Effect of the Jastrow Correlation Factor on Nuclear Charge Distributions

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It is shown that for nuclear charge distributions the dominant effect of the Jastrow correlation factor is to produce a new uncorrelated Slater determinant which is calculated explicitly. This is related to the absence of the Brueckner-Pauli operator in the Jastrow correlation factor.

There have been many attempts[1] to fit the elastic electron-scattering data by using charge densities calculated with Jastrow correlated wave functions[2]

$$|\Psi\rangle = \frac{1}{\sqrt{N}} \prod_{i<j} f(r_{ij}) |\Phi_0\rangle. \quad (1)$$

In the absence of the Jastrow correlation factor (JCF) the wave function $|\Psi\rangle$ of the nucleus is the Slater determinant $|\Phi_0\rangle$, the parameters of which should yield charge densities which fit the low-momentum-transfer data. The JCF is introduced so as to fit also the high-momentum-transfer data.[3] In doing so, however, one is forced to change appreciably the parameters of the original Slater determinant $|\Phi_0\rangle$. This shows that the JCF changes appreciably both the high and low Fourier components of the charge density. We show by an explicit calculation that as far as the charge density is concerned, the main effect of the JCF acting on the original Slater determinant $|\Phi_0\rangle$ is to produce a new (uncorrelated) Slater determinant. As an example, we calculate this new Slater determinant in the case of ^{40}Ca using harmonic oscillator wave functions. However our conclusions are independent of the basis functions used. The complete details of the theory and of the calculation will be published elsewhere.

We first calculate the density matrix,

$$\rho_{ij} = \langle\Psi| a_j^{\dagger} a_i |\Psi\rangle, \quad (2)$$

with the Jastrow wave function (1) and in the single-particle basis of oscillator wave functions. For the calculation of the density matrix a diagrammatic perturbation formalism was developed by Gaudin.[4] We included all terms up to second order in $h = f - 1$ and first order in $g = f^2 - 1$. In terms of ρ_{ij} the charge density is

$$\rho(r) = \sum_{i,j} \varphi_i(\vec{r}) \varphi_j^*(\vec{r}) \rho_{ij}, \quad (3)$$

where the sum is limited to proton single-particle states $\varphi_i(r)$. With the diagrams we have included to calculate ρ_{ij}, the expression for the charge density becomes the same as those used in Ref. 1.

We then diagonalize the density matrix ρ_{ij}:

$$\sum_j \rho_{ij} V_j^{\alpha} = n_\alpha V_i^{\alpha}. \quad (4)$$

This yields a set of new orbits $\varphi_\alpha'(r) = \sum_i V_i^{\alpha} \varphi_i(r)$. We then construct the new Slater determinant $|\Phi_0'\rangle$ with the A orbits φ_α' belonging to the eigenvalues which are close to unity. We can then separate the charge density (3) into two terms,

$$\rho(r) = \rho_0'(r) + \rho_c(r), \quad (5)$$

where $\rho_0'(r)$ is the charge density due to the new Slater determinant $|\Phi_0'\rangle$ and $\rho_c(r)$ is the remainder which we define as being due to the effect of correlations:

$$\rho_0'(r) = \sum_{\alpha(h)} |\varphi_\alpha(\vec{r})|^2,$$
$$\rho_c(r) = \sum_{\alpha(p)} n_\alpha |\varphi_\alpha(\vec{r})|^2 - \sum_{\alpha(h)} (1-n_\alpha) |\varphi_\alpha(\vec{r})|^2, \quad (6)$$

where the indices $\alpha(h)$ and $\alpha(p)$ denote, respectively, the occupied and unoccupied proton orbits in $|\Phi_0'\rangle$.

The definition of the new Slater determinant $|\Phi_0'\rangle$ together with the separation (5) of the charge density has the following two properties: (1) It is independent of the basis states used to calculate the density matrix ρ_{ij}. (2) It will yield $\rho_c = 0$ if the state $|\Psi\rangle$ is any Slater determinant. Indeed, it may be shown that the necessary and sufficient condition for a many-particle state $|\Psi\rangle$ to be a Slater determinant is that the density matrix ρ should satisfy the equation $\rho^2 = \rho$, in which case its eigenvalues are equal to either 0 or 1.

