

**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 the unitary correlation operator method and Brueckner methods for treating short-range correlations in double- $\beta$  decay are less significant than suggested by previous work.

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**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) [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 with high accuracy [2] by the ground-state-to-ground-state transition matrix element of a two-body operator,

$$\mathcal{M}^{0\nu} \equiv \sum_{a<b} \mathcal{M}_{ab}. \quad (1)$$

The matrix elements  $\langle f | \mathcal{M}^{0\nu} | i \rangle$  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  $\mathcal{M}$ ,

$$\mathcal{M}_{ab} \implies f[r_{ab}] \mathcal{M}_{ab} f[r_{ab}], \quad (2)$$

where  $r_{ab} \equiv |\mathbf{r}_a - \mathbf{r}_b|$  is the magnitude of the distance between the two nucleons. The Jastrow function almost always had the form prescribed in Ref. [3],

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

with  $r$  in femtometers. Recent work has questioned this prescription. References [4–6] treated short-range correlations through the unitary correlation operator method (UCOM), which has the advantages of wave-function overlap preserva-

tion and a range of successful applications [7]. References [8] and [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 ironclad guarantee.

In fact, all of these methods imply the existence of many-body effects that have always been neglected in applications to double- $\beta$  ( $\beta\beta$ ) decay. In Jastrow-based treatments, our subject here, one can write the full many-body correlated wave function (schematically) as

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

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. (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. (4). Cluster expansions and the Fermi-hypernetted-chain method [10,11] include three-body and higher 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 [12] and nuclear matter [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 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 the 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 the 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, obtained in the approach of Ref. [13], alongside the Miller-Spencer function. It also shows the effective scaling function, obtained from the ratio of calculations, with and without short-range correlations, that appears in the Brueckner-based treatment of the Argonne v18 potential in Ref. [9]. All of the functions go to unity at large  $r$ , but the Brueckner-based function has a sizable ‘‘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 result resembles the Miller-Spencer function, but has essentially no overshoot. If applied like the Miller-Spencer function via Eq. (2), it will produce an even smaller matrix element.

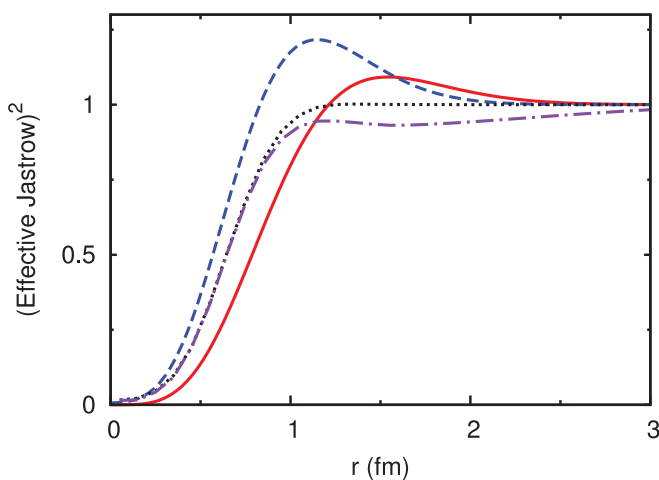


FIG. 1. (Color online) Squares of Jastrow functions  $F_{ab}$  from calculations following Ref. [13] (dotted black line, spin-singlet only), from Miller and Spencer [3] (solid red line), and from a fit to the results of a microscopic Brueckner-based calculation [9] (dashed blue line). The purple dot-dashed line comes from three-body and higher corrections to the dotted line.

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  $g_{01}(r)$  in the  $S = 0, T = 1$  channel, following Ref. [13], which incorporates the full product over all pair correlations of Eq. (4). This full  $g_{01}(r)$  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, reducing the number of singlet pairs slightly. 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,

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

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  $^{82}\text{Se}$  in Refs. [15] and [16]. The solid curve contains no Jastrow function and has an area of zero beneath it. The dashed curve is the result of the Brueckner-based

