Towards microscopic studies of survival probabilities of compound superheavy nuclei

Yi Zhu and J C Pei

State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, People’s Republic of China

E-mail: peij@pku.edu.cn

Received 10 May 2017, revised 31 July 2017
Accepted for publication 13 September 2017
Published 5 October 2017

Abstract

The microscopic approach of fission rates and neutron emission rates in compound nuclei have been applied to $^{258}\text{No}$ and $^{286}\text{Cn}$. The microscopic framework is based on the finite-temperature Skyrme-Hartree–Fock + BCS calculations, in which the fission barriers and mass parameters are self-consistently temperature dependent. The fission rates from low to high temperatures can be obtained based on the imaginary free energy method. The neutron emission rates are obtained with neutron gases at surfaces. Finally the survival probabilities of superheavy nuclei can be calculated microscopically. The microscopic approach has been compared to widely used statistical models. Generally, there are still large uncertainties in descriptions of fission rates.

Keywords: superheavy nuclei, fission, neutron emission, survival probability

(Some figures may appear in colour only in the online journal)

1. Introduction

To quest the heaviest nuclei, whose existences are merely due to quantum shell effects, is one of the major issues in nuclear physics [1–3]. Very recently, four elements with $Z = 113$, 115, 117 and 118 were officially named as nihonium (Nh), moscovium (Mc), tennesine (Ts), oganesson (Og), respectively by IUPAC [4]. To date, nuclei with proton numbers up to 118 have been experimentally discovered and confirmed. There are typical cold [5, 6] and hot fusion [7] reactions to synthesize superheavy nuclei. The key question is to find the optimal combination of beam-target and the bombarding energy in order to maximize the production cross sections. It will be a much harder challenge to synthesize new elements beyond $Z = 118$.

The synthesis procedure of superheavy nuclei can be described as the capture-fusion-evaporation reaction. The final production cross section (or evaporation residue cross section) can be written as [3]

$$\sigma_{\text{EVR}} = \sum_{J} \sigma_{E}(E_{\text{cm}}) P_{\text{CN}}(E^*) W_{\text{sur}}(E^*).$$

(1)

In equation (1), $\sigma_{E}$ is the capture cross section, $P_{\text{CN}}$ is the fusion probability of the compound nuclei, $W_{\text{sur}}$ is the survival probability of the compound nuclei. The survival probability is mainly determined by the competition between neutron emission rates and fission rates in compound nuclei. The $\alpha$ decays can provide critical information of ground states of superheavy nuclei but are negligible compared to the rapid fission and neutron emission processes in highly excited compound superheavy nuclei. Generally, there are large uncertainties in theoretical descriptions of these three steps although the total production cross section can be reproduced by various parameterized models. Experimentally, the measurement of survival probabilities is feasible. For example, very large survival probabilities of $^{258}\text{No}$ [8] and $^{274}\text{Hs}$ [9] have been directly obtained in hot fusion reactions, which provide a good opportunity to verify various theoretical models.

Conventionally, the statistical models have been widely applied to the calculations of survival probabilities $W_{\text{sur}}$ of highly excited nuclei [10–12]. The pioneer applications of statistical model can be traced back to Weisskopf for neutron evaporation in 1937 [13] and Bohr–Wheeler for fission in
1939 [14]. The statistical model of fission, also called transition state theory, involves fission barriers and level densities at ground state and saddle point, respectively. There are many developments on the statistical models with adjusted parameters and collective corrections. In particular, whether the fission barriers and level density parameters are temperature (or excitation energy) dependent is still a question [15, 16]. On the other hand, the microscopic descriptions of survival probabilities are based on effective nuclear forces and there are non-adjusted parameters needed [17]. The nuclear density functional theory is an ideal theoretical tool for descriptions of heavy and superheavy nuclei. The microscopic fission theory based on finite-temperature nuclear density functional theory can self-consistently describe the thermal properties of compound nuclei and the gradually decreased quantum effects. It is still worth to understand the microscopic fission mechanism [17] so as to make predictions for unknown experiments, although phenomenological statistical models have been widely used.

