Jastrow functions in double-beta decay

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We use simple analytic considerations and a Monte Carlo calculation of nucleons in a box to argue that the use of Jastrow functions as short-range correlators in the commonly employed two-body-cluster approximation causes significant errors in the matrix elements for double-beta decay. The Jastrow approach appears to agree with others, however, if many-body clusters are included.

A careful treatment of the charge-changing analog of the nuclear pair density shows, in addition, that differences between Unitary Correlator Operator Method and Brueckner methods for treating short-range correlations in double-beta are less significant than suggested by previous work.

I. INTRODUCTION

New experiments to measure the rate of neutrinoless double-beta ($0\nu\beta\beta$) decay will provide information about neutrino masses if neutrinos are Majorana particles. Unfortunately, one must know the value of the nuclear matrix element governing the decay to extract that information from an observed rate (or rate limit) \cite{1}. For that reason, attempts to better calculate the matrix elements appear regularly in the literature.

The matrix elements involve products of one-body decay operators and a sum over intermediate states, but the closure approximation allows them to be represented to high accuracy \cite{2} by the ground-state-to-ground-state transition matrix element of a two-body operator

$$M^{0\nu} \equiv \sum_{a<b} M_{ab}.$$ \hspace{1cm} (1)

The matrix elements $M_{fi} \equiv \langle f | M^{0\nu} | i \rangle$ can therefore be affected by the strong repulsive correlations that alter pair distribution functions at short distances.

For many years, theorists were satisfied to simulate these correlations by using a phenomenological Jastrow function $f(r_{ab})$ in the two-body cluster approximation to modify the operator $M$:

$$M_{ab} \rightarrow f(r_{ab}) M_{ab} f(r_{ab}),$$ \hspace{1cm} (2)

where $r_{ab} \equiv |r_a - r_b|$ is the magnitude of the distance between the two nucleons. The Jastrow function almost always had the form prescribed in Ref. \cite{3}:

$$f(r) = 1 - e^{-1.1r^2} (1 - 0.68r^2),$$ \hspace{1cm} (3)

with $r$ in fm. Recent work has questioned this prescription. Refs. \cite{4,5,6} treated short-range correlations through the Unitary-Correlation Operator Method (UCOM), which has the advantages of wave-function overlap preservation and a range of successful applications \cite{7}. Refs. \cite{8} and \cite{9} computed the effects of short-range correlations within well-defined Brueckner-based approximation schemes. All these papers found smaller effects on matrix elements than the phenomenological Jastrow function yields. Because they all limited their analysis to two-body correlations, however, their predictions for the size of short-range effects do not come with an iron clad guarantee.

In fact, all these methods imply the existence of many-body effects that are always neglected in applications to double-beta decay. In Jastrow-based treatments, our subject here, the full correlated wave function is written schematically as

$$|\Psi\rangle = \left(\prod_{a<b<c} T_{abc}\right) \left(\prod_{a<b} F_{ab}\right) |\Psi_0\rangle,$$ \hspace{1cm} (4)

where $|\Psi_0\rangle$ is a Slater determinant or a generalization thereof, $F_{ab}$ is a two-body Jastrow correlator depending on $r_{ab}$ and the spins and isospins of particles $a$ and $b$, and $T_{abc}$ is a similar three-body correlator, which we will ignore from here on. In recent years, practitioners have developed a range of techniques for moving beyond the two-body cluster approximation in Eq. \cite{2} and including many-body correlations generated by the product of $F$'s (in addition to explicit three-body correlations generated by a single $T$) in Eq. \cite{4}. Cluster expansions and the Fermi-hypernetted-chain method (see, e.g., Refs. \cite{10,11} and references therein) include three- and more-body clusters, and quantum Monte-Carlo methods allow an evaluation of the contributions of all clusters. The Jastrow approaches now yield accurate observables, including two-body density distributions with short-range correlations, in light nuclei \cite{12} and nuclear matter \cite{13}. Here, after analyzing the two-body cluster approximation in $\beta\beta$-decay, we see whether an initial application of quantum Monte Carlo with many-body correlations included supports the phenomenological two-body-cluster approximation.
Jastrow method used traditionally, or whether it supports one or more of the approaches introduced recently. We also point out that apparent differences between the results of UCOM and Brueckner methods are largely fictitious.

