Solutions to Tutorial 7

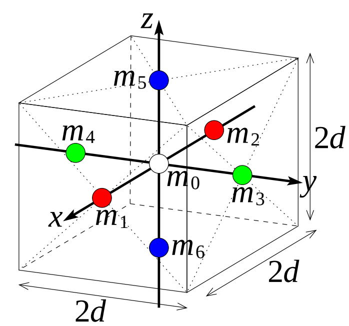
PHYS 2302 (Mechanics I); D. A. Clarke

Tutorial 7.1

Problem 1 (FC 4.19) The potential energy of interaction between any two atoms in a simple cubic lattice has the form $U(r) \sim cr^{-\alpha}$, where c and α are constants, and where r is the distance between the atoms. Show that the total energy of interaction of a given atom with its six nearest neighbours is approximately the potential of a 3-D harmonic oscillator, namely:

$$U(x,y,z) \;\sim\; A + B(x^2+y^2+z^2), \qquad (1)$$

where A and B are constants, and where (x,y,z) is the displacement of the given atom from its equilibrium position.



Hint: As shown in the diagram, place the atom of interest, m_0, at the origin, its six nearest neighbours ($m_1 \rightarrow m_6$) at $(\pm d,0,0)$, $(0,\pm d,0)$, and $(0,0,\pm d)$, and then displace m_0 by an arbitrary displacement (x,y,z) such that $x^2+y^2+z^2 \ll d^2$. Then,

$$U(x,y,z) \;=\; c\sum_{i=1}^{6} r_i^{-\alpha}, \qquad (2)$$

where $r_1 = \sqrt{(d-x)^2+y^2+z^2}$, and *etc.* for $r_2,\dots,r_6$. The approximation formulæ in Appendix D of the text may help.

Solution: As suggested in the problem statement, the displacements between m_0 and each of its six nearest neighbours are:

$$\begin{aligned}
\vec r_1 &= (d,0,0)-(x,y,z) = (d-x,-y,-z) &\Rightarrow\quad r_1 &= \sqrt{(d-x)^2+y^2+z^2};\\
\vec r_2 &= (-d,0,0)-(x,y,z) = (-d-x,-y,-z) &\Rightarrow\quad r_2 &= \sqrt{(d+x)^2+y^2+z^2};\\
\vec r_3 &= (0,d,0)-(x,y,z) = (-x,d-y,-z) &\Rightarrow\quad r_3 &= \sqrt{x^2+(d-y)^2+z^2};\\
\vec r_4 &= (0,-d,0)-(x,y,z) = (-x,-d-y,-z) &\Rightarrow\quad r_4 &= \sqrt{x^2+(d+y)^2+z^2};\\
\vec r_5 &= (0,0,d)-(x,y,z) = (-x,-y,d-z) &\Rightarrow\quad r_5 &= \sqrt{x^2+y^2+(d-z)^2};\\
\vec r_6 &= (0,0,-d)-(x,y,z) = (-x,-y,-d-z) &\Rightarrow\quad r_6 &= \sqrt{x^2+y^2+(d+z)^2}.
\end{aligned}$$

Now, neglecting all atoms beyond the six nearest neighbours of m_0, and assuming $m_1 \rightarrow m_6$ all remain fixed, the potential for m_0 is given by equation (2). To make progress, we must exploit the fact that $d^2 \gg x^2 + y^2 + z^2$ and, for this, we'll use the binomial expansion. Thus, for r_1,

$$r_1 = \sqrt{(d-x)^2 + y^2 + z^2} = \sqrt{d^2 - 2xd + x^2 + y^2 + z^2} = d\left(1 - \frac{2x}{d} + \frac{\rho^2}{d^2}\right)^{-1/2},$$

where $\rho^2 = x^2 + y^2 + z^2$. Thus,

$$\begin{aligned} r_1^{-\alpha} &= d^{-\alpha}\left(1 - \frac{2x}{d} + \frac{\rho^2}{d^2}\right)^{-\alpha/2} \\ &= d^{-\alpha}\left(1 + \underbrace{\left(-\frac{\alpha}{2}\right)\left(\frac{\rho^2}{d^2} - \frac{2x}{d}\right)}_{1^{\text{st}}\text{ order term}} + \underbrace{\frac{1}{2!}\left(-\frac{\alpha}{2}\right)\left(-\frac{\alpha}{2} - 1\right)\left(\frac{\rho^2}{d^2} - \frac{2x}{d}\right)^2}_{2^{\text{nd}}\text{ order term}} + \ldots\right) \\ &= d^{-\alpha}\left(1 + \frac{\alpha x}{d} - \frac{\alpha\rho^2}{2d^2} + \frac{\alpha(\alpha+2)}{8}\left(\frac{4x^2}{d^2} - \frac{4x\rho^2}{d^3} + \frac{\rho^4}{d^4}\right) + \ldots\right) \end{aligned}$$

This is an important example of the use of the binomial theorem, so listen up! If you are looking to a binomial expansion to give you a power series out to a particular order (here, we're looking for second order), then it is critical that you keep enough terms so that *all* the terms of the desired order are kept.

