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**Adhesion of small spheres**

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Only

## Adhesion of small spheres

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**ABSTRACT**

Bradley(1931) calculated the adhesive force between *rigid* spheres to be  $2\pi R\Delta\gamma$ , where  $\Delta\gamma$  is the surface energy of the spheres: Johnson, Kendall & Roberts (1971) calculated the adhesive force between *elastic* spheres to be  $(3/2)\pi R\Delta\gamma$  and independent of the elastic modulus. Derjaguin and colleagues published an alternative theory for elastic spheres ("DMT" theory), and concluded that Bradley's value for the pull-off force was the correct one. Tabor (1977) explained the discrepancy in terms of the range of action of the surface forces  $z_0$ , and introduced a parameter  $\mu \equiv (R\Delta\gamma^2 / E^2 z_0^3)^{1/3}$  determining which result is applicable. Subsequently detailed calculations by Derjaguin and his colleagues (Muller et al (1980) and others, assuming a surface force law based on the Lennard-Jones 6-12 potential law, covered the full range of the Tabor parameter. Johnson & Greenwood (1997) presented a map delineating the regions of applicability of the different theories.

Yao et al (2007) repeated the numerical calculations but using an exact sphere shape instead of the usual paraboloidal approximation. They found that the pull-off force could be less than one-tenth of the JKR value, depending on the value of a 'strength limit'  $\sigma_0 / E$ , and modified the Johnson & Greenwood map correspondingly.

Yao et al's numerical calculations for contact between an exact sphere and a elastic half-space are repeated and their values confirmed: but it is shown that the drastic reductions found occur only for spheres that are smaller than atomic dimensions.

The limitations imposed by large strain elasticity and by the 'Derjaguin approximation', are discussed.

**Keywords.** Contact mechanics, Surface energy, Adhesion, JKR theory

## INTRODUCTION.

Bradley(1932) calculated the adhesive force between rigid spheres in terms of a law of force between the ‘molecules’<sup>1</sup> : which he then related to the surface energy  $\Delta\gamma$  of the bodies.

Johnson, Kendall & Roberts (1971) calculated the adhesive force between elastic spheres directly in terms of the surface energy. Oddly, although both approaches predicted a pull-off force proportional to  $R\Delta\gamma$ , [where  $R$  is the radius of the sphere, or, for two spheres, the effective radius  $R_1R_2/(R_1 + R_2)$ ] they gave different coefficients,  $2\pi$  or  $3\pi/2$ , and no dependence on the elastic modulus. Thus, both values appear to be applicable to rigid spheres

The JKR theory gives a complete description of adhesive contact between spheres, with the dependence on load of the contact radius and approach/compression as well as the pull-off force. Derjaguin and colleagues subsequently postulated that adhesive contact is described by the Hertz equations except that the load includes a (negative) contribution from surface forces acting across the gap outside the contact ( the "DMT" theory, Derjaguin et al (1975) ). They rejected the JKR theory as neglecting the adhesive forces across the gap, and concluded that Bradley's value for the pull-off force was the correct one. Tabor (1977) explained this discrepancy in terms of the range of action of the surface forces  $z_0$ , and introduced a parameter  $\mu \equiv (R\Delta\gamma^2 / E^2 z_0^3)^{1/3}$ , where  $E$  is the elastic modulus, determining which result is applicable. Subsequently, detailed calculations by Derjaguin and his colleagues (Muller et al 1980), and more fully by Greenwood (1997) and Feng (2000, 2001) analysed the behaviour over the complete range of the Tabor parameter<sup>2</sup>, assuming a surface force law based on the Lennard-Jones 6-12 potential law. More precisely, they used the ‘3-9’ law governing the surface force between two half-spaces which results from the 6-12 potential law between particles,

$$\sigma(h) \equiv -p(r) = \frac{8\Delta\gamma}{3z_0} \left[ \left( \frac{z_0}{h} \right)^3 - \left( \frac{z_0}{h} \right)^9 \right],$$

together with the Derjaguin approximation that this law may be used between surface elements even when the elements are not plane or parallel. We note that while the surface force between two planar half-spaces is by symmetry a normal traction, between curved surfaces it is necessary to *assume* that the tractions are normal to the surface, or more specifically, that any tangential tractions have no effect.

<sup>1</sup> Hamaker (1937) obtained the same result rather more neatly.

<sup>2</sup> Replacing Tabor's  $E$  by the plane strain modulus  $E' \equiv E/(1-\nu^2)$

1 Interpretation of AFM measurements of nanoscale contacts has relied on the DMT  
 2 and JKR theories for the limiting values of the Tabor parameter, and on these detailed  
 3 numerical calculations, or more conveniently on an analytical theory by Maugis(1992)  
 4 which uses a simplified surface force law, to bridge the gap between these extremes. A map  
 5 delineating the regions of applicability of the different approaches in terms of the Tabor  
 6 parameter and a load parameter was presented by Johnson & Greenwood (1997)  
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12 Yao et al (2007) have recently argued that there is a 'strength limit'  $\sigma_0 / E'$  to these  
 13 theories of the adhesive elastic contact between a sphere and a elastic half-space<sup>3</sup>; and that  
 14 the Johnson & Greenwood map showing the areas of the applicability of the different  
 15 theories needs to be modified to allow for this strength limit. They repeated the numerical  
 16 calculations using the same law of surface force but using an exact sphere shape instead of  
 17 the paraboloidal approximation dating back to Hertz. They found that the pull-off force  
 18 could be considerably less than the accepted values lying between  $2\pi R\Delta\gamma$  (the Bradley  
 19 limit) and  $(3/2)\pi R\Delta\gamma$  (the JKR limit). and modified the Johnson & Greenwood map  
 20 correspondingly to include the dependence on the strength limit  $\sigma_0 / E'$ .  
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29 It is not clear that the term 'strength limit' is appropriate. Indeed, since the two  
 30 material properties involved in the 'strength limit' are an intrinsic part of the numerical  
 31 calculations, it is not clear how the strength limit can *also* be a limiting property. The  
 32 effect takes place when the contact radius becomes comparable with the radius of the  
 33 sphere: in other words, when the contact area no longer readily fits onto the sphere. Thus, a  
 34 better description is perhaps that there is a size effect associated with the finite size of a  
 35 sphere.  
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41 If we introduce the 'size ratio'  $\rho \equiv R / z_0$ , and note that for the Lennard-Jones  
 42 surface force law the surface energy is  $\Delta\gamma = 0.974 z_0 \sigma_0$  then the Tabor parameter can be  
 43 written  $\mu = (0.974)^{2/3} (R / z_0)^{1/3} (\sigma_0 / E')^{2/3}$ . Ignoring the numerical factor, then using Yao  
 44 et al's notation  $\varepsilon \equiv (\sigma_0 / E')$  for strength limit, we have  $\mu^3 = \rho \varepsilon^2$ . Clearly any two of these  
 45 three parameters may be taken as the independent variables, and there is a case for  
 46 abandoning the Tabor parameter and retaining the size ratio  $\rho \equiv R / z_0$  and the strength  
 47 ratio  $\varepsilon \equiv (\sigma_0 / E')$  as the real governing variables: only then can one be certain of obtaining  
 48 a realistic combination. For example, Yao et al combine a realistic strength ratio of  
 49  $\varepsilon = 0.01$  with an unexceptional Tabor parameter of  $\mu = 0.01$  to obtain a size ratio  $\rho = 0.01$ ,  
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<sup>3</sup>  $\sigma_0$  is the limiting 'surface force', equal to  $(16/9\sqrt{3})(\Delta\gamma / z_0)$  for the Lennard-Jones surface force law, and  
 $E'$  is the plane strain elastic modulus  $E/(1-\nu^2)$ .

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2 that is, for the usual range of action of the surface forces in the Lennard-Jones law, a  
3 sphere radius of 0.003 nm! However, abandoning the Tabor parameter is too drastic a step  
4 for the present author: this paper will use  $\mu$  and  $\rho$  as the parameters.  
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7 Yao et al's numerical calculations for contact between a rigid true sphere and a  
8 elastic half-space are repeated, but it is shown that the drastic reductions in pull-off force  
9 that they found occur only for spheres which are smaller than atomic dimensions. For any  
10 conditions for which continuum calculations can be believed, the reduction is rather small.  
11 It should be emphasised that in all the test cases, the present calculations completely  
12 reproduce Yao et al's *values*: the dispute is not about accuracy but about meaningfulness.  
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15 In addition to the numerical results, asymptotic equations agreeing well with the  
16 numerical results are found for  $\mu \rightarrow 0$  by the direct integration of the equations for a rigid  
17 sphere ("Bradley theory"), and for  $\mu \rightarrow \infty$  by using Maugis' (1995) extension of the JKR  
18 analysis for a true sphere<sup>4</sup>.  
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21 However, it is argued that the Maugis asymptote is physically wrong, or at best  
22 highly suspect. Lin & Chen (2006) performed a finite element analysis of the "Hertzian"  
23 contact between a rigid sphere and a neo-Hookean half-space (and show how this may be  
24 extended to give a "JKR" theory): but their calculations show that for their material, an  
25 ideal rubber, the Maugis true-sphere solution is rather less accurate than the simple  
26 (paraboloidal) Hertz theory. This provides an estimate of the error in using a true sphere  
27 with infinitesimal elasticity, *and the same error can be expected to be there in the full*  
28 *numerical solutions*.  
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31 In contrast, it is argued that the Bradley asymptote is accurate, and that in fact the  
32 "Derjaguin approximation" is exact when one of the bodies is a half-space, (as shown by  
33 Argento et al (1997)). It is less clear that the *second* Derjaguin approximation, that the local  
34 contribution to the total force between the two bodies may be treated as a local *surface*  
35 traction on an elastic body, is accurate, except when  $z_0 \ll R$ .  
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### 39 **Numerical calculations for a true hemisphere.**

40 The basic problem is to calculate the gap shape  $h = f(r)$  between a rigid body and  
41 an elastic half-space, when 'surface forces' (actually normal tractions)  $\sigma = \sigma(h)$  act on the  
42 half-space and so modify the gap shape. Until we know the gap shape  $h(r)$  we cannot  
43 calculate the surface traction, but until we know the surface traction we cannot calculate  
44 the gap shape. We note that the bodies never make 'contact' in the traditional sense:  
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<sup>4</sup> Note that this is *not* the well-known Maugis (1992) paper, in which the entire range of the Tabor parameter is analysed by the use of a simplified (Dugdale) law of force (and the paraboloidal approximation for the sphere).

