Shell Correction Energy for Bubble Nuclei

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The positioning of a bubble inside a many fermion system does not affect the volume, surface, or curvature terms in the liquid drop expansion of the total energy. Besides possible Coulomb effects, the only other contribution to the ground state energy of such a system arises from shell effects. We show that the potential energy surface is a rather shallow function of the displacement of the bubble from the center and in most cases the preferential position of a bubble is off-center. Systems with bubbles are expected to have bands of extremely low lying collective states, corresponding to various bubble displacements.

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There are a number of situations when the formation of voids is favored. When a system of particles has a net charge, the Coulomb energy can be significantly lowered if a void is created [1,2] and despite an increase in surface energy the total energy decreases. One can thus naturally expect that the appearance of bubbles will be favored in relatively heavy nuclei. This situation has been considered many times over the last 50 years in nuclear physics and lately similar ideas have been put forward for highly charged alkali metal clusters [3].

The formation of gas bubbles is another suggested mechanism which could lead to void(s) formation [4]. The filling of a bubble with gas prevents it from collapsing. Various heterogeneous atomic clusters [5] and halo nuclei [6] can be thought of as some kind of bubbles as well. In these cases, the fermions reside in a rather unusual mean field, with a very deep well near the center of the system and a very shallow and extended one at its periphery. Since the amplitude of the wave function in the semiclassical limit is proportional to the inverse square root of the local momentum, the single-particle (sp) wave functions for the weakly bound states will have a small amplitude over the deep well. If the two wells have greatly different depths, the deep well will act almost like a hard wall (in most situations).

Several aspects of the physics of bubbles in Fermi systems have not been considered so far in the literature. It is tacitly assumed that a bubble position has to be determined according to symmetry considerations. For a Bose system one can easily show that a bubble has to be off-center [7]. In the case of a Fermi system the most favorable arrangement is not obvious [8]. The total energy of a many fermion system has the general form

$$E(N) = e_v N + e_s N^{2/3} + e_c N^{1/3} + E_{sc}(N), \qquad (1)$$

where the first three terms represent the smooth liquid drop part of the total energy and E_{sc} is the pure quantum shell correction contribution, the amplitude of which grows in magnitude approximately as $\propto N^{1/6}$; see Ref. [9]. We consider in this work only one type of fermions with no electric charge. In a nuclear system the Coulomb energy depends rather strongly on the actual position of the bubble, but in a very simple way. In an alkali metal cluster, as the excess charge is always localized on the surface, the Coulomb energy is essentially independent of the bubble position. The character of the shell corrections is in general strongly correlated with the existence of regular and/or chaotic motion [10,11]. If a spherical bubble appears in a spherical system and if the bubble is positioned at the center, then for certain "magic" fermion numbers the shell correction energy $E_{sc}(N)$, and hence the total energy $E(N)$, has a very deep minimum. However, if the number of particles is not magic, in order to become more stable the system will in general tend to deform. Real deformations lead to an increased surface area and liquid drop energy. On the other hand, merely shifting a bubble off-center deforms neither the bubble nor the external surface and, therefore, the liquid drop part of the total energy of the system remains unchanged.

Moving the bubble off-center can often lead to a greater stability of the system due to shell correction energy effects. In recent years it was shown that in a 2-dimensional annular billiard, which is the 2-dimensional analog of spherical bubble nuclei, the motion becomes more chaotic as the bubble is moved further from the center [12]. One might thus expect that the importance of the shell corrections diminishes when the bubble is off-center. We show that this is not the case however.

One can anticipate that the relative role of various periodic orbits (diameter, triangle, square, etc.) is modified in unusual ways in systems with bubbles. In 3D systems the triangle and square orbits determine the main shell structure and produce the beautiful supershell phenomenon [10,13]. A small bubble near the center will affect only diameter orbits. After being displaced sufficiently far from the center, the bubble will first touch and destroy some triangle orbits. In a 3D system only a relatively small

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fraction of these orbits will be destroyed. Thus one might expect that the existence of supershells will not be critically affected but that the supershell minimum will be less pronounced. A larger bubble will simultaneously affect triangular and square orbits and thus can have a dramatic impact on both shell and supershell structure.

The change of the total energy of a many fermion system can be computed quite accurately using the shell corrections method, once the sp spectrum is known as a function of the shape of the system [9,11]. The results presented in this Letter have been obtained using the 3D version of the conformal mapping method described in [8] as applied to an infinite square well potential with Dirichlet boundary conditions. The magic numbers are hardly affected by the presence or absence of a small diffuseness [14]. The absence of a spin-orbit interaction leads to quantitative but to no qualitative differences.

