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Microscopic Theory of Nuclear Fission

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We describe the fission dynamics of ^{240}Pu within an implementation of the Density Functional Theory (DFT) extended to superfluid systems and real-time dynamics. We demonstrate the critical role played by the pairing correlations, which even though are not the driving force in this complex dynamics, are providing the essential lubricant, without which the nuclear shape evolution would come to a screeching halt. The evolution is found to be much slower than previously expected in this fully non-adiabatic treatment of nuclear dynamics, where there are no symmetry restrictions and all collective degrees of freedom (CDOF) are allowed to participate in the dynamics.

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Immediately after the epochal discovery of induced nuclear fission by Hahn and Strassmann [1] Meitner and Frisch [2], Bohr and Wheeler [3, 4] recognized that the main driving force leading to fission is the profile of the deformation nuclear energy arising form the competition between the nuclear surface and the Coulomb energies. The reasoning was based on a classical liquid charged drop model of a nucleus and the role of quantum mechanics started to became clear only with time. It was however soon realized that in nuclei nucleons form shells and behave in many instances as independent particles, like electrons in atoms, or in other words that the nucleons live on quantized orbits [5, 6], and that the spin-orbit interaction plays a critical role in the formation of the nuclear shells. Hill and Wheeler [7] were apparently the first to appreciate how the liquid drop deformation energy emerges from a quantum mechanical approach based on considering the quantized single-particle motion of nucleons in a slowly deforming potential well. The liquid drop potential deformation energy in their approach in the first approximation was an envelope of many intersecting parabolas, due to single-particle level crossings, see Figure 1. At single-particle level crossings of the last occupied level nucleons jump from one level to another, in order to maintain the sphericity of the Femi sphere. If a nucleus elongates on the way to scission into two fragments, without such a redistribution of nucleons at the Fermi level, the Fermi sphere would become oblate, while the spatial shape of the nucleus becomes prolate, and that would lead to a volume excitation energy of the nucleus. In the case of nuclei, which are saturating systems with a surface tension, while deforming by changing the shape of their surface only and while maintaining constant their volume, only the Coulomb and the surface contributions to the total energy changes. Each single-particle level is typically double degenerate, due to Kramers degeneracy, and nucleons would have to jump in pairs, otherwise the nuclear shape evolution towards scission would be hindered [8, 9]. Pairing interaction, which in spite of being relatively weak in nuclei, is very effective of promoting simultaneously two nucleons from time-reverse orbits into other time-reverse orbits and thus it greatly facilitates the evolution of the nuclear shape towards scission.

It was established later that single-particle level bunching exist in nuclear systems not only in the case of spherical nuclei (as in the case of atoms), but also in deformed and highly deformed nuclei. At first this phenomenon was experimentally observed in the case of fission isomers at very large

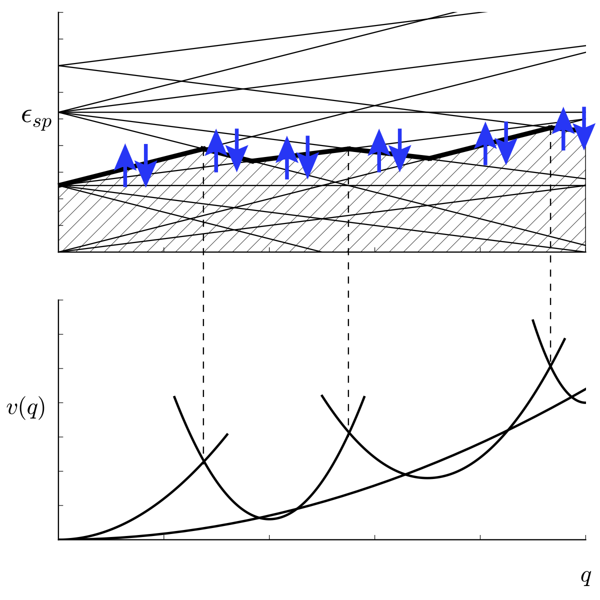

Figure 1: The qualitative evolution of the single-particle levels and of the total nuclear energy (lower panel) as a function of nuclear deformation [7, 8]. The Fermi level is shown with a thick line.

