Pairing effects in nuclear collective motion: Generator coordinate method

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The generator coordinate method for nuclear collective motion is studied in a simple model in which the dynamics is governed by the pairing interaction alone. A formula is derived for the overlap correlation length which exhibits the correct empirical dependence on nucleus mass number, pairing gap, and quadrupole deformation. The same analysis applied to the quadrupole inertia parameter provides an expression proportional to the square of the pairing gap, the same functional form as obtained from the cranking model. However, the simplified model differs numerically by a factor 2 to 4 from the results of a complete Hartree-Fock BCS calculation. The spectrum is well described by a hopping model based on the Hartree-Fock single-particle properties.

I. INTRODUCTION

Interest in nuclear collective motion has been renewed by the discovery of superdeformed bands and the attempt to understand their decays. One of us (H.F.) has been using the generator coordinate model (GCM) based on Hartree-Fock plus BCS (HFBCS) calculations of the potential-energy surfaces in heavy nuclei.[1,2] These calculations are technically somewhat complicated, and the relation of the resulting wave function to the physical input is far from transparent. It is therefore of interest to try to reduce the calculation to its simplest terms, keeping only the essentials of the Hamiltonian dynamics. The other author (G.B.) has held the point of view that the dynamics of large-amplitude shape changes is closely connected to the pairing interaction and the strength Δ of the pairing field. Indeed, in the cranking method the pairing is very important[3] and the inverse inertia is roughly proportional to Δ^2. A hopping model advocated by G.B. and collaborators[4,5] also depends quadratically on Δ, but is rather different in other respects.

In the GCM collective wave functions are built out of HFBCS wave functions labeled by a parameter q, the expectation value of an operator such as the mass quadrupole operator $\hat{Q}=3\hat{z}^2-\hat{r}^2$. Wave functions of different q are defined by including a constraining field in the HFBCS Hamiltonian. In order to establish a connection between the GCM and the Bohr collective Hamiltonian, one often introduces the so-called Gaussian overlap approximation (GOA).[6] An important quantity in the GCM is the overlap $\langle q|q'\rangle$ between states of different deformation. Within the GOA it is approximated by a Gaussian function:

$$\left\langle q+\frac{\delta q}{2}\middle|q-\frac{\delta q}{2}\right\rangle=\exp\left[-\frac{1}{2}\left[\frac{\delta q}{a(q)}\right]^2\right], \tag{1}$$

in which the quantity $a(q)$ measures the local correlation width between states of the nonorthogonal basis. The GOA also assumes that the ratio of the Hamiltonian kernel of the GCM to the overlap can be accurately reproduced by a quadratic expansion:

$$\left\langle q+\frac{\delta q}{2}|H|q-\frac{\delta q}{2}\right\rangle\Big/\left\langle q+\frac{\delta q}{2}\middle|q-\frac{\delta q}{2}\right\rangle = h_0(q)-\tfrac{1}{2}h_2(q)\delta q^2+\cdots . \tag{2}$$

Then it can be shown[6] that the GOA collective wave functions are the eigenvectors of a Bohr collective Hamiltonian with kinetic-energy operator

$$T=-\frac{1}{2}\frac{\partial}{\partial q}\frac{1}{I_q}\frac{\partial}{\partial q}=-\frac{1}{2}\frac{\partial}{\partial q}h_2(q)a^4(q)\frac{\partial}{\partial q} . \tag{3}$$

In our simplified treatment, we assume that the q dependence of both the overlap a and the function h_2 is determined by pairing correlations only. The first part of our derivation repeats that given in Sec. 4 of Ref. 1.

