Pairing Theory of the Wigner Cusp

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Abstract.

Subtracting the Coulomb energy from the mass of a nucleus results in what may be called the Coulomb reduced mass. In 1936, Bethe and Bacher suggested that the latter increases from \( N = Z \) approximately quadratically in \( N - Z \), where \( N \) and \( Z \) are the numbers of neutrons and protons. Myers and Swiatecki found in 1966 a marked deviation from this rule; for small \(|N - Z|\) the Coulomb reduced mass rises more rapidly. They called the apparent extra binding energy in the vicinity of \( N = Z \) the Wigner energy. It will be shown that this nonanalytic behaviour of the mass as a function of \( N - Z \), referred to as the Wigner cusp, arises naturally when the pairing force is treated in the random phase approximation (RPA). In the limit of equidistant single nucleon levels the increment of the Coulomb reduced mass from \( N = Z \) is approximately proportional to \( T(T+1) \), where \( T \) is the isospin, equal to \(|N - Z|/2\) in the ground state of a doubly even nucleus. This provides a microscopic foundation of taking the macroscopic symmetry energy to have this form.

Excitation energies proportional to \( T(T+1) \) resemble the spectrum of a quantal, axially symmetric rotor. In 1999, Frauendorf and Scheik identified the superfluid pair gap as the deformation which gives rise to an analogous rotation in isospace. Recent work by Bentley and Frauendorf in collaboration with the speaker applies a Strutinskij renormalised independent nucleons plus pairing Hamiltonian to the description of nuclei in the the vicinity of \( N = Z \). The theory includes a Strutinskij renormalisation of the RPA contribution to the total energy. This theory reproduces quite well the empirical masses in the vicinity of \( N = Z \) for \( A \geq 24 \), including the Wigner cusps and the splitting of the lowest levels with \( T = 0 \) and 1 in the doubly odd \( N = Z \) nuclei. While it is crucial for this result that the liquid drop symmetry energy is similar to the symmetry part of the Strutinskij counterterm to the RPA energy in being proportional to \( T(T+1) \) rather than \( T^2 \), large shell corrections modify this bulk behaviour. The RPA correction makes a contribution of about 1 MeV to the \( T = 0 \) doubly odd doubly even mass differences. For the relative masses of doubly even nuclei it is insignificant.

1 Introduction

In 1966, analysing the mass data of the time, Myers and Swiatecki discovered a “sharp trough along \( N = Z \) occurring in the masses of the lighter nuclei” remaining after “the experimental masses in the range \( A = 4 \) to \( A = 58 \) were
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corrected for all known effects (liquid-drop binding and shell effects deduced from nuclei with $N = Z$) [1]. It is important for the following to notice that the symmetry energy term in their “liquid-drop binding” is proportional to $(N - Z)^2$. Referring to Ref. [2], they name the extra term they include in their mass formula to account for this anomaly the “Wigner term”, and it is customary to refer accordingly to the trough itself as the “Wigner cusp”.

The reference to Wigner points to a result in Ref. [2] based on the supposition that the two-nucleon interaction is invariant under arbitrary unitary transformation of the four-dimensional space of the nucleonic spin and isospin. Under this and some other simplifying assumptions Wigner derives that the isospin dependent part of the total interaction energy of a nucleus is proportional to $T(T + 4)$, where $T$ is the isospin, in the ground state of a doubly even nucleus equal to $|N - Z|/2$. It is known by now that the two-nucleon interaction does not have this simple structure. Redoing Wigner’s derivation under the assumption of only isobaric invariance, I show in an appendix to Ref. [3] that in this case a factor $T(T + 1)$ replaces Wigner’s $T(T + 4)$. In both cases the estimate applies only to the interaction part of the total energy. Wigner estimates the contribution from the nucleonic kinetic energy by the Thomas-Fermi model. This gives a $T$-dependent term proportional to $T^2$ so that if the interaction energy is proportional to $T(T + 1)$ then the $T$-dependent part of the total energy is proportional to $T(T + X)$ with $X < 1$. Empirically, the kinetic and interaction terms make about equal contributions to the symmetry energy [4].

