{3}\frac{\hbar^2}{2m}\frac{\mathrm{d}\varrho}{\mathrm{d}r} = \sum_n (E_n - E_0)\int \mathrm{d}\Omega \cos\theta \langle 0|\varrho|n\rangle\langle n|z|0\rangle \,. \tag{7}$$

Both ϱ and z are one-body operators. Hence, they can connect the zero-particle–zero-hole state $|0\rangle$ with the one-particle–one-hole states $|n\rangle = |ph^{-1}\rangle$ only, as is well-known [3]. The indice p denotes the unoccupied states, whereas h labels the single-particle levels below the Fermi level. The transformation of the A-body matrix elements under consideration into one-body matrix elements is quite standard [3]. Equation (7) writes

$$-\frac{4\pi}{3}\frac{\hbar^2}{2m}\frac{\mathrm{d}\varrho}{\mathrm{d}r} = 2\sum_{n=ph^{-1}} (E_n - E_0)\int \mathrm{d}\Omega \cos\theta\, \psi_p(\boldsymbol{r})\psi_{\tilde{h}}^*(\boldsymbol{r})\langle p|z|\tilde{h}\rangle \,, \tag{8}$$

where $|\tilde{h}\rangle$ is the time-reversed of the single-particle state $|h\rangle$, and where ψ is the total single-particle wave function. The factor 2 accounts for the spin $\frac{1}{2}$ of the fermions.

The rest of the proof relies on the following property of the three-dimensional harmonic-oscillator wave functions. If n, l, m are the usual quantum numbers of the

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[2] J. V. NOBLE: *Ann. Phys.*, **67**, 98 (1971).

[3] A. BOHR and B. R. MOTTELSON: *Nuclear Structure* (New York, N. Y., 1969), Vol. I, Chapt. 3.

single-particle states, one has

$$(9)\qquad \langle n'l'm'|z|nlm\rangle = a_0\delta_{m'm}\left\{\delta_{nn'}\delta_{l'l+1}\left[\frac{(n+l+\frac{3}{2})(2l+1)}{(2l+3)}\right]^{\frac{1}{2}}\cdot\right.$$

$$\cdot(l\,0\,1\,0|l+1\,0)(l\,m\,1\,0|l+1\,m) -$$

$$-\delta_{n',n+1}(1-\delta_{l0})\delta_{l',l-1}\left[\frac{(n+1)(2l+1)}{(2l-1)}\right]^{\frac{1}{2}}(l\,0\,1\,0|l-1\,0)(l\,m\,1\,0|l-1\,m) +$$

$$+\delta_{nn'}(1-\delta_{l0})\delta_{l',l-1}\left[\frac{(n+l+\frac{1}{2})(2l-1)}{(2l+1)}\right]^{\frac{1}{2}}(l-1\,0\,1\,0|l\,0)\cdot$$

$$\left.\cdot(l-1\,m\,1\,0|l\,m) - (1-\delta_{n0})\delta_{n',n-1}\delta_{l',l+1}\left[\frac{n(2l+3)}{(2l+1)}\right]^{\frac{1}{2}}(l+1\,0\,1\,0|l\,0)(l+1\,m\,1\,0|l\,m)\right\}.$$

This relation may be derived by using the explicit expression of the harmonic-oscillator wave functions and the recurrence relations for the Laguerre functions. This is a rather combersome method. It is preferable to use second quantization techniques in the spherical representation. We refer the interested reader to the book by MOSHINSKY (4), which is one of the few textbooks to deal with the three-dimensional harmonic oscillator. It is interesting to note that the state $|nlm\rangle$ in the N-th major shell ($N = 2n + l$) can be connected, through the operator z, with a state in the major shells $N' = N \pm 1$ only. The first two terms in eq. (9) refer to $N' = N + 1$ and the last two terms correspond to $N' = N - 1$. This is a generalization of the one-dimensional case, for which the position operator has nonvanishing matrix elements between adjacent states only.