II. WAVE-FUNCTION OVERLAP

If one ignores the q dependence of the orbital wave functions, the overlap is given by

$$\left\langle q+\frac{\delta q}{2}\middle|q-\frac{\delta q}{2}\right\rangle=\prod_{i>0}(u_+u_-+v_+v_-)_i , \tag{4}$$

where the $u_{i\pm}$'s and $v_{i\pm}$'s are the BCS pairing amplitudes in the states $|q\pm\delta q/2\rangle$, and the product over i is taken over all the pairs (i.e., all doubly degenerate single-particle levels). The pairing amplitudes u_i and v_i depend on deformation q because of the varying single-particle energies ϵ_i. To expand the u's and v's in powers of δq, it is convenient to introduce the quantities $y_i=(\epsilon_i-\lambda)/\Delta$, in which λ denotes the Fermi energy. To second order in δq, the contribution of the pair i to the overlap is

$$(u_+u_-+v_+v_-)_i=1-\delta q^2\frac{y_i'^2}{8(1+y_i^2)^2} , \tag{5}$$

where y_i' denotes the derivative of y_i with respect to the

collective variable. This is expressed as an exponential and inserted in Eq. (4). Comparing with Eq. (1), one finds the formula for the correlation length given in Ref. 1:

$$\frac{1}{a^2}=\frac{1}{4}\sum_{i>0}\frac{y_i'^2}{(1+y_i^2)^2} . \tag{6}$$

To simplify this expression further, we evaluate the sum as an integral over single-particle energy divided by the level density $dn/d\epsilon$ at the Fermi energy. The result is

$$\frac{1}{a^2}=\frac{\pi}{8\Delta}\frac{dn}{d\epsilon}\left|\frac{\partial\epsilon}{\partial q}\right|^2 , \tag{7}$$

where $|\partial\epsilon/\partial q|$ denotes the average of the absolute value of the slope of single-particle orbitals at the Fermi energy. In Ref. 4 an approximate expression for this quantity was found for the case of quadrupole deformations of an axially symmetric nucleus. This required first determining the average separation Δq_0 between successive level crossings. A Fermi-gas estimate of this gives, for a nucleus of mass number A,

$$\Delta q_0=\frac{2\sqrt{3}\langle 3\hat{z}^2+\hat{r}^2\rangle}{A} . \tag{8}$$

Then the average of the absolute value of the slope of the levels can be written

$$\left|\frac{\partial\epsilon}{\partial q}\right|^{-1}=\Delta q_0\frac{1}{2}\frac{dn}{d\epsilon} , \tag{9}$$

where the factor $\frac{1}{2}$ accounts for the fact that, by definition, each crossing involves two levels.

Inserted in Eq. (8), this leads to the following expression for the overlap width:

$$a=\Delta q_0\left[\frac{2\Delta}{\pi}\frac{dn}{d\epsilon}\right]^{1/2} . \tag{10}$$

In order to display the A dependence of q, Δq_0, and a, we introduce a quantity r_0 which approximates the root-mean-square radius of the nucleus at $q=0$ and we measure the deformation by the ratio off the principal axes of the nucleus $\rho=(\langle\hat{z}^2\rangle/\langle\hat{x}^2\rangle)^{1/2}$:

$$\begin{aligned} r_0^2&=\tfrac{3}{5}(1.2A^{1/3})^2\ \text{fm}^2 ,\\ \langle\hat{z}^2\rangle&\approx\tfrac{1}{3}Ar_0^2\rho^{4/3} ,\\ \langle\hat{x}^2\rangle&=\langle\hat{y}^2\rangle\approx\tfrac{1}{3}Ar_0^2\rho^{-2/3} . \end{aligned} \tag{11}$$

The A dependence of the level density is obtained from the usual Fermi-gas expression:

$$\frac{dn}{d\epsilon}=\frac{3A}{4\epsilon_F} , \tag{12}$$

where ϵ_F is the Fermi energy measured from the bottom of the single-particle potential well. Inserting the expressions (11) and (12) in Eqs. (8) and (10), we obtain the following formulas:

$$\begin{aligned} q&\approx 0.58A^{5/3}\rho^{-2/3}(\rho^2-1)\ \text{fm}^2 ,\\ \Delta q_0&\approx 2.0A^{2/3}\rho^{-2/3}(2\rho^2+1)\ \text{fm}^2 ,\\ a&\approx 1.4A^{7/6}\sqrt{\Delta/\epsilon_F}\rho^{-2/3}(2\rho^2+1)\ \text{fm}^2 . \end{aligned} \tag{13}$$

