Nuclear fission as resonance-mediated conductance

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Abstract

For 75 years the theory of nuclear fission has been based on the existence of a collective coordinate associated with the nuclear shape, an assumption required by the Bohr-Wheeler formula as well as by the R-matrix theory of fission. We show that it is also possible to formulate the theory without the help of collective coordinates. In the new formulation, fission is facilitated by individual states in the barrier region rather than channels over the barrier. In a certain limit the theory reduces to a formula closely related to the formula for electronic conductance through resonant tunneling states. In contrast, conduction through channels gives rise to a staircase excitation function that is well-known in nanoscale electronics but has never been seen in nuclear fission.
I. INTRODUCTION

The theory of induced nuclear fission began with Bohr and Wheeler's landmark paper [1] that introduced the transition-channel formula for the fission decay rate $W$,

$$ W = \frac{1}{2\pi\hbar \rho_I} \sum_c T_c. $$

Here $\rho_I$ is the level density of the compound nucleus. The $T_c$ are the transmission coefficients of the channels and satisfy the condition $0 < T_c < 1$. The unit bound on the single-channel transmission coefficient is an important aspect of the theory, derived from detailed balance. In the Bohr-Wheeler theory the channel concept is applied at the barrier top which is far from the asymptotic region where the channels can be rigorously derived. There is an alternate formalism, the R-matrix theory, which forms the scaffolding of present-day phenomenological parameterization of reactions leading to fission [2–4]. This theory is also based on the channel concept, but there are no computational tools to calculate its basic ingredients such as the logarithmic derivative of the wave function [2, cf. p. 760]. The hallmark of well-developed channel physics is the staircase excitation function, increasing by one step as each new channel opens up. This is by now a well-known feature of quantum conductance, e.g., see Ref. [5], but conditions at the nuclear fission barrier are such such as to obscure it from being visible in the excitation function. Finally, we mention that there is a new appreciation of importance of diffusive dynamics in nuclear fission [11]; here channels play no role at all.

Besides the conductance through channels, there is another well-known limit of electron transport in which the electrons pass from one conductor to another through an intermediate resonance, which we shall call a “bridge state”. The formula for conductance is equivalent to the Bohr-Wheeler formula [12] but with a transmission coefficient $T_b$ given by the Breit-Wigner resonance expression [6]

$$ T_b = \frac{\Gamma_R \Gamma_L}{E_b^2 + (\Gamma_R + \Gamma_L)^2/4}. $$

Here $\Gamma_R, \Gamma_L$ are the decays widths of the bridge state into the two conductors and $E_b$ is its energy with respect to the Fermi level of the electrons in the conductors. The main object of the present study is to show how this structure arises in nuclear fission via a discrete-basis representation of the many-body Hamiltonian.
A very simplified picture of the energy landscape of a fissile nucleus is shown in Fig. 1. The ground state is somewhat deformed, but to fission the nucleus undergo a large shape changes that passes through or over a barrier. The colored regions in the left-hand graph show different conditions that need to be considered for a complete theory: the subbarrier tunneling region in green, the barrier-top region (most relevant to fission in nuclear power reactors) in blue, and the excited thermal region in red. The barrier-top region is most relevant to fission conditions in nuclear power reactions and is the focus of the present work. The dynamics for this region will be modeled using a discrete basis of configurations characterized by a shape variable as well as their energy.

In fact discrete-basis representations arise naturally in the theory of heavy nucleus structure. The most practical computational tool for that purpose is self-consistent mean field theory (SCMF) based on energy density functionals, and simplified approximations thereto. With the help of constraining fields, the theory yields a spectrum of configurations characterized by their energies and the expectation values of the constraining fields. Thus it naturally produces a spectrum for a fissionable nucleus such as that depicted on right-hand side of Fig. 1.

There is also a residual interaction between the configurations that is responsible for the dynamics. The important point for the discrete basis representation is that that a two-body residual interaction cannot change the shape by a a large amount, so the couplings are of limited range on the horizontal scale.

At excitation energies relevant for the fission dynamics in nuclear reactors, the configurations at the initial deformation form a compound nucleus. This means that the residual interactions produce a statistical distribution of amplitudes and energies as in random matrix theory. The statistical limit is approached when the residual interactions are uncorrelated and on average larger then the energy spacing between the levels. While this limit is achieved on the right and left-hand sides at moderate excitation energy, it will not be the case for configurations in the middle, at energies around the barrier energy.