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elongations [10, 11, 12] and subsequently in the case of superdeformed nuclei [13]. The existence of nucleonic shells at large deformations results in a potential energy deformation surface with significant maxima and minima, which are otherwise absent in the case of a classical charged liquid drop. The level crossings lead to a potential energy surface which appears quite rough, even though it can be smoothed out in the presence of pairing correlations, which results in avoided level crossings. The nuclear deformation potential energy surface appears in the end to have a rather complicated structure. The gross behavior is determined by the surface and Coulomb energy and resembles the deformation energy of a charged liquid drop and that is the main driving force leading to fission. Because nuclei are relatively small quantum systems made of a bit more than a couple hundred fermions, which to a large extend behave as being independent, a rather rich shell structure exists, even for large deformations. This shell structure imprints on the overall charged liquid drop energy hills and valleys [11, 12]. On the way to the scission configuration nucleons have to perform a large number of redistributions between the single-particle levels crossing at the Fermi level, in order to maintain the spherical symmetry of their local momentum distribution or of the Fermi sphere. Overall, the deformation potential energy surface acquires a profile somewhat similar to that of an uneven mountain, with little hills and valleys and covered by trees, and the evolution of the nuclear shape is in the end similar to the erratic motion of a pinball, not straight down the hill, but rather left and right, bouncing (mostly elastically) from the many obstacles on the way to the bottom of the valley, where the pinball breaks up. At the last stages of this complex nuclear shape evolution the independent character of the nucleons inside nuclei plays again a critical role, magic closed shells control the nuclear shape evolution. As our simulations demonstrate[15], the nucleus separates typically into two fission fragments, one bigger and the other somewhat smaller. The larger fragment fragment has properties very similar to the energetically very stable double-magic ^{132}Sn, emerges with an almost spherical shape, while the lighter fragment at the scission emerges into an elongated shape, with a ratio of the major to minor axes close to 3/2.

Overall the fission dynamics is a very complex process, which still did not reach a full microscopic description [14], in spite of almost eight decades of effort. In contrast the superconductivity, another remarkable quantum many-body phenomenon, required less than five decades to reach a microscopic understanding. Several reasons prohibited so far the formulation of a microscopic theory of fission (as opposed to phenomenological models), capable to produce results comparable to observations without introducing uncontrollable approximations, parameter fitting, and based on microscopic input. Two major relatively recent developments proved to be critical and created the conditions for the formulation of a microscopic theory of fission. The first element was the extension of the Density Functional Theory (DFT) to superfluid fermion systems, and extension in the spirit of the Kohn and Sham [16] Local Density Approximation (LDA) from normal systems to superfluid systems [17, 18, 19], the Superfluid Local Density Approximation (SLDA). A second major development was the mergence of powerful supercomputers capable of handling a time-dependent DFT (TDDFT) approach to nuclear fission.

Since fission dynamics is a truly non-stationary phenomenon a further extension was needed to its Time-Dependent version [19] and this approach was dubbed the Time-Dependent Superfluid Local Density Approximation (TDSLDA). According to the theorem of Hohenberg and Kohn [20] there is a one-to-one correspondence between the full ground state many-body wave function of a fermion system and the one-body density matrix: $\Psi(x_1,\dots,x_N) \leftrightarrow n(\mathbf{r})$, which directly leads