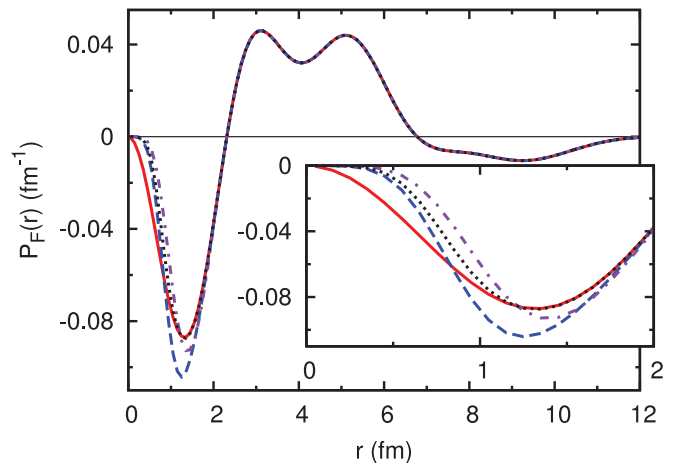


FIG. 2. (Color online) The charge-changing two-body density  $P_F(r)$  for the shell-model calculation of  $^{82}\text{Se}$  in Refs. [15] and [16]. The solid red line is the result without short-range correlations, the dashed blue line is that from the Brueckner-based calculation of Ref. [8], the dotted black line applies the Jastrow function from the approach in Ref. [13] in the two-body cluster approximation, and the dot-dashed purple line applies the Miller-Spencer Jastrow function. The inset magnifies the left-hand part of the figure.

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  $F_{01}$  as in 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  $g_{01}$  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. (4) and a general charge-changing operator  $\mathcal{M}_{ab}$ . Writing  $F_{ab}^2 \equiv 1 + h_{ab}$ , and expanding to first order in  $h$ , gives

$$\begin{aligned}
 \langle f | \mathcal{M} | i \rangle &= \langle f_0 | \sum_{a < b} \mathcal{M}_{ab} \prod_{c < d} (1 + h_{cd}) | i_0 \rangle \\
 &= \langle f_0 | \sum_{a < b} \mathcal{M}_{ab} | i_0 \rangle + \langle f_0 | \sum_{a < b} \mathcal{M}_{ab} h_{ab} | i_0 \rangle \\
 &\quad + \langle f_0 | \sum_{\substack{a < b \\ c \neq \{a, b\}}} \mathcal{M}_{ab} (h_{ac} + h_{bc}) | i_0 \rangle \\
 &\quad + \langle f_0 | \sum_{\substack{a < b \\ c < d \neq a, b}} \mathcal{M}_{ab} h_{cd} | i_0 \rangle + \mathcal{O}(h^2) \\
 &= \langle f_0 | \sum_{a < b} \mathcal{M}_{ab} \left( 1 + \sum_{c < d} h_{cd} \right) | i_0 \rangle + \mathcal{O}(h^2), \tag{6}
 \end{aligned}$$

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 involves 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  $\mathcal{M}_{ab} = \tau_a^+ \tau_b^+$ . 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 term, as we have seen, does not. The inclusion of all first-order terms in  $h$  must again yield 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 the 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

$$|\psi_v\rangle = \mathcal{N} \sum_{k_x, k_y, k_z \in K} |\mathbf{k}, -\mathbf{k}; S = 0\rangle, \tag{7}$$

where  $v$  stands for valence,  $\mathcal{N}$  is a normalization constant, and the set  $K$  contains vectors in which two  $k$  components are equal to  $\pm 2\pi/L$  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  $\pm 2\pi/L$  and the other two equal to zero.

We use quantum Monte Carlo calculations to evaluate  $P_F(r)$  between states of the form given by Eq. (4), where now the states  $|\Psi_0\rangle$  are the  $|i_0\rangle$  and  $|f_0\rangle$  just described, and the two-body correlators  $F_{ab}$  are again spin- and isospin-independent, with no three-body correlators  $T_{abc}$ . Figure 3 shows the results with the function correlator  $F_{ab}$  taken to be the Miller-Spencer Jastrow function. The two-body cluster approximation again has very little overshoot, but the full result, which includes clusters of all sizes, 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. [9] (which was done in finite nuclei). It 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, although we do not show it here, gives almost the same result as the Miller-Spencer function when many-body correlations are taken fully into account.