We call this the Fermi-gas estimate of Δq_0 and a. It depends parametrically on the quadrupole collective variable q. We first note that the predicted correlation length a is roughly proportional to A, in accordance with the findings of detailed GCM calculations by Bonche *et al.*[1,2]

We illustrate this formula numerically with the nucleus ^{194}Hg. For the quantities Δ and ϵ_F in Eq. (13), we take $\Delta\approx 1$ MeV and $\epsilon_F\approx 37$ MeV. At the spherical point ($\rho=1$), we find $\Delta q_0\approx 2.0$ b and a correlation length $a\approx 3.2$ b, which agrees to within a factor of 2 with the results of Ref. 1. Our correlation length is smaller than that of the microscopic calculation; we will return to this point shortly.

The q dependence of Eq. (13) is compared to the GCM results in Fig. 1. We see that a increases steadily over the range $-40\le q\le 70$ b, with a more pronounced effect at large prolate quadrupole moments. This is well described by Eq. (13), which has an explicit dependence on the shape of the nucleus. Indeed, Eq. (13) predicts that a is a growing function of q when $\rho\ge\frac{1}{2}$. For ^{194}Hg this corresponds to the oblate deformation $q=-45$ b. The formula also predicts that a will grow linearly with q at large prolate deformations, in accord with the findings of Ref. 1.

Although we have as good agreement here as one could expect from a crude model, it would be incorrect to conclude that the variation of the single-particle wave function with deformation is negligible. The authors of Ref. 1 evaluated Eq. (6) using the single-particle energies from the HFBCS calculations, shown as the dashed curve in Fig. 1. Here correlation length is too large, which should be expected since the neglected variation of the single-particle wave functions must decrease the correlation

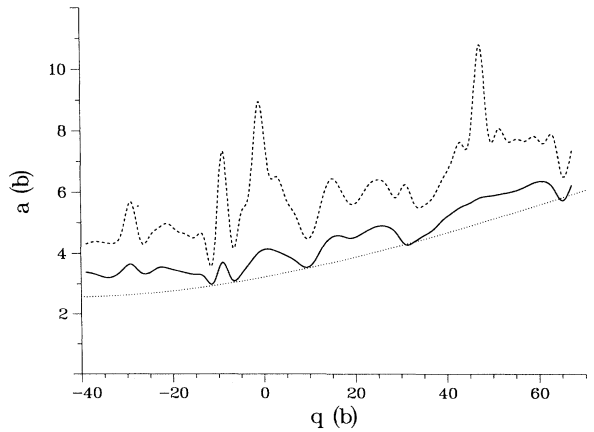

FIG. 1. Correlation length a. The solid line is the GCM value. The dotted line is the result of Eq. (13). The dashed line is evaluated from Eq. (6), using the pairing gaps and single-particle energies of the microscopic calculation.

