n-p Pairing, Wigner Energy, and Shell Gaps

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The diagonal correlation energy due to *n-n*, *p-p*, and *n-p* pairing is shown to resolve the discrepancies between shell gaps determined from binding energy differences and the gaps calculated with Woods-Saxon potentials or with other mean-field models. The difference in diagonal correlation energy between an $N = Z$ nucleus with filled shells and the nucleus with one less nucleon resolves this problem in lowest order. A previously derived result, that the diagonal correlation energy in the last occupied orbital for the latter nuclei is $1/2$ of the equivalent correlation energy for closed shell nuclei, is tested against observed binding energies and found to be fairly accurate.

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One of the great puzzles in nuclear structure studies is that mean-field potentials give accurate predictions of single-particle energy-level orderings and spacings within a shell, yet they substantially underestimate the "observed" gaps between shells. In this work, we resolve this striking discrepancy.

Bohr and Mottelson [1] note that the observed shell gap for $N = 8$ in ^{16}O is 11.5 MeV, and the gap obtained from a Woods-Saxon potential is 7.2 MeV. For ^{40}Ca the gap at $N = 20$ is 7.3 Mev, while a Woods-Saxon calculation gives 5.0 MeV. In ^{56}Ni the observed gap, for $N = 28$, is 6.2 MeV, and a Woods-Saxon potential gives 4.4 MeV. A Skyrme interaction [2] gives results similar to the Woods-Saxon estimates; a 6.8 MeV gap for $N = 8$ in ^{16}O; a 4.6 MeV gap for $N = 20$ in ^{40}Ca. This Skyrme interaction [2] has an effective mass close to 1.0, and gives a spectrum similar to Woods-Saxon estimates. Other Skyrme interactions have smaller effective masses and give larger shell gaps. However, Skyrme interactions with smaller effective masses give larger level spacings within a shell, usually worsening the agreement with experiment.

We can resolve these discrepancies by examining the meaning of observed spacing a little more closely. The observed level spacings are defined by taking differences of ground-state masses. Using ^{40}Ca as an example, the energy of the $f_{7/2}$ level, just above the $N = 20$ gap, is defined as the difference in ground-state mass of ^{41}Ca and ^{40}Ca. Similarly, the energy of the $d_{3/2}$ level, just below the $N = 20$ gap, is defined as the difference in mass of ^{40}Ca and ^{39}Ca. This method of assigning single-particle energies presupposes that there are no many-body effects involved in mass differences at closed shells. However, for nuclei having approximately equal numbers of neutrons and protons, there are large changes in binding energy due to many-body effects—even for closed shell nuclei. This was first noted by Wigner [3], and we refer to this energy as the Wigner energy in $N = Z$ even-even nuclei. Here, we note that there are also large correlation energy effects in the even-odd and odd-even nuclei, with one neutron or one proton less than the $N = Z$ even-even nucleus. The difference of these correlation energies accounts for much of the discrepancy between observed and calculated shell gaps.

For nuclei with almost equal numbers of protons and neutrons, *n-p* pairing, as well as like nucleon pairing, plays an important role in nuclear structure studies. The interplay of these pairing modes has been studied in the framework of extended quasiparticle approximations [4–13] and references therein, as well as in the framework of exact solutions [14–19].

The Hamiltonian that is used [7,20] to treat *n-p* pairing, both $T = 0$ and $T = 1$, as well as like particle pairing is

$$\begin{aligned} H = {} & \sum_{k>0} \varepsilon_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k} + b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) \\ & - \sum_{i,j} G_{i,j}^{T=1} [A_i^\dagger A_j + B_i^\dagger B_j + C_i^\dagger C_j] \\ & - \sum_{i,j} G_{i,j}^{T=0} [D_i^\dagger D_j + (M_i^\dagger M_j + N_i^\dagger N_j) \delta(\Omega_{i,j})], \end{aligned} \quad (1)$$