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to the fact that an energy density functional (EDF) exists: $E_{gs} = \langle\Psi[n]|H|\Psi[n]\rangle \equiv \int d^3r\varepsilon(\mathbf{r})$. The extension of these statements to both excited states and time-dependent phenomena has been performed for quite some time now and many aspects are well documented in monographs [21, 22]. Unfortunately so far no recipes have been produced on how to generate the energy density functional and only semi-phenomenological solutions, quite accurate though, have been suggested. For this reason many still in the nuclear physics community are still leveling an unwarranted criticism at the DFT. DFT, similarly to the Schrödinger equation in quantum mechanics, provides the theoretical framework within which one has to attack a variety of quantum many-body problems. In the Schrödinger equation one has to provide the potential, which in most cases we know only approximately, with various degrees of accuracy. The same is true in the case of DFT, the energy density functional is known only with some degree of accuracy. One would not stop using the Schrödinger equation if one would know the potential only approximately and instead would revert to some alternative methods. What are the minimal requirements a nuclear EDF (NEDF) has to meet in order to be used the fission dynamics within a TDDFT approach? Apart from the usual constraints (translational and rotational invariance, Galilean invariance, isospin symmetry, parity,etc.) it has to describe accurately the saturation properties on nuclear matter, have a correct surface tension and accurate spin-orbit interaction, and accurate pairing properties. Saturation properties, surface energy and Coulomb energy are needed to describe nuclear fission at the liquid drop model. The spin-orbit interaction and accurate pairing energies are needed in order to describe correctly the shell-corrections and the fact that the emerging heavy fission fragment in the fission of actinide has properties very close to the double-magic ^{132}Sn. Pairing correlations are also critical in order to have an efficient mechanism to maintain the sphericity of the Fermi surface while the shape of the mother nucleus evolves from a compact form up to scission. In the absence of an efficient mechanism, which would redistribute the nucleon pairs at the level-crossings occurring at the Fermi level, see Figure 1, a nucleus would fail to fission, unless excited to very large energies or elongated well beyond the our fission barrier [9, 24, 25].

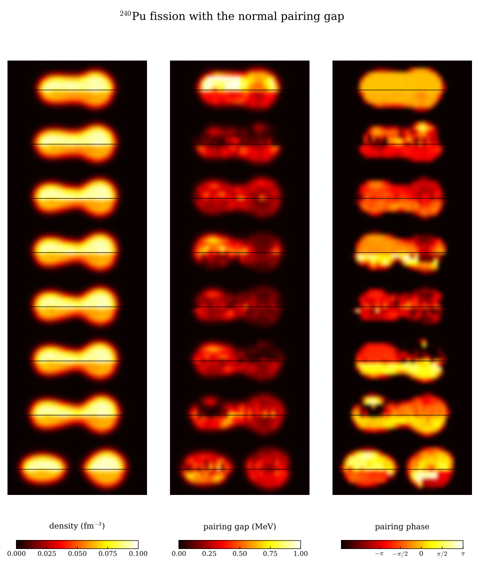

Figure 2: Induced fission of ^{240}Pu with normal pairing strength last about 14,000 fm/c from saddle-to-scission. The columns show sequential frames of the density (first column), magnitude of the pairing field (second column), and the phase of the pairing field (third column). In each frame the upper/lower part of each frame shows the neutron/proton density, the magnitude of neutron/proton pairing fields, and of the phase of the pairing field respectively [15]. At scission the heavy fragment is on the right and emerges almost spherical, while the light fragment is highly deformed with the ration of the axes $\approx 3/2$.

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An extension of the DFT to a TDDFT of superfluid systems requires the introduction of two new order parameters: the anomalous densities and currents. Pairing interaction in nuclei is short-ranged and that results in anomalous densities which converge very slowly with the upper cutoff energy, which is of the order of 100 MeV. It can be shown that if the pairing potential is local the anomalous density is actually divergent [17, 18]. Trying to eschew the presence of a divergent anomalous density by using finite short-range interactions makes the TDDFT approach practically impossible to implement in practice. An interaction such as the very successful Gogny interaction, has an phenomenological short-range, not resulting from any microscopic input. Moreover, a finite range interaction will render the TDDFT equations into partial differential-integral equations, which would require computations resources well beyond exascale computers. And last, but not least, there is no fundamental reason why the DFT equations have to be non-local in space in the case of nuclear interactions. It suffices to say that that was no need for non-local equations in the case of the electronic systems, for which the Coulomb interaction has an infinite range. We have used an NEDF based on the popular phenomenological SLy4 interaction [23], supplemented with a very accurate pairing anomalous contribution [18].

