

State-dependent equivalent local potentials for the Dirac equation*

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It is pointed out that previously published equivalent local representations of the relativistic Hartree-Fock exchange potentials are too small by a factor of 2. The implications of this error for the relativistic Hartree-Fock calculations of closed shell nuclei are discussed.

[NUCLEAR STRUCTURE Dirac equation, equivalent local potentials presented.]

Recently the concept of equivalent local potentials has been applied to the nonlocal exchange potentials which arise from the relativistic Hartree-Fock theory^{1,2} (based on the Dirac equation). In the present work, it is shown that the explicit expressions for the equivalent potentials given in Refs. 1 and 2 are too small by a factor of 2. The implications of this error for the relativistic Hartree-Fock calculations of closed shell nuclei that are reported in Ref. 2 are discussed. It is found that the conclusions based on those calculations are not affected by the correction of the error.

It is also shown that local state-independent potentials in the Dirac equation can be given equivalent local state-dependent forms. Aside from being a curiosity of the Dirac theory, these equivalent local state-dependent forms are useful in the present context because they can be used to illustrate the error which occurs in Refs. 1 and 2 while avoiding the complications associated with the nonlocal exchange interaction.

The basis of this work is the rotationally symmetric parity conserving Dirac equation:

$$\{c\vec{\alpha} \cdot \vec{p} + \beta[mc^2 + U_s + \gamma^0 U_v^0 - \gamma^r U_v^r - \gamma^0 \gamma^r U_t^r]\} \psi = E\psi. \quad (1)$$

The notations and conventions for the potentials and Dirac matrices are given in Ref. 2. Note is taken of the special nature of the potential U_v^r in that it cannot simultaneously satisfy the further restrictions of Hermiticity and time reversal invariance unless the potentials are state-dependent in a particular way. This fact was pointed out in Ref. 2 and is further elaborated in a forthcoming paper.³ Our interest is with the discrete eigenfunctions of this equation which can be labeled by the set of quantum numbers $(n\omega Jm)$ and can be

given the spatial representation

$$\psi_{Jm}^{n\omega}(\vec{r}) = \frac{1}{r} \begin{pmatrix} F_J^{n\omega}(r) \mathcal{Y}_{Jm}^{\omega}(\theta, \phi) \\ i G_J^{n\omega}(r) \mathcal{Y}_{Jm}^{\bar{\omega}}(\theta, \phi) \end{pmatrix}. \quad (2)$$

Again the quantum number notation and the definition of the spin-angular functions $\mathcal{Y}_{Jm}^{\omega}(\theta, \phi)$ are given in Ref. 2. Equation (1) may be reduced to radial form in which the radial large and small components F and G occur

$$\begin{aligned} \frac{dF}{dr} = & \left[i \frac{(U_v^r - U_t^r)}{\hbar c} - \frac{\omega(J + \frac{1}{2})}{r} \right] F \\ & + \left(\frac{2mc^2 + U_s - U_v^0 + E}{\hbar c} \right) G, \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{dG}{dr} = & \left[i \frac{(U_v^r + U_t^r)}{\hbar c} + \frac{\omega(J + \frac{1}{2})}{r} \right] G \\ & + \left(\frac{U_s + U_v^0 - E}{\hbar c} \right) F. \end{aligned} \quad (4)$$

The quantum number indices have been removed from the radial functions for simplicity. The rest energy has been subtracted from the energy eigenvalue as well.

One may obtain state-dependent equivalent potentials for a local state-independent potential (a scalar potential for example) by considering the following identity

$$\beta U_s \psi_i(\vec{r}) = \beta U_s \begin{bmatrix} \psi_i(\vec{r}) \psi_i^\dagger(\vec{r}) \\ \psi_i^\dagger(\vec{r}) \psi_i(\vec{r}) \end{bmatrix} \psi_i(\vec{r}). \quad (5)$$

