Proximity potential and the surface energy coefficient calculated using an energy density formalism

P. Chattopadhyay
Department of Physics, Guru Nanak Dev University, Amritsar, India

Raj K. Gupta
Department of Physics, Panjab University, Chandigarh, India

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Within a folding procedure, the universal function of the proximity potential is calculated by using the energy density functional of Vautherin and Brink for the Skyrme force interactions. The corrected Thomas-Fermi approximation is used for the nuclear density. Also, the surface energy coefficient in the nuclear binding energy expression (for a spherical nucleus) is calculated for making an estimate of the correction to the Thomas-Fermi kinetic energy density. Judging the performance of the various known Skyrme forces in giving a correct physical behavior of the proximity universal function and the surface energy coefficient, we obtain the correction parameter $\lambda \approx \frac{1}{36}$ for the original Skyrme force and the force SII of Vautherin and Brink.

I. INTRODUCTION

The concept of the proximity potential has come to play an important role in the physics of heavy ion collisions. First introduced by Blocki *et al.*[1] in the calculation of heavy ion potentials, it has now been extended to the collision of deformed, oriented nuclei.[2] The interesting feature of this approach is the separation of the force, between two gently curved surfaces in close proximity, into a geometrical factor representing the mean curvature of the interacting surfaces and a universal function of separation. The universal function gives the interaction potential per unit area between two flat surfaces. Various approaches have been used to calculate the universal function.[1,3] Since the proximity potential is a surface effect, in judging the effectiveness of such an approach (and of the interaction itself) it should be useful to examine not only the microscopic nucleus-nucleus interaction potential but also how well the method is able to reproduce the surface energy coefficient in the binding energy expression for the nuclei.

In the present work (which is an extension of a similar effort by Gupta *et al.*[4]) we calculate the universal function of the proximity as well as the surface energy coefficient for various Skyrme interactions, using the density functional method[5] with the Thomas-Fermi (TF) approximation for nuclear density. Within a folding procedure, the potential is obtained as the difference between the energies of the combined system and those of the isolated systems. This method of folding the densities ensures that the attractive nuclear proximity potential arises from the interaction of the surfaces only. As the overlap becomes large, the resulting potential becomes repulsive. The energy density functional used is the one derived by Vautherin and Brink[6] for the Skyrme interaction in which the energy density is given as a function of nucleon density $\rho=\rho_p+\rho_n$, the kinetic energy density $\tau=\tau_p+\tau_n$, and the spin orbit density $\vec{J}=\vec{J}_p+\vec{J}_n$; where p and n stand for proton and neutron, respectively. The potentials are calculated for various known Skyrme interactions and the relative contributions of the nucleon density and the kinetic energy density are investigated. Also, the surface energy coefficient is calculated and the performance of the various Skyrme interactions is judged for a best fit to the empirical value.[7]

II. UNIVERSAL FUNCTION OF THE PROXIMITY POTENTIAL

In the folding procedure, the ion-ion potential V, as a function of the separation degree of freedom, is calculated as a difference of the energies of the combined system and those of the isolated systems by considering the density ρ of the combined system as a superposition of the densities ρ_1 and ρ_2 of the individual nuclei:

$$V(\vec{r})=\int H(\vec{r},\rho,\tau)d\vec{r}-\left[\int H_1(\vec{r}_1,\rho_1,\tau_1)d\vec{r}_1+\int H_2(\vec{r}_2,\rho_2,\tau_2)d\vec{r}_2\right], \quad (1)$$

with

$$\rho=\rho_1+\rho_2 .$$

This means that the antisymmetrization effects are neglected. For the spin-orbit coupling and the Coulomb effects neglected, the energy density functional H of Vautherin and Brink,[6] for the even-even $N=Z$ nuclei, is given by

$$H(\vec{r},\rho,\tau)=\frac{\hbar^2}{2m}\tau+\tfrac{3}{8}t_0\rho^2+\tfrac{1}{16}t_3\rho^3+\tfrac{1}{16}(3t_1+5t_2)\rho\tau+\tfrac{1}{64}(9t_1-5t_2)(\vec{\nabla}\rho)^2 , \quad (2)$$

where m is the nucleon mass and t_0, t_1, t_2, and t_3 are the

TABLE I. The Skyrme force parameters together with the Fermi momentum k_f.