We thus a led to a Hamiltonian that consists of of two statistical reservoirs connected by a set of bridge configurations. This already simplifies the dynamics greatly. One first determines the boundaries of the reservoirs by calculation the level densities and average interaction energies as a function of energy and the shape parameter. The interactions of the bridge configurations still has to be determined. However, the coupling to the reservoirs can
FIG. 1: The fission barrier. Left: the black line depicts the potential energy surface (PES) as a function of some deformation parameter associated with the shape change during fission. The leftmost black dot on the PES indicates the ground state, which is moderately deformed. The other black dot indicates the barrier top. The shaded areas show regions of very different shape dynamics. At the ground state and low excitation energies fission occurs by tunneling through the barrier, (green area). At sufficiently high energy, diffusive dynamics is expected (red area). The region just around the barrier top (blue area) shows strong fluctuations and is the subject of the present study. Right: a magnified view of the barrier top region in a discrete-basis representation. Configurations are indicated by dots. The solid black line is the PES of the barrier top. We distinguish regions in the energy-deformation plane with low and high level densities. The high level-density regions are modeled by random matrix theory; the the levels in the low-density region at the barrier must be treated explicitly.

be treated statistically: the only relevant parameter is the decay width into the reservoir.

For the remainder of this letter, and in order to make contact with the Eq. (1) and (2), we simplify the Hamiltonian a single bridge state connecting the reservoirs. The configurations in the left and right reservoirs are labeled by \( l \) and \( r \), respectively. The bridge configuration is labeled by \( b \). The non-zero matrix elements of the Hamiltonian are:

\[
\langle l | H | l' \rangle = \delta_{l,l'} E_l
\]

\[
\langle r | H | r' \rangle = \delta_{r,r'} E_r
\]

\[
\langle l | H | b \rangle = v_{lb}
\]
FIG. 2: Survival probability in the left-hand reservoir as a function of time, starting from an eigenstate of the reservoir. Solid black line: regular Hamiltonians in both reservoirs. Dashed lines: two examples of decays when diagonal energies of the left-hand Hamiltonian are taken from random matrix theory. The time $t$ is given in units of $t_0$, Eq. (4).

$$\langle r|H|b \rangle = v_{rb}$$

$$\langle b|H|b \rangle = E_b.$$  

Eq. (2) of the mesoscopic theory can be recovered by taking equally spaced levels in the reservoirs and constant values for the coupling matrix elements to the reservoirs. We denote the parameters as $v_L = v_{lb}, v_R = v_{rb}, \Delta E_L = E_l - E_{l-1}$ and $\Delta E_R = E_r - E_{r-1}$. It is convenient to define decay widths of the bridge state to the right and left by Fermi’s Golden Rule, $\Gamma_{L,R} = 2\pi v_{L,R}^2/\Delta E_{L,R}$. This Hamiltonian is easily programmed and it reproduces the rate combining Eq. (1) and (2) nearly perfectly, provided and the energy bandwidths of the reservoirs, $N_L\Delta E_L$ and $N_R\Delta E_R$ is large compared to $\Gamma_R$ and $\Gamma_L$. This is illustrated in Fig. 2 taking a Hamiltonian with $N_L = 100$ levels in the left-hand reservoir, $N_R = 200$ levels in the right reservoir, and parameters chosen so that $\Delta E_L = 2\Delta E_R$ and $\Gamma_L = \Gamma_R = 0.12N_L\Delta E_L$. The initial wave function is taken as a pure configuration near the middle of the left-hand band. The energy of the bridge state is taken to be the same as the initial configuration. The wave function is evolved with the time-dependent Schrödinger equation. The solid line in the shows the probability remaining in the left-hand reservoir. It decreases linearly with time at a rate $W = \Delta E_L/2\pi$ up to the characteristic time

$$t_0 = \frac{2\pi}{\Delta E_L}. \quad (4)$$
This is in perfect agreement with the combined Eq. (1) and (2), since $T = 1$ for the given parameters. It may seem surprising that the probability current is constant up to the time $t_0$, but this can be easily understood. The uniform spacing of the levels in the left-hand reservoir simulates the middle of a band in a perfect one-dimensional conducting wire. The wave function of an eigenstate of the isolating wire has the particle uniformly over the length of the wire, and equal currents flowing to the left and to the right. When the interaction with the bridge state is turned on, the right-moving current passes without impediment to the other reservoir. The current only goes to zero after twice the transit time of the wire. If the parameters are changed so that $T < 1$, the only difference up to a time $t_0$ is that the slope changes from $t_0^{-1}$ to $T/t_0$.