The nuclear physics literature since 1966 has many attempts of explaining the Wigner cusp. My allotted time does not allow me to discuss it all; I must refer you to an extensive review in Ref. [3]. Presented here is my own take on the issue.

2 Superfluid isorotation

The empirical evidence points to something like a $T(T + 1)$ law for the $T$-dependent part of the Coulomb reduced mass of a nucleus. Thus, for example, the semiempirical mass formula of Duflo and Zuker [5] has symmetry terms of this form. Frauendorf and Sheikh noticed that this is similar to the spectrum of an axially symmetric rotor and identified the nuclear superfluidity as the deformation in isospace that could give rise to an analogous isorotation [6,7]. In fact, in a product of neutron and proton Bardeen-Cooper-Schrieffer (BCS) states the expectation value of the pair field isovector

$$\vec{P} = -2\hat{\tau}_i \sum_{p < q} \langle p | \vec{t} y \vec{t} | q \rangle a_p a_q$$

is perpendicular to the expectation value of the isospin $\vec{T}$. The pair field therefore precesses about $\vec{T}$ in a way analogous to the precession of the single-nucleon potential well of the axially deformed nucleus about the angular momentum. In Eq. (1) the vector $\vec{t}$ is the single-nucleon isovector, $a_p$ annihilates a nucleon in the
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member $|p\rangle$ of an orthonormal basis of single-nucleon states and the bar denotes time reversal.

A microscopic version of this picture is explored in Refs. [3,8–10]. I consider a Hamiltonian

$$H = \sum_j h_j - G \vec{P}^\dagger \cdot \vec{P} + \kappa \sum_{j<k} \vec{t}_j \cdot \vec{t}_k, \quad (2)$$

where $j$ and $k$ label the nucleons and $h$ is a single-nucleon Hamiltonian commuting with $\vec{t}$. By adding a constant, replacing $\sum_j h_j, \vec{P}$ and $\vec{T} = \sum_j \vec{t}_j$ by their expectation values in a Bogolyubov quasinucleon vacuum and constraining the expectation values of $N$ and $Z$ by Lagrangian multipliers, one arrives at the Routhian [11]

$$R = \left\langle \sum_j h_j \right\rangle - G|\langle \vec{P} \rangle|^2 + \frac{1}{2} \kappa |\langle \vec{T} \rangle|^2 - \lambda_n \langle N \rangle - \lambda_p \langle P \rangle. \quad (3)$$

Minimisation of $R$ gives essentially the BCS theory. Zero point oscillation about the minimal $R$ is taken into account in the random phase approximation (RPA). This gives for the total energy the expression

$$E = \sum v^2 \epsilon - \frac{\Delta^2}{G} + \frac{1}{2} \kappa T^2 + c + \frac{1}{2} \left( \sum \omega - \sum \omega_0 \right), \quad (4)$$

where $\epsilon$ is an eigenvalue of $h$ counted with multiplicity, $v^2$ is the BCS occupancy, possibly different for neutrons and protons, $\Delta = G\langle \vec{P} \rangle$, $T = |N-Z|/2$, the constant $c$, which does not depend on $T$, accounts for exchange contributions to $\langle H \rangle$ including a compensation for the constant added in the derivation of Eq. (3), $\omega$ denotes an RPA frequency and $\omega_0$ is a two-quasinucleon energy. The expectation values are taken in the BCS state. The BCS equations separate into independent ones for neutrons and protons and the RPA equations into independent ones for two-quasineutron, two-quasiproton and quasi-neutron-quasi-proton excitations.

If $\Delta_n = -2^{-\frac{1}{2}} G \langle P_- \rangle \neq 0$, a Nambu-Goldstone mode [12][13] arises from the invariance of $R$ under transformations $\exp i \alpha N$, and similarly if $\Delta_p = 2^{-\frac{1}{2}} G \langle P_+ \rangle \neq 0$. If $T > 0$ or $T = 0$ and $\Delta_n = \Delta_p \neq 0$, there is also a "quasi"-Nambu-Goldstone mode with frequency $|\lambda_n - \lambda_p|$ following from the relation

$$[-\lambda_n N - \lambda_p Z, T_-] = (\lambda_n - \lambda_p)T_-.$$

The last term in Eq. (4), which I call the symmetry force, turns out to have no other effect than adding its eigenvalue $\frac{1}{4} \kappa [T(T+1) - 3A/4]$ to the total energy. It may thus be included a posteriori. For the moment I set $\kappa = 0$ so that my Hamiltonian is the bare, isobarically invariant pairing Hamiltonian. The RPA theory of this Hamiltonian was first discussed by Ginocchio and Wesener [14].
3 Uniform single-nucleon spectrum

