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Heat pumping in nanomechanical systems

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We propose using a phonon pumping mechanism to transfer heat from a cold to a hot body using a propagating modulation of the medium connecting the two bodies. This phonon pump can cool nanomechanical systems without the need for active feedback. We compute the lowest temperature that this refrigerator can achieve.

Freezing out atomic motion by cooling matter to absolute zero temperature is a thought that has, for ages, fascinated both scientists and laymen alike. In atomic gases, techniques such as evaporative cooling can bring temperatures down to the submicrokelvin scale, allowing for the observation of quantum phenomena such as Bose-Einstein condensation. In solid state matter, the ionic motion takes the form of oscillations around equilibrium positions, and completely freezing the system (in the case of an insulator) means removing all lattice vibrations – phonons – leaving solely the quantum mechanical zero-point motion.

The quest for observing quantized mechanical motion in macroscopic systems has incited several experimental groups in recent years [1]. In most cases, cooling is obtained by a feedback mechanism which involves optical or electronic sensors and some control system that acts directly on a cantilever.

In this paper, we argue that it is possible to cool a nanomechanical system without relying on feedback control. The mechanism we propose acts directly on the acoustic phonons carrying heat in and out of the system without the need for monitoring its state. By deforming the lattice in the medium connecting the mechanical system to its phonon thermal reservoir, one can pump heat against a temperature gradient by extracting out phonons. The mechanism resembles a classical cooling cycle of a thermal machine and its physical basis is time-reversal symmetry breaking. The pump works in both coherent and incoherent phonon regime.

Quantum coherent electron pumps have been studied extensively since Thouless's original proposal [2]. For instance, using lateral quantum dots and quantum wires, charge [3], spin [4, 5], and heat [6] currents can be created in the absence of bias by modulating adiabatically and periodically in time two independent external parameters. In contrast, pumping massless bosons such as acoustic phonons is a much more subtle problem. For one, it is much harder to pump adiabatically phonons due to the lack of a large energy scale such as the Fermi energy. Moreover, phonons not only obey a different wave equation but are also not conserved when scattered by

external perturbations that couple linearly to the displacement field (*i.e.*, a driving force). The result in this case is entropy generation in addition to pumping.

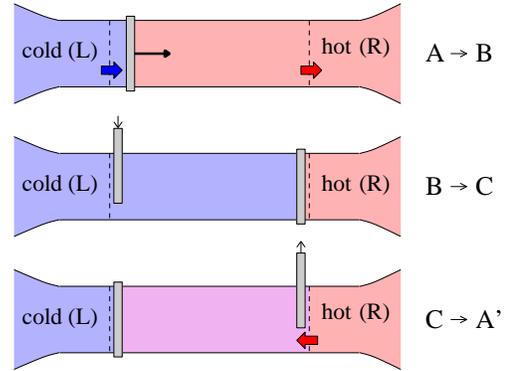


FIG. 1: Pumping cycle: $A \rightarrow B \rightarrow C \rightarrow A'$ (see text for an explanation). A traveling lattice perturbation acts as a semi-reflective barrier moving from cold to hot reservoir. The wide arrows indicate unimpeded heat flow.

In practice one can pump phonons with minimum heat generation by coupling quadratically to the displacement field, either by locally modulating the propagation velocity or by locally applying a pinning potential. An extreme example of a pinning perturbation, which preserves phonon number, is one that imposes Dirichlet boundary conditions to the displacement field at a given point in space. When such a perturbation travels along a quasi-one-dimensional medium, it works as a linear peristaltic pump. Below, we show that this mechanism allows for cooling down the system to a minimum temperature T_{\min} which, in one-dimension, is given by the expression

$$T_{\min} = \sqrt{\sqrt{\Theta_B^4 + T_H^4} - \Theta_B^2}, \quad (1)$$

with $\Theta_B = (\lambda/4\pi)\sqrt{5(1+\gamma)v_B/\pi c}$, where T_H is the temperature of the hot thermal reservoir, λ is the perturbation strength, c is the phonon velocity, v_B is the barrier speed, and γ is the Grüneisen parameter of the lattice.