length. However, taking into account this effect would make the Fermi-gas estimate worse, since it is already too small. Analyzing the situation more closely, an important difference between the Fermi-gas model and actual behavior of the levels in HFBCS is that number of level crossings differs by almost a factor of 2. For the nucleus ^{194}Hg, Eq. (8) predict 38 level crossings between $q=-30$ and $+60$ b, while by actual count there are only 23 in the HFBCS calculation. With fewer level crossings the overlap range extends to larger distances. There may be several reasons for the failure of the Fermi-gas estimate of the level density. The HFBCS calculation breaks axial symmetry and thus has more avoided crossings, but we explicitly restored these crossings to obtain the count of 23. The infinite-matter approximation might be too crude to describe this finite system. However, an explicit count of the level crossings in the Hill-Wheeler rectangular box model yields 38 crossings under the same conditions, very close to the Fermi-gas model. The surface contributions to the quadrupole moment might be more important than the crude model assumes. We examine this possibility using the Nilsson model with a pure harmonic-oscillator potential. For this model there are 30 level crossings when the deformation of ^{194}Hg is changed from -30 to $+60$ b. An additional reduction could come from the l- and spin-dependent terms in the full Nilsson Hamiltonian. In any case, the Fermi-gas model does not appear as reliable as assumed in Ref. 5.

III. HAMILTONIAN

We next turn to the matrix element of the Hamiltonian. In constrained HFBCS theory the Hamiltonian has the form

$$H=H_{\rm mf}-\lambda N-GPP^{\dagger}\ , \tag{14}$$

where $P=\sum_{i>0}c_i^{\dagger}c_{\bar{i}}^{\dagger}$ is the pair creation operator and $H_{\rm mf}-\lambda N=\sum_i(\epsilon_i-\lambda)c_i^{\dagger}c_{\bar{i}}$ is the mean-field Hamiltonian including the constraining field. The mean-field part is evaluated as

$$\left\langle q+\frac{\delta q}{2}\left|H_{\rm mf}-\lambda N\right|q-\frac{\delta q}{2}\right\rangle\Big/\left\langle q+\frac{\delta q}{2}\,\middle|\,q-\frac{\delta q}{2}\right\rangle = \sum_{i>0}\left[\frac{2(\epsilon-\lambda)v_+v_-}{u_+u_-+v_+v_-}\right]_i . \tag{15}$$

Expanding this to second order in δq, we find the following result for the second-order coefficient $(h_{\rm mf}-\lambda n)_2$:

$$(h_{\rm mf}-\lambda n)_2=\frac{\Delta}{4}\sum_{i>0}\left[\frac{y_iy_i''}{(1+y_i^2)^{3/2}}-\frac{y_i^2y_i'^2}{(1+y_i^2)^{5/2}}\right] . \tag{16}$$

The contribution of the pairing interaction is similarly evaluated from the matrix element of the pairing field,

$$\left\langle q+\frac{\delta q}{2}\left|P\right|q-\frac{\delta q}{2}\right\rangle\Big/\left\langle q+\frac{\delta q}{2}\,\middle|\,q-\frac{\delta q}{2}\right\rangle = \sum_{i>0}\left[\frac{v_+u_-}{u_+u_-+v_+v_-}\right]_i . \tag{17}$$

Again, this is expanded to second order in δq. In the pairing energy, we drop the linear term in δq, which vanishes in the limit of equal distributions of upward- and downward-sloping single-particle energies. The result of the second-order contribution to the Hamiltonian is

$$(h_p)_2=\frac{\Delta}{4}\sum_{i>0}\left[-\frac{y_iy_i''}{(1+y_i^2)^{3/2}}+\frac{(2y_i^2+1)y_i'^2}{(1+y_i^2)^{5/2}}\right] . \tag{18}$$

In deriving this result, we have used the consistency condition $\Delta=G\sum_{i>0}u_iv_i$. The sum of the mean-field and pairing contributions simplifies somewhat, and we find the result for the second-order contribution to the complete Hamiltonian:

$$(h_{\rm mf}-\lambda n+h_p)_2=\frac{\Delta}{4}\sum_{i>0}\frac{y_i'^2}{(1+y_i^2)^{3/2}} . \tag{19}$$

This expression is very similar to that obtained for a^{-2} in Eq. (6). We may evaluate it with the same approximations used before to obtain

$$h_2\sim\frac{1}{2}\frac{dn}{d\epsilon}\left|\frac{\partial\epsilon}{\partial q}\right|^2 . \tag{20}$$