Interaction	t_0 (MeV fm^3)	t_1 (MeV fm^5)	t_2 (MeV fm^5)	t_3 (MeV fm^6)	k_f[a] (fm^{-1})	Ref.
S	−1072.0	461.0	−40.0	8027.0	1.37	8
SI	−1057.3	235.9	−100.0	14463.5	1.32	6
SII	−1169.9	585.6	−27.0	9331.1	1.30	6
SIII	−1128.75	395.00	−95.00	14000.00	1.29	9
SIV	−1205.60	765.00	35.00	5000.00	1.31	9
SV	−1248.29	970.56	107.22	0	1.32	9
SVI	−1101.81	271.67	−138.33	17000.00	1.29	9

[a] $k_f=[(3\pi^2/2)\rho_0]^{1/3}$. This allows us to calculate ρ_0 for each interaction.

parameters of Skyrme interactions, listed in Table I. These parameters have been obtained in a self-consistent manner by fitting the binding energies, charge radii, and other single-particle properties of spherical nuclei. Besides the original force given by Skyrme[8] (denoted as S), the two sets of parameters (SI and SII) obtained by Vautherin and Brink[6] and the four sets of parameters (SIII to SVI) of Beiner *et al.*,[9] with quite different strengths, fit the nuclear properties in essentially an equally satisfactory manner. In Eq. (2) the first term is the kinetic energy contribution; the terms involving ρ^2 and ρ^3 are the volume effects arising from two- and three-body interactions; the term proportional to $\rho\tau$ is the interaction term and the last term involving the gradient of density is the surface term.

In the Thomas-Fermi (TF) approximation the nucleon density is of the form[6]

$$\rho=\begin{cases}\rho_0\tanh^2\dfrac{r-R}{2b} & \text{for } r\le R\\ 0 \text{ for } r>R\ , & \end{cases} \tag{3}$$

with

$$b=0.16\left[\frac{2m}{\hbar^2}\left[\frac{3\pi^2}{2}\right]^{-2/3}\rho_0^{1/3}(9t_1-5t_2)\right]^{1/2} \tag{4}$$

and R, the outer radius of the nucleus, given by

$$R=r_0A^{1/3}+2b;\ r_0=1.12 \text{ fm}\ . \tag{5}$$

In these expressions b is a measure of the surface diffusivity. The kinetic energy density τ_0 in this approximation is then given by

$$\tau_0=\tfrac{3}{5}(\tfrac{3}{2}\pi^2)^{2/3}\rho^{5/3}\ . \tag{6}$$

To this TF kinetic energy density τ_0, however, is added a correction τ_λ that involves additional surface effects, first suggested by von Weizsäcker.[10] Among other methods,[11] this correction can be calculated by using the gradient expansion method.[12,13] One obtains, to a first order, the following expression for the kinetic energy density:

$$\tau=\tau_0+\tau_\lambda=\tau_0+\lambda\left[\frac{\vec\nabla\rho}{\rho}\right]^2\ , \tag{7}$$

where λ is a constant. The value for λ has been a point of controversy in the literature and different authors[13] have suggested different values, lying between $\frac{1}{4}$ $(=\frac{9}{36})$ and $\frac{1}{36}$. In the present work, we start with the expression

$$\lambda=\tfrac{1}{9}\left[\frac{m^*}{m}+\frac{1}{4}\right] \tag{8}$$

that was derived recently by Barranco and Treiner.[14] Here m^* is the effective mass of the nucleon at the saturation point of the symmetric nuclear matter. A value for m^*/m lying between 0.95 and 1 has been indicated by these authors; this means $\lambda\approx\frac{5}{36}$. Our calculations, however, support the lower estimate of $\lambda=\frac{1}{36}$ for the reasonable set of Skyrme force parameters.

