Peierls-Nabarro potential for a confined chain of hard spheres under compression

A. Mughal, D. Weaire and S. Hutzler

1 Department of Mathematics, Aberystwyth University - Penglais, Aberystwyth, Ceredigion, Wales, SY23 3BZ, UK
2 School of Physics, Trinity College Dublin, The University of Dublin - Dublin, Ireland

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Abstract – Examples of bifurcation diagrams are presented for a chain of hard spheres under compression, which are confined by a transverse potential. The diagrams are modified in the presence of an axial force and show interesting topological rearrangements due to the reconnection of loci of different equilibrium solutions. The corresponding Peierls-Nabarro potential is defined and calculated for various values of compression. This relatively tractable and transparent system can illustrate in detail the general features of such a potential and its relation to experiment.

Introduction. – The Peierls-Nabarro (PN) potential originated in the theory of dislocations [1]. The motion of a dislocation through a crystal under an applied stress is subject to a potential arising from its discreteness: this is the PN potential.

The concept of the PN potential has found broad application in understanding a range of one-dimensional systems in which its significance is more straightforward. In all such systems there exists some sort of localised concentration or disturbance (often described as a kink or soliton) which may be moved from one position to another by the application of an appropriate force. A potential opposing the displacement may be adduced. The precise definition and procedure are somewhat arbitrary; consequently there is some slight arbitrariness in the choice of definition of the potential. Often this potential is defined and investigated for effectively infinite systems and emerges as a periodic potential. In finite systems, such as the one described below, the potential is of finite extent, and not periodic.

Examples of (quasi) one-dimensional systems in which the PN potential has been studied include the dynamics of vortex lattices in narrow channels [2], the sliding of chains of colloidal particles over corrugated surfaces [3, 4], the nanoscopic origins of friction [5], the mechanical unzipping of DNA [6], dynamics of polarons in one-dimensional molecular lattices [7] and solitons in Bose-Einstein condensates [8,9].

A prominent area in which the PN potential finds current applications is the study of ions confined in radio-frequency traps [10]. When cooled (by the use of laser radiation in the presence of an appropriate potential) ions condense into linear chains. In recent years these systems have attracted significant attention, not just because of their inherent scientific interest, but also for their applications in areas such as spectroscopy [11], frequency standards [12] and quantum computing [13–17].

Further examples and applications of the PN potential are given in [18]. Many of them can be related to the simpler system under consideration here which is exceptionally tractable and transparent. It concerns the buckling of a line of hard spheres under compression [19–21], in the presence of a transverse harmonic potential which opposes their displacement. This system has interesting properties; the linear chain buckles to form a variety of zigzag structures. The buckling is modulated and becomes increasingly localized as compression is increased. The equilibrium states of the system, stable and unstable, may be computed using a stepwise algorithm [19,21] and a continuum model has been adduced to help with the analysis of the results [21,22]. The present paper adds a further dimension to this study, the computation of the Peierls-Nabarro potential.

(a)E-mail: adil.m.mughal@gmail.com (corresponding author)
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well [21], which are also single peaked: these play a role
in what follows.

In this configuration of lowest energy the role of the dislocation is played instead by a localised peak. We therefore define the PN potential as the energy of the buckled chain as a function of buckling peak position $x_p$, for some fixed length $L$. In the theory of dislocations the PN potential is defined as the energy of the dislocated lattice as a function of the position of the dislocation (where the crystal has some fixed volume). In the case of our chain of hard spheres, the role of the dislocation is played instead by a localised peak. We therefore define the PN potential as the energy of the buckled chain as a function of buckling peak position $x_p$, for some fixed length ($i.e.$, compression).

To compute the Peierls-Nabarro (PN) potential we impose a longitudinal force $T$, which may be called “tilt” since it can be realised in experiments by tilting the apparatus, which displaces the localised buckling peak. The addition of the tilt force requires a simple modification of the equation used in the stepwise method [21]. Positive values of tilt displace the buckling peak towards the left-hand wall at $x = 0$ (as shown in fig. 2).

The energy $E$ of the structure, due to the displacement of the spheres, is given by summing the harmonic potential $-\frac{1}{2}y^2$ for all $N$ spheres. The stepwise “shooting method” (see [21]) enables (stable or unstable) equilibrium configurations to be readily computed, and hence $E$ and $x_p$ for each equilibrium configuration.

By keeping compression $\Delta$ fixed and varying the tilt force $T$ we can shift the position of the buckling peak. We are then able to compute the PN potential $E(x_p)$ for the chosen value of $\Delta$.