1  
2 however far apart they are, there is always an attraction between them: when the  
3 separation decreases to below  $h = z_0$  the local interaction becomes a pressure, and would  
4 become enormous if the separation were to become significantly less than  $z_0$  - which in  
5 practice it never does. A contact radius *could* be defined as the radius at which the surface  
6 force becomes zero, that is, where it changes from tensile to compressive: the more realistic  
7 definition seems to be the location of the maximum tensile traction<sup>5</sup>. This corresponds to  
8 the JKR contact radius, and to the crack tip location in fracture mechanics problems.

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10 The equations for the deformation of a half-space by axially symmetric pressure<sup>6</sup>  
11 distributions are well-known (see appendix 1): the surface traction law will be taken to be

12 Derjaguin's law  $\sigma(h) \equiv -p(r) = \frac{8\Delta\gamma}{3z_0} \left[ \left( \frac{z_0}{h} \right)^3 - \left( \frac{z_0}{h} \right)^9 \right]$ . This is derived from the Lennard-

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23 Jones 6-12 potential law acting between individual molecules of two half-spaces, assuming  
24 the forces to be completely additive, and that the density of 'molecules' is such that the  
25 summations can be replaced by integrations. The procedure dates back to the classic  
26 calculations of the force between two bodies by Bradley(1932) and Hamaker(1937),  
27 themselves based on principles set out by Maxwell and Rayleigh (see below). The law  
28 quoted for the force between two half-spaces follows readily from these earlier  
29 contributions, but its first appearance in the contact literature appears to be in Derjaguin's  
30 1980 paper (Muller et al(1980)) : the 'Derjaguin approximation' of assuming that a law of  
31 force between two half-spaces is applicable between surface elements of any two bodies,  
32 even when these elements are inclined and curved, was introduced much earlier (Derjaguin  
33 (1934)). Initially Derjaguin simply used his approximation to calculate the total force  
34 between two spheres (obtaining the same answer as found by Bradley and subsequently by  
35 Hamaker). Only later, in the 1980 paper, did Derjaguin made the further step of assuming  
36 the surface force law could be applied as a surface traction, *element by element*, to calculate  
37 the elastic deformation of the spheres.

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49 In the numerical calculations described by Greenwood (1997) or Feng (2000), the  
50 initial gap shape was (following Hertz) taken to be  $z(r) = r^2/2R$ . Following Yao et al, it is a  
51 straightforward matter to replace this using the exact equation for a hemisphere, so that

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54  $z(r) = R - \sqrt{R^2 - r^2}$ . We then need to solve the equation for the film shape

$$55 \quad h(r) = -\alpha + z_0 + z(r) + w(r);$$

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58 where the elastic deflection  $w(r)$  is

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5 The claim that classical contact theory defines the contact radius as where the pressure falls to zero seems misguided: the real classical definition is that it is the radius *beyond which* the pressure is zero.

$$w(r) = (4/\pi E') \int p(s) G(r,s) ds .$$

and the pressure depends on the gap height:  $p(r) = -\sigma(h)$ .

Here  $\alpha$  is the approach of the sphere and  $G(r,s)$  is the influence function giving the deflection at radius  $r$  due to a ring load at radius  $s$  (see appendix 1)

Feng's method of solving the equations by Newton-Raphson (Feng (2000)) is greatly superior to the simple iteration used by Greenwood, and was adopted here (see appendix 1) : however there seemed no need for his elaborate curve-following procedure - taking the minimum film thickness  $h(0)$  as the independent variable and using small steps in approach proved sufficient. In order to get solutions for higher values of the Tabor parameter, it was essential to use a variable radial spacing: this had the advantage that it was simple to extend the integration range out to the radius of the hemisphere. Details of the derivation of the compliance matrix for variable spacing are given in appendix 1.

Figure 1: Pressure distribution at pull-off.

The inset shows that the pressure spike really was resolved

The calculations reported here use the non-dimensional variables as used by Greenwood(1997): a reference radius  $r_0$  is defined as  $r_0 = (R^2 \Delta\gamma / E')^{1/3}$ ; then the radial variable  $r^*$  and the radius of contact  $a^*$  are defined by  $r^* = r / r_0$ ,  $a^* = a / r_0$ . Dimensionless pressures are defined by  $p^* \equiv (R / E'^2 \Delta\gamma)^{1/3} p$ , so that the maximum surface traction becomes  $(-p^*)_{\max} = 1.026\mu$ .

Figure(1) shows typical high-  $\mu$  behaviour, close to the singular pressure distribution of the JKR theory. It demonstrates the difficulty of resolving the pressure spike: here a radial spacing of  $dr^* = 0.0008$  was used, when the sphere radius  $r = R$  corresponds to  $r^* = 2.5$ . [ $r^*(R) = \sqrt{\rho l \mu}$ ]. The need for a variable spacing to avoid the need for 3 125 ordinates will be appreciated, as will the problem of correctly placing that fine-spacing!

Yao et al's calculations for a fixed strength ratio  $\varepsilon \equiv \sigma_0 / E^*$  were repeated for  $\varepsilon = 0.1$ , and produced results indistinguishable from theirs.

<sup>6</sup> The use of the Derjaguin approximation necessarily implies that the tangential tractions are zero: see 'Extension of Bradley's theory' below.

Pull-off forces for different size ratios are shown in Fig 2 below. For a parabolic contact ( $\rho = \infty$ ) the values are in good agreement with values given by Feng. [For  $\mu = 5, 7, 10$  Feng gives 1.5246, 1.5142, 1.5080: this paper 1.5260, 1.5160, 1.5093]

Figure 2. Pull-off forces for a true finite sphere.

The green lines are the JKR sphere theory (high  $\mu$ ), or the rigid hemisphere theory (low  $\mu$ ), and are clearly excellent asymptotes.

Greater reductions in the pull-off force could be obtained by taking lower values of the size ratio. It will be argued below that such calculations would be unjustified because the range of action of the surface forces would then exceed the diameter of the sphere, so that the surface force law would include the molecular interactions with non-existent molecules. The answers would not be the pull-off forces for a sphere, but for an infinite rod with a hemispherical end <sup>7</sup>!

In curve-fitting the results of AFM experiments, a frequently used parameter is the zero-load contact radius. The precise theoretical equivalent of the quantity obtained experimentally is uncertain: here contact radius is defined as the location of the maximum tensile stress. Figure 3 shows that for low values of  $\mu$  there is little dependence on the size ratio, but as the JKR region is approached the radii can be appreciably lower.

Figure 3. Contact radii at zero load.

For low  $\mu$  the radius is independent of the size ratio, but for  $\mu > 5$  the values for a finite sphere are lower.

Figure 4 brings out more clearly why this should be: for values of  $\mu$  greater than 5, the contact radius is restricted by the radius of the sphere. It also brings out a severe restriction on the plausibility of these calculations. The characteristic strain in a Hertzian contact is  $0.2a/R$ , and the same estimate should apply here: so we are applying linear elasticity for strains of around 0.2. The resulting errors are discussed below

Figure 4. Contact radii at zero load.

Values of  $a_0/R$  greater than 0.4 are highly suspect.

<sup>7</sup> Which may not be too far from some experimental configurations!

The contact radius at pull-off is of minor practical interest, as in experiments it is affected by the stiffness of the apparatus and by any trace of viscoelasticity: the significant point is that it is far from the zero value predicted by the DMT theory. Values are given in figure 5: while of course smaller, they are still worryingly high for the use of infinitesimal strain elasticity.

Figure 5. Contact radii at pull-off.

### JKR theory for a true sphere

Maugis(1995) has given an exact solution for the "Hertzian" contact between a rigid true sphere and a **linear elastic** half-space, and extended it to include the effect of surface energy as in the JKR analysis. The JKR equations become (see appendix 2):

$$P = \frac{1}{2} E' R^2 \left( \left\{ 1 + \left( \frac{a}{R} \right)^2 \right\} \ln \left\{ \frac{1+a/R}{1-a/R} \right\} - \frac{2a}{R} \right) - \sqrt{8\pi E' \Delta \gamma a^3}$$

and

$$\delta = \frac{a}{2} \ln \left\{ \frac{1+a/R}{1-a/R} \right\} - \sqrt{2\pi a \Delta \gamma / E'}$$

where  $P$  is the load and  $\delta$  the compression, *according to the equations of linear elasticity*.

Maugis does not give the pull-off force, but this is readily found from his equations in the form (see appendix):

$$P / R \Delta \gamma |_{\min} = f(\chi)$$

where  $\chi = \sqrt{E'R/\Delta\gamma} = (\rho/\mu)^{3/4}$ .

Fig 6 shows the results.

Figure 6 Pull-off forces according to Maugis' extended JKR theory.

The Lin & Chen curve is discussed below.