In this work, we introduce the microscopic framework for descriptions of the fission rates [18], neutron emission rates [19] and then survival probabilities based on the finite-temperature Skyrme–Hartree–Fock–Bogoliubov (HFB) (or BCS) theory [20]. In our approach, the fission barriers are given in terms of free energies and are temperature dependent [23]. The collective inertia mass parameters are calculated with the temperature-dependent cranking approximation [21, 22]. Then the fission rates are obtained with the imaginary free energy (IMF) method [24, 25] from low to high temperatures. The HFB solutions in coordinate spaces can self-consistently produce neutron gases around surfaces [26]. Then the neutron emission rates can be related to the neutron gas density [19]. For comparison, we also studied the survival probabilities with the widely used statistical models.

This paper is organized as follows. In section 2, we review the two theoretical methods to calculate the survival probability of the compound superheavy nuclei. In section 3, our results of $^{258}$No and $^{286}$Cn are presented and compared with experimental data. The summary and our perspectives are given in section 4.

2. Theoretical framework

2.1. Finite-temperature HFB (FT-HFB)

The FT-HFB theory was firstly derived by Goodman in 1981 [20]. We only display some relevant equations here. The FT-HFB equation in the coordinate space is written as [27]:

$$
\begin{bmatrix}
 h_T - \lambda \\
 \Delta_T
\end{bmatrix}
\begin{bmatrix}
 u_i \\
 v_i
\end{bmatrix}
= E
\begin{bmatrix}
 u_i \\
 v_i
\end{bmatrix},
$$

(2)

where $h_T(r)$ and $\Delta_T(r)$ are the temperature-dependent single-particle Hamiltonian and pairing potential, respectively. For the particle-hole interaction channel, the SKM* interaction [28] is employed. The density-dependent pairing interaction [29] is adopted in the particle–particle channel. The FT-HFB equation has the same form with the HFB equation at zero temperature, but the density $\rho(r)$ and pairing density $\tilde{\rho}(r)$ are modified as

$$
\rho(r) = \sum_i |u_i(r)|^2 f_i + |v_i(r)|^2 (1 - f_i),
$$

(3)

$$
\tilde{\rho}(r) = \sum_i v_i(r)^2 (1 - 2f_i) u_i(r),
$$

(4)

where the temperature-dependent factor $f_i$ is

$$
f_i = \frac{1}{1 + e^{E_i/kT}}.
$$

(5)

The entropy $S$ is evaluated with the finite-temperature HFB approximation as [20]:

$$
S = -k \sum_i [f_i \ln f_i + (1 - f_i) \ln(1 - f_i)].
$$

(6)

At a constant temperature $T$, the free energy is given as $F = E - TS$. We used the HFB-AX solver [30] with finite temperatures in deformed coordinate spaces to study neutron emission rates. The details of calculations can be found in the previous paper [19]. The finite-temperature Hartree–Fock +BCS equation can be solved similarly, which is computationally more efficient for thermal fission studies [18].

The essential inputs for the fission studies includes the fission barriers and mass parameters. The fission barriers are given in free energies. The fission barriers are self-consistently temperature-dependent, including the fission barrier heights and the barrier curvatures. The mass parameters as a function of deformation $\beta_2$ are calculated by the temperature-dependent cranking approximation [21, 22], is written as

$$
M(\beta_2) = \hbar^2 [M^{(1)}]^{-1} [M^{(3)}][M^{(1)}]^{-1},
$$

(7)

$$
M^{(k)}_{\mu \nu} = \frac{1}{2} \sum_{Q} \langle Q | Q \rangle_{\mu \nu} [Q | 0]
\times \left\{ \left( u_{\mu} u_{\nu} - v_{\mu} v_{\nu} \right)^2 \left[ \tan \left( \frac{E_{\mu}}{2kT} \right) - \tanh \left( \frac{E_{\mu}}{2kT} \right) \right] + \left( u_{\mu} v_{\nu} + u_{\nu} v_{\mu} \right)^2 \left[ \tanh \left( \frac{E_{\mu}}{2kT} \right) + \tan \left( \frac{E_{\mu}}{2kT} \right) \right] \right\},
$$

(8)

where $v_{\mu}^2$ is the BCS occupation number; $E_{\mu}$ is the BCS quasiparticle energy.

