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Effect of a fermion on quantum phase transitions in bosonic systems

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ABSTRACT

The effect of a fermion with angular momentum j on quantum phase transitions of a (s, d) bosonic system is investigated. It is shown that the presence of a fermion strongly modifies the critical value at which the transition occurs, and its nature, even for small and moderate values of the coupling constant. The analogy with a bosonic system in an external field is mentioned. Experimental evidence for precursors of quantum phase transitions in bosonic systems plus a fermion (odd–even nuclei) is presented.

Quantum phase transitions (QPT) are qualitative changes in the ground state properties of a physical system induced by a change in one or more parameters in the quantum Hamiltonian describing the system. Originally introduced in the 1970s [1,2], they have been the subject in recent years of many investigations and have found a variety of applications in many areas of physics and chemistry [3,4]. One of these applications is to atomic nuclei, where QPTs have been extensively investigated (for a review, see [5–7]) within the framework of the Interacting Boson Model (IBM), a model of even–even nuclei in terms of correlated pairs of valence nucleons with angular momentum $J = 0, 2$ treated as bosons (s, d) [8]. For this case also finite size effects [9–11] and scaling behavior [12–14] have been investigated, both analytically and numerically, showing that precursors of QPT can be seen even for relatively small values of N. QPTs have also been extended to excited states quantum phase transitions, that is qualitative changes in the properties of the system as a function of the excitation energy [15]. In this Letter we present results of an investigation of the effect of a fermion on QPTs in bosonic systems. We do this in atomic nuclei by making use of the Interacting Boson–Fermion Model (IBFM), a model of odd–even nuclei in terms of correlated pairs with angular momentum $J = 0, 2$ $(s, d$ bosons) and unpaired particles with angular momentum $J = j$ (j fermions) [16]. As an illustration we take $j = 11/2$. We note, however, that our method of analysis can also be used for systems with other values of the fermion, j, and boson, J, angular momenta, for example the spin–boson systems discussed in [17], the simplest case of which is a fermion with $j = 1/2$ (i.e., a single spin) in a bath of harmonic oscillator one-dimensional bosons of interest in dissipation and light phenomena. QPTs in IBFM for selected orbits have been investigated by Alonso et al. [18,19]. Here we focus on the effect of a fermionic impurity on QPTs in bosonic systems. Our main results are that, (1) the presence of a single fermion greatly influences the location and nature of the phase transition, the fermion acting either as a catalyst or a retarder of the QPT, and (2) there is experimental evidence for quantum phase transitions in odd–even nuclei (bosonic systems plus a single fermion).

Within the context of the geometric collective model of nuclei, the effect of an odd particle on collective properties was investigated years ago in core-particle models. However, both our results are novel, since (i) in the deformed phase the effect of the fermion is of order $1/N$ and thus vanishes in the geometric limit $N \to \infty$. However, we explicitly show that the effect is large in transitional nuclei even for small and moderate values of the coupling strength of the fermion to the bosons; (ii) the experimental evidence for QPTs in odd-nuclei has not been presented earlier and we show one of the key signatures of QPTs in nuclei, the two-neutron separation energies. This quantity is discontinuous for a first order phase transition at the transition point (or it has a sudden jump for a finite system). As shown below, this jump is observed experimentally.

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To prove our point, we consider the Hamiltonian of a system of N (s,d) bosons coupled (with a quadrupole interaction) to a single fermion with angular momentum j [16]

$$H = H_B + H_F + V_{BF}, \tag{1}$$

with

$$H_B = \varepsilon_0\left[(1-\xi)\hat{n}_d - \frac{\xi}{4N}\hat{Q}^\chi\cdot\hat{Q}^\chi\right],$$
$$H_F = \varepsilon_j,$$
$$V_{BF} = \Gamma\hat{Q}^\chi\cdot\hat{q}. \tag{2}$$

