Three-body monopole corrections to the realistic interactions

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It is shown that a very simple three-body monopole term can solve practically all the spectroscopic problems—in the $p$, $sd$ and $pf$ shells—that were hitherto assumed to need drastic revisions of the realistic potentials.

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The first exact Green’s function Monte Carlo (GFMC) solutions for $A > 4$ nuclei confirmed that two-body (2b) interactions fell short of perfectly reproducing experimental data [1]. The inclusion of a three-body (3b) force lead to excellent spectroscopy, but some problems remained for the binding and symmetry energies and spin orbit splittings. No core shell model calculations (NCSM) [2] have recently developed to the point of approximating the exact solutions with sufficient accuracy to provide a very important—though apparently negative—result in $^{10}$B [3]: While in the lighter systems the spectra given by a strict two-body potential are not always good—but always acceptable—in $^{10}$B, the spectrum is simply very bad.

My purpose is to show the striking analogy between this situation and what occurs in conventional ($0\hbar\omega$) shell model calculations with realistic G-matrices, and then explain how a very simple 3b term can solve practically all the spectroscopic problems—in the $p$, $sd$ and $pf$ shells—that were hitherto assumed to need drastic revisions of the realistic (R) 2b potentials.

The first realistic matrix elements [3], and the first large scale shell model codes [4] appeared almost simultaneously. Calculations for up to five particles in the $sd$ shell gave very satisfactory results, but the spectrum of $^{22}$Na (i.e., $(sd)^5 T = 0$) was very bad [5]. (Note that $^{10}$B is $(pf)^5 T = 0$). At the time nobody thought of 3b forces, and naturally the blame was put on the 2b matrix elements ($V_{stu}^{ff}$, $stu$ are subshells). The proposed phenomenological cures amounted to fit them to the experimental levels. Two “schools” emerged: One proposed to fit them all (63 in the $sd$ shell), and lead eventually to the famous USD interaction [6,7]. The alternative was to fit only the centroids, given in Eqs. (1,2).

$$ H_m = \sum_s \varepsilon_s n_s + \sum_{s \leq t} (a_{st} n_{st} + b_{st} T_{st}) $$

They are associated to the 2b quadratics in number ($n_s$) and isospin operators ($T_s$), Eqs. (3,4), and they define the monopole Hamiltonian, Eq. (5), in which we have added the single particle (1b) term. The idea originated in Ref. [10], where it was found that the Kuo Brown (KB) interaction in the $pf$ shell [11] could yield excellent spectroscopy through the modifications ($f \equiv f_{7/2}$, $r \equiv f_{5/2}$, $p_{3/2}$, $p_{1/2}$).

$$ V_{fr}^{ff}(KB) = V_{fr}^{ff}(KB) - (-)^T 300 \text{ keV}, $$
$$ V_{ff}^{ff}(KB) = V_{ff}^{ff}(KB) - 350 \text{ keV}, $$
$$ V_{ff}^{ff}(KB) = V_{ff}^{ff}(KB) + 110 \text{ keV}. $$

The validity of this prescription was checked in perturbative calculations [12], and convincingly confirmed for $A = 47 - 52$ once exact diagonalizations became feasible [13, 14, 15, 16, 17].

In what follows $f$ will stand generically for $(p_{3/2}, d_{5/2}, f_{7/2})$ in the $(p, sd, pf)$ shells respectively. Obviously $r = p_{1/2}$ and $r \equiv d_{3/2}, s_{1/2}$ for the $p$ and $sd$ shells.

Nowadays the 2b $NN$ potentials are nearly perfect, and the calculations are exact. Therefore, the blame for bad spectroscopy must be put on the absence of 3b terms. Which means that the monopole corrections must be 3b and Eq. (5) must be supplemented by

$$ \sum_{stu} (a_{stu} n_{stu} + b_{stu} T_{stu}) , $$

where $n_{stu} \equiv n_{rs} n_{rt} n_{at}$, or $n_s (n_r - 1)(n_t - 2)/6$ and similar forms for $T_{stu}$. To simplify matters we—tentatively—allow only contributions of the type $n_{st}(n - 2)$ and $T_{st}(n - 2)$, i.e., 2b terms modulated by the total number of particles $n$. It should be borne in mind that a 3b interaction also produces 2b pieces in the model space, exactly in the same way that the 2b interaction produces the single particle splittings by summing over the core orbits $c$ of degeneracy $D_c$,