To show the consequences of these distributions for  $0\nu\beta\beta$  decay, we write the associated nuclear matrix element as an integral over a radial distribution function  $C(r)$ :

$$\langle f | M^{0\nu} | i \rangle = \int_0^\infty C(r) dr, \quad C(r) \approx C_{GT}(r) - C_F(r), \tag{8}$$

where GT stands for Gamow-Teller and we have omitted the small contribution of a tensor term. The functions  $C_F$  and  $C_{GT}$  are the products of the densities  $P_F(r)$  and the analogous

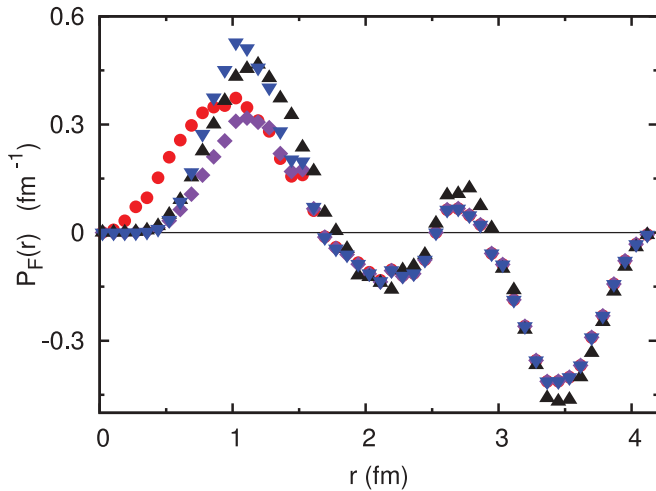


FIG. 3. (Color online) Monte Carlo calculation of  $P_F(r)$  for 2 protons and 16 neutrons in a box decaying to 4 protons and 14 neutrons. The red circles are the result with no Jastrow correlators, the purple diamonds include the Miller-Spencer Jastrow correlator in the two-body cluster approximation, 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 function from Ref. [9]. The numerical error associated with the values of  $P_F(r)$  is usually smaller than the size of the corresponding symbol.

density

$$P_{GT}(r) \equiv \langle f | \sum_{a<b} \delta(r - r_{ab}) \sigma_a \cdot \sigma_b \tau_a^+ \tau_b^+ | i \rangle, \quad (9)$$

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

$$C_K(r) \equiv 2H_K(r)P_K(r), \quad (10)$$

where  $K$  stands for either F or GT [and the factor of 2 compensates for our somewhat unconventional restriction to  $a < b$  in the sums in Eqs. (5) and (9)]. The  $H$ 's are given by [17,18]

$$H_K(r) = \frac{2R}{\pi r} \int_0^\infty \frac{h_K(q) \sin qr}{q + \bar{\omega}} dq, \quad (11)$$

where the  $h_K(q)$  contain the vector and axial-vector coupling constants, the form factors that account for the finite size of the nucleon, and the effects of forbidden currents (weak magnetism and the induced pseudoscalar term). The quantity  $\bar{\omega}$  is an average intermediate-nucleus excitation energy to which the  $H_K$  are not very sensitive.

Figure 4 displays  $C(r)$  from the full Monte Carlo and the various approximations to it exhibited in Fig. 3, with  $\bar{\omega} = 10$  MeV.<sup>1</sup> The full solution clearly corrects the substantial short-range suppression created by the two-body cluster approximation in a way consistent with the analysis of the

<sup>1</sup>In this simple calculation,  $P_{GT}$ , which determines  $C_{GT}$  through Eq. (10), is just proportional to  $P_F$  because the correlator is spin-independent and the two valence nucleons that participate in the decay are locked into a spin-zero configuration.

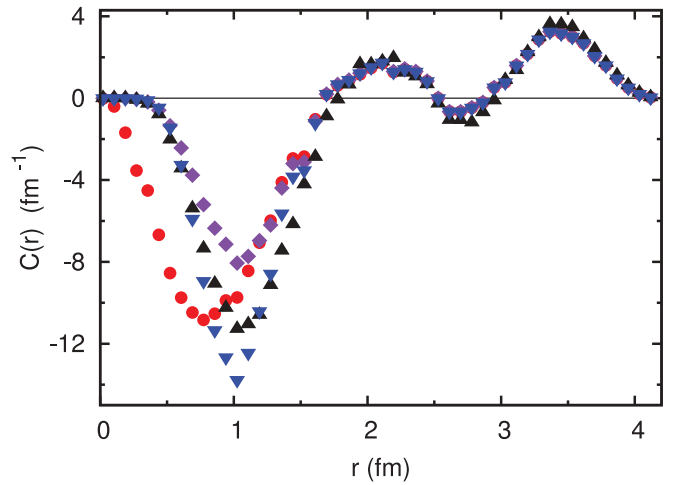


FIG. 4. (Color online) The radial functions  $C(r)$  from Eq. (8) that represent the contribution of internucleon distance  $r$  to the  $0\nu\beta\beta$  matrix element. Each curve corresponds to one of the distributions  $P_F(r)$  of Fig. 3. (The  $P_{GT}$  are just proportional to the  $P_F$  for the simple spin-zero pairs in our wave function.) The symbols indicate the same approximations as in Fig. 3.

integral in Sec. II. 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  $\beta\beta$  decay.