Here $\hat{n}_d = d^\dagger\cdot\tilde{d}$ is the number operator for d-bosons, $\hat{Q}^\chi = (d^\dagger\times s + s^\dagger\times\tilde{d})^{(2)} + \chi(d^\dagger\times\tilde{d})^{(2)}$ and $\hat{q} = (a_j^\dagger\times\tilde{a}_j)^{(2)}$, are quadrupole operators of bosons and fermion respectively, ε_0 is the scale of the boson energy, ε_j is the energy of the single fermion and Γ the strength of the quadrupole Bose–Fermi interaction. The dot and cross indicate scalar and tensor products and the adjoint operators for bosons and fermions are $\tilde{d}_\mu = (-)^\mu d_{-\mu}$ and $\tilde{a}_{j,m} = (-)^{j-m}a_{j,-m}$. QPTs of the purely bosonic part of the Hamiltonian H_B have been extensively investigated [20,21]. There are two control parameters ξ and χ. For fixed χ, as one varies ξ, $0\leqslant\xi\leqslant 1$, the bosonic system undergoes a QPT. The phase transition is first order for $\chi\neq 0$ and becomes second order at $\chi = 0$. No phase transition occurs as a function of χ. In this Letter, we take $\chi = -\frac{\sqrt{7}}{2}$, in which case the two "phases" of the system have U(5) symmetry ($\xi = 0$) and SU(3) symmetry ($\xi = 1$) [8]. The critical point, separating the spherical [U(5)] and axially-deformed [SU(3)] phases, occurs at $\xi_c \cong 1/2$.

A complete study of the properties of quantum phase transitions necessitates both a classical and a quantal analysis, and a consideration of other couplings of fermions to bosons in addition to quadrupole coupling [22]. In order to emphasize the main features of the results, we report here only the classical analysis. This amounts to constructing the combined Bose–Fermi potential energy surface (Landau potential) and minimizing it with respect to the classical variables. To this end, we introduce a boson condensate [8]

$$|N;\beta,\gamma\rangle = \frac{1}{\sqrt{N!}}\left[b_c^\dagger(\beta,\gamma)\right]^N|0\rangle, \tag{3}$$

$b_c^\dagger = (1+\beta^2)^{-1/2}[\beta\cos\gamma d_0^\dagger + \beta\sin\gamma(d_2^\dagger + d_{-2}^\dagger)/\sqrt{2} + s^\dagger]$, in terms of the classical variables β,γ. The expectation value of H_B of Eq. (2) in the condensate is [10]

$$\begin{aligned}E_B(N;\beta,\gamma) &= \langle N;\beta,\gamma|H_B|N;\beta,\gamma\rangle \\ &= \varepsilon_0 N\left\{\frac{\beta^2}{1+\beta^2}\left[1-\xi-(\chi^2+1)\frac{\xi}{4N}\right] - \frac{5\xi}{4N(1+\beta^2)}\right. \\ &\quad\left. - \frac{\xi}{(1+\beta^2)^2}\frac{N-1}{N}\left[\beta^2 - \sqrt{\frac{2}{7}}\chi\beta^3\cos 3\gamma + \frac{1}{14}\chi^2\beta^4\right]\right\}.\end{aligned} \tag{4}$$

We then evaluate the expectation value of H_F and V_{BF} in the condensate thus obtaining a fermion Hamiltonian

$$\mathcal{H}(N;\beta,\gamma) = E_B(N;\beta,\gamma) + \sum_{m_1,m_2}\left[\varepsilon_j\delta_{m_1,m_2} + g_{m_1,m_2}(N;\beta,\gamma)\right] \times\left(\frac{a_{j,m_1}^\dagger a_{j,m_2} + a_{j,m_2}^\dagger a_{j,m_1}}{1+\delta_{m_1,m_2}}\right). \tag{5}$$

The matrix $g_{m_1,m_2}(N;\beta,\gamma)$ is a real, symmetric matrix

$$\begin{aligned}g_{m_1,m_2}(N;\beta,\gamma) &= N\Gamma\left(\frac{\beta}{1+\beta^2}\right)(-)^{j+m_2} \\ &\quad\times\left\{\left[2\cos\gamma - \chi\sqrt{\frac{2}{7}}\beta\cos 2\gamma\right]C_{j,m_1;j,-m_2}^{2,0}\right. \\ &\quad\left. + \left[\sqrt{2}\sin\gamma + \chi\sqrt{\frac{1}{7}}\beta\sin 2\gamma\right]C_{j,m_1;j,-m_2}^{2,2}\right\},\end{aligned} \tag{6}$$

where $C_{j,m_1;j,-m_2}^{2,m}$ denotes a Clebsch Gordan coefficient. The eigenvalues e_i and eigenvectors ψ_i of the matrix g are the single-particle energies and wave functions of the fermion in the deformed (β,γ) field generated by the bosons. For $\gamma = 0°$ (field with axial symmetry), $\chi = 0$ and β small (i.e., neglecting β^2) they were obtained years ago by Nilsson [23]. For $\gamma\neq 0°$; $\chi = 0$ and β small, they were investigated by Meyer-ter-Vehn [24]. We have solved the problem in its generality and details are given in [22]. Here, we consider, for simplicity, the case $\gamma = 0°$ for which the eigenvalues are given in explicit analytic form [25]

$$\lambda_K(N;\beta;\chi;\Gamma) = -N\Gamma\left(\frac{\beta}{1+\beta^2}\right)\sqrt{5}\left(2-\beta\chi\sqrt{\frac{2}{7}}\right) \times P_j\left[3K^2 - j(j+1)\right], \tag{7}$$

where $P_j = [(2j-1)j(2j+1)(j+1)(2j+3)]^{-1/2}$. The quantum number $K = j, j-1, j-2, \ldots, \frac{1}{2}$ has the physical meaning of the projection of the angular momentum on the intrinsic z axis of the condensate.