We now go to Hamiltonians closer to the nuclear cases, modifying the reservoirs according to random matrix theory. In fact, the physics associated with the right-hand reservoir is insensitive to the fine details of its Hamiltonian. The levels spacings can be taken to be uniform or as extracted from the middle levels from Wigner’s random matrix ensemble. The coupling matrix elements $v_{rb}$ can be constant or Gaussian distributed, again from Wigner’s random matrix ensemble. The only important properties are:

- The width $\Gamma_R$. It may be computed from the Fermi Golden Rule using average level density and the root-mean-square average interaction matrix element.
- The average level spacing must be smaller than any other energy scale (or inverse time scale).

Under these conditions the coupling to the right-hand reservoir can be treated very simply. Instead of including it explicitly in the Hamiltonian, the absorptive effect of the right-hand reservoir can be computed adding an imaginary potential $-i\Gamma_R/2$ to $\langle b | H | b \rangle$. We have adopted this simplification for computing the rates shown later in Figs. 3 and 4.

In sharp contrast to the results of the above paragraph, the decay properties of a state of the left-hand reservoir are greatly affected by the level statistics. One aspect is well-understood: the decay width of a state $l$ is proportional to the square of the coupling matrix element $v_{lb}$ and this has a Gaussian distribution in random matrix models. But there is more. Fig. 2 shows two decay distributions when the level spectrum $E_l$ was taken from a random matrix ensemble but the couplings strengths were constant, as in the quantum wire conductance discussed earlier. One sees that the decay rates do not have any simple
behavior; they can neither be described as constant or as exponential decays.

Of course, for the physical problem we only care about the averages over many initial states. Fig. 3 shows such an average, for conditions that correspond to a unit transmission coefficient, $\Gamma_L = \Gamma_R$ and $E = E_b$. The average follows very well an exponential decay law, with an average decay rate given by Eq. (5) below. The error bars show the root mean square deviation of the individual probabilities $P(t)$; one sees that there are large fluctuations about the average. We have also examined the dependence of the decay profiles $P(t)$ on $\Delta E_L$, $v_L$, and $E_b$ and found that the average profiles are exponential and fairly well described by the formula

$$\Gamma_c = \frac{\Gamma_R \Gamma_L}{2\pi \rho \Gamma^2_E + \left(\Gamma_R + \Gamma_L\right)^2/4}. \quad (5)$$

As a final step to apply random matrix distributions to the left-hand reservoir, we taking the coupling strengths $v_b$ to be Gaussian distributed with variance $\langle v_{bL}^2 \rangle = v_0^2$. The expected average survival probability is then given by

$$\overline{P}(t) = \frac{1}{(2\pi v_0)^{1/2}} \int_{-\infty}^{\infty} dv e^{-v^2/2v_0^2 - 2\Gamma v^2\rho t} = \frac{1}{(1 + 2\Gamma_0 t)^{1/2}}. \quad (6)$$

Fig. 4 shows the computed $\overline{P}(t)$ as black dots, taking parameters such than $T_b = 1$. It agrees very well with Eq. (6), shown as the solid line in the Figure. For these parameters, $\Gamma_0 = 1/2\pi \rho \Gamma$.

Absent many-body calculations of properties of the bridge states, one can still see if proposed framework can give acceptable fits to parameterize experimental data. There is
very detailed data on the fission widths of compound nucleus states of $^{236}\text{U}$ just above the neutron threshold\cite{13,15} that we can try to fit. Assuming a set of independent bridge states, the rate formula is identical to Eq. (1) but with the sum over channels replaced by a sum over bridge states:

$$
\sum_c T_c \rightarrow \sum_b \frac{\Gamma_{bR}\Gamma_{bL}}{E_b^2 + (\Gamma_{bR} + \Gamma_{bL})^2/4}
$$