A scheme of the pumping cycle is shown in Fig. 1,

where the nanomechanical system to be cooled is represented by the left (cold) side. The local modulation in the phonon velocity or pinning potential works like a moving semi-reflective barrier to the phonons. In process $A \rightarrow B$, the barrier is translated from the cold to the hot side of a cavity-like region. After it reaches the endpoint, another barrier-like perturbation is activated at the opposite side of the cavity (process $B \rightarrow C$). Then, in $C \rightarrow A'$, the first barrier is deactivated and phonons from the hot reservoir free expand into the cavity. The procedure is then repeated.

Interesting issues arise out of this simple process of moving a reflective barrier (a “mirror”) for phonons, in particular that of phonon pressure across the barrier. Indeed, a similar process to the one described above was used by Bartoli when he attempted to show the applicability of thermodynamics to electromagnetism and raised the question of radiation pressure [7], which in turn inspired Boltzmann in his studies of blackbody radiation [8]. The issue of phonon pressure is not trivial (and more subtle than the case of photons) as phonons carry crystal momentum (\mathbf{q}) but not obviously physical linear momentum (denoted by \mathbf{p}). The connection between these two forms of momentum requires anharmonicity and is given by $\mathbf{p}_{\mathbf{q}} = \gamma \hbar \mathbf{q}$ [9–11].

Let us then start by discussing first the simpler case of a fully reflective barrier. In this case, we can treat the problem as a “gas” of phonons, which we cycle according to Fig. 1. Notice that the barrier does not let heat pass through and the cooling will be due to the removal of internal energy from the left-hand side, dumping it into the right-hand side, as explained below.

The expansion $A \rightarrow B$ is adiabatic and reversible ($\Delta S_{R,L} = 0$, i.e., no heat exchange between left- and right-hand sides), so if the barrier moves to the right, the change in internal energies on the two sides are $E_L^B = E_L^A - p_L V_{\text{pipe}}$ and $E_R^B = E_R^A + p_R V_{\text{pipe}}$, where V_{pipe} is the swept volume. Then, once we insert the other barrier to get to C , we redraw the boundary of what L is. The volume of L changes by a factor $(V_L - V_{\text{pipe}})/V_L$. So in C we have $E_L^C = \left(1 - \frac{V_{\text{pipe}}}{V_L}\right) E_L^B$, $E_R^C = E_R^B$, and $E_{\text{pipe}}^C = \frac{V_{\text{pipe}}}{V_L} E_L^B$, where the last energy is the one inside the “pipe”. Then, once the right barrier is removed in going $C \rightarrow A'$, one redraws the boundary of what R is, so $E_L^{A'} = E_L^C$ and $E_R^{A'} = E_R^C + E_{\text{pipe}}^C$. Putting it all together, we have

$$\begin{aligned} \Delta E_L^{A \rightarrow A'} &= \left(1 - \frac{V_{\text{pipe}}}{V_L}\right) (E_L^A - p_L V_{\text{pipe}}) - E_L^A \\ &= -(e_L + p_L) V_{\text{pipe}} + \dots, \end{aligned} \quad (2a)$$

$$\begin{aligned} \Delta E_R^{A \rightarrow A'} &= \frac{V_{\text{pipe}}}{V_L} (E_L^A - p_L V_{\text{pipe}}) + p_R V_{\text{pipe}} \\ &= (e_L + p_R) V_{\text{pipe}} + \dots, \end{aligned} \quad (2b)$$

where \dots stand for terms down by powers of $V_{\text{pipe}}/V_{L,R}$, and $e_{R,L} = E_{R,L}/V_{R,L}$ are the intensive energy densities

in the two sides. All the work done occurs between $A \rightarrow B$, and is given by

$$W^{A \rightarrow A'} = (p_R - p_L) V_{\text{pipe}} + \dots, \quad (2c)$$

where the leading term is insensitive to changes in the pressures $p_{L,R}$ as the volume expands. Notice that the first law of thermodynamics is clearly satisfied via Eqs. (2a,2b,2c). All entropy increase occurs when the barrier is removed in going $C \rightarrow A'$, and the second law is also satisfied.