Once the eigenvalues have been obtained, one can calculate the total energy functional (Landau potential for the combined Bose–Fermi system)

$$E_i(N;\beta,\gamma;\xi,\chi;\Gamma) = E_B(N;\beta,\gamma;\xi,\chi) + \varepsilon_j + e_i(N;\beta,\gamma;\chi;\Gamma). \tag{8}$$

This expression is the algebraic analog of the total potential energy surface, obtained in the macroscopic–microscopic Strutinsky procedure [26]. Minimization of E_i with respect to β and γ gives the equilibrium values β_e,γ_e (the classical order parameters) for each state. In the simple case of $\gamma = 0°$, $\chi = -\frac{\sqrt{7}}{2}$, $\varepsilon_j = 0$ the total energy functional becomes

$$E_K(N;\beta;\xi;\Gamma\gamma) = E_B\left(N;\beta,0;\xi,-\frac{\sqrt{7}}{2}\right) + \lambda_K\left(N;\beta;-\frac{\sqrt{7}}{2};\Gamma\right). \tag{9}$$

Minimization ($\frac{\partial E_K}{\partial\beta} = 0$) gives the equilibrium β_e values shown in Fig. 1 as a function of the control parameter ξ of the bosonic phase transition.

By comparing the top part of this figure (purely bosonic system) with the bottom part, one can see that the effect of the fermionic impurity is to wash out the phase transition for states with $K = 1/2, 3/2, 5/2$ and to enhance it for states with $K = 7/2, 9/2, 11/2$. In other words, the fermion acts as a catalyst for some states and as a retarder for others. Also, when the coupling strength becomes very large, the minima for some large K, in the figure $K = 11/2$, shift to negative values (oblate deformation). In addition to this result, also known qualitatively from particle-core models, the effect of the fermion is to move the location of the critical point even for small and moderate values of Γ. Physical values of Γ in

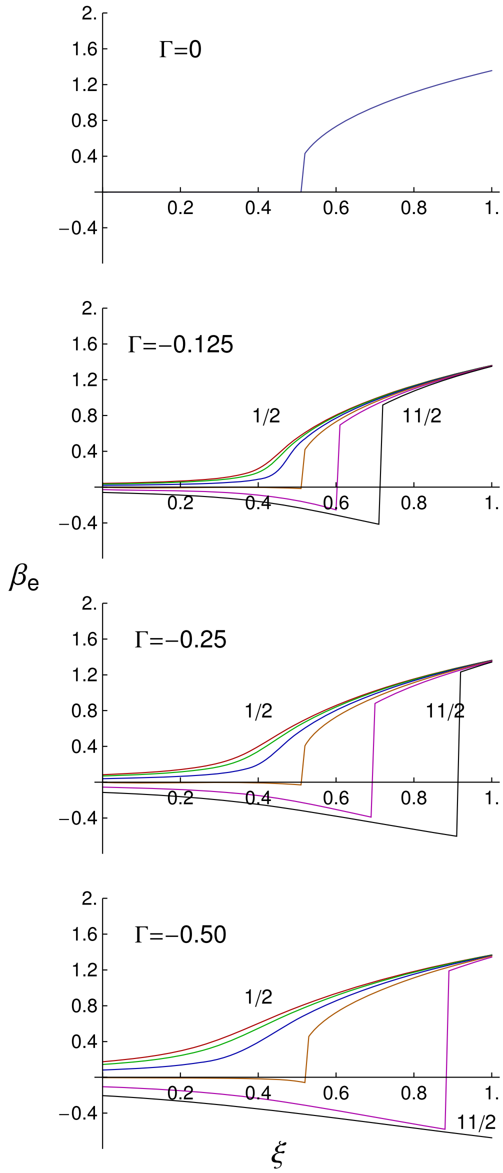

Fig. 1. (Color online.) Equilibrium values of the total boson plus fermion energy (classical order parameter) as a function of the control parameter ξ of the bosonic phase transition for various values of the coupling constant Γ in units of ε_0 and $N = 10$. The curves for $\Gamma \neq 0$ correspond, from left to right, to states with $K = 1/2, 3/2, 5/2, 7/2, 9/2, 11/2$. The value $\Gamma = 0$ gives the purely bosonic case.

the $_{61}$Pm, $_{63}$Eu, $_{65}$Tb nuclei, where the phase transition occurs, are $\Gamma \cong -0.125$ [27].