2.2. Neutron emission rates

In the coordinate-space FT-HFB calculation, the external neutron gas is produced naturally. The neutron emission width $\Gamma_n$ of the compound nucleus is given by the nucleosynthesis formula [31]:

$$
\frac{\Gamma_n}{\hbar} = n \langle \sigma v \rangle,
$$

(9)

where $\sigma$ is the neutron capture cross section defined as $\pi R^2$, $n$ denotes the neutron gas density, and $v$ is the average velocity of the external gas [19]. The calculations of neutron emission rates do not involve level densities and free parameters, see details in [19].
2.3. Nuclear fission rates

The WKB method has been widely used for descriptions of the spontaneous fission lifetime [32, 33]. There are two key inputs, the fission barriers and the collective mass parameters, for the WKB calculations. It is known that the SkM* force [28] can give reasonable fission barriers and has widely been used for fission studies. The mass parameters can be calculated by the cranking approximation and the temperature-dependent cranking approximation [21]. For thermal excited nuclei, the fission rates can be estimated by the IMF method [25, 34]. At low temperatures, the fission is mainly the barrier tunneling process. While at high temperatures, the fission is basically the barrier reflection process. The general IMF formula [35, 36] for the decay rates from excited systems is given as:

\[ \Gamma = Z^{-1} \int_{E_0}^{\infty} dE P(E) \exp(-\beta E), \]  

where \( P(E) \) is related to the transmission probability. \( Z \) indicates the normalization factor, and it is actually the partition function in the metastable system. The above formula applies to quantum systems in an ideal heating bath, which is suitable for chemical reactions but is not a good approximation for nuclear reactions. In this case, the integral upper limit may be modified to the excitation energy \( E^* \) to be consistent with the statistical model.

The temperature-dependent potential valley around the metastable equilibrium deformation can be approximated to be a harmonic oscillator well. Then the partition function can be derived as [25]:

\[ Z = \sum_{n=0}^{\infty} e^{-\frac{\hbar \omega_0}{kT}} = \left[ 2 \sinh \left( \frac{\hbar \omega_0}{2kT} \right) \right]^{-1}, \]  

where \( \beta = 1/kT \), \( \omega_0 \) is the curvature of the potential well. For realistic potential barriers and mass parameters, we can extract \( \omega_0 \) approximately by [18]:

\[ \omega_0 = \pi E/\int_{E_0}^{b} \sqrt{2M(s)(E-V(s))} ds. \]  

\( M(s) \) is the temperature-dependent mass parameter along the fission path, and it can be estimated by the temperature-dependent cranking approximation [21, 22].

At low temperatures, the fission probability at \( E^* \) is given by the WKB method as:

\[ P(E) = e^{-\frac{\pi}{\hbar \omega_b} \int_{E_0}^{E} \sqrt{2M(V(s)-E)} ds}. \]  

By combining equations (10), (11) and (13), the averaged low-temperature fission rates can be obtained.

We can approximate the temperature-dependent barrier as an inverted harmonic oscillator potential. The barrier curvature \( \omega_b \) at the saddle point can be extracted by [18]

\[ \omega_b = \pi (V_b - E)/\int_{E_0}^{E_s} \sqrt{2M(s)(V(s)-E)} ds, \]  

where \( V_b \) denotes the barrier height.

For fission rates at high temperatures, the contribution is dominated by reflections above the barriers. In this case, the fission probability \( P(E) \) can be estimated by

\[ P(E) = (1 + \exp[2\pi(V-V_0)/\hbar \omega_b])^{-1}. \]  

Finally the averaged fission rates at high temperatures can be written as [25]:

\[ \Gamma_f = \frac{\omega_b}{2\pi} \sinh \left( \frac{\hbar \omega_b}{2} \right) \exp \left( -\beta V_b \right). \]  