Here we assume ψ_i to be one of the eigenfunctions of Eq. (1) where only the scalar potential U_s is nonzero. All the quantum number indices are represented by the single index i . Now one may note that the matrix $\psi_i(\vec{r}) \psi_i^\dagger(\vec{r})$ may be expanded in

the 16 Dirac matrices

$$\psi_i(\mathbf{r})\psi_i^\dagger(\mathbf{r}) = \frac{1}{4} \sum_A [\psi_i^\dagger(\mathbf{r})\gamma_A\psi_i(\mathbf{r})]\gamma^A. \quad (6)$$

Inserting Eq. (6) into Eq. (5), one obtains an equivalence relation

$$\beta U_s = \frac{1}{4} \beta U_s \frac{\sum_A [\psi_i^\dagger(\mathbf{r})\gamma_A\psi_i(\mathbf{r})]\gamma^A}{\psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})}. \quad (7)$$

While this equivalence is formally exact insofar as the operation of either of the potentials upon one of the eigenstates ψ_i is concerned, it is complicated by the fact that all 16 elements of the sum over A on the right-hand side contribute. Furthermore, the right-hand side of Eq. (7) depends upon all of the single-particle quantum numbers ($n\omega Jm$). An analogous situation obtains in Refs. 1 and 2 where equivalent local forms for the Hartree-Fock exchange interaction were considered. There it was argued that the rotational invariance of the nonlocal interaction permits one to sum the nu-

merator and denominator of the equivalent local form over the magnetic quantum number m . To test this argument one may define a new potential U'_s by performing this magnetic averaging upon the right-hand side of Eq. (7),

$$\beta U'_s = \frac{1}{4} \beta U_s \frac{\sum_A \sum_{m_i} [\psi_i^\dagger(\mathbf{r})\gamma_A\psi_i(\mathbf{r})]\gamma^A}{\sum_{m_i} \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})}. \quad (8)$$

By utilizing the form of the wave functions given by Eq. (2) and the algebra of the Dirac matrices, one can reduce Eq. (8) to the form

$$\beta U'_s = \frac{1}{4} \beta U_s \left(1 + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} \gamma^0 + \frac{2i F_i G_i}{F_i^2 + G_i^2} \gamma^r \right). \quad (9)$$

Now only 3 terms of the original 16 are present and the dependence of the right-hand side upon the magnetic quantum number has disappeared.

To test the validity of this averaging procedure, one may calculate the matrix element of the right-hand side of Eq. (9) between two eigenstates (ψ_i

and ψ_j) of the original scalar potential,

$$\langle \psi_j | \beta U'_s | \psi_i \rangle = \frac{1}{4} \int \frac{1}{r} (F_j \mathcal{Y}_{jm}^\dagger, -i G_j \mathcal{Y}_{jm}^\dagger) \beta U_s \left(1 + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} \gamma^0 + \frac{2i F_i G_i}{F_i^2 + G_i^2} \gamma^r \right) \frac{1}{r} \begin{pmatrix} F_i & \mathcal{Y}_{jm}^\omega \\ i G_i & \mathcal{Y}_{jm}^\omega \end{pmatrix} d^3r. \quad (10)$$

Note that the quantum numbers ω , J , and m are not distinguished for the states i and j because the potential on the right-hand side of Eq. (9) cannot connect states of different ω , J , and m quantum numbers. Performing the angular integrations in Eq. (10), one obtains:

$$\langle \psi_j | \beta U'_s | \psi_i \rangle = \frac{1}{4} \int_0^\infty U_s \left[(F_j F_i - G_j G_i) + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} (F_j F_i + G_j G_i) + \frac{2F_i G_i}{F_i^2 + G_i^2} (F_j G_i - G_j F_i) \right] dr. \quad (11)$$

After a little algebra Eq. (11) may be reduced to the simple form

$$\langle \psi_j | \beta U'_s | \psi_i \rangle = \frac{1}{2} \int_0^\infty U_s (F_j F_i - G_j G_i) dr. \quad (12)$$