Heavy nuclei are still too complicated for Monte-Carlo methods in their current forms, so to evaluate many-body Jastrow effects we look instead at a simplified version of asymmetric nuclear matter. We make this choice with the idea that short-range correlations are nearly universal in nature, depending little on longer-range structure of the environment in which the correlated nucleons are embedded, provided that environment has the correct density.

II. TWO-BODY CLUSTER APPROXIMATION

In the $S = 0$ $T = 1$ channel that determines the contribution of short distances to the $\beta\beta$ amplitude, realistic variationally-determined correlation functions $F_{ab}$ are not so different from the Miller-Spencer Jastrow function. Figure 1 shows a typical nuclear-matter example, following the calculations of Ref. [13], alongside the Miller-Spencer function and the effective scaling function, obtained from the ratio of calculations with and without short-range correlations, that appears in the Brueckner-based work of Ref. [9]. All the functions go to unity at large $r$, but the Brueckner-based function has a sizeable "overshoot" near $r = 1$ fm. The Miller-Spencer function has a much smaller overshoot (occurring at larger $r$, which is made less important by the radial falloff of the $0\nu\beta\beta$ operator) leading to a significantly smaller $0\nu\beta\beta$ matrix element. The variational nuclear-matter resembles the Miller-Spencer function but has essentially no overshoot, and so if applied like that function via Eq. (2) it will produce an even smaller matrix element.

The use of the $F$ from Eq. (4) to multiply a two-body operator as in Eq. (2) is often called the two-body cluster approximation, because all terms are discarded except those in which the transition operator and the correlators act on the same pair of particles. This approximation appears to be reasonably good for number-conserving two-body densities. The dot-dashed line in Fig. 1 displays the distribution $g_{0\nu}(r)$ in the $S = 0, T = 1$ channel, following Ref. [13], which incorporates the full product over all pair correlations of Eq. (4). This full $g_{0\nu}(r)$ is somewhat smaller than the corresponding $F^2$ because many-body tensor correlations promote a fraction of the spin-singlet pairs to spin-triplet pairs, so that the number of singlet pairs is reduced. The reduction has also been seen in light nuclei [14], though the corrections are not large either there or here.

In $\beta\beta$ decay, the picture must be different, however. To see why, consider the charge-changing analog of the (spin-independent) two-body density:

$$ P_F(r) \equiv \langle f | \sum_{a<b} \delta(r-r_{ab}) \tau_a^+ \tau_b^+ | i \rangle, \tag{5} $$

where $F$ stands for Fermi. If we weight this function with $H_F(r)$, the radial part of the Fermi $0\nu\beta\beta$ operator (given approximately by $1/r$), and integrate, we get the Fermi piece of the $0\nu\beta\beta$ matrix element. If we integrate $P_F(r)$ without any weighting, we get $\langle f | \sum_{a<b} \tau_a^+ \tau_b^+ | i \rangle$, which must vanish because the isospins of $|i\rangle$ and $|f\rangle$ are different (in the very good approximation that isospin is conserved), while the operator between them is proportional to the square of the isospin-raising operator.

Figure 2 shows $P_F(r)$ for the shell-model calculation of the $\beta\beta$-decay of $^{82}$Se in Refs. [13] and [10]. The solid curve contains no Jastrow function and has area of zero beneath it. The dashed curve is the result of of the Brueckner-based calculations in Ref. [8]. Its overshoot at $r$ just greater than one causes the integral to stay very close to zero despite the suppression at very small $r$. But the use of the two-body Jastrow function $F_{0\nu}$ à la Ref. [13] (dotted curve) suppresses contributions at small $r$ without an overshoot and thus leads to an integral of 0.006. Substituting the pair distribution function $g_{0\nu}$ would only make the problem here worse. The Miller-Spencer Jastrow function yields a little bit of overshoot but not nearly enough, and results in an integral of 0.0075.