The 'paraboloidal' JKR theory is of course the limit as the Tabor parameter tends to infinity, so cannot be plotted on a  $(\mu, T_{\max})$  graph - essentially because there is no quantity  $z_0$  in the JKR theory. However, writing  $\rho \equiv R/z_0$ , the pull-off force for a *finite* sphere is seen to be a function of  $(\rho/\mu)$ , and so for given values of the size ratio  $\rho$  can indeed be plotted on the graph. The values have been added to Fig 2, and clearly represent the

1 asymptotic behaviour of the numerical solutions – confirming the self-consistency of the  
 2 calculations.  
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### 5 **A large strain solution.**

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 7 The Hertzian analysis of the elastic contact of a sphere and a elastic half-space fails  
 8 when the contact radius exceeds about  $0.4R$ . There are two reasons for this: the parabolic  
 9 approximation to the shape of the sphere breaks down, and so does the use of the equations  
 10 of linear elasticity. The Maugis solution just described includes only the first of these  
 11 effects: but is the second equally important? Fortunately a finite element solution by Lin &  
 12 Chen (2006) is available, in which the solid is treated as an ideal rubber with a constitutive  
 13 law best indicated by the tensile behaviour  $\sigma = G(\lambda - 1/\lambda^2)$  where  $\lambda$  is the stretch ratio  
 14 and  $G$  the low-strain shear modulus: the material is assumed to be incompressible. Lin &  
 15 Chen find that, for this material, the Maugis solution greatly overestimates the effect of  
 16 large  $a/R$ : so much so that a good approximation to their results is  $(1/3)*\text{Maugis} + (2/3)*$   
 17 Hertz.  
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27 Lin & Chen use their solution to obtain a large-strain JKR theory by assuming that  
 28 the relevant *punch* stiffness is equal to the derivative of load with respect to displacement  
 29 in their solution. They consider only adhesion in the high load region, where the load  
 30 change is relatively small and no problem arises: but near pull-off, where in the  
 31 paraboloidal JKR theory the effect of adhesion is to reverse the load from  $P = +\frac{3}{2}\pi R \Delta\gamma$  to  
 32  $P = -\frac{3}{2}\pi R \Delta\gamma$ , using the differential stiffness is less certainly correct. It is, of course, well-  
 33 known that the Hertz stiffness is equal to the small-strain punch stiffness for a contact of  
 34 the same radius: both are equal to  $2E'a$ . The same value is obtained from the Maugis  
 35 small-strain solution. Fortunately, for the case of a rigid sphere and an elastic half-space,  
 36 Lin & Chen find the stiffness to be close to  $2E'a$ , so that this value may safely be used.  
 37 Details of the calculation of the pull-off force are given in appendix 2, and the results are  
 38 shown above in figure 6.  
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53 Figure 7. Comparison of the two high-  $\mu$  asymptotes.  
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56 Figure 7 compares the two resulting high  $\mu$  asymptotes, and it is seen that the Maugis  
 57 solution does indeed exaggerate the effect of a finite radius sphere: the errors due to  
 58 simplifying the shape of the sphere and to simplifying the elastic behaviour largely cancel.  
 59 Since the numerical calculations equally include one effect but not the other, they are  
 60 presumably equally at fault.

### Rigid Sphere Analysis.

The detailed numerical calculations depend on the Derjaguin approximation that the surface traction between curved inclined elements of two surfaces is the same as if the elements were plane and parallel. Accepting the approximation, it is straightforward to evaluate the force/separation curve between a rigid sphere and a rigid half-space: we have simply

$T = \int_{r=0}^R 2\pi r \sigma(h) dr$  where  $\sigma(h)$  is given by the usual Lennard-Jones law

$$\sigma(h) = \frac{8\Delta\gamma}{3z_0} \left[ \left( \frac{z_0}{h} \right)^3 - \left( \frac{z_0}{h} \right)^9 \right] \text{ and } h = z_0 + R - \sqrt{R^2 - r^2}. \text{ Hence (see appendix 3) the pull-}$$

off force is found to be  $T / \pi R \Delta \gamma = 2 - \frac{18}{7} \frac{1}{\rho} + \frac{8}{3} \frac{1}{\rho(1+\rho)} + O(\rho^{-8})$ .

These values have been added to the pull-off graph, and once again form excellent asymptotes. But does this prove the correctness of the numerical calculations?

### Extension of Bradley's theory.

There are three suspect features of the use of the Derjaguin approximation. (a) when the element of the sphere is strongly inclined to the surface of the half-space, what is the distance between the two and hence the value of the surface force? (b) in what direction does the force act? (c) why should the integration be terminated at  $r = R$ ? Each of these may introduce an error, and it is unclear how large, or even in which direction, the final error will be.

Reconsideration of Bradley's papers suggests that all these worries are unnecessary, and perhaps derived from undue familiarity with magnetic lines of force around a magnetised sphere!

Bradley(1932) performs the exact analysis of the force between two rigid spheres, by assuming that the solids are composed of regular arrays of molecules<sup>8</sup>, and assuming that the forces between every pair of molecules may simply be added (and that the molecules are so densely packed that the summations may be replaced by integrals). It is not easy to give a simple physical interpretation of his results for two spheres, but straightforward and illuminating to do so when one of the bodies is a half-space. Bradley(1931) ( following Rayleigh(1890), who attributes the argument to Maxwell) shows that the force on a single

<sup>8</sup> Bradley refers to them as "molecules", Rayleigh (1890) as "particles". It is not clear which is the safer term: I would prefer "charges", but this might imply that the law of force is the electrostatic inverse square law.

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2 molecule of the first solid found by summing the interactions between that molecule and  
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4 every molecule of a half-space is simply  $Q(d) = 2\pi \int_d^\infty \phi(\rho) \rho d\rho$  where  $\phi(r)$  is the potential  
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6 between a pair of molecules a distance  $r$  apart and  $d$  is the distance of the single molecule  
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8 from the surface of the half-space. Integrating this over a single 'column' of molecules of  
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10 the first solid, the force per unit area on that solid is obtained as  $\int_{d_1}^{d_2} Q(h)dh$  when the  
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12 column extends from  $d_1$  to  $d_2$ . It will immediately be clear that the force will be  
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14 independent of the *lateral* position of the 'column', and that its direction will be normal to  
15  
16 the half-space. If the first solid is also a half-space, it follows that the force per unit area  
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18 between two half-spaces separated by  $d$  will be  $F(d) = \int_d^\infty Q(h)dh$ . In particular when the  
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20 potential between two individual molecules is a power law  $\phi = A_m / r^m$ , then  
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22  $Q(d) = 2\pi A_m / ((m-2)d^{m-2})$  and  $F(d) = [2\pi A_m / ((m-2)(m-3))] / d^{m-3}$ . Thus, the (6, 12)  
23  
24 Lennard-Jones potential gives rise to a (3, 9) law of force between two half-spaces: the  
25  
26 analysis by Bradley (1931) is readily extended to show that it will be  
27  
28  $F(d) = (8\Delta\gamma/3z_0) [(z_0/d)^3 - (z_0/d)^9]$  where  $z_0$  is the equilibrium spacing between the  
29  
30 two bodies<sup>9</sup>. [Note that this is not the equilibrium spacing between two isolated molecules,  
31  
32 which is  $(15)^{1/6} z_0 \sim 1.57z_0$ ].  
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37 The derivation of this force per unit area as the force on a single column of molecules  
38 makes it immediately clear that it applies equally whatever the shape of the body to which  
39 the column belongs. Even when the surface of the body is inclined or curved, still only the  
40 distance from the half-space to the first (and last) molecule is relevant. The surface slope  
41 does not affect the direction of the force. No force acts on the body from beyond its extent,  
42 for no relevant columns of molecules exist: the total force between the two bodies is  
43 correctly found by integrating out only as far as the radius of the sphere.  
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49 Why then does the exact result for the force between a rigid sphere and a half-space  
50 differ from the result found above? The answer is simply that the far ends of the columns of  
51 molecules have been ignored: the result of integrating 'round the back' of the sphere must  
52 be subtracted from the integral 'round the front'. This is readily done, to give the final  
53 answer as (see appendix 3)  
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$$58 \quad T / \pi R \Delta \gamma = 2 - \frac{18}{7} \frac{1}{\rho} + \frac{8}{3} \frac{1}{(1+2\rho)^2} + \frac{8}{3} \frac{1}{\rho(1+2\rho)} + O(\rho^{-8}).$$

59  
60  
<sup>9</sup> The first explicit statement I can find is Muller et al (1980).

1  
2 We note at once that to order  $(z_0/R)$  this agrees with the result of the simple integration  
3  
4 'round the front': figure 8 shows that the two methods are in excellent agreement even  
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6 down to  $R/z_0 = 5$   
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13 Figure 8. Comparison between the exact rigid-sphere answer and the  
14 value based on the 'Derjaguin approximation'.  
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18 Thus the usual Derjaguin calculation gives the exact result for a *hemisphere*, or  
19 more precisely, for a hemispherically ended infinite circular column. The modification for a  
20 sphere is straightforward: the accuracy of Derjaguin's approximation does not arise. The  
21 occurrence of terms in  $(2R + z_0)$  in the exact answer, but only terms in  $(R + z_0)$  in the  
22 approximate answer, is a sufficient clue to the correction.  
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### 31 Discussion

32 Is the 'Derjaguin approximation' an approximation? It is argued above that, when  
33 one body is a half-space, the calculation of the adhesive force by what is usually regarded as  
34 the approximation, ignoring the surface profile, is in fact no approximation. However, a  
35 warning is necessary. The result above is for the force the half-space exerts on the sphere.  
36 Newton's third law guarantees that it is also the force that the sphere exerts on the half-  
37 space. We note that Argento et al (1997) have also argued that when at least one of the  
38 bodies is a half-space, the Derjaguin approximation will lead to the correct total force.  
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45 However, there is no law guaranteeing that the surface traction distributions match:  
46 the correct surface traction distribution on body A does not imply that the surface traction  
47 distribution on body B is correct, and there is indeed some considerable doubt over this. The  
48 question only becomes serious when these *body* forces are used as *surface tractions* in an  
49 elastic calculation. Derjaguin's original 1934 paper, in which the 'approximation' first  
50 appears, considers only the total force: the widely quoted 1975 paper presenting the DMT  
51 theory merely adds the integral of the surface forces to the total force. Only in the ground-  
52 breaking 1980 paper by Derjaguin and his collaborators do the authors, without comment,  
53 treat the actual interaction as being a surface traction. Argento et al equally fail to discuss  
54 whether their general procedure for replacing volume integrals over individual molecules  
55 by surface integrals will yield surface traction distributions which can properly be used in  
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1  
2 elastic calculations<sup>10</sup>. There is clearly a matter for concern, even if the treatment of the  
3 body molecules as a continuum is accepted.  
4