The energy density functional H of Eq. (1), for ρ and τ given, respectively, by Eqs. (3) and (7), takes the form

$$H(\vec r,\rho,\tau_0)=\frac{\hbar^2}{2m}\tau_0+\tfrac{3}{8}t_0\rho^2+\tfrac{1}{16}t_3\rho^3+\tfrac{1}{16}(3t_1+5t_2)\rho\tau_0 +\alpha(\vec\nabla\rho)^2+\frac{\beta(\vec\nabla\rho)^2}{\rho}\ , \tag{9}$$

where

$$\alpha=\alpha_1+\alpha_2\ ,$$

with

$$\alpha_1=\tfrac{1}{64}(9t_1-5t_2)\ ,\qquad \alpha_2=\tfrac{1}{16}(3t_1+5t_2)\lambda\ , \tag{10}$$

and

$$\beta=\frac{\hbar^2}{2m}\lambda\ . \tag{11}$$

The last two terms in (9) correspond to the surface effects. We also notice in the above equations that the term proportional to $(\vec\nabla\rho)^2$ also contains a contribution from the correction to the TF kinetic energy, which arises via the $\rho\tau$ term.

Following the proximity approach,[1] the interaction potential between the two spherical ions, of radii C_1 and C_2, is given by

$$V=2\pi\bar R\int_S^\infty dD\, e(D)\ , \tag{12}$$

where $\bar R=C_1C_2/C_1+C_2$ and D is the gap width whose minimum value is S. For the crevice formation $S=0$.

$e(D)$ is the interaction energy per unit area between two flat parallel surfaces at separation D. Since $\int dD\, e(D)$ does not depend on the geometry of the systems involved, it is a universal function, $\Phi(D)$, characteristic of the matter. To calculate $\Phi(D)=\int dD\, e(D)$, we consider two slabs of semi-infinite nuclear matter with surfaces parallel to the XY plane moving in the Z direction. The two densities in the Thomas-Fermi approximation are then of the forms

$$\rho_1=\begin{cases}\rho_0\tanh^2\dfrac{Z-Z_1}{2b} & \text{for } Z_1\le Z\le\infty\\ 0 \text{ for } Z<Z_1\end{cases}$$

and (13)

$$\rho_2=\begin{cases}\rho_0\tanh^2\dfrac{Z-Z_2}{2b} & \text{for } -\infty\le Z\le Z_2\\ 0 \text{ for } Z>Z_2\ .\end{cases}$$

Here Z_1 and Z_2 are the parameters that determine the location of nuclear surfaces (see Fig. 1). $\rho=\rho_1+\rho_2$ is the density when the two systems overlap. The universal function is then given by

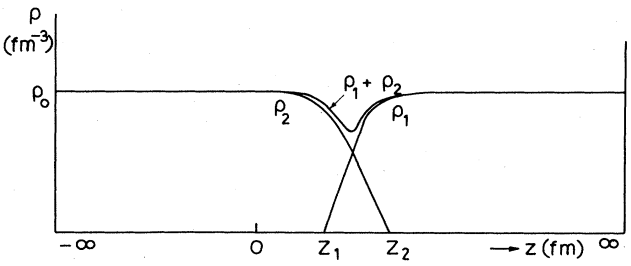

FIG. 1. Schematic Thomas-Fermi density distributions for two colliding nuclei, in a slab approximation.

$$\Phi(D)=\int e(D)dD=\int[H(\vec{r},\rho,\tau_0)-H(\vec{r},\rho_1,\tau_1)-H(\vec{r},\rho_2,\tau_2)]dz\ . \tag{14}$$

Combining (9) and (14) one gets the following expression for the universal function:

$$\Phi(D)=\frac{V}{2\pi\bar{R}}=\frac{3}{5}\frac{\hbar^2}{2m}\left[\frac{3}{2}\pi^2\right]^{2/3} I_{[5/3]}+\tfrac{3}{8}t_0I_{[2]}+\tfrac{1}{16}t_3I_{[3]}+\tfrac{1}{16}(3t_1+5t_2)\tfrac{3}{5}(\tfrac{3}{2}\pi^2)^{2/3}I_{[8/3]}+\Phi_{s\rho}+\Phi_{s\tau_\lambda}\ , \tag{15}$$

where the integrals, representing the volume, are

$$I_{[n]}=\int(\rho_1+\rho_2)^n dz-\int\rho_1^n dz-\int\rho_2^n dz \tag{16}$$

and the other two terms giving the surface contributions due to the nucleon density ρ and kinetic energy density τ_λ are