The emerging TDSLDA equations appear by design formally as TDHFB equations with local meanfield and pairing potentials. One has to remember that unlike TDHF or TDHFB equations, which are derived following specific approximations, the TDSLDA equations have an exact theoretical structure, and the only approximation is in the actual NEDF used, in our case a phenomenological one. The SLy4 NEDF provides quite an accurate description of the saturation properties of nuclear matter, of the surface properties of nuclei, and leads to a correct reproduction of the magic numbers, thus has a reasonably accurate spin-orbit contribution to the NEDF. The pairing part of the NEDF used by us is also quite accurate [18]. The time-dependent equations of the TDSLDA are discretized on a spatial lattice in a box large enough to contain both the initial mother nucleus as well as the separated fission fragments immediately after scission. The lattice constant corresponds to a momentum cutoff of ≈ 500 MeV/c, which is definitely large enough to describe accurately a large class of low-energy nuclear phenomena. Each single particle wave functions has four components: $u_{n\uparrow}(\mathbf{r}), u_{n\downarrow}, v_{n\uparrow}(\mathbf{r}), v_{n\downarrow}(\mathbf{r})$, where n runs over proton and neutron quasiparticle states. The total number of partial differential equations varies, depending on the size of the simulation box and the lattice constant, and runs from tens of thou-

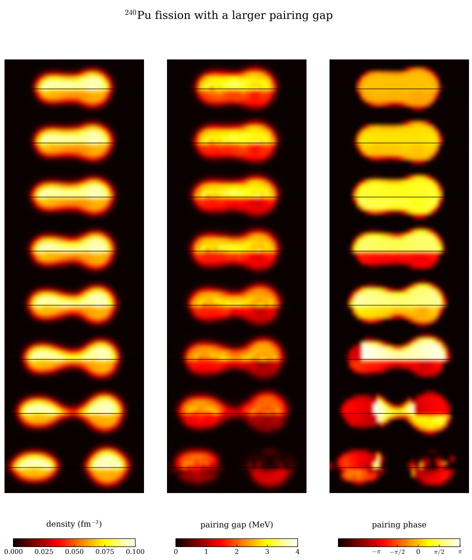

Figure 3: Induced fission of ^{240}Pu with enhanced pairing strength last about 1,400 fm/c from saddle-to-scission, thus about ten times faster than in the case of normal pairing strength.

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sands to hundreds of thousands. This very large number of coupled, non-linear time-dependent 3D partial differential equations and the very large number of time-steps required to complete the full evolution of the system explains why such a problem could not have been attacked numerically less than a decade ago. We initialize the fission nucleus to a state very close to the outer fission barrier and let the system evolve until scission. No restriction of any type are imposed on the dynamics and at all times the meanfield and the pairing potentials are determined by the instantaneous nucleon densities, and in this sense the dynamics is selfconsistent.

The most remarkable aspect of our work was that the chosen nucleus ^{240}Pu, with an excitation energy of about 8 MeV corresponding to the induced fission ^{239}Pu(n,f) with a neutron with an impinging kinetic energy of about 1.5 MeV reached the scission configuration and separated into two unequal fragments, see Figure 2. The average atomic mass $A_L \approx 105.3$, neutron number $N_L \approx 63.5$, and charge $Z_L \approx 39.7$ of the light fragment obtained in simulations compare surprisingly well with the systematic data $A_L^S \approx 100.6$, $N_L^S \approx 61$, and $Z_L^S \approx 39.7$, particularly considering that no effort or fitting was made. The light fragment emerges very deformed at scission, with the shape of an axially symmetric ellipsoid with the ratio of the major to the minor axes close to 3/2. The deformation energy of the light fission fragment is eventually converted into internal excitation energy and as a result most of the excitation energy resides in the light fission fragment. the total number of post-scission neutron emitted is estimated between 2-3 in reasonable agreement with experiment. The total kinetic energy of the fission fragments we obtain is 181.6 MeV to be compared with the value obtained from systematics 177.3 MeV. The time form the outer saddle-to-scission is surprisingly very large, of the order of 10,000 fm/c, which is about an order of magnitude larger that any previous estimate within various phenomenological models. The dynamics appears superficially as over damped, but in reality the down-the-hill roll of the nucleus can be compared with the motion of an electron in the Drude model of electric conduction. An electron collides with various ions in the lattice and it is forced to move in transversal directions to the electric field, and even though there is no dissipation, the total kinetic+potential energy of the "electron" is conserved and at any "height" the magnitude of the velocity in the presence and in the absence of the "ions" is the same, the actual length of the trajectory is significantly longer, which results in a much longer time to reach the bottom. This is exactly what happens in the case of the evolution of a fissioning nucleus while it rolls down from the outer saddle-to-scission. As there are no constraints on the dynamics (as usually practitioners enforce in semi-microscopic and phenomenological models), all collective degrees of freedom are allowed to participate. The fission fragments at the scission configuration are rather cold, any excitation is present mostly in the collective (shape and pairing) degrees of freedom, while the intrinsic nucleonic degrees of freedom follow essentially an adiabatic evolution.