5 But once we attempt to apply continuum theory to bodies whose size is of the order  
6 of the range of action of the surface forces  $z_0$ , a new worry arises. If a solid can indeed be  
7 treated as an array of 'molecules', the body forces do not form a continuous pressure but are  
8 separate forces at a lateral spacing of order  $z_0$ . Nor are they applied at the surface, but  
9 internally at individual molecules. It can be argued that a point force applied at a  
10 particular depth in an elastic solid may perhaps be regarded as a distributed pressure  
11 applied to a surface element of the solid whose width is of the order of that depth <sup>11</sup>. Both  
12 lines of thought suggest that the resolution of the continuum analysis can only be of order  
13  $z_0$ . Luan & Robbins (2005) compare continuum analysis with a molecular simulation of  
14 contact between a cylinder or sphere and a elastic half-space, and similarly find pressure  
15 fluctuations on a scale of  $z_0$ , dependent on the particular atomic structure considered, but  
16 even in the best case (a bent commensurate crystal) there are substantial differences within  
17  $\pm 2z_0$  from the contact edge. Converting  $z_0$  to the non-dimensional radius of the numerical  
18 calculations, we find that a width  $z_0$  corresponds to  $dr^* = 1/\sqrt{\rho\mu}$ . Thus, for the pressure  
19 distribution of figure 1 with  $\mu = 8$ ,  $\rho = 50$ , the molecular spacing<sup>12</sup> is  $dr^* = 0.05$  – rather  
20 considerably wider than the pressure spike, and enormously greater than the resolution  
21 thought necessary! Perhaps the pressures found by the Derjaguin approximation should be  
22 'smeared out' by introducing an intermediate step of replacing them by a suitable moving  
23 average?  
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#### 45 *The governing variables.*

46 This paper argues that  $R$  and  $z_0$  are measurable physical quantities, so that  
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48  $\rho \equiv (R/z_0)$  is a basic variable: and particularly that

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51 (a) values less than 1 are intrinsically absurd,  
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59 <sup>10</sup> The author has belatedly discovered a paper by Wu (2006) in which the present problem has been solved using the  
60 Argento surface tractions. The (minor) differences in results are being investigated.

<sup>11</sup> An idea perhaps envisaged by Derjaguin(1934): [das ist so lange berechtigt, wie die Durchmesser dieser  
Flächenelemente wesentlich grösser sind als die molekulare Wirkungsradius]. But at that time there was no question  
of elastic deformation.

<sup>12</sup> As noted earlier, the molecular spacing is not  $z_0$  but  $(15)^{1/6} z_0$ .

1  
2 (b) if the values of the surface force round the back of the sphere are still  
3 substantial, they should be taken into account – but certainly not by treating them  
4 as surface tractions on the *near* face of the sphere!  
5

6  
7 (c) the finite spacing of the molecules becomes significant for  $\rho$  small ( $\rho < 10$ ??).  
8

9 Yet  $\sigma_0$  and  $E^*$  are measurable physical quantities: is it unreasonable to specify their ratio?

10 Perhaps it is the Tabor parameter that is the artificial combination? It may be noted that  
11 many of the figures presented by Yao et al do indeed use  $(R/z_0)$  and  $(\sigma_0/E')$  as the  
12 governing variables, and no error can arise if this is done. If either is left to 'chance' by  
13 choosing  $\mu$  and either of the other two, a physically impossible combination may be chosen.  
14  
15 But the vast majority of experimental work uses spheres for which the paraboloidal  
16 approximation is entirely satisfactory: for this the Tabor parameter  $\mu$  remains the proper  
17 controlling variable.  
18  
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### 20 **Conclusion.**

21 When the radius of the sphere is no longer vastly greater than the equilibrium  
22 separation between the two bodies, the pull-off force will fall below, and the contact radii  
23 will be smaller than, the values for a large sphere. However, unless the reduction is trivial  
24 (ie for perhaps  $R > 50z_0$ ), attempts to calculate it by the methods of contact mechanics  
25 introduced by Derjaguin and his collaborators and followed by Greenwood, Feng, and others  
26 are highly suspect.  
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39 I am most grateful to Prof. M Ciavarella of the Politecnico di Bari for useful discussions,  
40 and for bringing to my attention the papers by Maugis and by Lin & Chen.  
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## Appendix 1: Numerical Solution

*Compliance matrix for axisymmetric loading of a half-space.*

The pressure distribution is approximated as piece-wise linear by the method of overlapping triangles (Johnson 1985). The influence function of a single triangle is found as follows.

Write the Green's function for a ring load  $P_1(s)$  acting on a half-space of unit plane strain modulus as  $(4/\pi)G(r,s)$ , so that the deformation at radius  $r$  due to a general axisymmetric pressure distribution will be

$$w(r) = \frac{4}{\pi E'} \int p(s)G(r,s) ds$$

The function  $G(r,s)$  is well-known, but will not be required.

For a triangular pressure distribution extending from  $s_{j-1}$  to  $s_{j+1}$ , with a maximum  $p_j$  at  $s_j$ , we integrate this equation by parts, to get

$$w(r) = \frac{4}{\pi E'} \int_{s_{j-1}}^{s_{j+1}} p'(s)H(r,s) ds \quad \text{where } H(r,s) = \int_0^s G(r,s) ds,$$

the integrated term vanishing since  $p(s_{j-1}), p(s_{j+1})$  both vanish.

But for the triangular pressures,  $p'(s) = p_j/(s_j - s_{j-1})$  for  $s_{j-1} < s < s_j$ , and  $p'(s) = -p_j/(s_{j+1} - s_j)$  for  $s_j < s < s_{j+1}$ , so that

$$w(r) = \frac{4p_j}{\pi E'} \left[ \frac{1}{s_j - s_{j-1}} \int_{s_{j-1}}^{s_j} H(r,s) ds - \frac{1}{s_{j+1} - s_j} \int_{s_j}^{s_{j+1}} H(r,s) ds \right]$$

or  $w(r_i) = \frac{4p_j}{\pi E'} [J_{ij} - J_{i,j=1}]$  where  $J_{ij} = \frac{1}{s_j - s_{j-1}} \int_{s_{j-1}}^{s_j} H(r_i, s) ds$ .

Now for a uniform pressure  $p_0$  over a circle of radius  $s$ , we have

$w(r) = \frac{4p_0}{\pi E'} \int_0^s G(r,s) ds = \frac{4p_0}{\pi E'} H(r,s)$ , and it is well-known (see, e.g. Johnson 1985) that the

answer is  $w(r) = \frac{4p_0}{\pi E'} [sE(r/s) \text{ or } (s^2/r)B(s/r)]$  depending on whether  $r < s$  or  $r > s$ . [ $E(k)$  and  $B(k)$  are elliptic integrals, see Jahnke & Emde]

To evaluate  $J_{ij}$ , we write  $s = s_{j-1} + \xi(s_j - s_{j-1})$  to get  $J_{ij} = \int_0^1 s \{ \quad \} d\xi$  where  $\{ \quad \}$

denotes either  $\{E(r/s)\}$  or  $\{(s/r)B(s/r)\}$ . This is conveniently integrated by 8-pt Gaussian quadrature, the integrand always being finite and well-behaved except that when  $s = r$  it has a logarithmically infinite slope {always at an end of the range since  $r_i, s_j$  are the same set of points!}. Note that the scale of the pressure distribution enters the equations only through the single factor  $s$ . Thus, for an unevenly spaced set of points  $0, s_1, s_2, s_3, s_4, s_5, \dots$  the integral is evaluated for  $s = 0, 1, (s_2/s_1), (s_3/s_1), (s_4/s_1), (s_5/s_1), \dots$  and the choice of scale left until later.

*Newton-Raphson Solution.*

The equations to be solved are (Greenwood 1997, Feng 2000)

<sup>1</sup> For comparison,  $\int_0^1 s \log(s) ds = -0.250149$  using 6-pt Gaussian,  $-0.250045$  using 8-pt gaussian.

$$h(r) = -\alpha + z_0 + z(r) + w(r); \quad p(r) = -\sigma(h)$$

$$\text{and} \quad w(r) = (4/\pi E') \int p(s) G(r, s) ds$$

Define a reference radius  $r_0$  as  $r_0 = (R^2 \Delta \gamma / E')^{1/3}$ , and define radial distances and the contact radius as  $r^* = r/r_0$ ,  $a^* = a/r_0$ . Note that this definition avoids the introduction of  $z_0$ , so that the JKR theory can be included. Normal distances are scaled by  $z_0$ , so that  $H(r^*) = (h(r) - z_0)/z_0$ ,  $\alpha^* = \alpha/z_0$ .

The dimensionless pressure is defined by  $p^* = p(R/E'^2 \Delta \gamma)^{1/3}$ , so that

$$p^* = \frac{8\mu}{3} \left[ \frac{1}{(H+1)^3} - \frac{1}{(H+1)^9} \right] \text{ and the height of the pressure spike will be } (16/9\sqrt{3})\mu,$$

ie  $(-p^*)_{\max} = 1.026\mu$  (which correctly becomes infinite for JKR conditions). Then

$$H = -\alpha^* + \frac{1}{2}\mu r^{*2} + \mu \int p^*(s^*) G(r^*, s^*) ds^* . \text{ We choose } H(0) \text{ as the independent variable}$$

in preference to the approach  $\alpha^*$  in order that the complete S-curve of  $P(\alpha)$  may be

followed, so we subtract  $H(0) = -\alpha^* + \mu \int p^*(s^*) G(0, s^*) ds^*$  to obtain

$$H(r^*) - H(0) = \frac{1}{2}\mu r^{*2} + \mu \int p^*(s^*) \{G(r^*, s^*) - G(0, s^*)\} ds^*$$

In discrete form this becomes

$$H_i = H_0 + \frac{1}{2}\mu r_i^2 + \mu \sum [G_{ij}^* - G_{0j}^*] p_j^* \text{ for } i=1:N, \quad j=0:N . \text{ More conveniently, since}$$

$p_0 = f(H_0)$  and so is known once  $H_0$  has been chosen, we separate off the  $j=0$  term and

$$\text{write } H_i = H_0 + \mu [G_{i0}^* - G_{00}^*] p_0^* + \frac{1}{2}\mu r_i^2 + \mu \sum [G_{ij}^* - G_{0j}^*] p_j^* \text{ for } i, j=1:N .$$

[The  $G_{ij}^*$  must contain a length scale corresponding to  $ds^*$ : conveniently taken as the

length of the first element.]