$$ \sum_c a_{sc} n_s n_c = n_s \sum_c a_{sc} D_c \equiv n_s \varepsilon_s . $$

Note that a 3b potential will produce both 1b and 2b terms. We need not worry about the former because

$$ V_{st}^T = \sum_J \frac{V_{st}^{JT}(2J + 1)[1 - (-)^{J+T}] \delta_{st}}{(2J + 1)[1 - (-)^{J+T}] \delta_{st}} , $$

$$ a_{st} = \frac{1}{4} (3 V_{st}^{T1} + V_{st}^{T0}) , $$
$$ n_{st} = \frac{1}{1 + \delta_{st}} n_r (n_s - \delta_{st}) , $$
$$ T_{st} = \frac{1}{1 + \delta_{st}} (T_r \cdot T_s - \frac{3}{4} n_s \delta_{st}) . $$
they correct \( \varepsilon_s \) which will be taken from experiment as traditionally done. The latter, together with the 3b part will transform the realistic (R) 2b centroid \( V_{\text{fr}}^T(R) \) into \( V_{\text{fr}}^T(R1) = \sqrt{\chi(1)}(R) + (\alpha_{\text{fr}}^T + \beta_{\text{fr}}^T n) \equiv V_{\text{st}}^T(R) + \chi_{\text{fr}}^T \).

\( H_m \) can be characterized by demanding correct single particle and single hole spectra around closed shell nuclei. This set \( (cs \pm 1) \) is taken to include the differences in binding energies (gaps) \( 2BE(cs) - BE(cs + 1) - BE(cs - 1) \). The major monopole correction involves the gaps around \( ^{12}\text{C}, ^{28}\text{Si}, ^{48}\text{Ca} \) and \( ^{56}\text{Ni} \) which are too small to produce the observed double magicity. It will be taken care by a single linear form \( \kappa \equiv \kappa(n) \). The generalization of Eq. (8) is then

\[
\begin{align*}
V_{\text{fr}}^T(R1) &= V_{\text{fr}}^T(R) - (-)^T \kappa + \chi_{\text{fr}}^T, \\
V_{\text{fr}}^T(R1) &= (V_{\text{fr}}^T(R) - 1.5 \kappa) \delta_{T0} + \chi_{\text{ff}}^T, \\
V_{\text{fr}}^T(R1) &= V_{\text{fr}}^T(R) + \chi_{\text{fr}}^T.
\end{align*}
\]

The single particle splittings above the \( f \) closures are quite well given by some R interactions. Hence the corrective term \( \chi_{\text{fr}}^T \)—which will prove useful in the \( sd \) shell—is most likely to have a 2b origin. \( \chi_{\text{ff}}^T \) is introduced only for completeness and will be altogether disregarded. \( \chi_{\text{fr}}^T \) must play an important role because the single hole states (at \( A = 15, 39 \) and 79) are severely missed. However, they have little influence on the nuclei we shall study (at the beginning of the shells).

For the \( ^{10}\text{B} \) spectrum in Fig. 1 the black squares show the results of Návratil and Ormand (NO) for the low lying \( T = 0 \) states in \( ^{10}\text{B} \). The black circles correspond to the bare KLS G-matrices used in \( ^{22}\text{Na} \). The agreement with experiment (lines) is poor but the agreement between the calculations is good. This is not a joke, but an important remark: NO provides the foundation for a conventional G-matrix study. As emphasized over the years, the realistic G-matrices are very close to one another and will provide good spectra once monopole corrected. Absolute energies and strength functions are another matter, and much remains to be learnt from exact and no-core results.

The open pentagons in Fig. 1 correspond to the classic Cohen Kurath fit (CK). The open squares and circles refer to the KLS interaction with a \( \kappa = 1.1 \) correction in Eq. (8). The open squares test the influence of the \( \chi_{\text{fr}}^T \) term through a uniform attraction of 1.5 MeV (in CK it is about 3 times as large). Conclusion: there is not much to choose between the two LKS corrected cases. Moreover, they are practically as good as CK except for the second \( J = 3 \) level.

