

To be submitted to
Phys. Rev. Comments

COMITATO NAZIONALE PER L'ENERGIA NUCLEARE
Laboratori Nazionali di Frascati

LNF-75/1 (P)
7 Gennaio 1975

A. Małecki and P. Picchi: FOR AND AGAINST THE
GARTENHAUS-SCHWARTZ TRANSFORMATION.

A. Małecki^(x) and P. Picchi: FOR AND AGAINST THE GARTENHAUS-SCHWARTZ TRANSFORMATION.

We examine the Gartenhaus - Schwartz procedure of imposing translational invariance. We point out the shortcomings of the original derivation and, at the same time, advocate the final result which has the virtue of preserving intrinsic dynamics.

The wave function or density of a nuclear state may be generally constructed as the linear combination of functions, each depending on a definite subset of nuclear coordinates. It is a common practice to use as the components also (and sometimes exclusively) functions which depend on the coordinates of a single nucleon.

There are good reasons for use of the single particle wave functions or densities. They reflect the nature of the average intranuclear field which is a convenient concept, greatly facilitating the description of nuclear interactions. The nuclear wave functions Ψ_{SP} , having as a basis the single particle functions (e. g. the shell model or Jastrow wave functions), are relatively easy in operation allowing their self-determination through the nucleon-nucleon interaction as well as the calculation of various nuclear observables. Also the application of the Pauli principle to these wave function is very easy.

The obvious drawback of the single particle wave functions consists in a lack of translational invariance. The correct nuclear wave function should have this property and must be an eigenfunction of the to

(x) - From Instytut Fizyki Jadrowej, Kraków, Poland.

2.

tal momentum operator

$$\vec{P} = \sum_{j=1}^A \vec{p}_j$$

which is the generator of infinitesimal translations. Such a wave function describes the motion of the centre-of-mass coordinate

$$\vec{R} = \frac{1}{A} \sum_{j=1}^A \vec{r}_j$$

as the plane wave. On the contrary, the wave functions Ψ_{SP} describe this motion as some fluctuation of the c. m. vector about the origin of the coordinate system.

The situation may be remedied by removing from Ψ_{SP} any dependence upon \vec{R} . This can, however, be done in a variety of ways (1, 2), e. g. :

$$(1) \quad \Psi_T([\vec{r}']) = \int d^3 R G(\vec{R}, [\vec{r}']) \Psi_{SP}(\vec{R}, [\vec{r}']),$$

$[\vec{r}']$ being the set of A-1 intrinsic coordinates and Ψ_T is the translationally invariant wave function of total momentum zero for any arbitrary choice of the function G. The ambiguity follows from the fact that the number of degrees of freedom is to be reduced by three.

At this point the question arises: what one would like to retain from the original wave function Ψ_{SP} while its \vec{R} - dependence is being removed.

If the functional form of the wave function is to be preserved:

$$(2) \quad \Psi_T = \Psi_{SP}(\vec{r}_j \rightarrow \vec{r}'_j), \quad \vec{r}'_j = \vec{r}_j - \vec{R},$$

one should use Eq. (1) with $G = \delta^{(3)}(\vec{R})$. It may be noted that in the case when the relative motion is to be described by A coordinates, the identity:

$$(3) \quad d^3 r_1 \dots d^3 r_A = A^3 d^3 R d^3 r'_1 \dots d^3 r'_{A-1} = d^3 R d^3 r'_1 \dots d^3 r'_{A-1} d^3 r'_A \delta^{(3)}\left(\frac{1}{A} \sum_{j=1}^A \vec{r}'_j\right)$$

implies the introduction of pseudometric in the Hilbert space of the wave functions⁽³⁾.

In fact, there is no reason for attaching importance to the form of Ψ_{SP} . Much more important is its content regarding the internal structure, i. e. the interrelations among nucleon coordinates. Even if Ψ_{SP} describes incorrectly the c. m. motion, the features relative to the intrinsic dynamics are valid and should be retained in the translationally invariant outcome.

Consider, for concreteness, the Jastrow wave functions which include the short-range correlations among the nucleons. The correlations are here superimposed on an average nuclear field, which is thought as determined by the long-range part of the nucleon-nucleon force. If one wants to maintain this convenient scheme of classification of nuclear interactions (short- and long - range effects) one should ensure that the translationally invariant partners of the Jastrow densities retain their intrinsic properties.