In Fig. 1 we show the unfolded sp spectrum for the case of a bubble of half the radius of the system, $a = R/2$, as a function of the displacement d/R of the bubble from the center. The size of the system is determined as usual from $R^3 - a^3 = r_0^3 N$. The unfolded sp spectrum is determined using the Weyl formula [15] for the average cumulative number of states.

$$\varepsilon_n = N_W(e_n), \tag{2}$$

where e_n are the actual sp energies of the Schrödinger equation, $N_W(e)$ is the Weyl formula for the total number of states with energy smaller than e in a 3D cavity, and ε_n are the unfolded eigenvalues, which by construction leads to a spectrum with a unit average level density. As the bubble is moved off-center, the classical problem becomes more chaotic [12] and one can expect that the sp spectrum would approach that of a random Hamiltonian [16] and that the nearest-neighbor splitting distribution would be given by the Wigner surmise [17]. A random Hamiltonian would imply that magic particle numbers are as a rule absent. There is a large number of avoided level crossings in Fig. 1 and one can clearly see a significant number of relatively large gaps in the spectrum. Note that levels with different symmetries (different angular momentum projection on the symmetry axis m) can cross. Even for extreme displacements large gaps in the sp spectrum occur significantly more frequently than in the case of a random (which is closer to a uniform) spectrum. A simple estimate, using the Wigner surmise, shows that gaps of the order of three units or larger should be absent in the portion of the spectrum shown in Fig. 1. The probability to encounter a nearest-neighbor energy spacing s greater than s_0 is given by $P(s > s_0) = \exp(-\pi s_0^2/4)$. For $s_0 = 3, 4, 5$ one thus obtains 8.5×10^{-4}, 3.5×10^{-6}, and 3×10^{-9}, respectively. Several very large gaps for $d/R \approx 0.45$ are unambiguously present. Higher in the spectrum even larger gaps could be found. These features are definitely not characteristic of a random Hamiltonian. If the particle number is such that the Fermi level is at a relatively large gap, then the system at the corresponding "deformation" is very stable. A simple inspection of Fig. 1 suggests that for various particle numbers the energetically most favorable configuration can have the bubble either on- or off-center. This situation is very similar to the celebrated Jahn-Teller effect in molecules. Consequently, a magic particle number could correspond to a "deformed" system. In this respect this situation is a bit surprising, but not unique. It is well known that many nuclei prefer to be deformed, and there are particularly stable deformed magic nuclei or clusters [11,13,14,18].

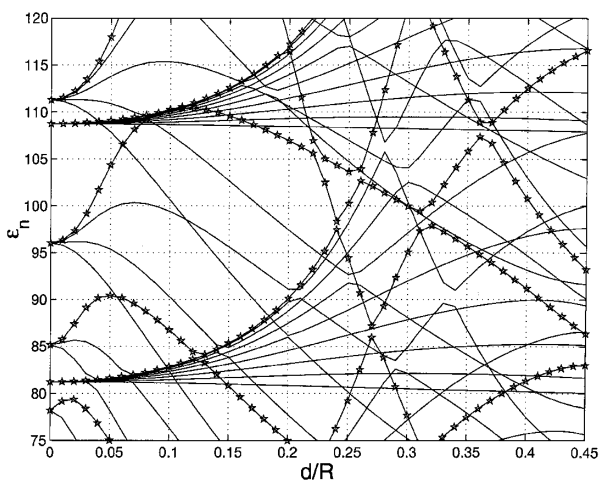

FIG. 1. A portion of the full unfolded sp spectrum (with unit average level density) for the case of a bubble of radius $a = R/2$ ($R = R_0 N^{1/3}$) as a function of the bubble displacement d/R. Energy levels with $m = 0$ (single-degenerate) are marked with pentagrams.

There is a striking formal analogy between the energy shell correction formula and the recipe for extracting the renormalized vacuum Casimir energy in quantum field theory [19] or the critical Casimir energy in a binary liquid mixture near the critical demixing point [20]. Note that even though Casimir energy is typically a smooth function of distance, it cannot be ascribed to the "smooth liquid drop" energy. Similarly, no part of the E_{sc} energy of a bubble near the surface can be ascribed to the smooth liquid drop energy. In Fig. 2 we show the contour plot of the E_{sc} energy for a system with $a = R/2$ as a function of the bubble displacement d/R versus $N^{1/3}$. The overall regularity of "mountain ridges" and "canyons" seem to be due to the interference effects arising from two periodic orbits along the diameter passing through the centers of the two spheres. Various mountain tops and valleys form an alternating network almost orthogonal to the mountain ridges and canyons. For some N's the bubble "prefers" to be in the center, while for other values that is the highest energy configuration.