There are two reasons not to dwell any longer in the \( p \) shell. The first is that the aim of this letter is to show that the monopole corrections must be 3b, i.e., \( \kappa \) must be linear in \( n \), which demands examining cases of sufficiently different \( n \). Unfortunately this is impossible without bringing in the other possible contributions: For example, \( \chi_{\text{fr}}^T \) is not very significant in \( ^{10}\text{B} \) \((n = 6)\), but it is important in \( ^{12}\text{C} \) \((n = 8)\) and crucial in \( ^{14}\text{N} \) \((n = 10)\). Therefore, there is no way of exploring what a single term in Eq. (8) does: all must contribute. As it happens—and this is the second reason—the full exploration has been done, and the results were excellent. At the time, the problem was that the 3b contributions turned out to be large and important, and the authors did not know what to do with them.

For the \( ^{22}\text{Na} \) spectrum in Fig. 2 the black squares show the results for the venerable KB. The black circles correspond to the BonnC (BC) G-matrices. The agreement with experiment (lines) is poor but the agreement between the calculations is good. Again, this is not a joke, but an important remark: as mentioned, there are very little differences between the realistic G-matrices. The open pentagons correspond to Wildenthal’s USD. The open squares and circles refer to the KB and BC interactions with \( \kappa = 0.9 \) and 0.85 corrections respectively. We shall come to the triangles soon. Though USD is closer to experiment, the corrected R interactions do definitely well.
The story repeats itself for $^{23}$Na and $^{24}$Mg in Fig. 3. The notations are the same as in Fig. 2. The agreement with experiment is now truly satisfactory, and the plotting technique adopted makes the physics quite evident: the trouble with a 2b-only description is that the excited band $K = 1/2$ in $^{23}$Na, and the $K = 2$ ($\gamma$) band in $^{24}$Mg are too low.

The open triangles in Figs. 2 and 3 show what happens with KB when—instead of keeping $\kappa$ fixed—we increase it by steps of 0.5 per $n$. Though there is an improvement, it is not sufficient to claim the irrefutability of a 3b mechanism. The proof comes when we move to Figs. 4: In $^{27}$Si, $^{28}$Si, and $^{29}$Si the local value of $\kappa$ (open squares and circles) has decreased to 0.60 for KB and to 0.55 for BC. A constant $\kappa$ is totally ruled out, while the linear law (triangles) does quite well. Clearly, the 3b terms are indispensable. The superb 2b-only USD fit was obtained mostly through the massacre of a strong $JT = 20$ pairing term that is a constant feature of the R interactions, which makes USD R-incompatible [25, Section V]. This has been known for some time and it is only occasionally that trouble may arise. The problem is that the intensity of the quadrupole force (in MeV, extracted as in [25]) is 2.7 for KB and 3.2 for BC. This discrep-
ancy is somewhat disturbing, but it does alter the basic fact that 3b monopole terms are necessary. Fig. 5 shows that for $\kappa = 0.43$, BC produces a backbending pattern in $^{48}\text{Cr}$ that is practically as good as the KB3 one. At $\kappa = 0.28$ — the correct value around $A = 56$ — the agreement with experiment is destroyed.

There are several other indications that a 3b interaction is essential. Perhaps the most significant is the following: The monopole centroids $V_{T_f}^{\ell} \langle s^d \rangle$ must be such that when $f_{7/2}$ fills the $d$, ($l = 2$) orbits are depressed with respect to the $s$, ($l = 0$) one. However, it is clear from the spectrum and the spectroscopic factors in $^{29}\text{Si}$ that the filling of $d_{5/2}$ favours the $p$, ($l = 1$) orbit(s) over the $f$, ($l = 3$) ones. A 2b-only assumption leads to a contradiction: if $f_{7/2}$ acting on the $sd$ shell favours the larger $l$ orbits, $d_{5/2}$ acting on the $pf$ shell must do the same. Without unacceptable ad-hoc assumptions, a 2b mechanism cannot do otherwise but a 3b one can.

From what we have seen, 3b monopole forces make things simpler, and there are good reasons to believe that the formidable task of a full treatment — including multipole terms — need not be inevitable. A recent generation of 3b potentials [1] has made it possible for the exact solutions to eliminate the more offending aspects of the 2b $^{10}\text{B}$ spectrum [2]. It will be of much interest to check whether the underlying mechanism corresponds to the one proposed in this letter. At any rate, a full characterization of the 3b potentials is not an easy matter, and it could be hoped that information coming from shell model studies may prove valuable. Especially at a time when GFMC and no-core calculations have rigorously established the basic reliability of such studies.

Several observations of Alfredo Poves and Frédérique Nowacki have been of great help.

[1] B. S. Pudliner, V. R. Pandharipande, J. Carlson, S. Pieper and R. W. Wiringa, Phys. Rev. C 56, 1720 (1997).