Define  $C_{ij} = G_{ij}^* - G_{0j}^*$  and write this  $H_i = H_0 + \mu C_{i0} p_0^* + \frac{1}{2}\mu r_i^2 + \mu \sum C_{ij} p_j^*$ , noting

that the only elements of the original matrix which need be retained are those of the first

row  $G_{0j}^*$ , used *after* the iteration to find the approach  $\alpha^* = -H_0 + \mu \sum G_{0j}^* p_j^*$ .

Define the residuals in an approximate solution as  $R_i = H_i - A_i - \mu \sum C_{ij} p_j^*$  where  $A_i$  are

the known quantities  $A_i = \{H_0 + \mu C_{i0} p_0^* + \frac{1}{2}\mu r_i^2\}$ . If a particular film thickness  $H_{(j)}$  is

varied, all the residuals will change, and we have  $\frac{\partial R_i}{\partial H_{(j)}} = \delta_{i(j)} - \mu C_{i(j)} \frac{\partial p_{(j)}^*}{\partial H_{(j)}}$ . Hence, the

Jacobian matrix describing the change is  $\mathbf{J} = \mathbf{I} - \mu \mathbf{C} \mathbf{D}$ , where  $\mathbf{D}$  is the diagonal matrix with elements  $f'(H_i)$ , the derivatives of the surface force law  $p = f(H)$ .

To reduce the residuals to (hopefully) zero, we change the film thicknesses such that  $\mathbf{JdH} = -\mathbf{R}$ : conveniently found in MATLAB by the matrix division  $\mathbf{dH} = -\mathbf{R} \setminus \mathbf{J}$  rather than by inverting  $\mathbf{J}$ . For low values of  $\mu$  ( $\mu < 1$ ) a few iterations suffice when taking the rigid shape as an initial guess: for higher values of  $\mu$  the process diverges unless a reasonable initial guess (the solution for a neighbouring value of  $H(0)$  or of  $\mu$ ) is available.

## Appendix 2: JKR theory for a true hemisphere.

### *Non-adhesive contact between an elastic plane and a rigid axisymmetric indenter*

The following method is taken directly from Barber's (1992) presentation of Collins' method. If the imposed displacements within a contact  $r < a$  are  $u(r)$ , (and the pressures are zero for  $r > a$ ), we define

$$g(t) = -\frac{E'}{\pi} \frac{d}{dt} \int_0^t \frac{r u(r)}{\sqrt{t^2 - r^2}} dr$$

Then according to Barber, the contact pressures will be

$$p(r) = \frac{1}{r} \frac{d}{dr} \int_r^a \frac{t g(t)}{\sqrt{t^2 - r^2}} dt \quad \text{and the load} \quad P = -2\pi \int_0^a g(t) dt$$

If the indenter shape is  $z = f(r)$ , the displacements will of course be  $u(r) = \delta - f(r)$  where the 'approach'  $\delta$  is unknown: it is found from the condition that if the pressure falls to zero at the contact edge, then  $g(a) = 0$ .

If we integrate the equation defining  $g(t)$  by parts and then perform the differentiation, we get an alternative form:

$$I(t) \equiv \int_0^t \frac{r u(r)}{\sqrt{t^2 - r^2}} dr = -u(r)\sqrt{t^2 - r^2} \Big|_0^t + \int_0^t u'(r)\sqrt{t^2 - r^2} dr = t u(0) + \int_0^t u'(r)\sqrt{t^2 - r^2} dr$$

$$\text{so that } g(t) = -\frac{E'}{\pi} \frac{dI}{dt} = -\frac{E'}{\pi} \left[ u(0) + \int_0^t \frac{t u'(r)}{\sqrt{t^2 - r^2}} dr \right] = -\frac{E'}{\pi} \left[ \delta - t \int_0^t \frac{f'(r)}{\sqrt{t^2 - r^2}} dr \right].$$

$$\text{Thus, the condition that } g(a) = 0 \text{ gives the approach as } \delta = a \int_0^a \frac{f'(r)}{\sqrt{a^2 - r^2}} dr$$

For a power law indenter  $f(r) = A_n r^{2n}$  this gives

$$\frac{\pi}{E'} g(t) = -\delta + 2n A_n t \int_0^t \frac{r^{2n-1}}{\sqrt{t^2 - r^2}} dr = -\delta + 2n A_n t^{2n} \int_0^1 \frac{s^{2n-1}}{\sqrt{1-s^2}} ds = -\delta + c_n A_n t^{2n}$$

$$\text{where } c_n = \frac{2 \cdot 4 \cdot 6 \dots (2n)}{1 \cdot 3 \cdot 5 \dots (2n-1)}.$$

$$\text{Then } \delta = c_n A_n a^{2n} \text{ and } P = -2E' \int_0^a \left( -\delta + c_n A_n t^{2n} \right) dt = 2E' A_n \left( \frac{2n}{2n+1} \right) a^{2n+1}$$

which are Steuermann's equations (Steuermann 1939, Johnson<sup>2</sup> 1985).

<sup>2</sup>Johnson also gives Steuermann's equations for the pressure, repeating the misprint in Steuermann's paper of an additional factor  $n$ .

Load/displacement relation for a hemispherical asperity.

The shape is  $f(r) = R - \sqrt{R^2 - r^2}$ , so that  $f'(r) = \frac{r}{\sqrt{R^2 - r^2}}$  and

$$g(t) = -\frac{E'}{\pi} \left[ \delta - t \int_0^t \frac{r}{\sqrt{R^2 - r^2} \sqrt{t^2 - r^2}} dr \right]$$

The integral is equal to  $\frac{1}{2} \ln\left(\frac{R+t}{R-t}\right)$ , so that  $g(t) = -\frac{E'}{\pi} \left[ \delta - \frac{t}{2} \ln\left(\frac{R+t}{R-t}\right) \right]$ .

$$\text{Thus } \delta = \frac{a}{2} \ln\left\{ \frac{1+a/R}{1-a/R} \right\}$$

$$\text{and } P = E' \int_0^a t \ln\left(\frac{R+t}{R-t}\right) dt = \frac{1}{2} E' R^2 \left\{ \left[ 1 + \left(\frac{a}{R}\right)^2 \right] \ln\left\{ \frac{1+a/R}{1-a/R} \right\} - 2a/R \right\}.$$

For  $a/R$  small, these reduce to the familiar Hertz equations  $\delta = a^2/R$ ;  $P = \frac{4}{3} E' a^3/R$ .

*Adhesive contact.*

To obtain the equations describing the effect of surface energy on the above contact, as in the JKR theory, we impose a uniform 'lift'  $\Delta$  over the contact area. The corresponding pressures are given by Boussinesq's solution for a stamp on a half-space:

$$p(r) = -\frac{E'\Delta}{\pi} \frac{1}{\sqrt{a^2 - r^2}} \quad (\text{the sphere geometry being irrelevant}), \text{ and the corresponding load}$$

is  $2 E' a \Delta$ . These pressures are infinite at the contact edges, with a stress intensity factor

$$N = \lim_{r \rightarrow a} (-\sqrt{a-r} p(r)) = \frac{E'\Delta}{\pi\sqrt{2a}}, \text{ and fracture mechanics theory requires that}$$

$$N = \sqrt{E'\Delta\gamma/\pi}. \text{ Thus } \Delta = \sqrt{2\pi a \Delta\gamma/E'}$$
 and the load change is  $-\sqrt{8\pi E'\Delta\gamma} a^3$ .

Combining these results with the non-adhesive solution gives the Maugis equations

$$P = \frac{1}{2} E' R^2 \left\{ \left[ 1 + \left(\frac{a}{R}\right)^2 \right] \ln\left\{ \frac{1+a/R}{1-a/R} \right\} - 2a/R \right\} - \sqrt{8\pi E'\Delta\gamma} a^3$$

$$\text{and } \delta = \frac{a}{2} \ln\left\{ \frac{1+a/R}{1-a/R} \right\} - \sqrt{2\pi a \Delta\gamma/E'}.$$

*Pull-off force.*

$$\text{Write } x = a/R: \text{ then } P/R\Delta\gamma = \frac{1}{2} \frac{E'R}{\Delta\gamma} \left[ \{1+x^2\} \ln\left\{ \frac{1+x}{1-x} \right\} - 2x \right] - \sqrt{8\pi \frac{E'R}{\Delta\gamma}} x^3, \text{ or}$$

$$P/R\Delta\gamma = \chi^2 F(x) - \chi \sqrt{8\pi} x^3$$

$$\text{where } F(x) = \frac{1}{2} \{1+x^2\} \ln\left\{ \frac{1+x}{1-x} \right\} - x \text{ and } \chi = \sqrt{E'R/\Delta\gamma} = (\rho/\mu)^{3/4}.$$

Then the pull-off force is when  $dW/dx = 0$ , ie when  $\chi^{-1} = F'(x)/3\sqrt{2\pi} x$ . Here this

$$\text{becomes } \chi^{-1} = \left[ x^{1/2} \ln\left\{ \frac{1+x}{1-x} \right\} - \frac{2x^{3/2}}{1-x^2} \right] / 3\sqrt{2\pi}.$$

It will be seen that it is easier to obtain  $\chi$  as a function of  $x$ , [ and hence

$a/R|_{\text{crit}}, T/\pi R\Delta\gamma|_{\text{max}}$  as functions of  $(\rho/\mu) \equiv \chi^{4/3}$ ] than to insist on choosing  $(\rho/\mu)$ .