Important qualitative insight is gained from the case of a uniform single-nucleon spectrum with constant level density $g$. This is studied in Ref. [10]. Presently, let it be assumed for simplicity that the Kramers degenerate single-nucleon levels are $\epsilon = 1/(2g), 3/(2g), 5/(2g), \ldots, (2\Omega - 1)/(2g)$, where $\tau = n, p, np$ refer to the neutron and proton BCS + RPA and neutron-proton RPA calculations, respectively, and $\Omega_n = N, \Omega_p = Z, \Omega_{np} = A/2$. Displacing the single-nucleon spectrum adds $A$ times the displacement to the total energy. It is understood that $N$ and $Z$ are even.

The result of replacing summation over $\epsilon$ by integration is

$$E = \sum_{\tau = n, p} \left( g \int_0^{\Omega_\tau/2g} \epsilon \, d\epsilon + E_{\text{BCS},\tau} \right) + \sum_{\tau = n, p, np} E_{\text{RPA},\tau}, \quad (6)$$

where $E_{\text{BCS},\tau}$ and $E_{\text{RPA},\tau}$ are given by closed, analytic expressions. For $\tau = n$ and $p$ these expressions are functions of $G$, $g$ and $\Omega_\tau$ while $E_{\text{RPA},np}$ also depends on $\delta\lambda_{np} = \lambda_n - \lambda_p$. By expressing $E$ as a function of $T$ for a constant $A$ one gets

$$\sum_{\tau = n, p} \left( g \int_0^{\Omega_\tau/2g} \epsilon \, d\epsilon + E_{\text{BCS},\tau} \right) \approx \frac{A^2}{4} + \frac{T^2}{2g}, \quad (7)$$

$$E_{\text{RPA},n} + E_{\text{RPA},p} + E_{\text{RPA},np, T = 0} = \text{constant}, \quad (8)$$

$$E_{\text{RPA},np} - E_{\text{RPA},np, T = 0} \approx \frac{T}{2g}. \quad (9)$$

The contribution (9) comes from the quasi-Nambu-Goldstone mode. It is seen to add a term to the “kinetic” symmetry energy $T^2/(2g)$ which renders also this part of the total symmetry energy proportional to $T(T+1)$. Eq. (8) is a special case of a general relation

$$\omega_{\text{quasi-NG}} = \frac{d}{dT} E_{\text{mean field}}. \quad (10)$$

Hence if $E_{\text{mean field}} - E_{\text{mean field}, T = 0} \propto T^2$—which holds necessarily when the mean field state is not an eigenstate of $T_z$ and $T$ is sufficiently small—then $E_{\text{mean field}} - E_{\text{mean field}, T = 0} + \omega_{\text{quasi-NG}} \propto T(T+1)$ [9]. Marshalek made the analogous observation for spatial rotation [15]. As the RPA energy atop a mean field theory has always the form of the last term in Eq. (4), it follows that if the mean field energy rises quadratically in $T$ and the remainder of the RPA energy is constant then the $T(T+1)$ proportionality of the symmetry energy is exact in the mean field plus RPA approximation. In fact this remainder is, in the uniform case, not a constant but adds a negative term, which is proportional to $T^2$ to the lowest order of $T$. This correction is largest in the lightest nuclei. With realistic parameters its absolute value amounts to at most 3 MeV for $T \leq 0.2A$, $A \geq 24$. 