$$\Phi_{s\rho}=\alpha_1\Phi_0=\alpha_1\left[\int\left|\frac{\partial}{\partial z}(\rho_1+\rho_2)\right|^2dz-\int\left|\frac{\partial\rho_1}{\partial z}\right|^2dz-\int\left|\frac{\partial\rho_2}{\partial z}\right|^2dz\right] \tag{17}$$

and

$$\Phi_{s\tau_\lambda}=\alpha_2\Phi_0+\beta\left[\int\frac{\left|\frac{\partial}{\partial z}(\rho_1+\rho_2)\right|^2}{(\rho_1+\rho_2)}dz-\int\frac{\left|\frac{\partial\rho_1}{\partial z}\right|^2}{\rho_1}dz-\int\frac{\left|\frac{\partial\rho_2}{\partial z}\right|^2}{\rho_2}dz\right]. \tag{18}$$

For the TF densities (13), one obtains an analytical expression for the universal function Φ, which is given in the Appendix.

III. SURFACE ENERGY COEFFICIENT

The energy density functional (9) for the corrected TF approximation can also be used to calculate the surface energy of a spherical nucleus,

$$E_s=\alpha\int(\vec{\nabla}\rho)^2d\vec{r}+\beta\int\left[\frac{\vec{\nabla}\rho}{\rho}\right]^2d\vec{r}\ . \tag{19}$$

The contributing terms are apparently the gradient terms due to both the nucleon density and the kinetic energy density. Using for ρ the TF density given by Eq. (3), we obtain for the surface energy of a spherical nucleus

$$E_s=E_{s\rho}+E_{s\tau_\lambda}\ , \tag{20}$$

where the contributions from the nucleon density and from the correction to the TF kinetic energy density are given, respectively, as

$$E_{s\rho}=\alpha_1 E_0=\alpha_1\left\{4\pi\left[\frac{\rho_0}{b}\right]^2[0.877\,28b^3+0.606\,00b^2R+0.266\,67bR^2]\right\} \tag{21}$$

and

$$E_{s\tau_\lambda}=\alpha_2 E_0+\beta\left\{8\pi\left[\frac{\rho_0}{b}\right][0.859\,92b^2+1.181\,72bR+0.666\,67R^2]\right\}. \tag{22}$$

This allows us to study the relative importance of the two terms. We notice that whereas the term $E_{s\rho}$ is independent of λ, $E_{s\tau_\lambda}$ depends on the λ value through α_2 and β.

Equating the total E_s to $4\pi R^2\gamma$ (or equivalently to $a_s A^{2/3}$) the surface energy coefficient γ can be estimated and compared with the most accepted empirical value of 0.9517 MeV/fm^2 due to Myers and Swiatecki.[7] Other authors have used larger γ values in their mass formula fits; the largest one being $\gamma=1.3527$ MeV/fm^2 ($a_s=24.49$ MeV) due to Bauer.[15] Apparently, these different estimates for the γ value should have a strong bearing on the choice of a value for the parameter λ.

IV. RESULTS AND DISCUSSION

Table II gives the universal function Φ, as a function of the separation distance D, for various Skyrme interactions whose parameters are summarized in Table I. The λ values chosen are $\frac{5}{36}$ and $\frac{1}{36}$. We first analyze the results of the calculation for $\lambda=\frac{5}{36}$ and notice that for the forces SIV and SV, the potentials remain attractive even up to an overlap distance of $D=-2$ fm. This is unrealistic because already for $D=-1.75$ fm the compression limit of nuclear matter is reached (i.e., for $D=-1.75$ fm, $\rho_1+\rho_2=\rho_0$, the central nuclear density). Also, for the Skyrme interactions with large values of the three-body parameter t_3 (i.e., SI, SIII, and SVI), the potentials are shown to behave unrealistically since they become repulsive within a short distance of only about -1 fm and are also quite shallow. The remaining two forces, S and SII, however, seem to give potentials with acceptable behaviors. It is interesting to find that the potential due to the original Skyrme force[8] S becomes repulsive at exactly the compression limit of $D=-1.75$ fm. As we take a smaller value for the parameter $\lambda(=\frac{1}{36})$, we notice that though the qualitative behaviors of the potentials do not change significantly, the reaching of the compression limit, etc., does get modified. For $\lambda=\frac{1}{36}$, Table II shows that still only the forces S and SII are well behaved, but the performance of SII over S is now somewhat improved.

