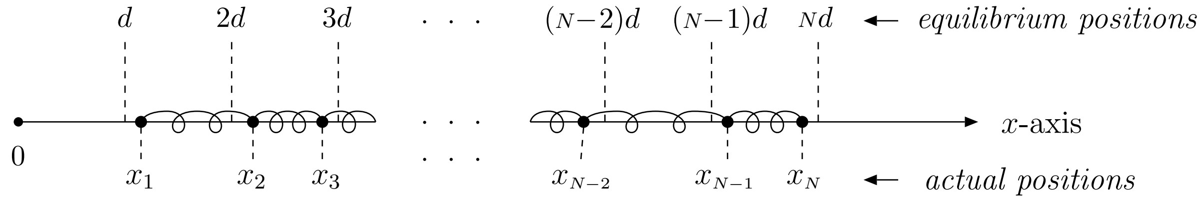
Exercises for Quantum Mechanics 3
Set 3

Exercise 5: Acoustic phonons in a 1-dimensional mono-atomic lattice

Consider a 1-dimensional mono-atomic lattice (chain) comprised of a very large odd number N of almost localized atoms of the same type. In equilibrium these atoms have a fixed lattice distance d to their nearest neighbours in the chain. For moderate deviations from the atomic equilibrium positions, the lattice vibrations can be modelled quite well by a chain of coupled springs.



This model is obtained by using at each atomic equilibrium position a parabolic approximation for the potential that the corresponding atom is experiencing due to the neighbouring atoms. As generalized coordinates we will use the deviations of the atoms with respect to the fixed equilibrium positions, $q_n = x_n - nd$ for $n = 1, \cdots, N$. For convenience finite-size effects are neglected by assuming that the very long atomic chain is periodic (ring shaped), so that $q_n = q_{n+N}$. This results in the following effective Hamilton operator:

$$\sum_{n=1}^{N} \Big[\frac{\hat{p}_n^2}{2m} + \frac{m\omega^2}{2} (\hat{q}_n - \hat{q}_{n-1})^2 \Big] = \boxed{\sum_{n=1}^{N} \Big[\frac{\hat{p}_n^2}{2m} + \frac{m\omega^2}{2} (2\hat{q}_n^2 - \hat{q}_n\hat{q}_{n-1} - \hat{q}_n\hat{q}_{n+1}) \Big] = \hat{H}} \, ,$$

where m is the atomic mass and $\sqrt{m\omega^2}$ the effective spring constant. Together the coordinate q_n and momentum p_n form a conjugate pair, which implies that the corresponding operators satisfy the usual (canonical) quantum mechanical quantization conditions

$$\big[\hat{q}_n, \hat{p}_{n'}\big] = i\hbar\delta_{nn'}\hat{1} \qquad \text{and} \qquad \big[\hat{q}_n, \hat{q}_{n'}\big] = \big[\hat{p}_n, \hat{p}_{n'}\big] = 0 \, .$$

Subsequently we diagonalize the Hamilton operator in an attempt to determine the vibrational eigenmodes. Due to translational symmetry over the fixed lattice distance d and the ensuing Bloch condition, it pays off to switch to normal coordinates u_k and conjugate momenta π_k by means of a discrete Fourier decomposition:

$$\hat{q}_n \;\equiv\; \frac{1}{\sqrt{N}} \sum_{k\,\in\,\text{B.Z.}} \mathrm{e}^{iknd}\,\hat{u}_k \qquad \text{and} \qquad \hat{p}_n \;\equiv\; \frac{1}{\sqrt{N}} \sum_{k\,\in\,\text{B.Z.}} \mathrm{e}^{-iknd}\,\hat{\pi}_k \;,$$

$$\hat{u}_k \;\equiv\; \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \mathrm{e}^{-iknd}\,\hat{q}_n \qquad \text{and} \qquad \hat{\pi}_k \;\equiv\; \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \mathrm{e}^{iknd}\,\hat{p}_n \;,$$

with corresponding orthonormality relation

$$\frac{1}{N} \sum_{n=1}^{N} \mathrm{e}^{i(k-k')nd} \;=\; \delta_{kk'} \;.$$

As a result of the periodicity condition $q_{n+N} = q_n$ we have to impose that $\mathrm{e}^{ikdN} = 1$, which implies that the wave number k can take N different values only. For odd N these values are distributed symmetrically around 0:

$$\underline{\text{1}^{\text{st}}\ \text{Brillouin zone (B.Z.)}}: \quad k \;=\; 0\,, \pm\frac{2\pi}{Nd}\,, \pm\frac{4\pi}{Nd}\,, \cdots, \pm\frac{(N-1)\pi}{Nd} \qquad (N\ \text{odd})\;.$$

(i) To what generic class of transformations does this Fourier decomposition belong?