4
4 Woods-Saxon levels, $\kappa > 0$

Calculations with a Woods-Saxon single-nucleon spectrum and $\kappa > 0$ are reported in Ref. [3]. I refer to Figs. 3 and 4 of that article. When the single-nucleon spectrum is derived from a deformed Woods-Saxon potential ($A = 48, 68, 80$) the expectations from the uniform case are roughly borne out as seen, for example, from $\frac{\omega_{\text{quasi-NG}}}{(E(T) - E(0))} \approx 1/3 = T/(T(T + 1))$ for $T = 2$. But when the $N = Z$ nucleus is doubly magic ($A = 56, 100$) an entirely different picture emerges. Then the kinetic symmetry energy is almost linear in $T$. Quadric terms arise from the symmetry force and to some extent from the onset of BCS pairing when the neutron and proton Fermi levels move from the magic gap into the shells above and below. This gives rise to a large $X$ in an approximation of the total symmetry energy by an expression proportional to $T(T + X)$.

The reason for the linearity in $T$ is that the neutron excess is generated by a promotion of nucleons across the magic gap in the single-nucleon spectrum. Each proton transformed into a neutron adds to the total independent-nucleon energy an amount approximately equal to the width of the gap.

5 Accuracy of the BCS + RPA, BCS criticality

It is well known that the BCS gap parameter $\Delta_n$ vanishes for coupling constants $G$ below a critical value $G_{\text{crit}, n}$ of the order of the spacing of the single-nucleon levels surrounding the neutron Fermi level, and similarly for protons. (It follows that $G_{\text{crit}, \tau} = 0$ if the Fermi level is within a spherical subshell and also in the uniform approximation.) The accuracy of the BCS + RPA can be tested by comparison with a numeric minimisation of the Hamiltonian. Bentley and Frauendorf made such minimisations in valence spaces of six and seven Kramers and isospin degenerate single-nucleon levels [16], and comparisons with the BCS + RPA were done by Bentley et al. [17]; see Fig. 1 of the latter article for at fairly extreme case.

It turns out that globally, the BCS + RPA reproduces the exact energy very well. It can be shown to be asymptotically exact for $G \to \infty$ [14, 17]. However, a plot of $E$ as a function of $G$ has sharp dips at the critical $G$ while the exact curve goes smoothly through these points. This gives rise to fairly large local deviations. As a remedy Bentley et al. introduce an interpolation of the last term in Eq. (4). In the calculations reported below interpolation is applied for $0.5 G_{\text{crit}, \tau} < G < 2 G_{\text{crit}, \tau}$ when $\tau = n$ or $p$, and in the union of these intervals when $T = 0$ and $\tau = np$.

The singularity of the RPA energy at $G = G_{\text{crit}, \tau}$ is well known from the literature [18] and has a natural explanation in terms of the emergence of Nambu-Goldstone modes at these point [17].
6 Strutinskij renormalisation

Bentley et al. apply a Strutinskij renormalisation to the theory presented so far [17]. My present rendering of the method and its results includes some as yet unpublished updates.

The total energy is written

\[ E = E_{\text{mic}} - \tilde{E}_{\text{mic}} + E_{\text{LD}}. \]  

(11)

where \( E_{\text{mic}} \) and \( \tilde{E}_{\text{mic}} \) are given by Eqs. (4) and (6), respectively, except that the first term in the bracket in Eq. (6) is replaced by

\[ \int_{-\infty}^{\tilde{\lambda}_\tau} \tilde{g}_\tau(\epsilon) \epsilon \, d\epsilon. \]  

(12)

Here \( \tilde{g}_\tau(\epsilon) \) and \( \tilde{\lambda}_\tau \) are Strutinskij's smooth level density and chemical potential [19]. For clarity I write in the present context \( \tilde{E}_{\text{BCS},\tau} \) and \( \tilde{E}_{\text{RPA},\tau} \) for the terms \( E_{\text{BCS},\tau} \) and \( E_{\text{RPA},\tau} \) in Eq. (6). In these terms I use \( g = \tilde{g}_\tau(\tilde{\lambda}_\tau) \) with \( \tilde{g}_{np}(\epsilon) \) and \( \tilde{\lambda}_{np} \) to be defined below. In Ref. [17] a heuristically based approximation of \( \tilde{E}_{\text{RPA},np} \) is employed.