The requirement of preserving intrinsic dynamics leads to the following prescription for the nuclear densities:

$$(4) \quad |\Psi_T|^2 = \int d^3 R |\Psi_{SP}|^2$$

The prescription (4) is very simple in use, when the expectation values of operators, which depend only on intrinsic variables, are to be calculated. One has then^(x):

$$(5) \quad \langle \Psi_T | O(\vec{r}') | \Psi_T \rangle = \langle \Psi_{SP} | O(\vec{r}') | \Psi_{SP} \rangle$$

for any intrinsic operator O , not involving the derivatives.

The range of applicability of Eq. (5) is rather large. In fact, in any measurement which refers to the internal dynamics, the operators of interest can involve only the relative positions of the particles^(o).

- (x) - In the case of excitations the transition densities may be introduced. Then the prescription analogous to Eq. (4) would not change the transition matrix elements of intrinsic operators, and, in particular, will secure the relations of orthogonality.
- (o) - From this point of view not all nuclear operators are correctly defined. For example, frequently one states that the electron-nucleus interaction is described by the one-body operator $\sum_j^A e_j \exp(i\vec{q} \cdot \vec{r}_j)$, \vec{q} being the momentum transfer. But this is only an approximate manner of speaking, the correct operator is $\sum_j^A e_j \exp[i\vec{q} \cdot (\vec{r}_j - \vec{R})]$. Having this in mind, the objections raised against the elastic electron scattering as a tool for studying the nucleon-nucleon correlations⁽⁴⁾ are unjustified.

4.

The prescription (5) has been established many years ago by Gartenhaus and Schwartz⁽⁵⁾. Their arguments, however, were different from ours. Recently, it has been noted⁽⁶⁾ that ref. (5) contains an error. Our aim is twofold. We would like to clarify some misunderstandings connected with the Gartenhaus-Schwartz transformation, formulating the shortcomings of the original derivation in another way. At the same time we advocate the result (5); the qualitative arguments have already been given, then a numerical example will be presented.

Gartenhaus and Schwartz⁽⁵⁾ constructed the translationally invariant wave function as the following limit:

$$(6) \quad \Psi_{GS} = \lim_{\Lambda \rightarrow \infty} \Psi_{GS}^{\Lambda}, \quad \Psi_{GS}^{\Lambda} = U_{\Lambda} \Psi_{SP}, \quad U_{\Lambda} = e^{-i \frac{\Lambda}{2} (\vec{R} \cdot \vec{P} + \vec{P} \cdot \vec{R})}$$

This can be rewritten also this way⁽⁵⁾:

$$(7) \quad \Psi_{GS} = \lim_{\Lambda \rightarrow \infty} U_{\Lambda} \Psi_{SP} U_{\Lambda}^{-1} U_{\Lambda} = \lim_{\Lambda \rightarrow \infty} e^{-\frac{3}{2} \Lambda} \Psi_{SP} (\vec{R} e^{-\Lambda} [\vec{r}'])$$

Let us analyse the convergence of the sequences (6) and (7). Recall that there are two types of convergence for vectors in the Hilbert space - strong or weak. The convergence would be strong if

$$(8) \quad \lim_{\Lambda, \Lambda' \rightarrow \infty} \langle \Psi_{GS}^{\Lambda} - \Psi_{GS}^{\Lambda'} / \Psi_{GS}^{\Lambda} - \Psi_{GS}^{\Lambda'} \rangle = 0$$

for any two independent sequences of Λ and Λ' .

The expression

$$(9) \quad \begin{aligned} \langle \Psi_{GS}^{\Lambda} / \Psi_{GS}^{\Lambda'} \rangle &= \int d^3 R d^3 r'_1 \dots d^3 r'_{A-1} e^{-\frac{3}{2} \Lambda} e^{-\frac{3}{2} \Lambda'} \Psi_{SP}^x (\vec{R} e^{-\Lambda} [\vec{r}']) \\ &\quad \Psi_{SP} (\vec{R} e^{-\Lambda'} [\vec{r}']) \\ &= e^{-\frac{3}{2} (\Lambda - \Lambda')} \int d^3 R d^3 r'_1 \dots d^3 r'_{A-1} \Psi_{SP}^x (\vec{R} e^{-(\Lambda - \Lambda')} [\vec{r}']) \\ &\quad \Psi_{SP} (\vec{R}, [\vec{r}']) \end{aligned}$$

however, depends on the way in which the two limits $\Lambda \rightarrow \infty$, $\Lambda' \rightarrow \infty$ are realized, hence the convergence cannot be strong.