where the indices i, j, and k denote values of j_z for spherical nuclei or the projection of angular momentum on the nuclear symmetry axis for deformed nuclei. Here, $a_k^\dagger (b_k^\dagger)$ denotes a neutron (proton) creation operator; $A_i^\dagger = (a_i^\dagger a_{-i}^\dagger)$ and $B_i^\dagger = (b_i^\dagger b_{-i}^\dagger)$. The $T = 1$ *n-p* pair creation operator is $C_i^\dagger = \frac{1}{\sqrt{2}} [a_i^\dagger b_{-i}^\dagger + a_{-i}^\dagger b_i^\dagger]$ and the $T = 0$ *n-p* pair creation operator is $D_i^\dagger = \frac{i}{\sqrt{2}} [a_i^\dagger b_{-i}^\dagger - a_{-i}^\dagger b_i^\dagger]$.

The terms $M_i^\dagger = (a_i^\dagger b_i^\dagger)$ and $N_i^\dagger = (a_{-i}^\dagger b_{-i}^\dagger)$ are relevant only for states having the same value of $|j_z|$ or Ω, the Nilsson quantum number in the case of deformed nuclei. The $M_i^\dagger$ and $N_i^\dagger$ terms do not lead to collective correlations but their diagonal matrix elements are important.

Our ordering convention is to put neutron creation operators before proton creation operators in the $C^\dagger$, $D^\dagger$, $M^\dagger$, and $N^\dagger$ operators that appear in the Hamiltonian and in the wave functions. We define the proton wave function with positive j_z as the negative of the equivalent neutron wave function to retain the usual plus sign in $C^\dagger$.

Our variational wave function [20] is a product form

$$\Theta = \prod^{k} \Psi_k \prod^{m} \Phi_m |0\rangle, \tag{2}$$

where the index k runs over the unblocked orbitals, the index m runs over all blocked orbitals (orbitals with one or three nucleons), and $|0\rangle$ is the physical vacuum.

For unblocked orbitals, Ψ_k is given by

$$\Psi_k = [1 + U(1,k)A_k^\dagger + U(2,k)B_k^\dagger + U(3,k)C_k^\dagger + U(4,k)D_k^\dagger + U(5,k)W_k^\dagger], \tag{3}$$

where $U(i,k)$ are variational amplitudes. $W_k^\dagger$ denotes the configuration in which level k is occupied by two neutrons and two protons. The ordering of creation operators in $W_k^\dagger$ is $A_k^\dagger B_k^\dagger$.

For blocked orbitals, Φ_m is given by

$$\Phi_m = [T(1,m)a_m^\dagger + T(2,m)b_m^\dagger + T(3,m)A_m^\dagger b_m^\dagger + T(4,m)a_m^\dagger B_m^\dagger], \tag{4}$$

where $T(i,m)$ are variational amplitudes. The proton number and neutron number are projected from the wave functions before the variational amplitudes are determined. It should be noted that there is pair scattering between the one-particle and the three particle configurations in Φ_m, but there is no scattering between configurations in Φ_{m0} and configurations in Ψ_{m0}, because this two-body interaction preserves particle number parity in all levels.

For the purposes of this analysis, it is most important to note that there are large diagonal contributions to the energies of the different configurations. Taking protons and neutrons in the same orbit to have the same single-particle energy ϵ_i, we obtain

$$E(A_i^\dagger) = E(B_i^\dagger) = E(C_i^\dagger) = 2\epsilon_i - G_{i,i}^{T=1}, \tag{5}$$

$$E(D_i^\dagger) = 2\epsilon_i - G_{i,i}^{T=0}, \tag{6}$$

$$E(W_i^\dagger) = 4\epsilon_i - 3(G_{i,i}^{T=0} + G_{i,i}^{T=1}), \tag{7}$$

where $E(A_i^\dagger)$ is the energy of two neutrons in orbital i.

