Assignment 12

The due date for submitting this assignment has passed.

Due on 2021-04-14, 23:59 IST.

As per our records you have not submitted this assignment.

Use the following information for all the question below

Consider calculating the Lennard-Jones interaction energy E_s of a spherical surface $S : (a\cos\theta\sin\theta, a\sin\theta\sin\phi, a\cos\phi), -\pi < \theta \le \pi, 0 \le \phi \le \pi$ with radius a and atomic desnity η_s with some point at a distance δ from the centre of the sphere (i.e the point is $(0,0,\delta)$, assuming $\delta > a$) , assuming the continuum appproximation and Lennard-Jones constants of A and B

1) After adopting an appropriate parameterisation , which of the following is/are an integral for the interaction energy E_s *1 point*

- $E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-6} + B\rho^{-12}\right) a^2 \sin\phi \, d\theta d\phi$
- $E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-6} + B\rho^{-12}\right) a^2 \sin\theta \, d\theta d\phi$
- $E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-6} + B\rho^{-12}\right) a \sin\phi \, d\theta d\phi$
- $E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-16} + B\rho^{8}\right) a^2 \sin\phi \, d\theta d\phi$
- $E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-6} + B\rho^{-12}\right) a \sin\phi \sin\theta \, d\theta d\phi$
- $E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-16} + B\rho^{8}\right) a \sin\phi \, d\theta d\phi$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$E_s = \eta_s \int_0^\pi \int_{-\pi}^\pi \left(-A\rho^{-6} + B\rho^{-12}\right) a^2 \sin\phi \, d\theta d\phi$

2) Integrate the expression from question 1 by treating the integral as a hypergeometric integral , which of the following is/are the expression for this interaction in terms of hypergeometric functions. *1 point*

- $E_s = \pi a^2 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^2} F\left(6,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$
- $E_s = 2\pi a^2 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^{12}} F\left(6,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$
- $E_s = 2\pi a^2 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^2} F\left(6,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$
- $E_s = 3\pi a^2 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^{12}} F\left(6,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$
- $E_s = 3\pi a^3 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^{12}} F\left(6,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$
- $E_s = 2\pi a^2 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^2} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$E_s = 2\pi a^2 \eta_s \left[-\frac{A}{(\delta-a)^6} F\left(3,1;2;-\frac{4a\delta}{(\delta-a)^2}\right) + \frac{B}{(\delta-a)^{12}} F\left(6,1;2;-\frac{4a\delta}{(\delta-a)^2}\right)\right]$

3) Which of the following is/are quadratic transformation which will convert the hypergeometric function into a form which relates to the Chebyshev polynomial of the second kind *1 point*

$$U_m(x) = (m+1)F\left(-m, m+2; \tfrac{3}{2}; \tfrac{1-x}{2}\right)$$

- $F(a,b;2b;z) = \left(\frac{1+\sqrt{1-z}}{2}\right)^{-2a} F\left(a, a-b+\frac{1}{2}; b+\frac{1}{2}; \left(\frac{1-\sqrt{1-z}}{1+\sqrt{1-z}}\right)^2\right)$
- $F(a,b;2b;z) = \left(\frac{1+\sqrt{1-z}}{2}\right)^{2a} F\left(a, a+b+\frac{1}{2}; b-\frac{1}{2}; \left(\frac{1-\sqrt{1-z}}{1+\sqrt{1-z}}\right)^2\right)$
- $F(a,b;2b;z) = (1-z)^{\frac{a}{2}} F\left(a, 2b-a; b+\frac{1}{2}; -\frac{(1-\sqrt{1-z})^2}{4\sqrt{1-z}}\right)$
- $F(a,b;2b;z) = (1-z)^{-\frac{a}{2}} F\left(a, 2b-a; b+\frac{1}{2}; \frac{(1+\sqrt{1-z})^2}{\sqrt{1-z}}\right)$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$F(a,b;2b;z) = (1-z)^{\frac{a}{2}} F\left(a, 2b-a; b+\frac{1}{2}; -\frac{(1-\sqrt{1-z})^2}{4\sqrt{1-z}}\right)$

4) Which of the following is/are the expression for E_s in terms of the parameters a and δ and Chebyshev polynomials of the second kind $U_1(x)$ and $U_4(x)$ *1 point*

- $E_s = 3\pi a^2 \eta_s \left[-\frac{A}{(\delta^2-a^2)^3} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^6} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$
- $E_s = 3\pi a^2 \eta_s \left[-\frac{A}{2(\delta^2-a^2)^3} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^3} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$
- $E_s = 3\pi a^2 \eta_s \left[-\frac{A}{(\delta^2-a^2)^6} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^3} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$
- $E_s = 2\pi a^2 \eta_s \left[-\frac{A}{2(\delta^2-a^2)^3} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^6} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$
- $E_s = 2\pi a^2 \eta_s \left[-\frac{A}{2(\delta^2-a^2)^6} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^3} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$
- $E_s = 2\pi a^2 \eta_s \left[-\frac{A}{(\delta^2-a^2)^3} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^3} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$E_s = 2\pi a^2 \eta_s \left[-\frac{A}{2(\delta^2-a^2)^3} U_1\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right) + \frac{B}{2(\delta^2-a^2)^6} U_4\left(\frac{\delta^2+a^2}{\delta^2-a^2}\right)\right]$