#### 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 the UCOM. Figure 2 of Ref. [4], Fig. 9 of Ref. [18], and Fig. 4 of Ref. [9] present  $0\nu\beta\beta$  distribution functions 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 the UCOM correlations are considered than when other methods are used. The UCOM prescription [7] 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 does not depend on momentum. Thus, to evaluate the  $0\nu\beta\beta$  matrix element, one replaces  $H_K(r_{ab})$  with  $H_K(R_+(r_{ab}))$ .

The shifting implies that the UCOM produces functions  $C_K$  given by

$$\begin{aligned} C_K^U(r) &= 2 \sum_{a<b} \langle f | H_K(R_+(r_{ab})) \delta(r - R_+(r_{ab})) O_K^{ab} \tau_a^+ \tau_b^+ | i \rangle \\ &= H_K(r) \langle f | \sum_{a<b} \delta(r - R_+(r_{ab})) O_K^{ab} \tau_a^+ \tau_b^+ | i \rangle \\ &\equiv H_K(r) P_K^U(r), \end{aligned} \quad (12)$$

where  $O_F^{ab} = 1$ ,  $O_{GT}^{ab} = \sigma_a \cdot \sigma_b$ , and  $U$  stands for UCOM. In prior work on the UCOM in  $\beta\beta$  decay, however, the “contribution from a given  $r$ ” was defined instead by simply

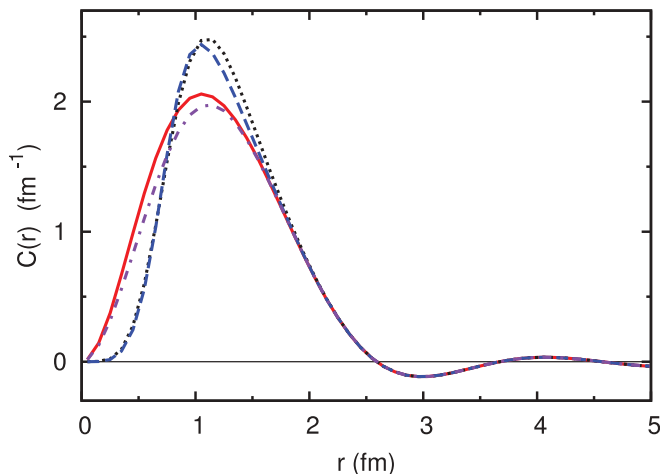


FIG. 5. (Color online) The function  $C(r)$ , defined in Eq. (8) (solid red curve); the corresponding UCOM function  $C^U(r)$ , defined through the use of Eq. (12) in Eq. (8), with  $R_+(r)$  from Ref. [7] (dashed blue curve); the previously used UCOM function  $C^{U'}(r)$ , defined through the use of Eq. (13) (dot-dashed purple curve); and the Brueckner-based version (dotted black curve). The new UCOM and Brueckner curves are very similar.

replacing  $r_{ab}$  with  $R_+(r_{ab})$  in  $H$  as follows:

$$\begin{aligned} C_K^{U'}(r) &= \langle f | \sum_{a < b} H_K(R_+(r_{ab})) \delta(r - r_{ab}) O_K^{ab} \tau_a^+ \tau_b^+ | i \rangle \\ &= H_K(R_+(r)) P_K(r). \end{aligned} \quad (13)$$

This definition, which leaves  $r_{ab}$  unshifted in the  $\delta$  function, gives the correct result for the matrix element  $\langle f | \mathcal{M}^{0\nu} | i \rangle$  when  $r$  is integrated over, but does not define an observable and is not what is calculated in other approaches. The correct expression, given by Eq. (12), is a bit more complicated to evaluate but has a pronounced overshoot. Figure 5 compares the distribution  $C(r)$  from the shell-model–Brueckner treatment of  $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$  in Ref. [8] to the properly defined UCOM distribution for the same decay. The two curves are extremely close to one another, and quite different from  $C^{U'}(r)$ , which is also shown. The UCOM and Brueckner pictures are therefore more similar than previously thought.

## 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 quasiparticle random phase approximation (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 the important effects at the intermediate range  $r \approx 1$  fm. The UCOM procedure generates three-body and higher correlations that have been neglected in almost all applications to date, and the Brueckner-based  $\beta\beta$  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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