Table III gives the calculated surface energy contributions $E_{s\rho}$ and $E_{s\tau_\lambda}$ ($E_s=E_{s\rho}+E_{s\tau_\lambda}$) for various Skyrme interactions, taking an illustrative spherical nucleus with $A=200$. Once again for the parameter λ, we have chosen $\lambda=\frac{5}{36}$ and $\frac{1}{36}$. We notice that the contribution to the term $E_{s\tau_\lambda}$, which is solely due to the correction to Thomas-Fermi kinetic energy density, is quite large. For $\lambda=\frac{5}{36}$, $E_{s\tau_\lambda}$ is larger than $E_{s\rho}$ for almost all the Skyrme

TABLE II. Universal function $\Phi(D)$ for various Skyrme interactions and for different λ values.

Separation D (fm)	S	SI	SII	SIII	SIV	SV	SVI
			$\Phi(D)$ in (MeV/fm) for $\lambda=\frac{5}{36}$				
−0.25	−2.41	−1.18	−3.58	−1.90	−5.84	−9.12	−1.28
−0.50	−4.62	−2.28	−6.86	−3.86	−10.76	−16.37	−2.64
−0.75	−6.15	−1.37	−9.43	−4.87	−14.58	−21.57	−2.28
−1.00	−6.00	4.64	−10.39	−2.98	−17.06	−25.08	2.88
−1.25	−3.84	16.56	−9.38	−2.50	−18.19	−27.36	13.71
−1.50	−0.23	32.27	−6.86	10.50	−18.23	−28.73	28.29
−1.75	3.93	48.80	−3.57	19.33	−17.54	−29.38	43.81
−2.00	7.98	63.94	−0.07	27.77	−16.35	−29.40	58.18
			$\Phi(D)$ in (MeV/fm) for $\lambda=\frac{1}{36}$				
−0.25	−2.03	−0.70	−3.24	−1.51	−5.53	−8.84	−0.84
−0.50	−3.90	−1.37	−6.20	−3.12	−10.16	−15.82	−1.81
−0.75	−5.13	−0.13	−8.50	−3.84	−13.72	−20.76	−1.14
−1.00	−4.77	6.12	−9.26	−1.75	−15.99	−24.07	4.23
−1.25	−2.48	18.17	−8.13	3.86	−16.99	−26.20	15.18
−1.50	1.18	33.94	−5.55	11.90	−16.98	−27.51	29.81
−1.75	5.35	50.47	−2.25	20.75	−16.27	−28.15	45.33
−2.00	9.36	65.59	1.22	29.15	−15.12	−28.21	59.68

TABLE III. Calculated surface energy contributions from ρ and from τ for different λ values and the surface energy coefficient γ for various Skyrme interactions, taking the spherical nucleus with $A=200$.

		Skyrme interactions						
		S	SI	SII	SIII	SIV	SV	SVI
$E_{s\rho}$ (MeV)		605.58	416.98	716.50	571.59	851.11	1002.99	474.52
$E_{s\tau_\lambda}$ (MeV)	$\lambda=\frac{5}{36}$	845.37	887.85	833.43	825.09	853.61	886.21	835.02
γ (MeV/fm^2)	$\lambda=\frac{5}{36}$	1.82	1.78	1.87	1.78	1.97	2.09	1.74
$E_{s\tau_\lambda}$ (MeV)	$\lambda=\frac{1}{36}$	169.07	177.57	166.68	165.02	170.72	177.24	167.00
γ (MeV/fm^2)	$\lambda=\frac{1}{36}$	0.97	0.81	1.06	0.94	1.18	1.30	0.85