The strong convergence would permit a convenient transformation in the expectation value of an operator O in the state Ψ_{GS} :

$$(10) \quad \langle \Psi_{GS} O / \Psi_{GS} \rangle = \lim_{\Lambda, \Lambda' \rightarrow \infty} \langle \Psi_{SP} / U_{\Lambda}^+ O U_{\Lambda'} / \Psi_{SP} \rangle = \langle \Psi_{SP} / \lim_{\Lambda \rightarrow \infty} U_{\Lambda}^+ O U_{\Lambda} / \Psi_{SP} \rangle$$

As we have seen, this simplification in taking the limits, being an important point in the paper of Gartenhaus and Schwartz, is not justified^(x).

The limit of the Gartenhaus-Schwartz sequence, defined in Eq. (6), exists but in the meaning of weak convergence. In fact, using the same trick as in (9), it may be seen that

$$(11) \quad \lim_{\Lambda \rightarrow \infty} \langle \Psi_{GS}^{\Lambda} / \Psi \rangle = \langle \Psi_{GS} / \Psi \rangle$$

$$\Psi_{GS} = \frac{1}{V} \int d^3 R \Psi_{SP}(\vec{R}, [\vec{r}])$$

for any wave function Ψ , the normalization coefficient V being allowed to become infinite.

It should be pointed out that the above limit is different from the prescription (2) which was sometimes erroneously identified with the G-S transformation^{(1), (6)}. This may be illustrated using the example of a wave function of two particles moving in the harmonic oscillator wells of different sizes R_1, R_2 . The intrinsic wave function corresponding to Eq. (11) is then $\exp(-(1/2) r^2/R_1^2 + R_2^2)$, r being the relative distance, while Eq. (2) gives $\exp(-(1/8)r^2 R_1^2 R_2^2 / R_1^2 + R_2^2)$ ^(o).

Let us notice that the forms of Eqs. (11) and (4) are very similar. This observation leads immediately to the following conclusion: the prescription (4) may be thought as the result of the modified G-S transformation, defined as in (6) but for the densities rather than for the wave functions. It is this redefinition which one should have in mind when the results (4) and (5) are referred to the G-S procedure.

(x) - Of course, this is also true of the transition amplitudes. Here, the additional argument for having two independent limits would follow from the requirement that the initial and final wave function each be separately translationally invariant⁽⁶⁾. We would like to stress that the lack of strong convergence in the G-S limit is a sufficient obstacle, invalidating the simplification made in (10).

(o) - In this particular case the density corresponding to Eq. (11) coincides with the prescription (4). In general the two densities are different, hence the calculation with the wave function (11) may differ from the result (5).

6.

At the same time it should be realized that the operator of Gartenhaus and Schwartz is only one of a continuous family of operators which impose the translational invariance on the wave function or density⁽²⁾. Hence the use of their transformation does not remove the problem of ambiguity.

We want to advocate the prescription (4) by invoking its physical meaning, and not the way of "derivation". The translationally invariant density (4) is nothing else as the intrinsic density corresponding to the single particle wave function Ψ_{SP} . Hence the prescription (4) (and the analogous prescriptions concerning the transition densities) has the very important virtue of preserving internal dynamics.