On the other hand, Eq. (3) shows that the physically interesting quantity is not h_2, but rather h_2a^4. Combining Eqs. (20) and (6), we find

$$I_q=\frac{\pi^2}{32\Delta^2}\frac{dn}{d\epsilon}\left|\frac{\partial\epsilon}{\partial q}\right|^2 . \tag{21}$$

The expression for I_q has the same functional form as found in the cranking model.[3,4] However, the numerical coefficient is slightly different from that obtained in Eq. (5.29) of Ref. 4. There, instead of $\pi^2/32\sim0.31$, the coefficient is $\frac{1}{3}$.

Evaluating Eq. (21) with the same approximations as

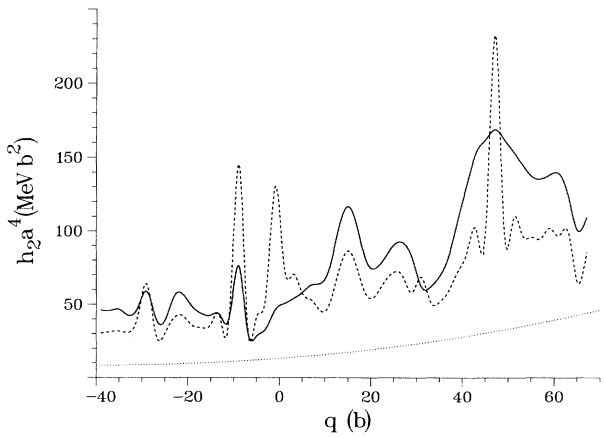

FIG. 2. Inverse inertia h_2a^4. The solid line is the GCM value. The dashed and dotted lines are the result of Eqs. (6), (19), and (22), respectively.

were used to obtain Eq. (13), we find

$$I_q^{-1} = \frac{4\Delta}{\pi} a^2$$
$$= 2.4 \frac{\Delta^2}{\epsilon_F} A^{7/3} \rho^{-4/3} (2\rho^2 + 1)^2 \text{ MeV fm}^4 . \quad (22)$$

This Fermi-gas estimate is compared with the microscopic calculation in Fig. 2. The trend with q is reasonable, but the magnitude is too small by roughly a factor of 5. Part of the discrepancy is due to the pairing gap Δ, which is somewhat higher for protons than the estimate we used, $\Delta \sim 1$ MeV. Even so, it is clear that overestimate of the number of level crossings in the Fermi-gas model produces an inertia which is much too large. The figure also shows the result from evaluation of Eq. (6.19) using the single-particle energies and pairing gaps from Ref. 1. The agreement is good, but somewhat fortuitous, as one should not expect a better description of the inertia than of the overlap distance.

IV. HOPPING MODEL

Reference 4 also discusses a different treatment of pairing-dominated collective motion, in which a discrete chain of states is constructed. These states have diagonal energies determined from Hartree-Fock theory. The off-diagonal interaction connects only neighboring states on the chain, hence the same "hopping model." The magnitude of the off-diagonal interaction v is a constant given by

$$v = \frac{\Delta_n^2 + \Delta_p^2}{4G} . \quad (23)$$

The global systematics of pairing[7] yield a value of v near

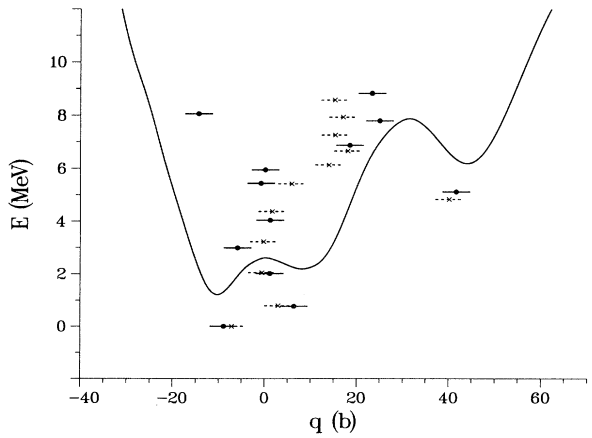

FIG. 3. Spectrum of collective states in ^{194}Hg. The solid curve gives the HFBCS constrained energy. The solid dots with short horizontal bars indicate the average quadrupole moment and the energy of the GCM eigenstates (Ref. 2). The crosses with the dashed lines give the same information for the states obtained with the hopping model. The energy of the hopping model ground state has been adjusted to that of the GCM ground state.