For the levels having odd number parity configurations, the diagonal energies are

$$E(a_i^\dagger) = E(b_i^\dagger) = \epsilon_i, \tag{8}$$

and

$$E(A_i^\dagger b_i^\dagger) = E(a_i^\dagger B_i^\dagger) = 3\epsilon_i - \tfrac{3}{2}(G_{i,i}^{T=0} + G_{i,i}^{T=1}). \tag{9}$$

Denoting the energy of the $N = Z = A/2$ nucleus as E_0^0, the single-particle energy of the last occupied orbital as ϵ_0 and the energy of the first unoccupied orbital as ϵ_1, we immediately get the usual result for the neutron addition energy

$$B(A/2, A/2+1) - B(A/2, A/2) = \epsilon_1, \tag{10}$$

where $B(Z,N)$ denotes a binding energy. However, the neutron removal energy has a correlation contribution

$$B(A/2, A/2) - B(A/2, A/2-1) = \epsilon_0 - \tfrac{3}{2}[G_{i,i}^{T=0} + G_{i,i}^{T=1}]. \tag{11}$$

The extra term in the neutron removal energy comes from pairing.

To extract these correlation energies from experimental data, we utilize the function [21,22], $\delta V(Z,N)$,

$$\delta V(Z,N) = B(Z,N) - B(Z-2,N) - B(Z,N-2) + B(Z-2,N-2), \tag{12}$$

for e-e nuclei. The use of $\delta V(Z,N)$ was first applied to the analysis of Wigner correlation energies by Van Isacker *et al.* [23] and soon after by Satula *et al.* [24].

For odd mass nuclei, e.g., the nuclide with $Z = (A/2 - 1)$ and $N = A/2$, we define a similar quantity

$$\delta K(Z-1,N) = B(Z-1,N) - B(Z-1,N-2) - B(Z-2,N) + B(Z-2,N-2). \tag{13}$$

$\delta K(Z, N-1)$ is defined similarly. Note that $\delta V(Z,N)$ can be rewritten as three terms

$$\delta V(Z,N) = [B(Z,N) - B(Z-2,N-2)] - [B(Z,N-2) - B(Z-2,N-2)] - [B(Z-2,N) - B(Z-2,N-2)]. \tag{14}$$

The first term is the binding energy gained by adding two protons and two neutrons to the nuclide $(Z-2, N-2)$ and the last two terms are the binding energies gained by adding a neutron pair and a proton pair separately. $\delta V(Z,N)$ gives the extra binding due to the four nucleon correlation. $\delta K(Z-1,N)$ can be rewritten in a similar way and it gives the difference in binding energy gained by adding a proton and two neutrons together, as compared to adding the proton and neutron pair separately.

In lowest order, i.e., assuming that the wave-function is a Slater determinant, we calculate for an $N = Z = A/2$ even-even nucleus

$$\delta V(A/2, A/2) = 3G_{i,i}^{T=0} + G_{i,i}^{T=1}, \tag{15}$$

and for the odd mass nuclide, we get

$$\delta K(A/2-1, A/2) = \delta K(A/2, A/2-1) = \tfrac{3}{2}G_{i,i}^{T=0} + \tfrac{1}{2}G_{i,i}^{T=1}. \tag{16}$$

In order to extract these quantities from the experimental data, we first subtract out all smooth contributions to the binding energies such as the symmetry energy. Our subtraction procedure is a symmetrized version of one given earlier [24]. For $N = Z = A/2$, we have

$$E_{\text{smooth}} = 0.25[\delta V(Z-2,N) + \delta V(Z+2,N) + \delta V(Z,N-2) + \delta V(Z,N+2)], \quad (17)$$

for e-e nuclei. For odd mass nuclides, we replace δV by δK to calculate E_{smooth}. For the case $Z = (A/2 - 1)$, note that all values of Z in E_{smooth} are odd. For both odd mass and even mass nuclides, the number parity of both neutrons and protons is the same for all terms in E_{smooth} as it is in the nuclide of interest. Having defined E_{smooth}, the Wigner correlation energy is then defined as

$$E_{\text{Wigner}} = 0.25[\delta V(Z,N) - E_{\text{smooth}}] \quad (18)$$

In lowest order, the predicted correlation energy calculated in this way for the nuclide $(A/2 - 1, A/2)$ or $(A/2, A/2 - 1)$ is $1/2$ the value for $(A/2, A/2)$. Configuration interaction can change this value. In Fig. 1, we present the ratios $\delta\tilde{K}(A/2-1, A/2)/\delta\tilde{V}(A/2, A/2)$ and $\delta\tilde{K}(A/2, A/2-1)/\delta\tilde{V}(A/2, A/2)$ as a function of mass, where the tilde indicates that E_{smooth} has been subtracted out. The quantities $\delta\tilde{V}(A/2, A/2)$ and $\delta\tilde{K}(A/2, A/2-1)$ are strictly experimental quantities, depending only on nuclear ground-state masses. The values cluster nicely near 0.5, the lowest order estimate. Note the expanded scale in the figure.