The deformation potential energy surface however is still full of local little hills and valleys, arising from the partially avoided level crossing as a result of the pairing correlations. To demonstrate how essential the role of the pairing correlations is in the fission dynamics, in spite of the fact that in magnitude the contribute very little, we performed a fission study where we artificially increased the strength of the pairing gaps, see Figure 3. The main result of this is that the magnitude of the roughness of the deformation potential energy surface is greatly reduced and the deformation potential energy surface is thus almost smooth. A nucleus now at the top of the barrier will start rolling down the hill towards scission configuration straight down, without significant excursions

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sideways. The time from saddle-to-scission in this case is a factor ten smaller and almost identical to the time one would obtain in a fully hydrodynamic approach of an ideal nuclear fluid [26]. This results agrees with the known behavior of well developed superfluid systems, which at zero temperature behave as ideal or perfect fluids. There is another remarkable difference between the dynamics illustrated in Figures 2 and 3. While the evolution of the neutron and proton densities appear superficially similar, the evolution of the pairing field is qualitatively different. In Figure 2 the paring field is seen to fluctuate quite a lot both in magnitude and in phase, a signature of a not very well developed condensate. In Figure 3 however, prior to scission the pairing fields of both neutrons and protons hardly fluctuate either in magnitude or phase, and as in stationary ground states, the phase is essentially uniform throughout the entire nuclear system, which is a signature of a well defined adiabatic evolution of the entire system. This is an example of the recently described mechanism of phase-locking in the evolution of superfluid systems [27], when the strength of the interaction leading to superfluidity (both in Fermi and Bose systems) exceeds a critical value. We can thus conclude that the pairing interaction, in spite of being rather weak, plays a crucial role in the nuclear large amplitude dynamics. In its absence a nuclear system would come to screeching halt [24, 25], as in the presence of large static friction in classical systems.

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References

[1] O. Hahn and F. Strassmann, *Über den Nachweis und das Verhalten der bei der Bestrahlung des Urans mittels Neutronen entstehenden Erdalkalimetalle*, Naturwissenschaften **27**, 11 (1939).

[2] L. Meitner and O.R. Frisch, *Disintegration of Uranium by Neutron: a New Type of Nuclear Reaction,* Nature (London), **143**, 239 (1939).

[3] N. Bohr, *Disintegration of Heavy Nuclei,* Nature (London), **143**, 330 (1939).

[4] N. Bohr and J.A. Wheeler, *The Mechanism of Nuclear Fission,* Phys. Rev. **56**, 426 (1939).

[5] Maria Goeppert Mayer, *On closed shells in nuclei. II,* Phys. Rev. **75**, 1969 (1949).

[6] O. Haxel, J.H.D. Jensen, and H.E. Suess, *On the "magic numbers" in nuclear structure,* Phys. Rev. **75**, 1766 (1949).

[7] D.L. Hill and J.A. Wheeler, *Nuclear Constitution and the Interpretation of Fission Phenomena,* Phys. Rev. **89**, 1102 (1953).

[8] G.F. Bertsch, *The nuclear density of states in the space of nuclear shapes,* Phys. Lets. **B 95**, 157 (1980).