It is interesting to note that the effect of the fermionic impurity is similar to the effect of an external field with linear coupling on a thermodynamic phase transition investigated by Landau and Lifshitz years ago [28, p. 456]. They considered the potential

$$\Phi(\eta) = \Phi_0 + A\eta^2 + B\eta^4 + \alpha\eta, \tag{10}$$

where α is the strength of the coupling to the external field and η a classical variable (order parameter). (The bosonic part of this potential $A\eta^2 + B\eta^4$ has only a second order transition.) After a projective transformation $\frac{\beta^2}{1+\beta^2} = \eta^2$ which does not change the nature of the phase transition and some rearrangement, the IBFM potential can be written for small η, in the form

$$E_K(\eta) = \Delta_0 + A\eta^2 + C\eta^3 + B\eta^4 + \alpha_K\left(2\eta + \frac{\eta^2}{\sqrt{2}}\right), \tag{11}$$

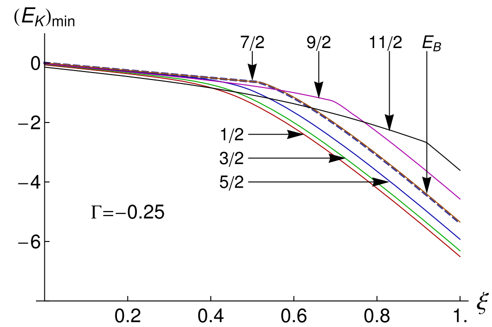

Fig. 2. (Color online.) The total energy at the equilibrium value, $(E_K)_{\min}$ Eq. (9), as a function of the control parameter ξ for an intermediate value of the strength of the Bose–Fermi interaction, $\Gamma = -0.25$, with $\varepsilon_0 = 1$ and $N = 10$. The dashed curve, labeled by E_B, is the corresponding energy of the purely bosonic system.

where α_K is the strength of the coupling for each K value. By comparing the couplings in Eqs. (10) and (11), one can see that the IBFM $E_K(\eta)$ is more general than $\Phi(\eta)$ since it has a linear and quadratic coupling, but for small η (note that $|\eta| \leqslant 1$), the quadratic term is negligible and the two expressions become identical. Also, in the IBM the bosonic part has a cubic term leading to the possibility of a first order transition. The analogy with bosonic systems in an external field also suggests that our results apply to the study of phase transition in superconductors in the presence of magnetic fields.

Finally, having computed the equilibrium values, one can compute the total energies $E_i(N; \beta_e, \gamma_e; \xi, \chi)$ which for the special case discussed here are given by $E_K(N; \beta_e; \xi; \Gamma)$ and shown in Fig. 2. One can see again by comparing E_K with the energy of the purely bosonic system, E_B, that there is an effect especially close to the critical value, ξ_c. The effect is not so much in the total energy E_K (where it is of order $1/N$) but in the derivative of the total energy with respect to the control parameter, $\frac{\partial E_K}{\partial \xi}$.

An important property of atomic nuclei is that they provide experimental evidence for shape QPTs, in particular, of the spherical to axially-deformed transition (U(5)–SU(3) symmetry) [5–7]. Three signatures have been used to experimentally verify the occurrence of shape phase transitions in nuclei: (a) the behavior of the order parameter (β_e) as a function of the control parameter, measured through the B(E2) values proportional to β_e^2; (b) the behavior of the ground state energies, measured through the two-neutron separation energies, S_{2n}; and (c) the behavior of the gap between the ground state and the first excited 0^+ state. Here for conciseness we concentrate only on $S_{2n} = -[E_0(N+1) - E_0(N)]$, which can be related to the derivative of the ground state energy, E_0, with respect to the control parameter, $\frac{\partial E_0}{\partial \xi}$. S_{2n} can be written as a smooth contribution linear in the boson number N, plus the contribution of the deformation [8,29]