It seems, then, that a realistic treatment of short-range correlations must yield an overshoot in $P_F(r)$ if it is to preserve isospin (The UCOM procedure does this exactly, by construction). When Jastrow functions are extended beyond the two-body cluster approximation, the effective functions that result must therefore look different.
for charge-changing densities, which involve only valence nucleons, than for like-particle densities, to which all nucleons contribute coherently.

It is not hard to get an idea of how this happens. Let us consider spin-and-isospin-independent two-body correlators $F_{ab}$ (with no three-body correlators $T_{abc}$) in Eq. (1) and a general charge-changing operator $M_{ab}$. Writing $F_{ab}^2 = 1 + h_{ab}$, and expanding to first order in $h$ gives

$$\langle f | M | i \rangle = \langle f_0 | \sum_{a<b} \sum_{c<d} h_{cd} (1 + h_{cd}) | i_0 \rangle \quad (6)$$

$$= \langle f_0 | \sum_{a<b} M_{ab} | i_0 \rangle + \langle f_0 | \sum_{a<b} M_{ab} h_{ab} | i_0 \rangle + \langle f_0 | \sum_{c < b} M_{ab} (h_{ac} + h_{bc}) | i_0 \rangle$$

$$+ \langle f_0 | \sum_{c < d} M_{ab} h_{cd} | i_0 \rangle + O(h^2)$$

where $|i_0\rangle$ and $|f_0\rangle$ are Slater determinants, and in the third and fourth lines, $h_{mn} \equiv h_{nm}$ if $n < m$.

The second line in Eq. (6) involves the bare two-body transition operator and the two-body-cluster correction. The third line involves an effective three-body operator, and the fourth line an effective four-body operator. Terms of higher-order in $h$ generate even higher many-body operators.

Now let the neutron number exceed the proton number so that the Slater determinants $|i_0\rangle$ and $|f_0\rangle$ have well-defined isospins that differ from each other, and consider the operator $M_{ab} = T^{s}_{a} T^{s}_{b}$. The matrix element above is then the integral of $P_F(r)$, i.e., zero. Although the first term in the second line indeed gives zero, the second, as we’ve seen, does not. The inclusion of all terms first-order in $h$ must restore the value zero, however, because, as the last line shows, the result can be obtained by acting on $|i_0\rangle$ with the isospin-preserving two-body operator $\sum_{a<b} h_{ab}$ before acting with the transition operator. It is not hard to show that effective four-body term contributes the same amount as the two-body-cluster correction, and the effective three-body term contributes twice that amount with the opposite sign, so that the sum of terms indeed vanishes. But this also means that, at least to first order in $h$, three- and four-body effective operators are just as important for the quantity $\int P_F(r) dr$ as is the effective two-body correction generated by the two-body-cluster approximation. This perhaps surprising conclusion leads us to examine the charge-changing density itself and the higher order corrections in a model amenable to numerical solution.

### III. MANY NUCLEONS IN A BOX

We consider a cubic box with each side $L = 4.85$ fm and periodic boundary conditions. In the box are 2 protons and 16 neutrons (so that the nucleon density is very near nuclear-matter density), which decay to 4 protons and 14 neutrons. The protons in the initial state and all but the last two neutrons in that state are in filled fermi levels, and the last two (valence) neutrons are in the spin-zero two-body pairing wave function:

$$|\psi_v\rangle = N \sum_{K} \sum_{\mathbf{k}, -\mathbf{k}; S = 0} |\mathbf{k}, -\mathbf{k}; S = 0\rangle ,$$

where $v$ stands for valence, $N$ is a normalization constant, and the set $K$ contains vectors in which two $k$ components are equal to $\pm2\pi/L$ and the third is zero. In the final state the neutrons and all but the last two protons are in filled fermi levels; the two valence protons are in the configuration $\psi_v$, above, but with the set $K$ containing vectors with one component equal to $\pm2\pi/L$ and the other two equal to zero.