2.4. Statistical model

Statistical models have been widely used for calculating the survival probabilities of superheavy nuclei [10, 12]. In the statistical model, the width of neutron evaporation is:

\[ \Gamma_n(E^*) = \frac{2\hbar R^2}{\pi \hbar^2 \rho(E^*)} \times \int_{0}^{E^*-B_n} \rho \left( E^*-\varepsilon_n \right) T_f(\varepsilon_f) d\varepsilon_n, \]  

where \( B_f \) is the fission barrier; \( \rho_d \) is the level density at the ground state. The barrier transmission probability \( T_f(\varepsilon_f) \) is defined as:

\[ T_f(\varepsilon_f) = \left[ 1 + \exp \left( \frac{2\pi \varepsilon_f}{\hbar \omega_{sd}} \right) \right]^{-1}. \]  

The curvature is \( \hbar \omega_{sd} = 2.2 \text{ MeV} \), as suggested in [11, 12]. Usually the level density is calculated by the Fermi-gas model with several corrections according to [12],

\[ \rho(E^*) = \frac{\exp[2\sqrt{a(E^*-\delta)} - \delta]}{2\pi \sigma^{d/4} (E^*-\delta)^{3/4}} \]  

with

\[ \sigma^2 = 6m^2 \sqrt{a(E^*-\delta)}/\pi^2, \quad m^2 \approx 0.24A^{1/3}. \]  

In this work, the level density parameter is \( a = A/12 \text{ MeV}^{-1} \). The level density parameter at the saddle point is \( a_{sd} = 1.1A/12 \text{ MeV}^{-1} \). The pairing correction adopts \( \delta = 12/\sqrt{A} \) for even-even nuclei.
3. Results and discussions

In this section, we study the survival probabilities of $^{258}\text{No}$ and $^{286}\text{Cn}$, for which the experimental data are available. Therefore we can comparatively analyze the microscopic approach and the statistical model in details.

Figure 1 shows the temperature-dependent fission barriers of $^{258}\text{No}$ as a function of quadrupole deformation $\beta_2$. The unit of the temperature is MeV.

![Figure 1](image1.png)

Figure 1. Calculated temperature-dependent fission barriers of $^{258}\text{No}$ as a function of quadrupole deformation $\beta_2$. The unit of the temperature is MeV.

The mass parameter is an essential input for the microscopic fission approach. In this work, the temperature-dependent cranking approximation is employed [21, 22]. We show in figure 2 the mass parameters of the compound nucleus $^{258}\text{No}$ for temperatures ranging between 0 and 1.5 MeV. Based on the discussion of [40], the mass parameter is inversely proportional to the square of the pairing gap. As the temperatures increase, the pairing gaps are gradually reduced and finally disappeared at 0.5–0.8 MeV [27, 41]. Consequently, it can be understood that the mass parameters increase at $T = 0.75$ MeV in figure 2. At a higher temperature of $T = 1.5$ MeV, the disappearance of shell effects [38] leads to reduced mass parameters.

![Figure 2](image2.png)

Figure 2. The mass parameters of $^{258}\text{No}$ obtained by the temperature-dependent cranking approximation as a function of the deformations.

The fission widths are not only dependent on the heights of the fission barriers but also on the shapes of the barriers. In figure 3 the curvatures at the equilibrium point ($\omega_0$) and the barrier saddle point ($\omega_b$) as a function of temperature are shown. We can see that at the equilibrium point, $\omega_0$ firstly increases and then decreases. At the barrier point, $\omega_b$ changes slightly. For different nuclei, the curvatures behavior very differently [18].

![Figure 3](image3.png)

Figure 3. For $^{258}\text{No}$, the calculated potential curvatures (or frequencies) around the equilibrium point ($\omega_0$) and the barrier saddle point ($\omega_b$) as a function of temperature.