As a function of the particle number N and at fixed d/R, the oscillation amplitude of the shell correction energy is maximal for on-center configurations. For a given particle

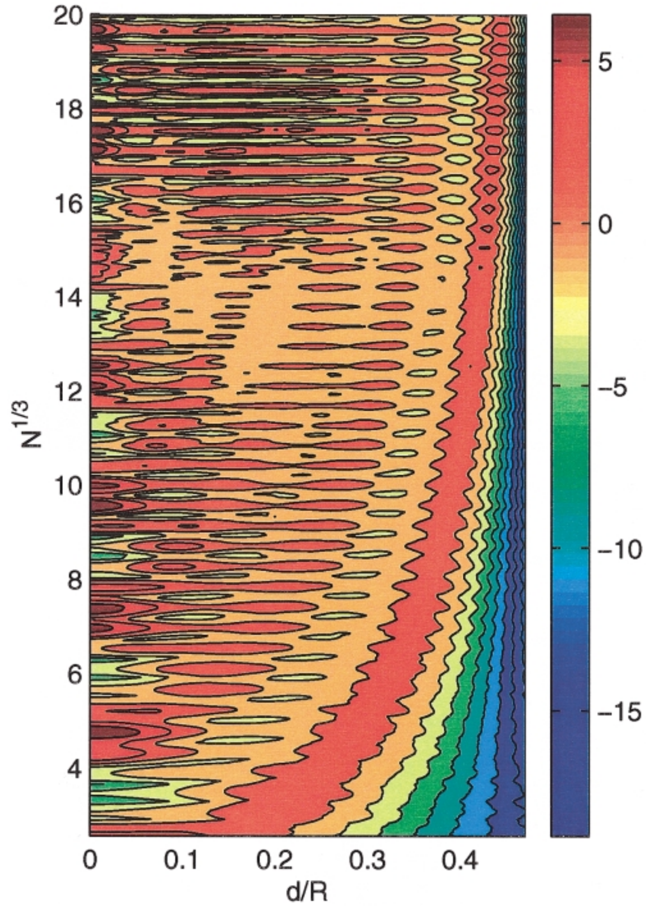

FIG. 2 (color). Contour plot of the shell correction energy for the case of a bubble of radius $a = R/2$ for up to $N = 8000$ spinless fermions. Energy is measured in units of $\hbar^2/2mr_0^2$.

number N the energy is an oscillating function of the displacement d and many configurations at different d values have similar energies. However, in all cases, moving the bubble all the way to the edge of the system leads to the lowest values of $E_{sc}(N)$. This drop in the shell correction energy as a function of d is preceded by the highest "mountain range." A practitioner of the Strutinsky method might be tempted to ascribe these features to the smooth part of the total energy. One should remember, however, that the Strutinsky recipe requires a smearing energy γ, which is supposed to be chosen larger than the typical energy separation between two consecutive energy shells. In a semiclassical language, such a difference is determined by the shortest periodic orbit in the system. In the present case the length of the shortest orbit $2(R - d - a) \to 0$, when the bubble approaches the edge of the system. This would require an even longer smearing interval γ in order to perform the Strutinsky procedure. In the absence of analytical results for this system a comparison with a simpler situation is extremely illuminating. When the inner and outer surfaces are very close one can ignore in the first approximation their curvatures and consider instead the case of matter between two infinite parallel planes. It can be shown explicitly that the shell correction energy is inversely proportional to the separation between the two surfaces [21], a behavior which is similar to that seen in Fig. 2. For a small bubble one can easily agree that it is more cost effective to make a hole closer to the edge, where the sp wave functions are smaller. Once again, we note here the analogy with the Casimir energy [19,20]. Moreover, at least qualitatively, this shortest orbit and the one diametrically opposed to it suffice to explain the pattern of "valleys" and "ridges" in Figs. 2 and 3. It is not entirely clear to us whether this final drop in the total energy could occur in a self-sustaining system. When the bubble is close to the outer surface, matter density in the region of the closest approach decreases, which in turn leads to a decrease of the self-consistent potential. In this case the square well potential model used by us becomes then inadequate. Physical systems where such configurations can nevertheless be realized are briefly mentioned at the end. In the case of a bubble with a smaller radius $a = R/5$ the number of level crossings is significantly smaller than in Fig. 1. As a result, the shell correction energy contour plot has less structure, see Fig. 3, and thus a system with a smaller bubble is also significantly softer.