The liquid drop energy \( E_{\text{LD}} \) is taken in the form [5]

\[ E_{\text{LD}} = - \left( a_w - a_{wt} \frac{T(T+1)}{A^2} \right) A \]

\[ + \left( a_s - a_{st} \frac{T(T+1)}{A^2} \right) A^{2/3} B_s + a_c \frac{Z(Z-1)}{A^{1/3}} B_c, \]

(13)

where \( B_s \) and \( B_c \) are the usual functions of deformation [20]. A conventional Nilsson-Strutinskij calculation [21] supplies the deformations and single-nucleon spectra, and the different spectra for neutrons and protons are used everywhere except in the calculation of \( \tilde{E}_{\text{RPA},np} \), where average neutron and proton levels are employed. The calculations reported in Ref. [17] use average levels throughout. The variable \( \delta\lambda_{np} \) in \( \tilde{E}_{\text{RPA},np} \) (see the text after Eq. (6)) is set to \( \lambda_n - \lambda_p \) with \( \tilde{\lambda}_n \) and \( \tilde{\lambda}_p \) calculated from \( \tilde{g}_{np}(\epsilon) \) while \( \tilde{\lambda}_{np} \) corresponds to filling \( A/2 \) nucleons into the smooth average spectrum. In all parts of \( E_{\text{mic}} \) the \( A/2 \) lowest levels of either kind of nucleon are included in the calculation, and I take accordingly \( \Omega = A/2 \) for all \( \tau \) in the calculation of \( \tilde{E}_{\text{mic}} \).

In the calculation of \( E_{\text{mic}} \) for odd \( N = Z \) and \( T = 0 \) one neutron and one proton contribute the Fermi energy and the BCS and RPA schemes are applied to the remaining nucleons populating the remaining levels. The lowest state with \( T = 1 \) in such nuclei is assumed to differ in energy from its isobaric analogue with \( Z - 1 \) protons only by the difference in liquid drop Coulomb energy.

7 Data and parameters

I denote by \( E(A,T) \) the ground state energy for \( N + Z = A, (N-Z)/2 = T \), where \( N \) and \( Z \) are even, while \( E^*(A,T) \) is the lowest energy for odd
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\( N = Z = A/2 \) and isospin \( T \). The following combinations of these energies are considered.

- \( \Delta_{oo-ee} = E^*(A, 0) - \frac{1}{2}[E(A-2, 0) + E(A+2, 0)] \).
- \( E^*(A, 1) - E^*(A, 0) \).
- The constants \( \theta \) and \( X \) defined by

\[
E(A, T) = E_0 + \frac{T(T + X)}{2\theta} + a_c \frac{Z(Z - 1)}{A^{1/3}} B_c,
\]

\[
T = \begin{cases} 
0, 2, 4, & A \equiv 0 \mod 4, \\
1, 3, 5, & A \equiv 2 \mod 4.
\end{cases}
\]

The five parameters in Eq. (13) were fitted to the the values of \( E(A, T) \) for \( 24 \leq A \leq 100, 0 \leq N - Z \leq 10 \) that were measured according to the 2012 Atomic Mass Evaluation (AME12) [22]. The resulting rms deviation is 0.875 MeV, which is somewhat better than 0.950 MeV achieved in the calculations of Ref. [17]. The parameters \( G_1 \) and \( \chi \) in \( G = G_1 A^\chi \) were fitted to the empirical values of \( \Delta_{oo-ee} \) and \( E^*(A, 1) - E^*(A, 0) \) for \( 26 \leq A \leq 98 \) in so far as they can be derived from data from AME12 and the National Nuclear Data Center [23]. Here the resulting rms deviation is 0.708 MeV. Because the two sets of parameters are not independent, the fits were repeated alternately until both converged. The complete set of resulting parameters is \( a_v, a_{vt}, a_s, a_{st}, a_c, G_1, \chi = 15.07, 107.4, 16.04, 133.6, 0.6506, 7.232, -0.7604 \), all of them except \( \chi \) in MeV.

8 Results

Figure 1 shows comparisons of the calculated and measured values of \( \Delta_{oo-ee}, E^*(A, 1) - E^*(A, 0), 1/\theta \) and \( X \). While no perfect agreement is achieved, the model evidently accounts well for qualitative aspects of the variations with \( A \). In the calculations, these aspects have simple explanations in terms of the shell structure. I discuss in particular the peaks in the plot of \( X \); see the figure.