Figure 1 shows charge densities of ^{40}Ca (uncorrected for the proton form factor and center-of-mass motion) using a harmonic oscillator constant $(m\omega/\hbar)^{1/2} = 0.55$ fm^{-1} and a Jastrow function $1 - f^2(r) = \exp(-\beta^2 r^2)$ with $\beta = 1.4$ fm^{-1}. We have verified that these parameters yield a charge density [Eq. (3) or (5)] which, at high momentum transfer $q \sim 3.5$ fm^{-1}, fits the form factor given in Ref. 3 and derived from the 750-MeV elastic

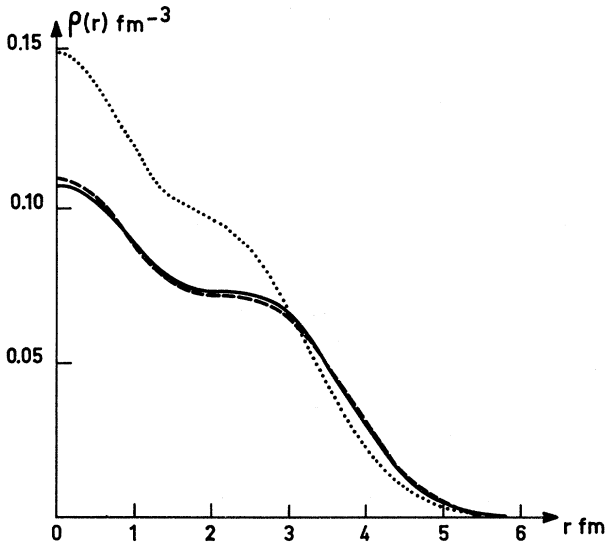

FIG. 1. Charge densities of ^{40}Ca.

electron scattering on ^{40}Ca. The dotted line shows the charge density ρ_0 of the original Slater determinant $|\Phi_0\rangle$ made up of oscillator orbits. The solid line is the charge density [Eq. (3) or (5)] of the Jastrow wave function (1). The dashed line is the charge density ρ_0'[Eq. (6)] of the new Slater determinant $|\Phi_0'\rangle$.

The reason why the JCF produces a new Slater determinant is essentially due to the fact that the Jastrow factor $f(r)$ scatters particles into all states and not only into states in which both particles are outside the Fermi sea of $|\Phi_0\rangle$ as in the case in Brueckner theory. Indeed if we replaced the function $f-1$ by the operator $Q(f-1)$, where Q projects pairs of particles outside the Fermi sea,[6] then (to the order in which we have calculated ρ_{ij}) all the particle-hole elements of the density matrix ρ_{ij} would vanish; the diagonalization (4) would then yield orbits φ_α which are linear combinations of the occupied orbits in $|\Phi_0\rangle$ so that $|\Phi_0'\rangle = |\Phi_0\rangle$ and $\rho_0' = \rho_0$. For this reason it is not possible to compare $\rho-\rho_0$ obtained with a Jastrow wave function (1) with the change in density due to Brueckner correlations [Fig. 24(b) of Ref. 5] which also yields zero particle-hole elements for the density matrix.

Finally we write the expressions used to calculate the density matrix ρ_{ij} in terms of the (not antisymmetrized) matrix elements of the Jastrow factors $h=f-1$ and $g=f^2-1$:

$$\rho_{ij}-(\rho_0)_{ij}=\rho_{ij}{}^A-\rho_{ij}{}^B+\rho_{ij}{}^C,$$

$$\rho_{ij}{}^A=\sum_{m,n<F}\sum_k[4(mn|h|ik)-(mn|h|ki)](jk|h|mn)$$

$$\rho_{ij}{}^B=\sum_{m\le F}[4(jm|g|im)-(jm|g|mi)] \text{ if } i,j\le F,$$

$$=0 \text{ otherwise.}$$

$$\rho_{ij}{}^C=\epsilon_{ij}\sum_{m<F}[4(jm|h|im)-(jm|h|mi)],$$

where

$$\epsilon_{ij}=1 \text{ if } i>F, j\le F, \text{ or } i\le F \text{ and } j>F,$$

$$=2 \text{ if } i,j\le F,$$

$$=0 \text{ otherwise.}$$

The sums run over all the spatial orbits and F denotes the last filled orbit of $|\Phi_0\rangle$.

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