interactions. This is completely unrealistic since $E_{s\tau_\lambda}$ is only a correction term. However, for $\lambda=\frac{1}{36}$, $E_{s\tau_\lambda}$ is reasonably small compared to the main term $E_{s\rho}$ and is more of the order of a correction. Furthermore, a calculation of the surface energy coefficient γ shows that only $\lambda=\frac{1}{36}$ give the estimates comparable with the empirical number 0.9517 MeV/fm^2 of Myers and Swiatecki.[7] Once again, the original Skyrme force S stands out to be the best. Even if one accepts the largest value of $\gamma=1.3527$ MeV/fm^2 due to Bauer,[15] it is evident from Table III that the parameter λ must have a value smaller than $\frac{5}{36}$. A similar situation is presented in Fig. 2 by the two contributions to the universal function, plotted for the Skyrme force S. The contribution of the term $\Phi_{s\tau_\lambda}$ decreases with the decrease of the λ value and becomes more reasonable for $\lambda=\frac{1}{36}$.

Finally, two earlier results are also worth quoting here: (i) von Dewitz[16] could reproduce the binding energies of nuclei reasonably well for $\lambda=\frac{1}{36}$, and (ii) Skyrme[17] had taken the total kinetic energy density to contribute as much as one-half to the total surface energy, which apparently rules out the value $\frac{5}{36}$ and suggests a much smaller value of the order of $\frac{1}{36}$ for the parameter λ.

V. CONCLUSIONS

We have shown that for judging the effectiveness of the proximity approach and the relative performance of the various known Skyrme force parameters, an estimation of the surface energy coefficient in the semiempirical mass formula is as important as the calculation of the ion-ion proximity potential itself. Interestingly enough, only the parameters of the original force due to Skyrme[8] and the widely used SII force of Vautherin and Brink[6] generate realistic results. They demonstrate not only reasonable behaviors for the universal functions of the proximity potential but also give the calculated value of the surface energy coefficient γ in nice agreement with the usually accepted empirical number.[7]

The correction to the Thomas-Fermi kinetic energy density, representing additional surface effects, is shown to be always quite appreciable and very sensitive to the choice of its parameter λ. Though a λ value lying between $\frac{1}{36}$ and $\frac{5}{36}$ does not change the qualitative structure of the ion-ion interaction potential (the universal function of proximity) but for a quantitative estimate of the surface energy coefficient γ our calculations support a value of $\lambda=\frac{1}{36}$.

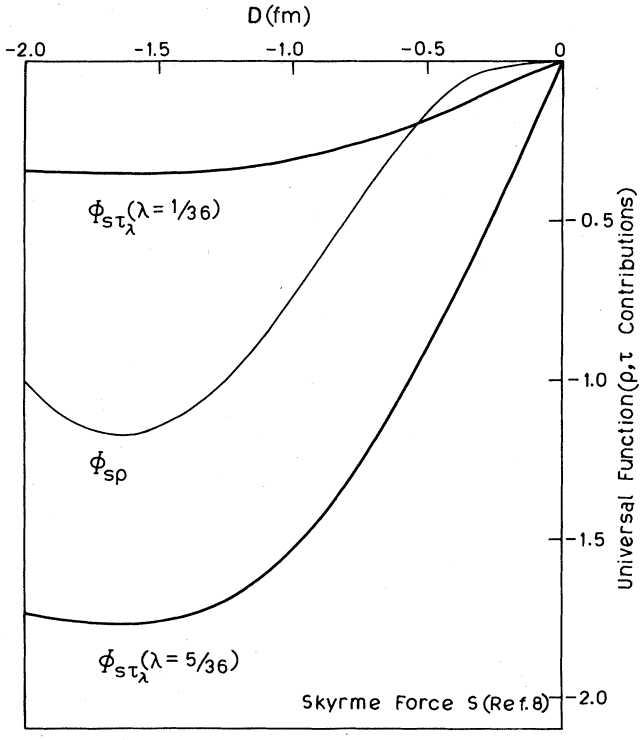

FIG. 2. The surface contributions to the universal function due to the Thomas-Fermi nucleon density and the surface correction to the kinetic energy density for the correction parameters $\lambda=\frac{1}{36}$ and $\frac{5}{36}$. The Skyrme force parameters used are of Skyrme (Ref. 8).