Pairing correlations can lead to a further softening of the potential energy surface of a system with one or more

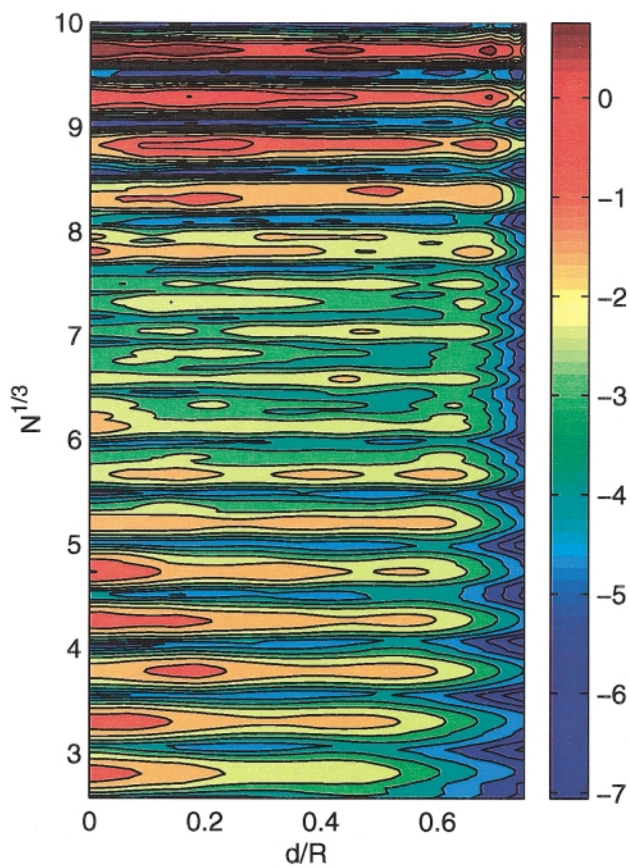

FIG. 3 (color). The same as in Fig. 2 but for $a = R/5$ and for up to $N = 1000$ spinless fermions.

bubbles. We have seen that the energy of a system with a single bubble is an oscillating function of the bubble displacement. When the energy of the system as a function of this displacement has a minimum, the Fermi level is in a relatively large gap, where the sp level density is very low. When the energy has a maximum, just the opposite takes place. Pairing correlations will be significant when the Fermi level occurs in a region of high sp level density and it is thus natural to expect that the total energy is lowered by pairing correlations at "mountain tops," and be less affected at "deep valleys." All this ultimately leads to a further leveling of the potential energy surface. With increasing temperature the shell correction energy decreases in magnitude, but the most probable position of a bubble is still off-center. The reason in this case is, however, of a different nature, the "positional" entropy of such a system favors configurations with the bubble off-center, as a simple calculation shows, namely, $S_{\text{pos}}(\mathbf{d}) = 2 \ln d + \text{const}$, where **d** is the position vector of the center of the bubble with respect to the center of the sphere. Moreover, making more bubbles could lead to a further decrease of the free energy, even though the total energy might increase.

A system with one or several bubbles should be a very soft system. The energy to move a bubble is parametrically much smaller than any other collective mode. All other familiar nuclear collective modes, for example, involve at least some degree of surface deformation. For this reason, once a system with bubbles is formed, it could serve as an extremely sensitive "measuring device," because a weak external field can then easily perturb the positioning of the bubble(s) and produce a system with a completely different geometry. There are quite a number of systems where one can expect that the formation of bubbles is possible [8]. Known nuclei are certainly too small and it is difficult at this time to envision a way to create nuclei as big as those predicted in Ref. [2]. On the other hand, voids, not always spherical though, can be easily conceived to exist in neutron stars [22]. Metallic clusters with bubbles, one or more fullerenes in a liquid metal, or a metallic ball placed inside a superconducting microwave resonator [23] in order to study the ball energetics and maybe even dynamics are all very promising candidates.