**Bifurcation diagrams for position.** – Here we will focus on bifurcation diagrams in terms of compression $\Delta$ and buckling peak position $x_p$ (rather than energy as in previous work [21]). The effect of tilt $T$ is to modify the bifurcation diagrams as described below.

In the absence of tilt, the bifurcation diagram of peak position $x_p$ is shown in fig. 3 for the case of ten spheres. For low values of compression there is only one solution, the structure with a buckling peak at $x_p = 0$.

With increasing compression the off-centre solutions emerge in pairs via “blue sky” bifurcations. One solution

\[
x_p = \frac{\sum_{n=1}^{N} y_n^2 (x_n - L/2)}{\sum_{n=1}^{N} y_n^2}.
\] (1)

We have adopted the following for the definition of the position $x_p$ of the localised buckling for a given equilibrium state, relative to the centre:

\[
x_p = \frac{\sum_{n=1}^{N} y_n^2 (x_n - L/2)}{\sum_{n=1}^{N} y_n^2}.
\]

In this configuration of lowest energy the profile of displacement has a single peak, which is antisymmetric (in displacement) about the centre. All lowest-energy structures for a given compression have such symmetry. As compression is increased, off-centre solutions arise as well [21], which are also single peaked: these play a role in what follows.

Our interest in this case of buckling arose from its experimental realisation using a lathe to create a centrifugal force (for buoyant spheres) [19,23] to supply the transverse restoring force [19]. We have subsequently shown that much more elementary set-ups can be employed [20,21]. The present paper is entirely theoretical but we intend to undertake its experimental counterpart in due course.

**The buckled chain.** – A line of hard spheres in contact is unstable with respect to infinitesimal compression (that is, reduction in length). This is still the case when a harmonic potential is introduced in the transverse direction, opposing the lateral displacement of each sphere. With hard wall boundary conditions on both ends the effect of compression is to produce a modulated zigzag structure [21]: an example of such a structure is shown in fig. 1, along with a plot of the amplitude of displacement for each sphere in the $y$-direction. We define the dimensionless compression as $\Delta = N - L/d$, where $d$ is the sphere diameter and $L$ is the chain length.

In this configuration of lowest energy the profile of displacement has a single peak, which is antisymmetric (in displacement) about the centre. All lowest-energy structures for a given compression have such symmetry.
is mechanically stable (continuous line) while the other is unstable (dashed line). An unstable state generally has a profile of displacement that is peaked on a single sphere, while it is shared more or less equally between two adjacent spheres in the case of a doublet state (this latter type of profile shown in fig. 1). Nevertheless, the two states emerge together at the same position, when a bifurcation appears. This is readily interpreted, in terms of the quadratic form of the confining potential and the minimisation/maximisation of energy by varying peak position.

The locus of each stable or unstable state is terminated at the point at which a sphere comes into contact with a second nearest neighbour, we are not concerned here with structures that are formed beyond such a point [21]. In the case of the stable structures all of the branches terminate in an arrangement which we have called the doublet [21]. It corresponds to two spheres arranged side by side in the transverse direction while the remaining spheres form an unbuckled linear chain. There are nine such possible configurations for a doublet for a chain of $N = 10$ spheres and tilt $T = 0$. The solutions terminate at points indicated by coloured dots, as defined in [21]. The solution indicated in the above diagram (with $\Delta = 0.7$ and $T = 0$) is shown in fig. 1.

In the presence of tilt the bifurcation diagram defined by position $x_p$ and compression $\Delta$ is modified; an example for tilt $T = 1.7 \times 10^{-4}$ is shown in fig. 4. In general there exists only one solution for low values of compression, but the effect of the tilt is to shift the location of its peak (as measured by $x_p$) so that it is no longer located at the midpoint of the system (see fig. 4)—even for an infinitesimal compression. With increased tilt the peak is further displaced. It migrates in such a way as to “leap-frog” the other (off-centre) modes via a topological change as illustrated in fig. 5. An example of a structure with an off-centre peak is shown in fig. 2.

Figure 6 shows in detail the manner in which this rearrangement is achieved. With increasing tilt $T$ two curves in the bifurcation diagram are brought ever closer to each other (as indicated by the blue arrows). They make contact at an osculation point, whereupon they are connected as shown. Increasing tilt drives the newly formed curves further apart (as indicated by the red arrows). Note, as shown in fig. 5(b), there is a slight doubling-back in the shape of the newly formed curve.

**Peierls-Nabarro potential.** For any given value of compression we can construct the Peierls-Nabarro potential as outlined above. Several examples are shown in fig. 7.