$$S_{2n} = -A_{2n} - B_{2n}N + S(2n)_{\text{def}}. \tag{12}$$

In order to emphasize the occurrence of the phase transition it is convenient to plot the deformation contribution only, obtained from the data by subtracting the linear dependence, as a function of N. In previous studies of the purely bosonic part it has been shown that N is approximately proportional to the control parameter ξ [5]. The experimental values of $S(2n)_{\text{def}}$ are shown in the top part of Fig. 3 for even–even nuclei (purely bosonic) and in the bottom part for odd–even nuclei (bosonic plus one fermion). They are obtained from the data [30] with $A_{2n} = -14.61$, -15.82, -16.997 MeV for Nd–Sm–Gd, respectively, and $B_{2n} = 0.657$ MeV, and with $A_{2n} = -15.185$, -16.37, -17.672 MeV for Pm–Eu–Tb, and $B_{2n} = 0.670$ MeV. Precursors of the phase transition are visible in all six nuclei between neutron numbers 88 and 90 in both,

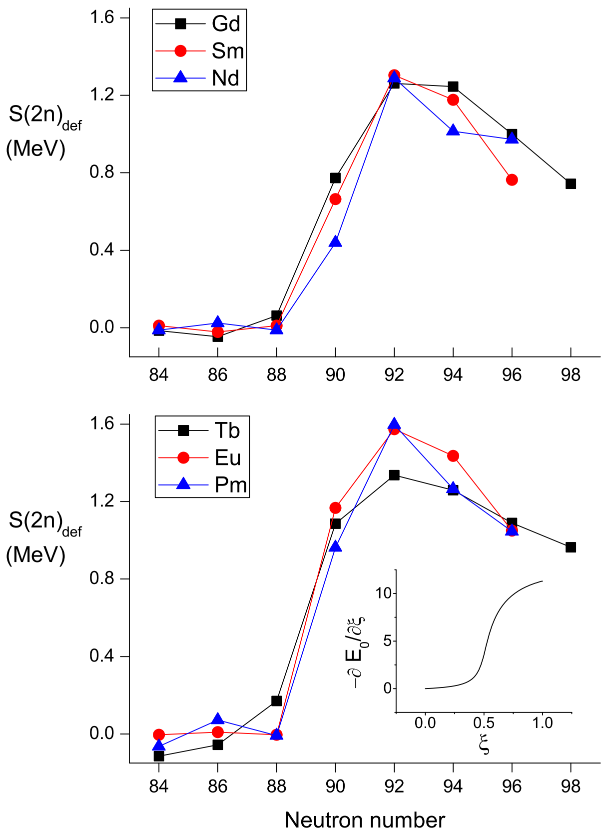

Fig. 3. (Color online.) The contribution of deformation to the two-neutron separation energies, $S(2n)_{\mathrm{def}}$ for even–even $_{60}$Nd–$_{62}$Sm–$_{64}$Gd nuclei (top) and odd–even $_{61}$Pm–$_{63}$Eu–$_{65}$Tb nuclei (bottom), plotted as a function of neutron number. The contribution is enhanced in odd–even nuclei by approximately 300 keV (at neutron number 92). Also the rise between neutron numbers 88 and 90 is sharper in odd–even nuclei than in even–even nuclei. In the limit $N \to \infty$ (no finite size scaling) the quantity $S(2n)_{\mathrm{def}}$ should be zero before the critical value and finite and large after that. The expected behavior of $-\frac{\partial E_0}{\partial \xi}$ for the U(5)–SU(3) transition and $N = 10$ is shown in the inset.

and, most importantly, appears to be enhanced in odd–even nuclei relative to the even–even case.

In conclusion, we have presented here a classical analysis of quantum phase transitions in a system of N bosons and one fermion (spin–boson system) and shown that (i) the addition of a fermion greatly modifies the critical value at which the phase transition occurs, and in some cases its nature; (ii) the effect is similar to that of adding an external field; (iii) there is experimental evidence for these phase transitions in odd–even nuclei at neutron number 88–90. The effect of the odd fermion is about 20% in $S(2n)_{\mathrm{def}}$. A quantal analysis, in which the Hamiltonian H is diagonalized numerically for finite N, produces results similar to those of the classical analysis [22]. Our results are of interest not only for applications to nuclei, but also for applications to other systems in which a fermion is immersed in a bath of bosons, for example, the simple case of a spin 1/2 particle in a bath of harmonic oscillator bosons [17]. Our analysis opens the way for a systematic study of QPTs in Bose–Fermi systems, in particular, of shape phase transitions in odd–even nuclei. This includes experimental studies and microscopic investigations using Density Functional Theory and/or other methods, in a way similar to what it has been done recently for the study of QPTs in purely boson systems (even–even nuclei) [6,31].

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