(ii) Show that $\big[\hat{u}_k, \hat{\pi}_{k'}\big] = i\hbar\delta_{kk'}\,\hat{1}$ and argue that $\big[\hat{u}_k, \hat{u}_{k'}\big] = \big[\hat{\pi}_k, \hat{\pi}_{k'}\big] = 0$.

(iii) Give a simple argument why it was to be expected that also the normal coordinates and associated momenta satisfy canonical quantization conditions.

(iv) Use the orthonormality relation to derive that

$$\hat{H} \;=\; \sum_{k\,\in\,\text{B.Z.}} \Big(\frac{1}{2m}\,\hat{\pi}_k\hat{\pi}_{-k} \;+\; \frac{m\omega_k^2}{2}\,\hat{u}_k\hat{u}_{-k} \Big) \qquad \text{with} \qquad \omega_k \;=\; \omega\sqrt{2\big[1-\cos(kd)\big]}\;.$$

The lattice vibrations have been decoupled almost completely in this way.

(v) In analogy with the linear harmonic oscillator we now introduce a suitable set of raising and lowering operators:

$$\hat{a}_k \;=\; \Big(\hat{u}_k + \frac{i\hat{\pi}_{-k}}{m\omega_k}\Big)\sqrt{\frac{m\omega_k}{2\hbar}} \qquad \text{and} \qquad \hat{a}_k^\dagger \;=\; \Big(\hat{u}_{-k} - \frac{i\hat{\pi}_k}{m\omega_k}\Big)\sqrt{\frac{m\omega_k}{2\hbar}}$$

$$\Rightarrow \quad \hat{u}_k \;=\; \big(\hat{a}_k + \hat{a}_{-k}^\dagger\big)\sqrt{\frac{\hbar}{2m\omega_k}} \qquad \text{and} \qquad \hat{\pi}_k \;=\; \big(i\hat{a}_k^\dagger - i\hat{a}_{-k}\big)\sqrt{\frac{m\hbar\omega_k}{2}}\;,$$

using that $\hat{u}_k^\dagger = \hat{u}_{-k}$ and $\hat{\pi}_k^\dagger = \hat{\pi}_{-k}$.

– Show that these operators satisfy bosonic commutation relations

$$\big[\hat{a}_k, \hat{a}_{k'}^\dagger\big] \;=\; \delta_{kk'}\,\hat{1} \qquad \text{and} \qquad \big[\hat{a}_k, \hat{a}_{k'}\big] \;=\; \big[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger\big] \;=\; 0\;.$$

– Prove that the Hamilton operator decouples into N independent oscillator modes:

$$\hat{H} \;=\; \sum_{k\,\in\,\mathrm{B.Z.}} \hbar\omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \tfrac{1}{2}\,\hat{1}\right) \;.$$

The associated bosonic vibration quanta, with energy $\hbar\omega_k$ and momentum $\hbar k$, are called acoustic phonons (quantized sound waves).

– How will the Fourier component $\hat{u}_k$ influence the total momentum of the system?

– Determine the operator $\hat{q}_{n_H}(t)$ in the Heisenberg picture.

(vi) Plot the relation between ω_k and k (dispersion relation) on the interval $k \in [0, \pi/d]$. Do the same for the speed of propagation $\omega_k/|k|$ of the harmonic sound waves.

(vii) A sound that is comprised of a packet of sound waves with exclusively low ω_k-values can propagate through the lattice without appreciable deformation. However, for increasingly larger contributions from higher frequencies in the sound-wave packet progressively more deformation (dispersion) will occur. Why is that?

(viii) Which property of the considered system is responsible for this?

(ix) Presentation assignment. There are models of gravity for which space is discrete (granular) on very small length scales, in analogy with the lattice discussed above.

On May 10 2009 a gamma-ray burst was observed involving light that had traveled for at least 10 billion years before reaching us. Within a second after the initial pulse of the burst a very energetic photon with $|k| = 1.5 \times 10^{17}\ \mathrm{m}^{-1}$ was detected (see Fig. 1). Assume that this photon was emitted in coincidence wih the initial pulse.[1] Use the formula on page 2 for the speed of wave propagation on a lattice to describe the k-dependence of the speed of light and derive from this an upper limit on the "lattice distance of discrete space". In this example the photons play the role of "the lattice phonons of discrete space". [*Nature* **462**, *331–334 (19 November 2009)*]

To clarify: the presentation (mini-lecture) of 10 − 15 minutes will count towards the bonus as one additional exercise set. It should be prepared by a group of 3-4 students and presented at the start of the next exercise class. In total there will be four or five of these presentation assignments and the idea is that everybody participates once. If you are not on the presentation team, you can treat the assignment as a bonus exercise and hand in the corresponding solution along with the solutions to the rest of the exercises.