For small $\Delta$ the potential only has a single minimum, corresponding to the single solution at low compression in the bifurcation diagram, fig. 3. The minimum of $E(x_p)$ is located at the middle of the system and increases (in a roughly parabolic manner) as the buckling peak is pushed towards either wall, this implies that the buckling peak is “repelled” by the walls.

As $\Delta$ increases the localised buckling peak (as shown in fig. 1(b)) narrows until it has a width comparable to the spacing between spheres, whereupon oscillations develop in the PN potential. The minima and maxima correspond respectively to stable and unstable equilibria for zero tilt, as may be identified by comparing with fig. 1. Thus, in the case of $N = 10$ for high values of compression the potential has nine minima. The two extreme minima for $\Delta = 1.0$ are not shown in fig. 7.

It can be seen that the magnitude of these oscillations increases with compression $\Delta$. For low values of $\Delta$ these can be thought of as shallow undulations superimposed over the underlying parabolic trend. However, for higher values of $\Delta$ the oscillations have the effect of suppressing the parabolic trend so that in the example of $\Delta = 1$, as shown in fig. 7, the parabolic trend can no longer

![Peierls-Nabarro potential](image_url)
Fig. 5: Bifurcation diagram for peak position $x_p$ (relative to the center) for $N = 10$ spheres and tilt (a) $T = 8.0 \times 10^{-4}$ and (b) $T = 8.7 \times 10^{-4}$. Below a critical tilt, as shown in (a) the branch indicated by the arrow ultimately terminates close to $x_p = -1$; however, as shown in (b), above a critical value of tilt the same branch instead terminates close to $x_p = -2$. The topological rearrangement occurs when two curves osculate, meeting at a point. Immediately after the transition they reconnect, as shown in (b).

Fig. 6: Approach to the topological change in fig. 5. The relevant curves meet at an osculation point and are reconnected.

Fig. 7: Examples of the Peierls-Nabarro potential calculated for various values of compression $\Delta = N - L/d$ for 10 hard spheres. For convenience we plot $E(x_p)/E_s$ where $E_s = E(x_p = 0, T = 0)$. For $\Delta = 1.0$ the two extreme minima are not shown in the diagram.

Fig. 8: An example of hysteresis, peak position varies as shown when tilt is varied - including abrupt jumps as indicated by vertical arrows. Red and blue arrows indicate increasing and decreasing tilt, respectively. The start and end points of the hysteresis loop are indicated by red and blue dots, the green dot is the point at which the tilt is reversed. See also the animation included in the supplementary video supp.mp4.

be discerned in the PN potential near the middle of the system.

The combination of the parabolic and oscillatory potentials can lead to hysteresis as described immediately below.

**Implications for experiments.** – The PN potential provides a convenient basis for prediction or interpretation of experimental results. For example, take the case $N = 10$ and $\Delta = 0.8$ which is included in fig. 7. We begin a gedanken experiment with the system in its lowest-energy state ($x_p = 0$) with zero tilt.

In the presence of tilt the dependence on energy becomes

$$E(x_p, T) = E(x_p) + Tx_p,$$

(2)
shifting the equilibrium position as shown in fig. 8 (red arrow) and the animation which is included in the supplementary video supp.mp4. This continues until the adjacent point of inflection of the PN potential is reached, whereupon the equilibrium becomes unstable, and we expect the system to fall into the neighbourhood of the adjacent stable equilibrium state. If the tilt continues to increase, a second abrupt change causes a further transition. In the example shown, the change of tilt is then reversed, resulting in a return path (blue arrows) with strong hysteresis.

Note that although the above details can be extracted from the bifurcation diagrams, nevertheless, the PN potential provides a more condensed and transparent basis for prediction of experimental results.

Conclusion. – Since the PN potential is readily calculated for this system it provides a convenient prototype for the wider discussion of the concept and its implications. It also provides an elementary platform for experimental investigations such as that suggested by [20,21] which we intend to pursue.

Hard spheres may be inappropriate for this, as some friction is involved, but small bubbles can provide a suitable alternative. The use of bubbles will entail a generalisation to interacting soft (elastic) particles but we expect qualitatively similar results to those described here. (Chains of colloids are for example being used to create moving density kinks when driven over a sinusoidal energy landscape [3].) Moreover, it should be possible to use bubbles of sufficiently small size (comparable to the capillary length) to ensure that the hard sphere limit is closely approached [24]. Indeed, a preliminary bubble experiment (without tilt) was described in [20].

These developments should extend the general understanding of the potential, by no means confined to the elementary hard sphere system presented here, which may be considered as a baseline for the development of a wider understanding of PN potentials.

Data availability statement: The data that support the findings of this study are available upon reasonable request from the authors.

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