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[1] H. A. Wilson, Phys. Rev. **69**, 538 (1946); J. A. Wheeler (unpublished); P. J. Siemens and H. A. Bethe, Phys. Rev. Lett. **18**, 704 (1967); C. Y. Wong, Ann. Phys. (N.Y.) **77**, 279 (1973); W. J. Swiatecki, Phys. Scr. **28**, 349 (1983); W. D. Myers and W. J. Swiatecki, Nucl. Phys. **A601**, 141 (1996).
[2] K. Pomorski and K. Dietrich, Nucl. Phys. **A627**, 175 (1997); K. Dietrich and K. Pomorski, Phys. Rev. Lett. **80**, 37 (1998); J. Dechargé *et al.*, Phys. Lett. B **451**, 275 (1999).
[3] K. Pomorski and K. Dietrich, Eur. J. Phys. D **4**, 353 (1998).
[4] L. G. Moretto *et al.*, Phys. Rev. Lett. **78**, 824 (1997).
[5] S. Saito and F. Yabe, in *Chemistry and Physics of Fullerenes and Related Materials*, edited by K. M. Kadish and R. S. Ruoff (Electrochem. Soc., Pennington, NJ, 1998), Vol. 6, pp. 8–20; T. P. Martin *et al.*, J. Chem. Phys. **99**, 4210 (1993); U. Zimmermann *et al.*, Phys. Rev. Lett. **72**, 3542 (1994).
[6] S. M. Austin and G. F. Bertsch, Sci. Am. **272**, No. 6, 90 (1995).
[7] S. A. Chin and H. A. Forbert, Los Alamos e-print cond-mat/9810269.
[8] A. Bulgac *et al.*, in *Proceedings of the International Workshop on Collective Excitations in Fermi and Bose Systems*, edited by C. A. Bertulani, L. F. Canto, and M. S. Hussein (World Scientific, Singapore, 1999), pp. 44–61; Los Alamos e-print nucl-th/9811028.
[9] V. M. Strutinsky and A. G. Magner, Sov. J. Part. Nucl. Phys. **7**, 138 (1976).
[10] R. Balian and C. Bloch, Ann. Phys. (N.Y.) **69**, 76 (1972); M. Brack and R. K. Bhaduri, *Semiclassical Physics* (Addison-Wesley, Reading, MA, 1997).
[11] V. M. Strutinsky, Sov. J. Nucl. Phys. **3**, 449 (1966); Nucl. Phys. **A95**, 420 (1967); **A122**, 1 (1968); M. Brack *et al.*, Rev. Mod. Phys. **44**, 320 (1972).
[12] O. Bohigas *et al.*, Phys. Rep. **223**, 43 (1993); O. Bohigas *et al.*, Nucl. Phys. **A560**, 197 (1993); S. Tomsovic and D. Ullmo, Phys. Rev. E **50**, 145 (1994); S. D. Frischat and E. Doron, Phys. Rev. E **57**, 1421 (1998).
[13] H. Nishioka *et al.*, Phys. Rev. B **42**, 9377 (1990); J. Pedersen *et al.*, Nature (London) **353**, 733 (1991); M. Brack, Rev. Mod. Phys. **65**, 677 (1993), and references therein.
[14] A. Bulgac and C. Lewenkopf, Phys. Rev. Lett. **71**, 4130 (1993).
[15] R. T. Waechter, Proc. Cambridge Philos. Soc. **72**, 439 (1972); H. P. Baltes and E. R. Hilf, *Spectra of Finite Systems* (Bibliographisches Institut, Wissenschaftsverlag, Mannheim, Wien, Zürich, 1976).
[16] O. Bohigas *et al.*, Phys. Rev. Lett. **52**, 1 (1984).
[17] M. L. Mehta, *Random Matrices* (Academic Press, Boston, 1991).
[18] A. Bohr and B. Mottelson, *Nuclear Structure* (Benjamin, New York, 1974), Vol. II.
[19] H. B. G. Casimir, Proc. K. Ned. Akad. Wet. **51**, 793 (1948); V. M. Mostepanenko and N. N. Trunov, Sov. Phys. Usp. **31**, 965 (1988), and references therein.
[20] M. E. Fisher and P. G. de Gennes, C.R. Acad. Sci. Ser. B **287**, 207 (1978); A. Hanke *et al.*, Phys. Rev. Lett. **81**, 1885 (1998), and references therein.
[21] A. Bulgac and P. Magierski (unpublished).
[22] G. Baym *et al.*, Nucl. Phys. **A175**, 225 (1971); C. P. Lorentz *et al.*, Phys. Rev. Lett. **70**, 379 (1993); C. J. Pethick and D. G. Ravenhall, Annu. Rev. Nucl. Part. Sci. **45**, 429 (1995), and references therein; H. Heiselberg *et al.*, Phys. Rev. Lett. **70**, 1355 (1993).
[23] H. D. Graf *et al.*, Phys. Rev. Lett. **69**, 1296 (1992).