[9] G.F. Bertsch and A. Bulgac, *Comment on "Spontaneous Fission: A Kinetic Approach",* Phys. Rev. Lett. **79**, 3539 (1997).

[10] S.M. Polikanov, V.A. Druin, V.A. Karnaukov, V.L. Mikheev, A.A. Pleve, N.K. Skobelev, V.G. Subotin, G.M. Ter-Akopian, and V.A. Fomichev, *Spontaneous fission with an snomalous short period,* JETP (Sov. Phys.) **42**, 1016 (1962)

[11] M. Brack, J. Damgaard, A.S. Jensen, H.C. Pauli, V.M. Strutinsky, and C.Y. Wong, *Funny Hills: The Shell-Correction Approach to Nuclear Shell Effects and its Applications to the Fission Process,* Rev. Mod. Phys. **44**, 320 (1972).

[12] S. Bjørnholm and J.E. Lynn, The Double-Humped Fission Barrier, Rev. Mod. Phys. **52**, 725 (1980).

[13] P.J. Twin, B.M. Nyakó, A.H. Nelson, J. Simpson, M.A. Bnentley, H.W. Cramer,-Gordon, P.D. Forsyth, D. Howe, A.R. Mokhtar, J.D. Morrison, J.F. Sharpey-Schafer, and G. Sletten, *Observatrion of a Discreete-Line Superdeformed Band up to* $60\hbar$ *in* ^{152}Dy*,* Phys. Rev. Lett. **57**, 811 (1986).

[14] N. Schunck and L.M. Robledo, *Microscopic Theory of Nuclear Fission: A review,* Rep. Prog. Phys. **79**, 116301 (2016).

[15] A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu, I*nduced Fission of* ^{240}Pu *within a Real-Time Microscopic Framework,* Phys. Rev. Lett. **116**, 122504 (2016).

[16] W. Kohn and L.J. Sham, Self-Consistent Equations *Including Exchange and Correlation Effects, Phys. Rev.* **140***,* A1133 (1965).

[17] A. Bulgac and Y. Yu, *Renormalization of the Hartree-Fock-Bogoliubov Equations in the Case of a Zero Range Pairing Interaction,* Phys. Rev. Lett. **88**, 042504 (2002)

[18] Y. Yu and A. Bulgac, *Energy Density Functional Approach to Superfluid Nuclei,* Phys. Rev. Lett. **90**, 222501 (2003).

[19] A. Bulgac, *Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids,* Ann. Rev. Nucl. Part. Sci. **63**, 97 (2013).

[20] P. Hohenberg and W. Kohn, *Inhomogeneous Electron Gas,* Phys. Rev. **136**, B864 (1964).

[21] R.M. Dreizler and E.K.U. Gross, *Density Functional Theory: An Approach to the Quantum Many-Body Problem*, (Springer-Verlag, Berlin, 1990).

[22] *Fundamentals of Time-Dependent Density Functional Theory*, Eds. M.A.L. Marques, N.T. Maitra, F.M.S. Nogueira, E.K.U. Gross, and A. Rubio, Lecture Notes in Physics, vol. 837 (Springer-Verlag, Berlin, 2012).

[23] E. Chabanat, P. Bonche, P. Haensel, J. Meyer, R. Schaeffer, *A Skyrme parametrization from subnuclear to neutron star densities Part II. Nuclei far from stabilities,* Nucl. Phys. **A635**, 231 (1998).

[24] P. Goddard, P. Stevenson, and A, Rios, *Fission Dynamics within Time-Dependent Hartree-Fock: Deformation Induced Fission,* Phys. Rev. C **92**, 054610 (2015).

[25] P. Goddard, P. Stevenson, and A, Rios, *Fission Dynamics within Time-Dependent Hartree-Fock: Boost Induced Fission,* Phys. Rev. C **93**, 014620 (2016).

[26] A. Bulgac. M.M. Forbes, and S. Jin, *Nuclear energy density functionals: what do we really know?*, arxiv:1506.09195.

[27] A. Bulgac, *Dynamics of Fragmented Condensates and Macroscopic Entanglement*, arXiv:1701.06683.

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