In this case, the first order term actually contains terms proportional to $1/d$ *and* $1/d^2$. Thus, the second order term, being proportional to the first order term squared, contains terms proportional to $1/d^2$, $1/d^3$, and $1/d^4$. Thus, if we want a power series complete to $1/d^2$, we must keep all of the first order term *plus* the leading term in the second order term, namely the one proportional to $1/d^2$. The terms proportional to $1/d^3$ and $1/d^4$, being very much smaller, we can safely discard.

OK, back to the solution: Keeping all terms proportional to $1/d$ and $1/d^2$, we get:

$$r_1^{-\alpha} \approx d^{-\alpha}\left(1 + \frac{\alpha x}{d} - \frac{\alpha\rho^2}{2d^2} + \frac{\alpha(\alpha+2)x^2}{2d^2}\right) = d^{-\alpha}\left(1 + \frac{\alpha x}{d} + \alpha\frac{(\alpha+2)x^2 - \rho^2}{2d^2}\right)$$

Similarly, we find:

$$\begin{aligned} r_2^{-\alpha} &\approx d^{-\alpha}\left(1 - \frac{\alpha x}{d} + \alpha\frac{(\alpha+2)x^2 - \rho^2}{2d^2}\right) \\ r_3^{-\alpha} &\approx d^{-\alpha}\left(1 + \frac{\alpha y}{d} + \alpha\frac{(\alpha+2)y^2 - \rho^2}{2d^2}\right) \\ r_4^{-\alpha} &\approx d^{-\alpha}\left(1 - \frac{\alpha y}{d} + \alpha\frac{(\alpha+2)y^2 - \rho^2}{2d^2}\right) \\ r_5^{-\alpha} &\approx d^{-\alpha}\left(1 + \frac{\alpha z}{d} + \alpha\frac{(\alpha+2)z^2 - \rho^2}{2d^2}\right) \end{aligned}$$

$$r_6^{-\alpha} \approx d^{-\alpha}\left(1 - \frac{\alpha z}{d} + \alpha\frac{(\alpha+2)z^2 - \rho^2}{2d^2}\right)$$

Substituting all these into equation (2), we get:

$$\begin{aligned} U(x,y,z) \approx cd^{-\alpha}\Bigg(&1 + \cancel{\frac{\alpha x}{d}} + \alpha\frac{(\alpha+2)x^2-\rho^2}{2d^2} + 1 - \cancel{\frac{\alpha x}{d}} + \alpha\frac{(\alpha+2)x^2-\rho^2}{2d^2} + \\ &1 + \cancel{\frac{\alpha y}{d}} + \alpha\frac{(\alpha+2)y^2-\rho^2}{2d^2} + 1 - \cancel{\frac{\alpha y}{d}} + \alpha\frac{(\alpha+2)y^2-\rho^2}{2d^2} + \\ &1 + \cancel{\frac{\alpha z}{d}} + \alpha\frac{(\alpha+2)z^2-\rho^2}{2d^2} + 1 - \cancel{\frac{\alpha z}{d}} + \alpha\frac{(\alpha+2)z^2-\rho^2}{2d^2}\Bigg) \end{aligned}$$

$$\Rightarrow \quad U(x,y,z) \approx cd^{-\alpha}\left(6 + \alpha\frac{(\alpha+2)2\rho^2 - 6\rho^2}{2d^2}\right) = cd^{-\alpha}\left(6 + \alpha\frac{\alpha-1}{d^2}\rho^2\right)$$

$$= \boxed{6cd^{-\alpha} + cd^{-(\alpha+2)}\alpha(\alpha-1)\big(x^2+y^2+z^2\big),}$$

which has the form of a 3-D harmonic oscillator, as suggested by equation (1).

Note that all the terms proportional to $1/d$ cancelled, and thus, had we only aimed for a power series to first order (proportional to $1/d$) only, we would have found only the constant term, $6cd^{-\alpha}$, which would have been insufficient for this problem. If, in using the binomial expansion, you find that all the "interesting terms" go away, this often means you have to go back to where you made the binomial expansion and carry it to another order in smallness.

Tutorial 7.2

Problem 2 Show that despite depending upon velocity, the Lorentz force as given by Eq. (3.5.1) is conservative. That is, show that $\nabla \times \vec{F} = 0$.

Solution: Start by writing down the Lorentz force as given by Eq. (3.5.1):

$$\vec{F} = qB_0\big(\dot{y}(t)\hat{\imath} - \dot{x}(t)\hat{\jmath}\big) = qB_0\omega\big(-A\cos(\omega t+\delta)\hat{\imath} + A\sin(\omega t+\delta)\hat{\jmath}\big), \tag{1}$$

using Eq. (3.5.5) and the second of Eq. (3.5.6) from the class notes. But, from Eq. (3.5.4) and the first of Eq. (3.5.6), we have:

$$x - a = A\cos(\omega t+\delta) \qquad \text{and} \qquad y - b = -A\sin(\omega t+\delta),$$

and Eq. (1) becomes:

$$\vec{F} = -qB_0\omega(x-a, y-b, 0) \quad \Rightarrow \quad \nabla\times\vec{F} = 0,$$

and Lorentz force is conservative.

Indeed, because $\vec{F} \perp \vec{v}$ (like a centripetal force), $\vec{F}$ cannot change speed (and thus K) of particle, just its direction.