To get a feeling for the magnitudes of the various quantities involved in this ratio, we consider ^{40}Ca in detail. The quantity $\delta V(20, 20)$ is 8.30 Mev and $E_{\text{smooth}}(20, 20)$ is 3.59 Mev. The quantity $\delta K(20, 19)$ is 4.50 Mev and $E_{\text{smooth}}(20, 19)$ is 1.81 MeV.

The lowest order estimate of the decrease in the shell gaps for $(A/2, A/2)$ nuclides is

$$\Delta(\text{gap}) = \tfrac{3}{2}[G_{i,i}^{T=0} + G_{i,i}^{T=1}], \quad (19)$$

i.e., for the neutron gaps that we consider here,

$$\Delta(\text{gap}) = \tfrac{3}{2}[\delta\tilde{V}(A/2, A/2) - \delta\tilde{K}(A/2, A/2-1)], \quad (20)$$

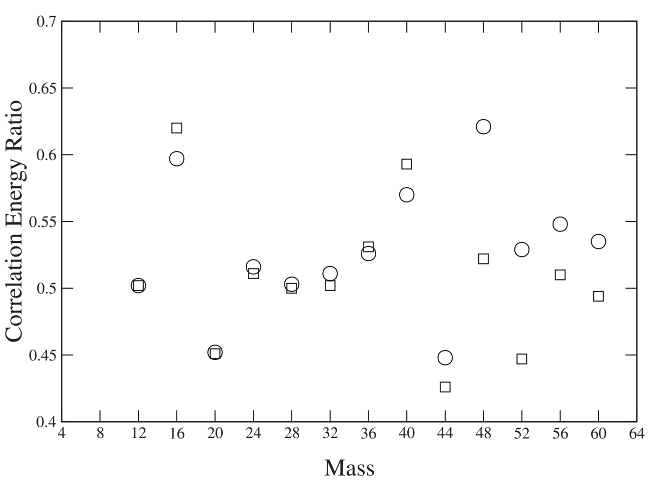

FIG. 1. Correlation energy ratios as a function of mass. The x axis is the mass of the nuclide $(A/2, A/2)$. Open circles are for $(A/2, A/2 - 1)$; open squares for $(A/2 - 1, A/2)$.

where we assume equal $T = 0$ and $T = 1$ pairing strengths. In addition to extracting shell gaps, we have also extracted sub-shell gaps for $N = Z$ nuclides; the six neutron subshell $p_{3/2} - p_{1/2}$ gap in ^{12}C; the 14 neutron subshell $d_{5/2} - s_{1/2}$ gap in ^{28}Si and the 16 neutron $s_{1/2} - d_{3/2}$ subshell gap in ^{32}S. In Fig. 2, we compare shell gaps for nuclides ranging from $A = 12$ to $A = 56$. For each nuclide, we show the observed gap and the gap extracted from the experimental data, when the correlation energy is subtracted. We compare these gaps with spacings obtained from a Woods-Saxon (WS) potential. The Woods-Saxon potential parameters were slightly modified from the values obtained [25] for nuclides near $A = 250$. The potential depth was adjusted to give the observed binding energy for the orbital just above the gap of interest. The magnitude of the spin-orbit potential was increased by 1 MeV. The calculated gaps differ slightly from those cited [1,2]. The comparison illustrates that the extracted gaps are much more reasonable than the observed gaps for fixing nuclear single-particle potentials. In fact, the agreement between the extracted gaps and the Woods-Saxon calculations is quite good, with the exception of ^{12}C. Even for ^{12}C, the value of 1.95 MeV for the extracted gap is much more reasonable than the observed value of 13.77 MeV.