Because of relation (9), the summation over h in eq. (8) is restricted to the single-particle states of the last occupied major shell ($N = F$) and the indice p runs only on the single-particle states of the first nonoccupied major shell. Consequently $E_n - E_0$ is equal to $\hbar\omega$. After some simple Racah algebra, eq. (8) can be put in the form

$$(10)\qquad a_0\frac{\mathrm{d}\sigma}{\mathrm{d}r} = -\frac{1}{\pi}\sum_{\substack{n,l\\2n+l=F}}\left\{\left(n+l+\frac{3}{2}\right)^{\frac{1}{2}}(l+1)R_{nl}(r)R_{n,l+1}(r) -\right.$$

$$\left. -(1-\delta_{l0})(n+1)^{\frac{1}{2}}lR_{nl}(r)R_{n+1,l-1}(r)\right\},$$

where $R_{nl}(r)$ is the radial wave function.

An expression similar to (10) is also valid, when a subshell is filled, like it is often the case in nuclear physics. For instance, the neutrons in the ^{48}Ca nucleus occupy the $N = 0$ and $N = 1$ shells and the $1f_{\frac{7}{2}}$ subshell of the $N = 2$ major shell. Then it is appropriate to consider the j-representation. One has

$$(11)\qquad \frac{\hbar^2}{2m}\frac{\mathrm{d}\varrho}{\mathrm{d}r} = -\hbar\omega\frac{a_0}{4\pi}\sum_{[nlj]}(2j+1)\left\{\left[(2l+1)(2l+3)\left(n+l+\frac{3}{2}\right)\right]^{\frac{1}{2}}\begin{pmatrix} l & 1 & l+1\\ 0 & 0 & 0\end{pmatrix}\cdot\right.$$

$$\left.\cdot\sum_{[j']}(2j'+1)\begin{Bmatrix} j' & j & 1\\ l & l+1 & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} j & 1 & j'\\ -\frac{1}{2} & 0 & \frac{1}{2}\end{Bmatrix}R_{n,l+1}(r)R_{nl}(r) -\right.$$

(4) M. MOSHINSKY: *The Harmonic Oscillator in Modern Physics: From Atoms to Quarks* (New York, N. Y., 1969), p. 20.

$$-(1-\delta_{l,0})[(n+1)(2l-1)(2l+1)]^{\frac{1}{2}}\begin{pmatrix} l & 1 & l-1 \\ 0 & 0 & 0 \end{pmatrix}\sum_{[j']}(2j'+1)\begin{Bmatrix} j' & j & 1 \\ l & l-1 & \frac{1}{2} \end{Bmatrix}\cdot$$

$$\cdot\begin{pmatrix} j & 1 & j' \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} R_{nl(r)}R_{n+1,l-1}(r)\Bigg\}\,.$$

The summation over n, l is restricted as before, to the values for which either the subshell $n, l+1$ or $n+1, l-1$ is partially or totally empty. The summation over $j(j')$ is restricted to the occupied (unoccupied) subshells. In the limit of the magic nuclei (all lowest major shells occupied) the summation over j and j' in eq. (11) can be performed and the expression (10) is recovered.

Expressions (10) and (11) embody a curious property of the harmonic oscillator, since the derivative of the density (and therefore the density itself) is determined by just a few wave functions around the Fermi level. This property is of no practical usefulness, but it may have some important connection with nuclear physics. The three-dimensional harmonic-oscillator potential have been used extensively for many years in the development of the nuclear shell model. These days, more realistic potential wells like the Saxon-Woods potential, are used. However, it is well known that the corresponding single-particle wave functions are not very different from those of a harmonic-oscillator potential, provided the oscillator parameter is suitably chosen ([3]). Hence, expressions like (11) can perhaps be extended to realistic potentials, for which it could be approximately valid. Of course, it has to be modified, since the parameter ω looses its meaning. A possible modification is