Figure 4 displays the level density parameter $a$ of $^{258}\text{No}$ calculated by the $E^*/T^2$, $S/2T$ and $S^2/4E^*$ [31], respectively. In panel (a) the level density parameters at equilibrium point ($a_{g.s.}$) with different temperatures are shown. The results of three different methods have similar trends. We observe a rapid increase of level density parameters at the temperature $T = 0.75$ MeV. The level density parameters at saddle point ($a_{s.d.}$) from three methods are shown in panel (b). It can be seen that $a_{s.d.}$ is larger than $a_{g.s.}$ because the level density parameter increases with deformation [42]. The different level density parameters between the ground state and the saddle point have been considered phenomenologically in statistical models. In the microscopic study, it can be seen that the deformation and temperature-dependent level density can be self-consistently taken into account. The deformation dependence of level densities are related to specific shell structures. At high excitation energies, the shell effects would disappear and the deformation dependence of level densities would be much reduced. Indeed, at high temperatures, the
The level density parameters at the equilibrium point and the saddle point are close, as shown in figure 4. In [8], the extracted value of $G_{n\text{tot}} = 0.840 \pm 0.050$ for the first-chance fission of $^{258}$No at $E^* = 61$ MeV in the $^{26}$Mg+$^{232}$Th. In figure 5, the $\Gamma_n/\Gamma_{\text{tot}}$ calculated by our approach and the statistical model are plotted versus excitation energies of $^{258}$No. In our approach for $E^* = 56.9$ MeV, we obtain the neutron emission width $\Gamma_n = 2.09 \times 10^{-2}$ MeV, and the fission width $\Gamma_f = 2.22 \times 10^{-2}$ MeV. The final survival probability $G_{\text{final}} = 0.515$ that is smaller than experimental value. For the statistical model, results with two sets of barrier parameters are shown, for which one adopts a constant barrier height of 4.54 MeV [8] and the other is from our temperature-dependent calculations in figure 1. Figure 5 demonstrated that the fission barrier heights have a significant influence on $\Gamma_n/\Gamma_{\text{tot}}$.

The survival probabilities of $^{286}$Cn have also been studied by the statistical model and our microscopic method, as shown in figure 6. $^{286}$Cn has been studied by the hot fusion experiment [3] and the excitation energy of the compound nuclei are about 40 MeV. The experimental data of the residual cross section are given for $3n$ and $4n$ evaporation channels. There is no direct measurements for the survival probabilities and a lower limit of $7 \times 10^{-11}$ is obtained [3]. In this work, we calculate the survival probabilities after the first neutron evaporation, as given by $G_{n\text{tot}}$. Microscopic calculations of survival probabilities after multiple neutron emissions would be extremely time consuming. In figure 6, the survival probabilities are also calculated by the statistical model as described in section 2.4. The microscopic fission rates are obtained by the equation (16). In figure 6, our results are generally comparable to the statistical model. The microscopic results are larger than that of the statistical model although the same fission barrier heights are adopted. This is mainly because the curvatures $\omega_0$ (or frequency) at the equilibrium point of $^{286}$Cn are very small. The potential energy
surface of the compound $^{286}$Cn is very flat around the equilibrium point. The decreased $\omega_0$ can reduce the fission widths about one order.

In order to analyze the difference between the microscopic approach and statistical model, we plot the neutron emission widths of $^{286}$Cn in figure 7. It can be seen that results of the two methods are comparable within a factor of 3, while the microscopic method underestimates the neutron widths in particular at high energies. Based on our studies, we can say that the uncertainties of neutron emission rates are smaller than that of fission rates. In the future, to improve the reliability of microscopic fission theory, we should improve the effective nuclear force [43] and also perform multi-dimensional fission calculations.

4. Summary

In summary, the microscopic framework for descriptions of survival probabilities of compound superheavy nuclei has been proposed. Our motivation is to study the microscopic fission rates and neutron emission rates without free parameters, in contrast to the widely used phenomenological statistical models. The thermal fission rates are based on the temperature-dependent fission barriers from Skyrme-Hartree–Fock–BCS calculations. We studied the survival probability of compound nuclei $^{258}$No and $^{286}$Cn. The survival probability of $^{258}$No are comparable to the experimental data. Generally there are still large uncertainties in fission rates compared to neutron emission rates. In the future, the microscopic fission rates should be studied in multi-dimensional deformation spaces.

Acknowledgments

We thank Professors G Adamian, A Nasirov and Xiaojun Sun for useful discussions. This work was supported by the National Natural Science Foundation of China under Grants No. 11375016, 11522538, 11235001.