One may note that the right-hand side of Eq. (12) is exactly one-half of the matrix element of the original scalar potential. Since this is the most general nonzero matrix element in this basis, one concludes that the angle averaging procedure used

in defining Eq. (8) is rendered exact by a multiplication of the result by a factor of 2. Thus one has proved the following equivalence for a scalar potential U_s acting upon an eigenstate ψ_i of the Dirac Hamiltonian:

$$\beta U_s = \frac{1}{2} \beta U_s \left(1 + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} \gamma^0 + \frac{2i F_i G_i}{F_i^2 + G_i^2} \gamma^r \right). \quad (13)$$

For the sake of completeness, the more general equivalence relation which includes all three potentials which satisfy the usual shell model type

restrictions is given below without proof:

$$\begin{aligned} \beta [U_s + \gamma^0 U_v^0 - \gamma^0 \gamma^r U_t^r] = & \frac{1}{2} \beta \left[\left(U_s + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} U_v^0 \right) + \left(U_v^0 + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} U_s + \frac{2i F_i G_i}{F_i^2 + G_i^2} U_t^r \right) \gamma^0 \right. \\ & \left. + \left(\frac{2i F_i G_i}{F_i^2 + G_i^2} U_s + \frac{F_i^2 - G_i^2}{F_i^2 + G_i^2} U_t^r \right) \gamma^r + \left(-U_t^r + \frac{2i F_i G_i}{F_i^2 + G_i^2} U_v^0 \right) \gamma^0 \gamma^r \right]. \end{aligned} \quad (14)$$

As is shown by Eq. (14), these equivalent state-dependent potentials in general include a component which transforms like the unusual U_v^r potential.

While the equivalence relation given, for example, by Eq. (13) is amusing, it is probably not of any practical importance since it is far easier to work with the original state-independent local potential than with the state-dependent form. The exercise of deriving Eq. (13) is useful, however, in that it illustrates the factor of 2 error in the angle averaging procedure which was erroneously represented as being exact in Refs. 1 and 2. Although the details are too lengthy to present in a short communication of this nature, it is straightforward to show that a similar factor of 2 error occurs in the state-dependent equivalent local potentials which are presented in Refs. 1 and 2.

The concept of equivalent potentials has been investigated within the framework of the Dirac equation and it has been shown that local state-independent potentials which are rotationally invariant and parity conserving may be given local state-dependent representations. With respect to the nonlocal exchange potentials of relativistic Hartree-Fock theory, it is shown that the local state-dependent representations given in Eqs. (14)–(17) of Ref. 1 and in Eqs. (41)–(44) of Ref. 2 must be multiplied by a factor of 2 in order for the potentials to be exact representations of the original nonlocal potentials.

One should also note that the right-hand side of Eq. (53) of Ref. 2, which gives the exchange contribution to the total binding energy, should be multiplied by a factor of $\frac{1}{2}$ inasmuch as the erroneously defined exchange potential U_v^{oi} occurs there.

As far as the author knows, no numerical calculations have been published which are based upon the erroneous equations in Ref. 1. In Ref. 2,

however, some numerical calculations were presented for the nuclei ^{16}O , ^{40}Ca , and ^{48}Ca and it is of interest to consider to what extent this error affects the numbers published and the conclusions drawn from them. The corrections to the exchange contributions to the total binding energies published in Ref. 2 will be due to second order effects coming from changes in the single-particle wave functions rather than from changes in the equations used to calculate the binding energies. The corrections to the total binding energies given in Table II of Ref. 2 should be no more than a few percent since the exchange energies themselves are only about 15% of the total binding energy. The corrections to the rms radii and single-particle eigenvalues can be estimated by noting the differences between the Hartree and Hartree-Fock values quoted in Ref. 2. This amounts to a decrease of about 0.03 fm for the rms radii.

The exchange potentials which are plotted in Figs. 1–4 of Ref. 2 for ^{16}O , for example, are expected to be doubled in value. They will, nevertheless, still remain very small in comparison to the direct potentials. For the exchange potentials from the inclusion of the one-pion exchange (Figs. 6–8), a doubling is also expected and this should further increase the stability problems associated with these potentials which were noted in Ref. 2. One concludes then that the conclusions reached in Ref. 2 will not be significantly altered by the correction of the error in the exchange potential expression.

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