$$(12)\qquad \frac{\mathrm{d}\varrho}{\mathrm{d}r}=-\frac{1}{2\pi}\frac{\sqrt{m}}{\hbar}\sum_{[nlj]}(2j+1)\Bigg\{\Bigg[(2l+1)(2l+3)\left(n+l+\frac{3}{2}\right)\Bigg]^{\frac{1}{2}}\begin{pmatrix} l & 1 & l+1 \\ 0 & 0 & 0 \end{pmatrix}\cdot$$

$$\cdot\sum_{[j']}(2j'+1)\begin{Bmatrix} j' & j & 1 \\ l & l+1 & \frac{1}{2} \end{Bmatrix}\begin{pmatrix} j & 1 & j' \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}(\varepsilon_{nl+1j'}-\varepsilon_{nlj})^{\frac{1}{2}}\cdot$$

$$\cdot R_{nl+1j'}(r)R_{nlj}(r)-(1-\delta_{l0})[(2l+1)(2l-1)(n+1)]^{\frac{1}{2}}\cdot$$

$$\cdot\sum_{[j']}(2j'+1)\begin{Bmatrix} j' & j & 1 \\ l & l-1 & \frac{1}{2} \end{Bmatrix}\begin{pmatrix} j & 1 & j' \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}(\varepsilon_{n+1l-1j'}-\varepsilon_{nlj})^{\frac{1}{2}}R_{n+1l-1j'}(r)R_{nlj}(r)\Bigg\}\,,$$

where ε_{nlj} is the single-particle energy and where the radial wave function $R_{nlj}(r)$ now depends upon the quantum number j because of the spin-orbit interaction. We have tested the likelihood of such a relation on a specific example. We have chosen a Saxon-Woods potential with the parameters of ref. ([5]). Figure 1 shows the results of the calculation for the ^{40}Ca nucleus. Relation (12) is strikingly fulfilled for $r \geqslant 3$ fm, whereas departures appear for smaller values of r.

These considerations put some enlightment on a well-known observation first made by LIU and BROWN ([6]). They draw the attention to the fact that in order to provide a good description of the excitations of nuclei, it is important to use a single-particle potential which gives a good description of the single-particle states *near the Fermi energy*. On the other hand, it is known that the coupling to low-lying excitations is

([5]) K. BEAR and P. E. HODGSON: *J. Phys. G*, **4**, L287 (1978).

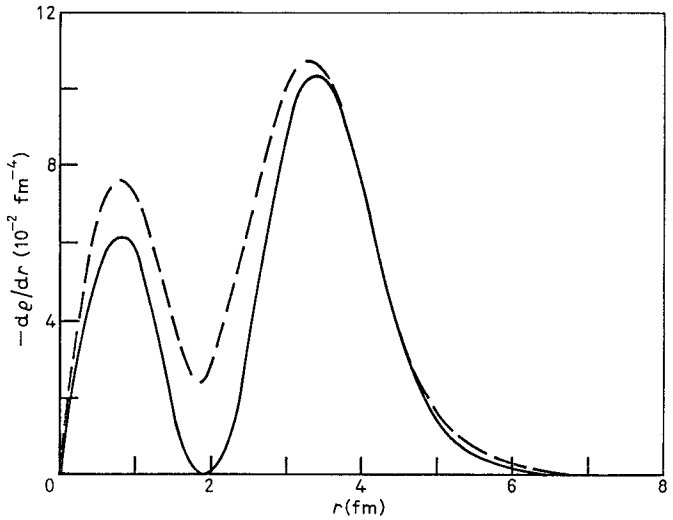

Fig. 1. – Comparison of formula (11) with the exact derivative of the nuclear density in ^{40}Ca. —— exact, — — — eq. (12).

often proportional to the derivative of the density (7) (multiplied by some power of r, according to the angular momentum of the excitation). Our result makes the observation of ref. (6) understandable. Having a good description of the single-particle states in the vicinity of the Fermi level amounts to having a good description of the transition operator.

(6) K. F. LIU and G. E. BROWN: *Nucl. Phys. A*, **265**, 385 (1976).
(7) A. BOHR and B. R. MOTTELSON: *Nuclear Structure* (New York, N. Y., 1969), Vol. II, Chapt. 6.