The retention of intrinsic properties may be illustrated on the example of statistical correlations in the shell model. The antisymmetry correlations, contained in the determinantal wave functions, can be described by the Jastrow-like density which in the approximation of two-particle correlations takes the form⁽⁷⁾:

$$\begin{aligned}
 (12) \quad \left| \Psi_{STAT} \right|^2 &= \prod_{j=1}^A \rho(r_j) \left\{ 1 + \sum_{\ell=1}^{A/2} (2^\ell \ell!)^{-1} \sum_{\substack{j_1 \neq k_1 \neq \dots \\ j_\ell \neq k_\ell}}^A [\Delta(j_1, k_1) \dots \Delta(j_\ell, k_\ell)] \right\} \\
 \Delta(j, k) &= \frac{\rho^A(\vec{r}_j, \vec{r}_k)}{\rho(r_j)\rho(r_k)} - 1
 \end{aligned}$$

where $\rho(r)$ is the average one-body density and $\rho^A(\vec{r}_1, \vec{r}_2)$ - the two-body density calculated with the Slater determinant. The density (12) describes antisymmetrization as the short-range interaction. This is justified since the statistical correlations are, indeed, most effective at small distances.

In the case of harmonic oscillator model one has for ^{16}O :

$$\begin{aligned}
 (13) \quad \rho(r) &= \rho(0) \left(1 + 2 \frac{r^2}{R^2} \right) \exp \left(- \frac{r^2}{R^2} \right) \\
 \rho^A(\vec{r}_1, \vec{r}_2) &= \frac{16}{15} \rho(r_1) \rho(r_2) - \frac{4}{15} \rho^2(0) \left(1 + 2 \frac{\vec{r}_1 \cdot \vec{r}_2}{R^2} \right)^2 \exp \left(- \frac{r_1^2 + r_2^2}{R^2} \right)
 \end{aligned}$$

R being the oscillator size parameter.

We have calculated the charge form factor of ^{16}O for the density $|\Psi_{STAT}|^2$ and the density $|\Psi_A|^2$ given by the Slater determinant of the oscillator orbitals. In the latter case, as is well known, the c. m. problem may be solved univocally. For the density (12) we have used the two prescriptions for removing the c. m. coordinate: Eq. (4) (conventionally named "CM averaged") and Eq. (2) ("CM fixed"). The results presented in Table

clearly favor the use of Eq. (4). Only in this case the properties of statistical correlations are reproduced correctly.

TABLE - Charge form factor of ^{16}O (q_{μ} -four-momentum transfer) corresponding to various treatments of the statistical correlations in the harmonic oscillator model ($R = 1.66$ fm). The nucleon form factor taken from ref. (8).

q_{μ}^2 (fm $^{-2}$)	^{16}O CHARGE FORM FACTOR		
	A	STAT CM averaged	STAT CM fixed
0	1.0	1.0	1.0
2	0.70 10^{-1}	0.69 10^{-1}	0.67 10^{-1}
4	-0.20 10^{-1}	-0.20 10^{-1}	-0.18 10^{-1}
6	-0.13 10^{-1}	-0.13 10^{-1}	-0.11 10^{-1}
8	-0.50 10^{-2}	-0.51 10^{-2}	-0.42 10^{-2}
10	-0.17 10^{-2}	-0.17 10^{-2}	-0.13 10^{-2}
12	-0.52 10^{-3}	-0.53 10^{-3}	-0.40 10^{-3}
14	-0.15 10^{-3}	-0.16 10^{-3}	-0.11 10^{-3}

REFERENCES. -

- (1) - H. J. Lipkin, Phys. Rev. 110, 1395 (1958).
- (2) - J. L. Friar, Nuclear Phys. A173, 257 (1971).
- (3) - F. Miglietta, Nuovo Cimento 4A, 144 (1971).
- (4) - G. Ripka and J. Gillespie, Phys. Rev. Letters 25, 1624 (1970);
M. Fink, H. Hebach and H. Kümmel, Phys. Rev. C3, 2075 (1971).
- (5) - S. Gartenhaus and C. Schwartz, Phys. Rev. 108, 482 (1957).
- (6) - D. J. Ernst, C. M. Shakin and R. M. Thaler, Phys. Rev. C7, 1340 (1973);
F. Palumbo, Phys. Letters 37B, 341 (1971).
- (7) - A. Małecki and P. Picchi, Riv. Nuovo Cimento 2, 119 (1970);
E. Bieszyńska, M. Bieszyński, A. Małecki and P. Picchi, Phys. Letters 43B, 355 (1973).
- (8) - T. Janssens, R. Hofstadter, E. B. Hughes and M. R. Yearian, Phys. Rev. 142, 922 (1966).