We use quantum Monte Carlo to evaluate $P_F(r)$ between states of the form Eq. (1), where now the states $|i_0\rangle$ and $|f_0\rangle$ are those just described, and with simple spin-and-isospin two-body correlators $F_{ab}$ and no three-body correlators $T_{abc}$, as considered previously. Figure 3 shows the results with the Miller-Spencer Jastrow function. The two-body-cluster approximation again has very little overshoot, but the full results, including clusters of all size, has considerably more, so that the integral vanishes as it should. Also shown is the result with the effective Jastrow function fit to the Brueckner-based calculation of Ref. [3] (which was done in finite nuclei).
We use the simplified forms here because they are sufficient to make our point.

Figure 4 displays \( C_F(r) \) from the Monte Carlo. (In this simple calculation \( C_{GT} \) is just proportional to \( C_F \) because the correlator is spin-independent and the two valence nucleons that participate in the decay are locked into a spin-zero configuration). The full solution clearly corrects the extreme suppression of the \( 0\nu\beta\beta \) matrix element created by the two-body-cluster approximation, in a way consistent with the analysis of the integral in section III. Differences with the Brueckner treatment are fairly small and due once again at least in part to the unusual system we analyze here. Effects beyond the two-body cluster approximation are thus both required and apparently sufficient to describe short-range correlations in \( \beta \) decay.

FIG. 3. (Color online) Monte-Carlo calculation of \( P_F(r) \) for 2 protons and 16 neutrons in a box decaying to 4 protons and 14 neutrons. The red circles are the result with no Jastrow correlators, the purple diamonds include the Miller-Spencer Jastrow correlator in the two-body-cluster approximation, the black upward-pointing triangles are the full result with that correlator, and the blue downward-pointing triangles apply the effective Brueckner based two-body-cluster Jastrow from Ref. [17]. The numerical error associated with the values of \( P_F(r) \) are usually smaller than the size of the corresponding symbols.

is now quite close to the full many-body Miller-Spencer result, and the remaining discrepancy is probably mostly due to the simplicity of our model. Surprisingly, the use of a Jastrow function with no overshoot at all gives almost the same result as the Miller-Spencer function when many-body correlations are taken fully into account.

To show the effects of these various functions on \( 0\nu\beta\beta \)-decay, we define functions \( C_K(r) \), \( K = F, GT \), for the Fermi and Gamow-Teller parts of the \( 0\nu\beta\beta \) operator. (If we wanted to be accurate we would also define one for the very small tensor term.) These functions are the products of the densities \( P_F(r) \) and the analogous density

\[
P_{GT}(r) \equiv \langle f | \sum_{a < b} \delta (r - r_{ab}) \sigma_a \cdot \sigma_b \tau_a^+ \tau_b^+ | i \rangle
\]

with functions \( H_F(r) \) and \( H_{GT}(r) \) that specify the radial dependence of the \( 0\nu\beta\beta \) operators. In other words

\[
C_K(r) = H_K(r) P_K(r), \tag{9}
\]

with

\[
H_F(r) = H_{GT}(r) \approx \frac{2R}{\pi r} \int_0^\infty dq \frac{\sin qr}{q + \tilde{E} - (E_i + E_f)/2}. \tag{10}
\]

The quantities \( \tilde{E}, E_i, \) and \( E_f \) are energies to which the \( H_K \) are not very sensitive. Equation (10) holds only if we neglect nucleon form factors and forbidden currents; in the complete, more complicated expressions \( H_F \neq H_{GT} \)

FIG. 4. (Color online) The curves \( C_F(r) \) corresponding to the distributions \( P_F(r) \) of Fig. 3 without forbidden currents or nucleon form factors. The symbols indicate the same approximations as in Fig. 3.

IV. UCOM

In this section we digress from our main line of inquiry to take up apparent differences between the results of Brueckner methods and UCOM. Fig. 2 of [1] and Fig. 9 of Ref. [17] present \( 0\nu\beta\beta \) distribution functions (similar to the function \( C_0^F(r) \) presented here in Fig. 4 with the UCOM (and other) treatments of short-range correlations. Unlike the Brueckner-based curves in our Figs. 2, 4 the UCOM curves show no overshoot. But the reason is that the “contribution from distance \( r \)” has been treated differently when UCOM correlations are considered than when other methods are used. The UCOM prescription requires that the operator \( r_{ab} \) be replaced by a shifted version \( R_+(r_{ab}) \) (where the function \( R_+ \) is usually determined variationally) in any operator that doesn’t depend on momentum. Thus, to evaluate the \( 0\nu\beta\beta \) matrix element, one replaces \( H_K(r_{ab}) \) by