APPENDIX

The universal function of the proximity potential, for Thomas-Fermi densities with additional surface correction to the kinetic energy density, is obtained to be of the form:

$$\Phi(d)=\frac{V}{2\pi\bar{R}}=\frac{3}{5}\frac{\hbar^2}{2m}\left[\frac{3\pi^2}{2}\right]^{2/3} I_{[5/3]}+\tfrac{3}{8}t_0 I_{[2]}+\tfrac{1}{16}t_3 I_{[3]}+\tfrac{1}{16}(3t_1+5t_2)\tfrac{3}{5}(\tfrac{3}{2}\pi^2)^{2/3} I_{[8/3]}+\Phi_{s\rho}+\Phi_{s\tau_\lambda}\,, \tag{A1}$$

where the integrals $I_{[n]}$, representing the volume, are

$$I_{[2]}=2\rho_0^2\tanh^{-1}(2bk)-4\rho_0^2 bk-\frac{4b\rho_0^2}{k^3}[k^2(2-k^2)+2(1-k^2)\ln(1-k^2)]\,, \tag{A2}$$

$$\begin{aligned} I_{[3]}=&6\rho_0^3\tanh^{-1}(2bk)-4b\rho_0^3k^3-\frac{12b\rho_0^3}{k^3}[k^2(2-k^2)+2(1-k^2)\ln(1-k^2)]-12b\rho_0^3k(1-\tfrac{1}{3}k^2)\\ &-\frac{12b\rho_0^3}{k^5}\left\{-(1-k^2)^2+(1-k^2)+2(1-k^2)(2-k^2)\ln(1-k^2)\right.\\ &\left.+[(1-k^2)^2+4(1-k^2)+1]k^2-(2-k^2)^2k^2+\tfrac{1}{3}-\tfrac{1}{3}(1-k^2)^3\right\}, \end{aligned} \tag{A3}$$

$$\begin{aligned} I_{[5/3]}=&(2\rho_0)^{5/3}\left\{\tanh^{-1}(2bk)-\tfrac{10}{3}bk+\tfrac{5}{18}(-\tfrac{1}{3}k^3+k)\right.\\ &\left.+\tfrac{5}{9}b\left[k-\frac{1}{k}(2-k^2)-\frac{2}{k^3}(1-k^2)\ln(1-k^2)\right]+\tfrac{5}{324}[\tfrac{1}{5}k^5-\tfrac{2}{3}k^3+k]\right\}\\ &+(2\rho_0)^{5/3}\tfrac{5}{108}\left[2bk(1-\tfrac{1}{3}k^2)-\frac{2b}{k}(2-k^2)-\frac{4b}{k^3}(1-k^2)\ln(1-k^2)\right.\\ &\left.+\frac{2b}{k^5}\left\{k^2(1-k^2)+2(1-k^2)(2-k^2)\ln(1-k^2)+[(1-k^2)^2+4(1-k^2)+1]k^2\right.\right.\\ &\left.\left.-(2-k^2)^2k^2+\tfrac{1}{3}-\tfrac{1}{3}(1-k^2)^3\right\}\right]+2\rho_0^{5/3}\left[\frac{6b}{7}\right]k^{7/3}\\ &-\rho_0^{5/3}\left[\int_{z_1}^{z_2}\tanh^{4/3}\frac{z-z_1}{2b}dz+\int_{z_1}^{z_2}\tanh^{4/3}\frac{z-z_2}{2b}dz\right], \end{aligned} \tag{A4}$$