TABLE I. Off diagonal quadrupole matrix elements. The quadrupole matrix element between the superdeformed and ground states, divided by the expectation value in the superdeformed state, is compared. The first column is from the wave function in the generator coordinate calculation (Ref. 1). The second column is the hopping model discussed in the text.

	GCM	Hopping model
^{190}Hg	$\frac{1}{300}$	$\frac{1}{150}$
^{198}Hg	10^{-4}	10^{-4}

-2.9 MeV, and in previous applications[5] this value was adopted. The hopping model can be easily compared with GCM using the potential-energy curves given in Ref. 2 to fix the diagonal energies of the states. The only question is how far the states should be spaced. We can either use the Fermi-gas estimate [Eq. (8)] or the explicit counting of level crossings obtained in the microscopic calculation. If we use the Fermi-gas estimate, we find that the level spectrum is much more compressed than obtained with the GCM. This should be expected from the results of the previous section, where the Fermi-gas estimate was seen to give too high an inertia. If we use for Δq_0 the value extracted from the actual count of level crossings ($\Delta q_0 \sim 23$ crossings over a 60-b range), the model works remarkably well. In Fig. 3 we show the spectrum of levels in ^{194}Hg, comparing the hopping model and the full generator coordinate calculation. The energy of the states are shown on the vertical axis and the expectation of the quadrupole moment on the horizontal axis. As in the case of the inertia calculated from the HFBCS single-particle spectrum in the previous section, the good agreement may be somewhat fortuitous.

The off-diagonal matrix elements of the quadrupole operator are of interest in discussing the decay of the superdeformed band. For example, Ref. 2 found a non-negligible quadrupole matrix element between ground and superdeformed bands in ^{190}Hg, suggesting that this nucleus might decay out of the deformed band by an $E2$ transition. These matrix elements can easily be evaluated in the hopping model from the finite-basis wave functions. The comparison for ^{190}Hg and another case with a very small matrix element, ^{198}Hg, is shown in Table I. The agreement is remarkably close.

V. CONCLUSION

We have found that a simplified treatment of pairing can explain the qualitative behavior of the correlation length and the inertia parameter in the generator coordinate model of nuclear collective motion. Besides the pairing field, it is important to know the level density and energy dependence of the single-particle levels on the collective coordinate. Closed expressions for these can be derived in the Fermi-gas model, and the resulting formulas display the qualitative dependence on mass number, pairing gap, and deformation. However, on a quantitative level the Fermi-gas model appears to be too crude, predicting a steeper slope of the single-particle energies

and more level crossings than is obtained in the Nilsson model or the microscopic HFBCS calculations. If the empirical single-particle properties are put into the simplified model, the correlation length is somewhat too large, but the inertia agrees rather well with the microscopic GCM result. The omitted physics of the changing single-particle wave function seems to be more important for the correlation than for the inertia. Another simplified treatment that assumes pairing dominance is the hopping model in a discrete basis. As with the other treatment, good agreement is obtained with the empirical single-particle properties as input, while the results with the Fermi-gas estimates yield too large an inertia.

Thus it may be the case that some form of the pure pairing model may describe the overall dynamics in the shape degree of freedom. The hopping model, using a microscopic level density parameter rather than a Fermi-gas model, may be useful for estimation when the problem does not warrant the full apparatus of the GCM.

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