- \( A = 40, 56, 100 \): The \( T = 0 \) nucleus is doubly magic. The mechanism that gives rise to a large \( X \) is discussed in Sec. 4.

- \( A = 30 \): Here the mechanism is similar. For \( T = 1, 3, 5 \) a pair of neutrons occupy the \( 2s_{1/2} \) spherical orbit and isospin beyond \( T = 1 \) is generated by a promotion of nucleons from the \( 1d_5/2 \) to the \( 1d_3/2 \) shell.

- \( A = 24, 48 \): Deformation is important. The \( T = 0 \) nucleus has a large deformation while for \( T = 2 \) and 4 the nucleus is almost or completely spherical. The cost in deformation energy required to make \( T = 2 \) and 4 gives the large \( X \).
Given these microscopic explanations of some large $X$ one might ask whether the $T(T + 1)$ proportionality of the liquid drop symmetry energy is required. The answer is affirmative as seen from what happens if it replaced by a $T^2$ proportionality and the liquid drop parameters are refitted: (1) The rms deviation of the doubly even masses increases from 0.875 MeV to 1.073 MeV.
(2) $E^*(A, 1) - E^*(A, 0)$ decreases by 1–2 MeV thus becoming negative also in the lightest nuclei. (3) $X$ decreases by 0–2 units rendering the calculation mostly below the data.

The marked underestimate of the $X$ measured for $A \approx 100$ might reflect an inaccurate representation by the Nilsson model of the shell gaps at $N = Z = 50$.

9 Role of the RPA correction

The RPA correction $\delta E_{RPA} = \sum_{\tau=n,p,pn} (E_{RPA,\tau} - \tilde{E}_{RPA,\tau})$, where $\sum_{\tau=n,p,pn} E_{RPA,\tau}$ is the last term in Eq. (4), is plotted in Fig. 2 in several cases. It is seen that in the doubly even nuclei it is largely constant with an average of about 0.7 MeV. Therefore differential quantities like $1/\theta$ and $X$ are mainly unaffected by $\delta E_{RPA}$. The changes in the plots of these quantities when $\delta E_{RPA}$ is set to zero are barely visible. In other words, the shape of the Wigner cusp is well reproduced by a Nilsson-Strutinskij calculation with only a BCS pairing correction.

In the doubly odd $T = 0$ states $\delta E_{RPA}$ is considerably larger, decreasing from about 2.3 MeV to about 1.2 MeV in the range of the plot. This influences
the fit of the pair coupling constant \( G \) to the measured \( \Delta_{oo-ee} \). More precisely, the RPA correction reduces the required pair coupling constant.

Both the general positivity of \( \delta E_{\text{RPA}} \) and its larger value in the doubly odd nuclei can be understood as a result of an effective dilution of the single-nucleon spectra near the Fermi levels [10]. In the doubly even nuclei this dilution stems from the equilibration of the deformation. In the doubly odd nuclei a further dilution results from the inaccessibility of the Fermi levels to the pairing force.

10 Conclusions

The insight gathered on this tour may then be summarised as follows.

- Calculations with an RPA correction added to the BCS pairing correction conventionally employed in Nilsson-Strutinskij calculations account well for the variation with \( A \) of the pattern of masses near \( N = Z \).

- The RPA correction is insignificant for reproducing the doubly even masses and hence for the shape of the Wigner cusp.

- It is important, however, that the macroscopic (liquid drop) symmetry energy be proportional to \( T(T + 1) \).

- This form of the macroscopic symmetry energy is understood microscopically, in terms of the RPA, to result from the nuclear superfluidity.

- The variation of the shape of the Wigner cusp is dominated by shell effects.

- The RPA correction significantly reduces the \( T = 0 \) binding in doubly odd nuclei, thus reducing the required pair coupling constant.
It is due to mention that work by Negrea and Sandulescu based on a picture of quartet condensation addresses the same differential mass combinations except $E^*(A, 1) - E^*(A, 0)$ and reproduces them equally well [24]. Noteworthy are the traits both approaches have in common: Both employ states constructed from isovector Cooper pairs and both take measures to ensure isobaric invariance.

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