*The large-strain solution.*

Lin & Chen give a Finite Element solution of the problem of the contact between a rigid sphere and an elastic half-space, taking the material of the half-space to be an ideal rubber. They find that an excellent curve-fit to their load-radius equation is

$$P = \frac{4}{3} \frac{E' a^3}{R} \phi_4(a/R)$$

where

$$\phi_4(x) = \exp(0.225x^3 + 0.275x^{10})$$

If we again assume the punch stiffness in the large strain solution to be the standard  $2E' a$  rather than the incremental stiffness of their FE solution, the analysis above for the Maugis solution can be applied if we write

$$F_{LC}(x) = \frac{4}{3} x^3 \phi_4(x). \text{ Again we may readily find } \chi(x) \text{ and hence the pull-off force.}$$

**Appendix 3. Rigid Sphere Analyses.**

As discussed in the text, the surface force between a half-space and a column of molecules extending from  $h_1$  to  $h_2$  will be  $\sigma(h) = \frac{8\Delta\gamma}{3z_0} \left[ \left\{ \left( \frac{z_0}{h_1} \right)^3 - \left( \frac{z_0}{h_1} \right)^9 \right\} - \left\{ \left( \frac{z_0}{h_2} \right)^3 - \left( \frac{z_0}{h_2} \right)^9 \right\} \right]$ . It will be

convenient to treat the two terms separately, in effect by first integrating round the front face of the sphere, which is precisely what is done in the 'Derjaguin approximation', but then subtracting the result of integrating round the back.

Thus, the Derjaguin result is  $T(h_0) = \int_0^R 2\pi r \sigma(h) dr$  where  $h = h_0 + R - \sqrt{R^2 - r^2}$ . Then

$$R^2 - r^2 = (h_0 + R - h)^2 \text{ and } r dr = (h_0 + R - h) dh \text{ so that } T(h_0) = \int_{h_0}^{h_0+R} 2\pi \sigma(h) (h_0 + R - h) dh.$$

The greatest force, as in the Bradley and Derjaguin analyses, is when  $h_0 = z_0$ . Write  $h = y z_0$  and recall that  $R = \rho z_0$ : then

$$\begin{aligned} T_{\max} = T(z_0) &= \frac{16\pi \Delta\gamma}{3} z_0 \int_1^{\rho+1} \left[ (1+\rho) \{y^{-3} - y^{-9}\} - \{y^{-9} - y^{-8}\} \right] dy \\ &= \frac{16\pi R \Delta\gamma}{3\rho} \left[ (1+\rho) \left\{ \frac{1}{2} - \frac{1}{8} - \left( \frac{1}{2(1+\rho)} \right)^2 - \frac{1}{8} \left( \frac{1}{1+\rho} \right)^8 \right\} - \left\{ 1 - \frac{1}{7} - \left\{ \left( \frac{1}{1+\rho} \right) - \frac{1}{7} \left( \frac{1}{1+\rho} \right)^7 \right\} \right\} \right] \end{aligned}$$

Neglecting terms of order  $\rho^{-7}$  we get

$$T_{\max} = 2\pi R \Delta\gamma \left[ 1 - \frac{9}{7\rho} + \frac{4}{3\rho(1+\rho)} \right]$$

For the round the back integration, we have  $h = h_0 + R + \sqrt{R^2 - r^2}$ , so that now

$R^2 - r^2 = (h - (h_0 + R))^2$  and  $r dr = -(h - (h_0 + R)) dh$ , and the only change is the integration limits, which become  $(h_0 + R)$  to  $(h_0 + 2R)$ . Thus, taking  $h_0 = z_0$ ,

$$T_{\text{rear}} = \frac{16\pi R \Delta\gamma}{3\rho} \left[ (1+\rho) \left\{ \left( \frac{1}{2} \left( \frac{1}{1+\rho} \right)^2 - \frac{1}{8} \left( \frac{1}{1+\rho} \right)^8 \right) - \left( \frac{1}{2} \left( \frac{1}{1+2\rho} \right)^2 - \frac{1}{8} \left( \frac{1}{1+2\rho} \right)^8 \right) \right\} - \left\{ \left( \frac{1}{1+\rho} \right) - \frac{1}{7} \left( \frac{1}{1+\rho} \right)^7 \right\} - \left\{ \left( \frac{1}{1+2\rho} \right) - \frac{1}{7} \left( \frac{1}{1+2\rho} \right)^7 \right\} \right]$$

Neglecting terms of order  $\rho^{-7}$ :

$$\begin{aligned} T_{\text{rear}} &= \frac{16\pi R \Delta\gamma}{3\rho} \left[ \frac{1}{2} \left( \frac{1}{1+\rho} \right) - \frac{1+\rho}{2(1+2\rho)^2} - \frac{1}{1+\rho} + \left( \frac{1}{1+2\rho} \right) \right] \\ &= 2\pi R \Delta\gamma \left[ -\frac{4}{3} \frac{1}{\rho(1+\rho)} + \frac{4}{3\rho(1+2\rho)} + \frac{4}{3(1+2\rho)^2} \right] \end{aligned}$$

Combining,

$$T = 2\pi R \Delta\gamma \left[ 1 - \frac{9}{7\rho} + \frac{4}{3\rho(1+2\rho)} + \frac{4}{3(1+2\rho)^2} \right] + O(\rho^{-8}).$$

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2 [More directly, we could use

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4 
$$T = \int_{h_0}^{h_0+R} 2\pi \sigma(h)(h_0 + R - h) dh + \int_{h_0+R}^{h_0+2R} 2\pi \sigma(h)(h_0 + R - h) dh = \int_{h_0}^{h_0+2R} 2\pi \sigma(h)(h_0 + R - h) dh ]$$
  
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**Nomenclature.**

$a$  contact radius (location of maximum tensile stress)

$d$  minimum gap between two bodies

$h = h(r)$  gap between two bodies

$m$  (negative) power law exponent: here either 6 or 12

$p(r) = -\sigma(h)$  pressure applied to surface of half-space.

$p^* \equiv p / (E'^2 \Delta\gamma / R)^{1/3}$  non-dimensional pressure.

$r$  radial co-ordinate

$r_0 \equiv (R^2 \Delta\gamma / E')^{1/3}$  reference radius

$r^* = r / r_0$  non-dimensional radial co-ordinate

$z_0$  Qualitatively, range of action of surface forces. Specifically, equilibrium separation of two half-spaces in the Lennard-Jones surface force law

$\sigma(h) = (8\Delta\gamma / 3z_0) \left( (z_0 / h)^3 - (z_0 / h)^9 \right)$ .

$E, E'$  Young's modulus, plane strain modulus  $E / (1 - \nu^2)$

$E^*$  "contact modulus"  $\left[ \text{usually } 1/E^* = (1 - \nu_1^2)/E_1 + (1 - \nu_2^2)/E_2 : \text{here } E^* = E' \right]$

$G$  low-strain shear modulus for ideal rubber ( $= E/3$ ).

$P$  Load applied to contact

$R$  Sphere radius, or for two spheres,  $1/R = 1/R_1 + 1/R_2$ .

$T$  Tensile load ( $T = -P$ )

$T_{\max}$  maximum value of  $(-P)$ , ie pull-off force.

$r_0 = (R^2 \Delta\gamma / E')^{1/3}$  reference radius for non-dimensionalising horizontal distances

$\alpha$  approach of centre of sphere: for a rigid sphere, maximum deflection of surface of half-space

$\varepsilon \equiv (\sigma_0 / E')$  strength limit

$\Delta\gamma$  Work of adhesion, also called the Dupré surface energy

$\mu \equiv (R \Delta\gamma^2 / E^2 z_0^3)^{1/3}$  Tabor parameter. Originally used  $E$ : now usually  $E'$

$\rho \equiv R / z_0$  size ratio

$\sigma_0$  maximum value of surface force, equal to  $(16/9\sqrt{3})(\Delta\gamma/z_0)$

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$\sigma(r) = (8\Delta\gamma/3z_0) \left[ (z_0/h)^3 - (z_0/h)^9 \right]$  "Lennard-Jones" surface force law

$\chi = \sqrt{E'R/\Delta\gamma} = (\rho/\mu)^{3/4}$  parameter in Maugis' exact sphere analysis

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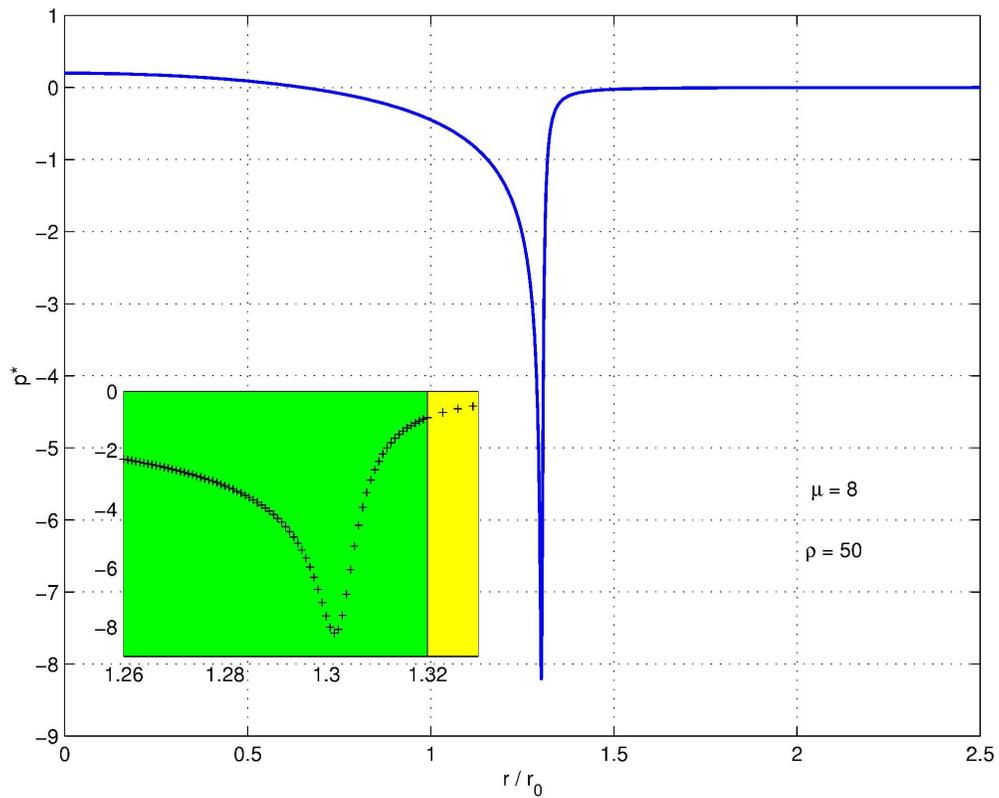


Figure 1. Pressure distribution at pull-off.