The information available comprise the energies, angular momentum, and fission widths of the individual levels of compound nucleus in a narrow energy window\cite{14}. The level density $\rho_I$, and average fission width $\Gamma_f$ obtained by Ref. \cite{14} are given in Table I. The extracted $\sum T$ is shown in the last column. In principle, both could be attributed to a single bridge state at resonance. However, the fluctuations in the individual fission width would be much larger than observed if that were the case. On an energy scale of several keV, variations in $\sum T$ are seen that are reminiscent of of resonant peaks\cite{14, Fig. 16,17}. Their extracted excitation function for the $J^\pi = 4^-\text{ levels}$ is shown as the solidline in Fig. 5. We have attempted to fit the curve with Eq. (7) in Eq.(1). A fit using 13 independent bridge states is

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$J^\pi$ & $1/\rho_I$ (keV) & $\Gamma_f$ & $\sum T$ \\
\hline
3- & 0.95 ± 0.08 & 0.18 ± 0.02 & 1.2 \\
4- & 0.81 ± 0.07 & 0.09 ± 0.01 & 0.7 \\
\hline
\end{tabular}
\caption{Average fission widths from Ref. \cite{14}}
\end{table}
FIG. 5: Average fission widths of 4− states in $^{236}U$ as a function of neutron energy measured in the $^{235}U(n,f)$ reaction. The black line shows the experimental data abstracted from Ref. [14], see also Ref. [15]. The dashed line shows the width for a single very broad bridge state with $\Gamma_R = \Gamma_L$ and at resonance. The dotted line shows a fit using Eq. (7) as discussed in the text.

shown as the dotted line in Fig. 5. We see that a reasonable fit is possible, although there are discrepancies. In particular, the depths of the valleys are deeper than can be accounted for by independent bridge states.

Of course the theory as implemented with independent bridge states is a great oversimplification of nuclear fission dynamics. We mention two of the important ingredients for a predictive theory that have been neglected here. The first is that the barrier region very likely requires many bridge configurations to be considered explicitly. The fission barrier has at least two humps [16]. Besides bridge states crossing the two humps, the states in the middle, called class II states, are visible as resonances in the fission excitation functions. Once we go beyond the individual bridge state linking the two reservoirs, the properties of the interaction linking the bridge states becomes very important. It is well-known that in the sub-barrier region the fission lifetimes are very sensitive to the pairing interaction [10]. This gives a coherence to the matrix elements of the lowest bridge states, and if the pairing strength were large enough would allow the linked states to act as channels. However, nuclear pairing is rather weak and is easy blocked in excited states. For that reason, the discrete basis picture seems closer to the physical reality than the channel picture.
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[1] N. Bohr and J.A. Wheeler, Phys. Rev. 56 426.
[2] S. Bjornholm and J.E. Lynn, Rev. Mod. Phys. 52 725 (1980).
[3] O. Bouland, J.E. Lynn, and P. Talou, Phys. Rev. C 88 054612 (2013).
[4] O. Bouland, J.E. Lynn, and P. Talou, Nucl. Data Sheets 118 211 (2014).
[5] B.J. van Wees, et al. Phys. Rev. Lett. 60 848 (1988)
[6] Y. Alhassid, Rev. Mod. Phys. 72 895 (2000).
[7] R. Landauer, IBM J. Res. Dev. 1 223 (1957).
[8] M. Bender, P.-H. Heenen, and P-G. Reinhard, Rev. Mod. Phys. 75 121 (2003).
[9] M. Zirnbauer, J. Verbaarschot, and H.A. Weidenmüller, Nucl. Phys. A411 161 (1983).
[10] R. Rodriguez-Guzmann and L.M. Robledo, Phys. Rev. C 89 054310 (2014).
[11] J. Randrup and P. Möller, Phys. Rev. Lett. 106 132503 (2011).
[12] G.F. Bertsch, J. Phys. Condens. Matter 3 373 (1991).
[13] R.B. Perez, G. de Saussure, E.G. silver, R.W. Ingle, and H. Weaver, Nucl. Sci. Eng. 55 203 (1974).
[14] M.S. Moore, J.D Moses, G.A. Keyworth, J.W. Dobbs and N.W.Hill, Phys. Rev. C 18 1328 (1978).
[15] M.S. Moore, L. Calabretta, F. Corvi, and H. Weigmann, Phys. Rev. C 30 214 (1984).
[16] M. Brack, et al., Rev. Mod. Phys. 44 320 (1972).