[1] This assumption need not be true, of course. However, it will provide a conservative upper limit on the "lattice distance of discrete space", bearing in mind that the energetic photon will not have been emitted prior to the first pulse.

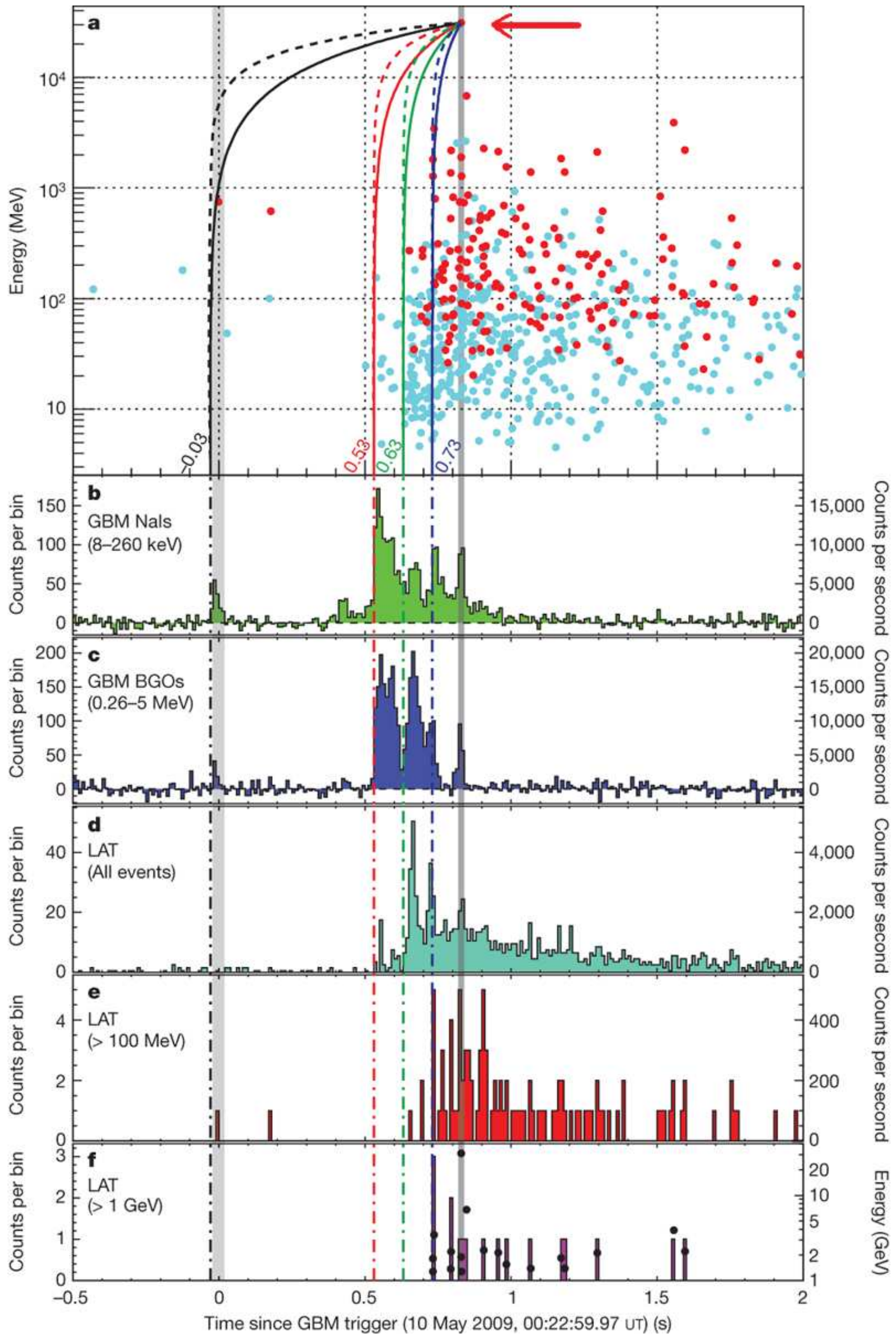


Figure 1: *Photons of the gamma-ray burst GRB090510 as observed by the Gamma-ray Burst Monitor (GBM) and the Large Area Telescope (LAT) on board the Fermi Gamma-ray Space Telescope. In panel* **a** *the energy of the high-energy LAT photons is plotted against the time of arrival in seconds. The zero of time is taken to coincide with the onset of the burst as seen by the GBM. The remaining panels show the light curves of the burst for several energy brackets, displayed as histograms that count the number of photons per time bin. Official source: Nature volume 462, pages 331–334 (19 November 2009).*