The inset shows that the pressure spike really was resolved.  
171x138mm (600 x 600 DPI)

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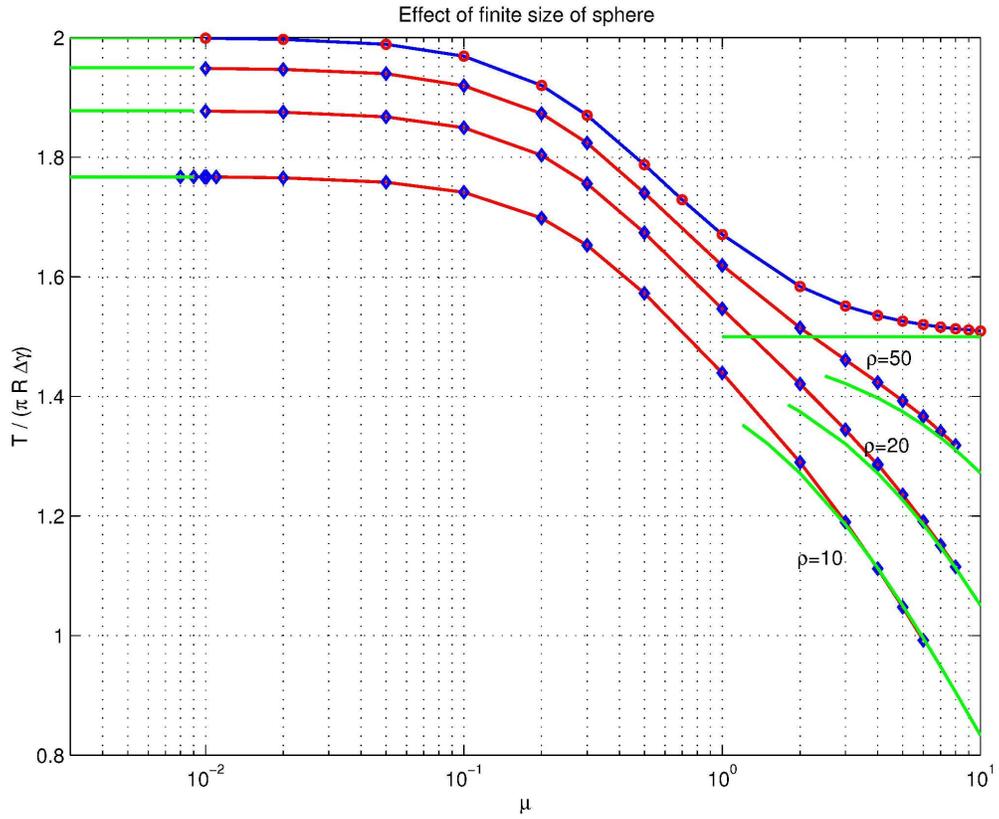


Fig 2 Pull-off forces for a true finite sphere  
172x142mm (600 x 600 DPI)

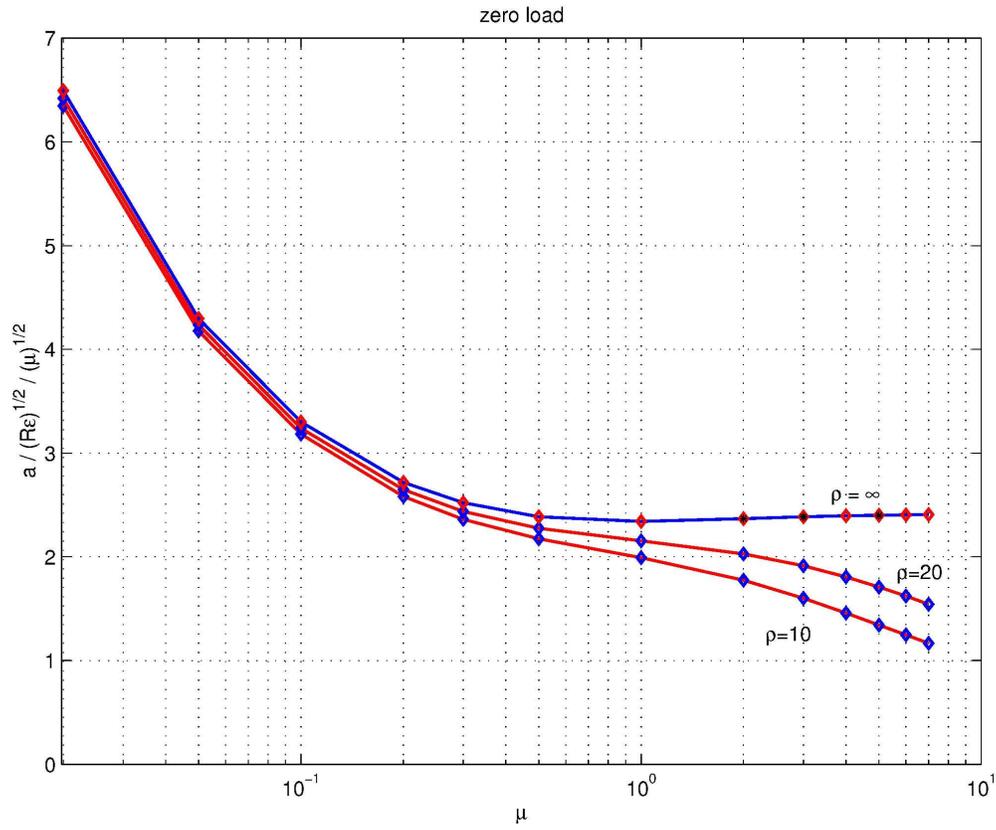


Figure 3. Contact radii at zero load.  
 For low  $\mu$  the radius is independent of the size ratio, but for  $\mu > 5$  the values for a finite sphere are lower.  
 170x142mm (600 x 600 DPI)

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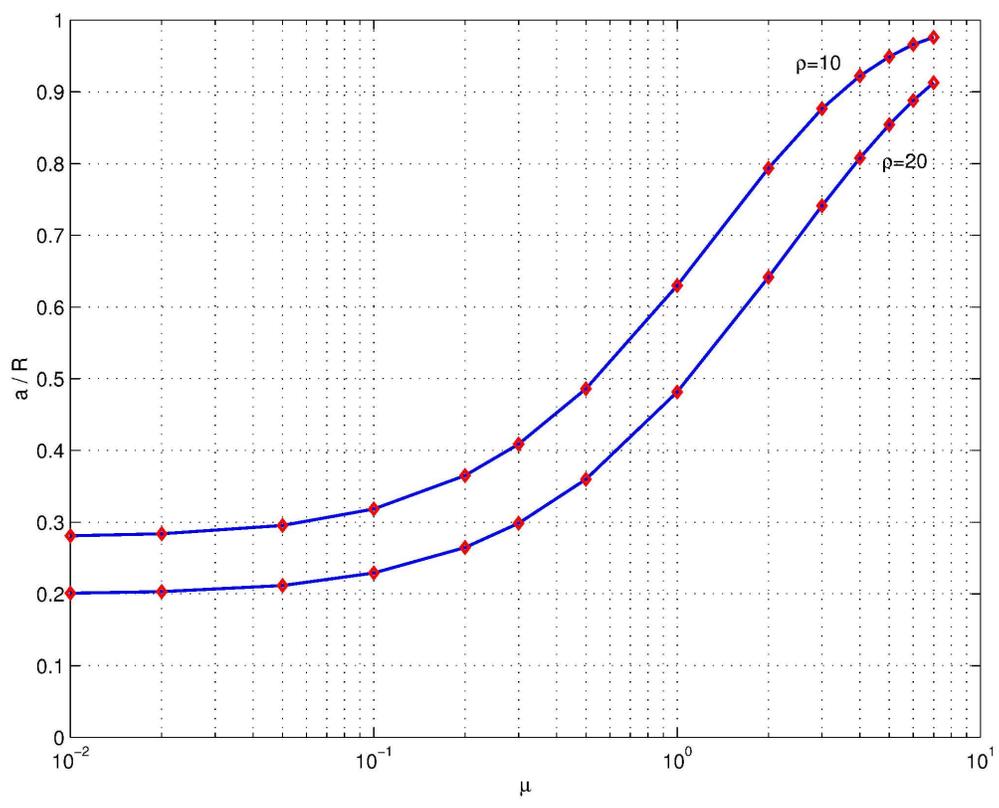
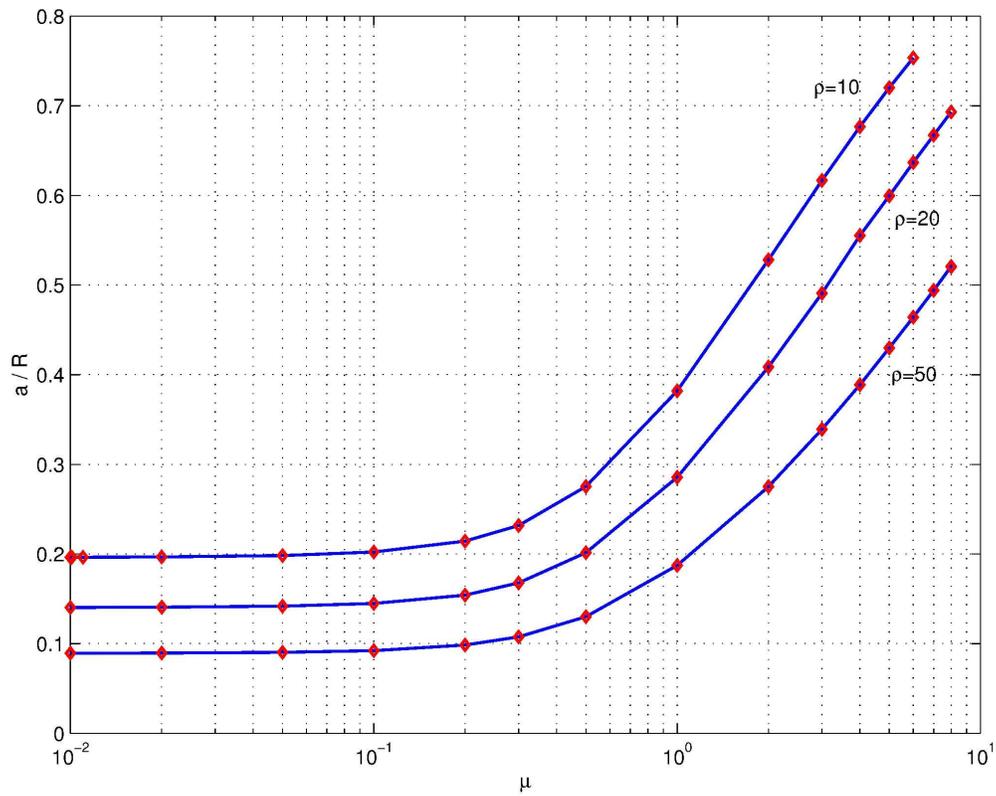