[17]
The shifting implies that UCOM produces a function $C_F$ (which we use as an example because it is simpler than $C_{GT}$) given by

$$C_F^{U}(r) = \sum_{a<b} \langle f | H_F(R_{+}(r_{ab})) \delta(r-R_{+}(r_{ab})) \tau_a^+ \tau_b^+ | i \rangle$$

$$= H_F(r) \sum_{a<b} \delta(r-R_{+}(r_{ab})) \tau_a^+ \tau_b^+ | i \rangle$$

$$\equiv H_F(r)P_F^U(r), \quad (11)$$

(where $U$ stands for UCOM). In prior work on UCOM $\beta\beta$-decay, however, the “(Fermi) contribution from a given $r$" was defined instead by simply replacing $r_{ab}$ with $R_{+}(r_{ab})$ in $H$, viz:

$$C_F^{U'}(r) = \langle f | \sum_{a<b} H_F(R_{+}(r_{ab})) \delta(r-r_{ab}) \tau_a^+ \tau_b^+ | i \rangle$$

$$= H_F(R_{+}(r))P_F(r). \quad (12)$$

This definition, which leaves $r_{ab}$ unshifted in the delta function, gives the correct result for the Fermi matrix element when $r$ is integrated over, but does not define an observable and is not what is calculated in other approaches. The correct expression, Eq. (11), is a bit more complicated to evaluate, but has a pronounced overshoot.

Figure 5 compares the distribution $C_{GT}(r)$ from the shell-model-Brueckner treatment of $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$ in Ref. [8] (with no forbidden currents or nucleon form factors) to the properly defined UCOM distribution for the same decay. The two curves are extremely close to one another, and quite different from $C_F^{U'}(r)$, which is also shown. The UCOM and Brueckner pictures are therefore more similar than previously thought.

![Graph showing comparison of $C_{GT}(r)$ distributions](image)

**FIG. 5.** (Color online) The function $C_{GT}(r)$, defined in Eqs. [8] and [11] (solid red curve), the corresponding UCOM function $C_F^{U}(r)$, defined as in Eq. [11] (dashed blue curve), the previously-used UCOM function $C_F^{U'}(r)$, defined as in Eq. [12] (dot-dashed purple curve), and the Brueckner-based version (dotted black curve). The new UCOM and Brueckner curves are very similar.

### V. DISCUSSION

The main point of this paper, to which we now return, is that the use of Jastrow functions in the two-body-cluster approximation suppresses short-range contributions too much, and that the problem is fixed by including many-body correlations. This discovery raises the question of whether existing treatments are adequate. They include long-range many-body correlations in shell-model or QRPA wave functions but allow only two particles to be correlated at short distances. Is that sufficient?

It is hard to answer the question definitively because the approach taken here is so different from the others. We can say that the very-short-range correlations are unlikely to be altered; our figs. 3 and 4 show that corrections to the two-body-cluster approximation are barely noticeable below about $r = 0.7$ fm. But corrections are large at 1 fm or so. It is far from obvious that the marriage of UCOM or Brueckner treatments of short-range correlations to shell-model or QRPA treatments of longer-range correlations incorporates all important effects at the intermediate range $r \approx 1$ fm. The UCOM procedure generates three- and higher-body correlations that have been neglected in almost all applications to date, and the Brueckner-based double-beta work has so far not included contributions from, e.g., three-particle ladders. As for the shell model and QRPA, they leave untreated a significant range of single-particle energies between those contained in the calculation and those represented as short-range effects. Whether these omissions are significant is still an open question.

In the meantime, however, it appears that the UCOM and Brueckner methods give reasonable short-range correlations. Like the full Jastrow calculations here, they supply the overshoot required to preserve isospin symmetry. Higher-body corrections in these schemes appear unlikely to be as large as they are in the Jastrow approach, which violates isospin symmetry in the two-body cluster approximation. Short-range effects in $\beta\beta$-decay thus seem to be mostly under control.

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