$$\begin{aligned} I_{[8/3]}=&(2\rho_0)^{8/3}\left\{\tanh^{-1}(2bk)-\tfrac{16}{3}bk+\tfrac{10}{9}(-\tfrac{1}{3}k^3+k)\right.\\ &\left.+\tfrac{10}{9}\left[2bk-\frac{2b}{k}(2-k^2)-\frac{4b}{k^3}(1-k^2)\ln(1-k^2)\right]-\tfrac{10}{81}[\tfrac{1}{5}k^5-\tfrac{2}{3}k^3+k]\right\}\\ &-(2\rho_0)^{8/3}\tfrac{10}{27}\left[2bk(1-\tfrac{1}{3}k^2)-\frac{2b}{k}(2-k^2)-\frac{4b}{k^3}(1-k^2)\ln(1-k^2)\right.\\ &\left.+\frac{2b}{k^5}\left\{k^2(1-k^2)+2(1-k^2)(2-k^2)\ln(1-k^2)+[(1-k^2)^2+4(1-k^2)+1]k^2\right.\right.\\ &\left.\left.-(2-k^2)^2k^2+\tfrac{1}{3}-\tfrac{1}{3}(1-k^2)^3\right\}\right]+2\rho_0^{8/3}\left[\frac{6b}{7}k^{7/3}+\frac{6b}{13}k^{13/3}\right]\\ &-\rho_0^{8/3}\left[\int_{z_1}^{z_2}\tanh^{4/3}\frac{z-z_1}{2b}dz+\int_{z_1}^{z_2}\tanh^{4/3}\frac{z-z_2}{2b}dz\right], \end{aligned} \tag{A5}$$

with

$$k=\tanh d$$

and

$$d=(z_2-z_1)/2b=-D\ . \tag{A6}$$

For the integral

$$\int_{z_1}^{z_2}\left[\tanh^{4/3}\frac{z-z_1}{2b}+\tanh^{4/3}\frac{z-z_2}{2b}\right]dz$$

in (A4) and (A5), the following approximate analytical expressions can be obtained. If $d\leq 0.8$,

$$\int_{z_1}^{z_2}\left[\tanh^{4/3}\frac{z-z_1}{2b}+\tanh^{4/3}\frac{z-z_2}{2b}\right]dz\approx 4b\,[0.428\,57(\tanh^{-1}k)^{7/3}-0.102\,56(\tanh^{-1}k)^{13/3}$$
$$+0.031\,97(\tanh^{-1}k)^{19/3}+0.010\,78(\tanh^{-1}k)^{25/3}]\ , \tag{A7}$$

and if $d>0.8$

$$\int_{z_1}^{z_2}\left[\tanh^{4/3}\frac{z-z_1}{2b}+\tanh^{4/3}\frac{z-z_2}{2b}\right]dz\approx 4b[\tanh^{-1}k-\tfrac{2}{3}k+\tfrac{1}{27}(k^3-3k)-\tfrac{4}{81}(\tfrac{1}{5}k^5-\tfrac{2}{3}k^3+k)]\ . \tag{A8}$$

The terms giving the surface contributions are

$$\Phi_{s\rho}=\alpha_1\Phi_0=\alpha_1\left\{\frac{4\rho_0^2}{k^5}[12k^2-14k^4+2k^6+12(1-k^2)\ln(1-k^2)-8k^2(1-k^2)\ln(1-k^2)]\right\} \tag{A9}$$

and

$$\Phi_{s\tau_\lambda}=\alpha_2\Phi_0+\beta\frac{4\rho_0}{b}\left\{k(1-k^2)\ln k+\frac{(1-k^2)(1+k^4)}{k^3}\ln(1-k^2)-\frac{(1-k^2)}{6k^3}(2k^4-k^2+11)\right.$$
$$+\frac{1}{6k^3}(11-6k^2)-(k-\tfrac{1}{3}k^3)-\ln k\,(k-k^3)$$
$$-\mathrm{Re}\left[-(1-3y_1^2)(z\ln z-z)-6y_1\left[\frac{z^2}{2}\ln z-\frac{z^2}{4}\right]+3\left[\frac{z^3}{3}\ln z-\frac{z^3}{9}\right]\right]_{y_1}^{y_1-k}$$
$$\left.-\mathrm{Re}\left[(1-3y_2^2)(z\ln z-z)-6y_2\left[\frac{z^2}{2}\ln z-\frac{z^2}{4}\right]-3\left[\frac{z^3}{3}\ln z-\frac{z^3}{9}\right]\right]_{-y_2}^{k-y_2}\right\}, \tag{A10}$$

with $y_1(k)$ and $y_2(k)$ as the roots of the equation

$$y^2-\frac{(1+i)}{k}y+i=0\ . \tag{A11}$$

The expression for $\Phi_{s\rho}$ is the same as already obtained in Ref. 4, where the contribution of the kinetic energy density was not included.

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