Figure 4. Contact radii at zero load.  
Values of  $a/R$  greater than 0.4 are highly suspect.  
172x138mm (600 x 600 DPI)

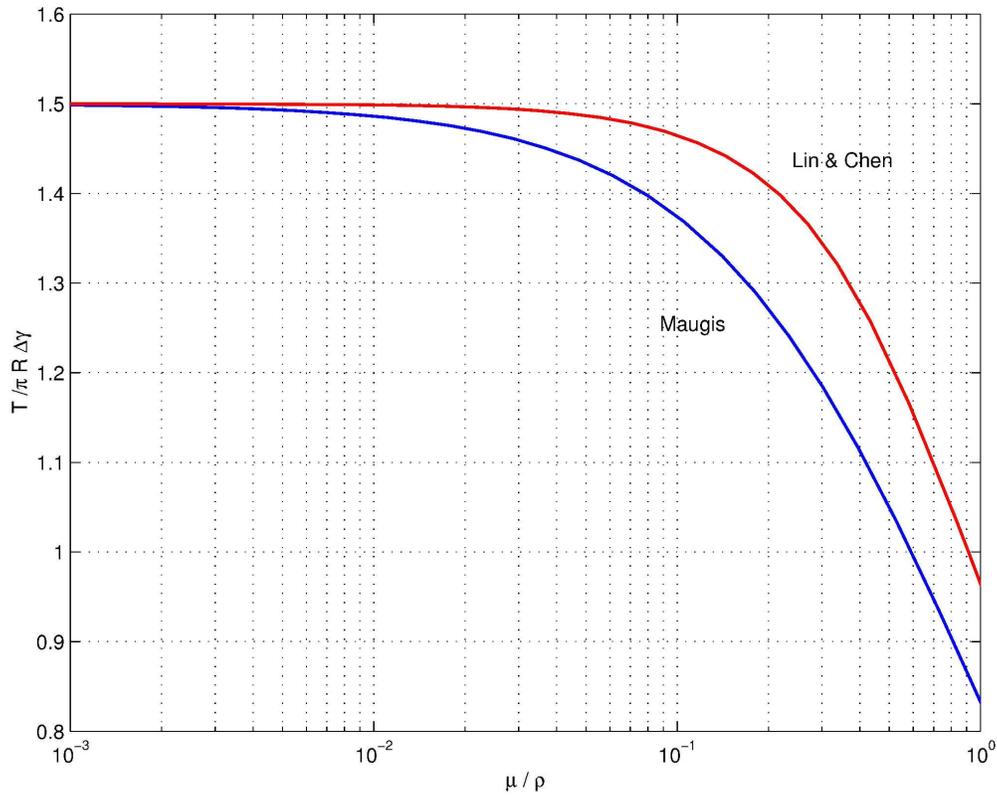
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Contact radii at pull-off  
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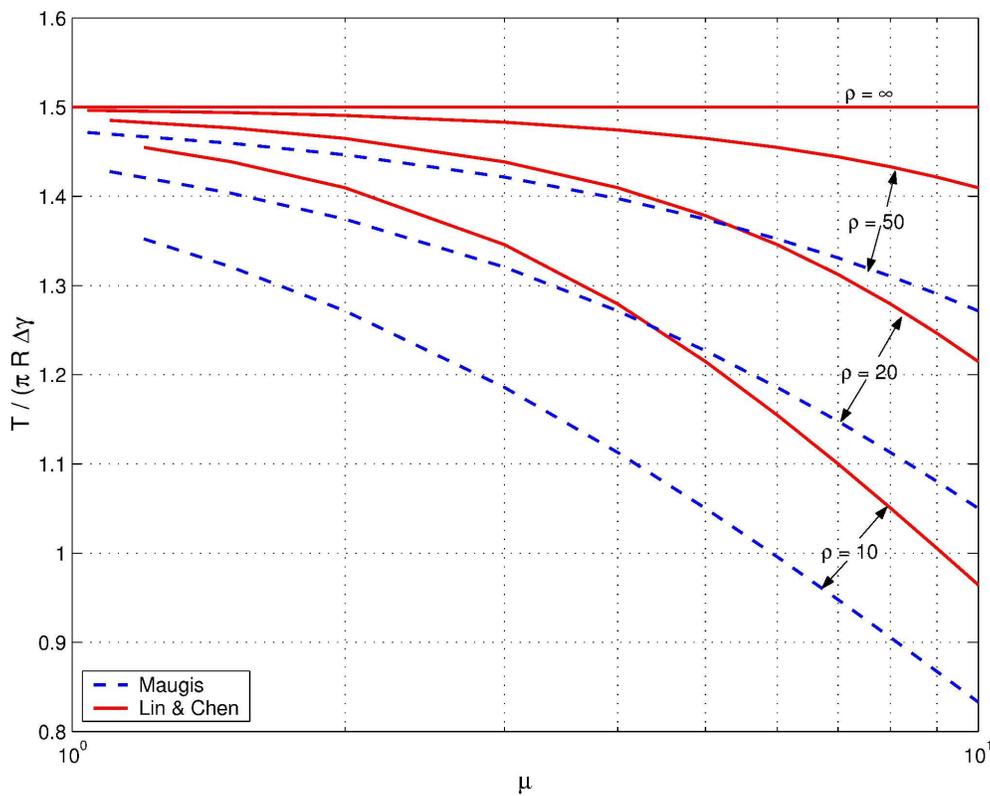
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Pull-off forces according to Maugis' extension of the jkr theory.  
The Lin & Chen curve is discussed below.  
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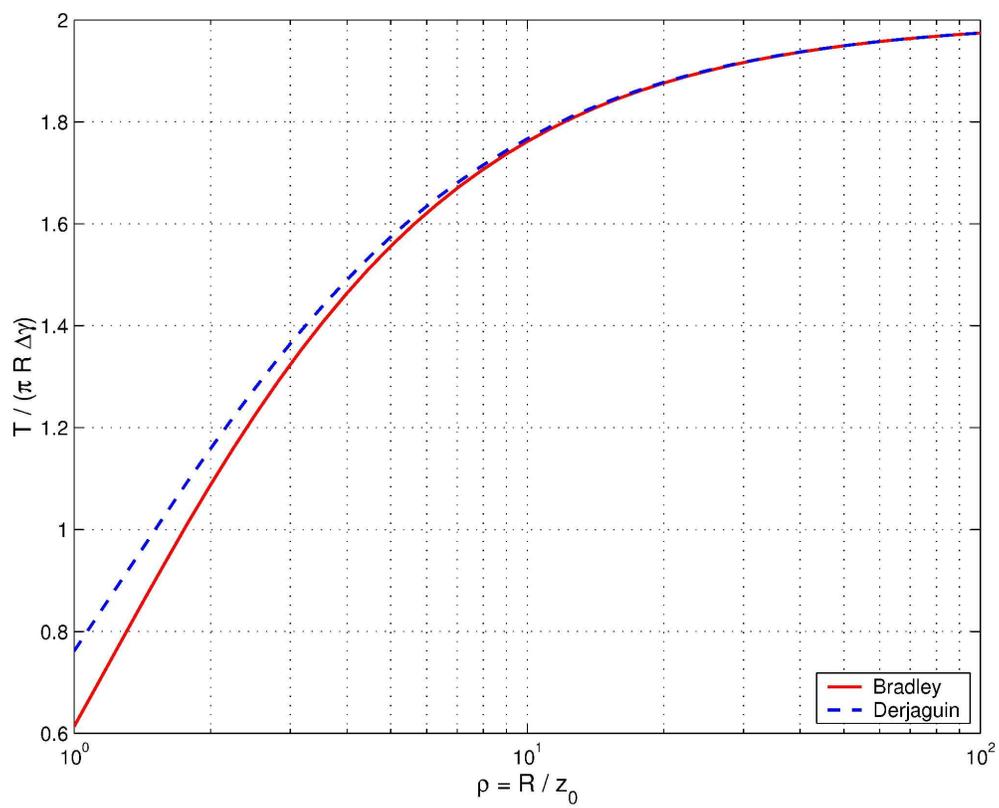
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Comparison of the two high- $\mu$  asymptotes  
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Comparison of exact rigid-sphere answer with value from the Derjaguin approximation  
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3 Figure 1. Pressure distribution at pull-off.

4 The inset shows that the pressure spike really was resolved

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7 Figure 2. Pull-off forces for a true finite sphere.

8 The green lines are the JKR sphere theory (high  $\mu$ ), or the rigid  
9 hemisphere theory (low  $\mu$ ), and are clearly excellent asymptotes.

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13 Figure 3. Contact radii at zero load.

14 For low  $\mu$  the radius is independent of the size ratio,  
15 but for  $\mu > 5$  the values for a finite sphere are lower.

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19 Figure 4. Contact radii at zero load.

20 Values of  $a_0 / R$  greater than 0.4 are highly suspect.

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24 Figure 5. Contact radii at pull-off.

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28 Figure 6. Pull-off forces according to Maugis' extended JKR theory.

29 The Lin & Chen curve is discussed below.

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33 Figure 7. Comparison of the two high- $\mu$  asymptotes.

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37 Figure 8. Comparison between the exact rigid-sphere answer and the  
38 value based on the 'Derjaguin approximation'.  
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