References

[1] Oganessian Y T, Sobizcewski A and Ter-Akopian G M 2017 Phys. Scr. 92 023003
[2] Hofmann S and Münzenberg G 2000 Rev. Mod. Phys. 72 733
[3] Itkis M G, Vardaci E, Itkis I M, Knazycheva G N and Kozulin E M 2015 Nucl. Phys. A 944 204
[4] Öhrström L and Reedijk J 2016 Pure Appl. Chem. 88 1225
[5] Armbruster P 1985 Annu. Rev. Nucl. Part. Sci. 35 135
[6] Hofmann S et al 2002 Eur. Phys. J. A 14 147
[7] Oganessian Y T et al 2010 Phys. Rev. Lett. 104 145202
[8] Peterson D et al 2009 Phys. Rev. C 79 044607
[9] Yanez R et al 2014 Phys. Rev. Lett. 112 152702
[10] Zubov A S, Adamian G G, Antonenko N V, Ivanova S P and Scheid W 2002 Phys. Rev. C 65 024308
[11] Zubov A S, Adamian G G, Antonenko N V, Ivanova S P and Scheid W 2005 Eur. Phys. J. A 23 249
[12] Xia C J, Sun B X, Zhao E G and Zhou S G 2011 Sci. China Phys. Mech. Astron. 54 109
[13] Weisskopf V 1937 Phys. Rev. 52 295
[14] Bohr N and Wheeler J A 1939 Phys. Rev. 56 426
[15] Świątecki W J, Siwek-Wilkzyńska K and Wilczyński J 2008 Phys. Rev. C 78 054604
[16] Adamian G G and Antonenko N V 2010 Phys. Rev. C 81 019803
[17] Schunck N and Robledo L M 2016 Rep. Prog. Phys. 79 116301
[18] Zhu Y and Pei J C 2016 Phys. Rev. C 94 024329
[19] Zhu Y and Pei J C 2014 Phys. Rev. C 90 054316
[20] Goodman A L 1981 Nucl. Phys. A 352 30
[21] Iwamoto A and Greiner W 1979 Z. Phys. A 292 301
[22] Baran A and Lojevski Z 1994 Acta Phys. Pol. B 25 1231
[23] Sheikh J A, Nazarewicz W and Pei J C 2009 Phys. Rev. C 80 011302
[24] Langer J S 1967 Ann. Phys., NY 41 108
[25] Affleck I 1981 Phys. Rev. Lett. 46 388
[26] Pei J C, Nazarewicz W, Sheikh J A and Kerman A K 2010 Nucl. Phys. A 834 381c
[27] Khan E, Van Giai N and Sandulescu N 2007 Nucl. Phys. A 789 94
[28] Bartel J, Quentin P, Brack M, Guet C and Håkansson H-B 1982 Nucl. Phys. A 386 79
[29] Dobaczewski J, Nazarewicz W and Stoitsov M V 2002 Eur. Phys. J. A 15 21
[30] Pei J C, Stoitsov M V, Fann G I, Nazarewicz W, Schunck N and Xu F R 2008 Phys. Rev. C 78 054316
[31] Bonche P, Levi S and Vautherin D 1984 Nucl. Phys. A 427 278
[32] Baran A, Sheikh J A, Dobaczewski J, Nazarewicz W and Stasiewicz A 2011 Phys. Rev. C 84 054321
[33] Erler J, Langunké K, Loens H P, Martinez-Pinedo G and Reinhard P-G 2012 Phys. Rev. C 85 025802
[34] Hagino K, Takigawa N and Abe M 1996 Phys. Rev. C 53 1840
[35] Miller W H 1975 J. Chem. Phys. 62 1899
[36] Hänggi P, Talkner P and Borkovec M 1990 Rev. Mod. Phys. 62 251
[37] Reinhard P-G private communication
[38] Egidio J L, Robledo L M and Martin V 2000 Phys. Rev. Lett. 85 26
[39] Pei J C, Nazarewicz W, Sheikh J A and Kerman A K 2009 Phys. Rev. Lett. 102 192501
[40] Bertsch G and Flocard H 1991 Phys. Rev. C 43 2200
[41] Martin V and Robledo L M 2009 Int. J. Mod. Phys. E 18 861
[42] Pomorski K, Nerlo-Pomorska B and Bartel J 2007 Int. J. Mod. Phys. E 16 566
[43] Xiong X Y, Pei J C and Chen W J 2016 Phys. Rev. C 93 024311