The mechanism that explains the difference between observed gaps and extracted gaps plays an additional role in nuclear structure studies. It predicts that the excitation energy of four-particle four-hole (4p-4h) configurations in $N = Z$ even-even nuclei, is reduced substantially relative to the excitation energy of 1p-1h configurations. The excitation energy of the 1p-1h configuration is

$$E(\text{1p-1h}) = \epsilon_1 - \epsilon_0 + \tfrac{3}{2}[G_{i,i}^{T=0} + G_{i,i}^{T=1}], \quad (21)$$

while

$$E(\text{4p-4h}) = 4\epsilon_1 - 4\epsilon_0. \quad (22)$$

The fact that the $T = 1$, $I^\pi = 0^+$ state and the $T = 0$, $I^\pi = 1^+$ states are close in energy in $N = Z$ odd-odd nuclei indicates that the pairing strengths are roughly

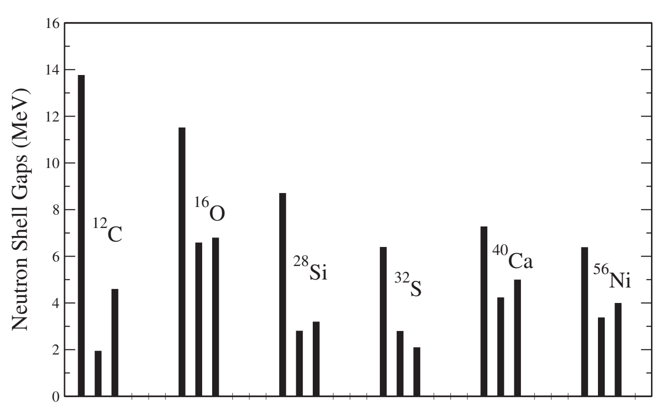

FIG. 2. Comparison of gaps. For each nuclide, the ordering is observed gap, extracted gap, and calculated WS spacing.

equal. The two levels would be degenerate if the strengths were equal. This near equality of pairing strengths is suggestive of SU(4) symmetry. Our analysis of shell gaps, however, includes regions where the $\mathbf{l} \cdot \mathbf{s}$ splittings are large and the SU(4) symmetry is no longer strictly valid.

To make an estimate of shell-gaps that takes off-diagonal pairing effects into account, requires rather detailed assumptions. Single-particle energy-level spacings and the relative magnitudes of diagonal and off-diagonal pairing matrix elements are needed. Using the variational wave function of Eq. (2), we consider ^{40}Ca in detail, to get some feeling for how large such effects might be. We assume that protons and neutrons have the same single-particle energies and that the spectra are those given by Bohr and Mottelson [1], with the change that the gap at $N = 20$ is set to 4.24 MeV, as determined by our procedure. It has long been known [26–28] that the diagonal pairing matrix elements of a δ interaction or a density dependent δ interaction are roughly twice as strong as the off-diagonal pairing matrix elements. Using a D1S Gogny interaction, [29], one gets a ratio of 2.4, which we have used [20] previously, together with an off-diagonal pairing strength of $(19.6/A)$ MeV, based on systematics of the Wigner correlation energy [24]. Making these assumptions for the interaction strengths, we find that the relative shift in the binding energies of ^{39}Ca and ^{41}Ca is roughly 100 kev.

In this work, we have resolved the long standing puzzle of the discrepancy between observed shell gaps and the shell gaps obtained from mean-field calculations. By taking into account the Wigner energy in even-even $N = Z$ nuclides, and the counterpart of this energy in nuclides with one less nucleon, we obtain shell gaps and sub-shell gaps that are in very good agreement with mean-field calculations, apart from ^{12}C. We have shown that the ratio of correlation energies in nuclides with one nucleon less than the $N = Z$ even-even nuclides, divided by the $N = Z$ nuclide correlation energy is in good agreement with the ratio of 0.5, predicted by the n-p pairing force wave functions [20] that take three-body and four-body correlations into account. This correlation energy effect also gives a substantial decrease in the excitation energy of 4p-4h configurations relative to 1p-1h excitations in $N = Z$ even-even nuclei.

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