From this analysis, we can compute the energy flux out of the left reservoir per unit time of operation of the cycle:

$$\mathcal{J}_L^E = (e_L + p_L) v_B, \quad (3)$$

where v_B is the barrier speed. Here we use for total time the duration of the $A \rightarrow B$ stroke, assuming that the equilibration in the entropy production part $C \rightarrow A'$ is fast compared to this time.

The expression in Eq. (3) holds for a gas of particles, photons, or phonons. For our case of interest, $e_L = \eta_d T_L^{d+1}/c^d$ and $p_L = \gamma e_L/d$, where d is the spatial dimension, c is the phonon velocity and $\eta_d = 2g d! \zeta(d+1)/[(4\pi)^{d/2} \Gamma(d/2)]$. The Riemann zeta function and the Gamma function are denoted by $\zeta(z)$ and $\Gamma(z)$, respectively while g is a degeneracy factor. Notice that the energy flux depends only on the intensive quantities for the system on the left (and thus on T_L), and not on any property on the right-hand side of the barrier, in particular its temperature. Of course, this is a straightforward consequence of the fact that the barrier is perfectly reflective, so one is not faced with the difficulty of fighting a thermal gradient between the hot and cold reservoirs. The idealized situation, however, serves the purpose of displaying clearly the main principle for the cooling mechanism we discuss in this paper.

Let us then turn the discussion to the less idealized situation when the barrier is not perfectly reflective, allowing some heat to be transmitted from the hot to the cold side. In this case, we intuitively expect that the slower we move the barrier, the more difficult it becomes to cool, because the energy transferred in the operation $A \rightarrow B \rightarrow C \rightarrow A'$ depends only on the volume swept by the barrier, but not on the rate (as long as the $A \rightarrow B$ stroke is done in a quasi-equilibrium situation, allowing for thermal equilibration on both sides of the barrier). In addition, the longer we take to move the barrier to the right in the $A \rightarrow B$ stroke, the more heat is transferred through the transmitting barrier (the total transfer scales linearly with the sweeping time). So let us now compute the heat flow through the moving barrier, and the conditions to attain net cooling for a semi-reflective barrier moving with speed v_B . Hereafter, for the sake of simplicity, we focus on a purely one-dimensional case.

For concreteness, consider a “moving mirror” corresponding to a region in space where the atoms are coupled to an external short-range potential, which is localized in space. The position of this pinning potential is modulated in time so as to make it travel at speed v_B , causing the reflection and transmission coefficients to depend on the red and blue shifted frequencies of the phonons coming from the two reservoirs. Acoustic phonons in a one-dimensional chain, interacting with such a “moving mirror” potential of strength λ , obey the following wave equation in the continuum limit:

$$\partial_t^2 u(x, t) - c^2 \partial_x^2 u(x, t) = -\lambda c \delta(x - v_B t) u(x, t), \quad (4)$$

It is simpler to work in the reference frame of the barrier, $t' = t$ and $x' = x - v_B t$, where the wave equation becomes

$$\left[(\partial_{t'} - v_B \partial_{x'})^2 - c^2 \partial_{x'}^2 \right] u(x', t') = -\lambda c \delta(x') u(x', t'). \quad (5)$$

The function $u(x', t')$ and its partial time derivatives are continuous, but its partial space derivative is not. Then, integrating Eq. (5) between 0^- and 0^+ , we get the following boundary conditions in the barrier reference frame:

$$u(0^-, t') = u(0^+, t'), \quad (6a)$$

$$(v_B^2 - c^2) [\partial_{x'} u(0^+, t') - \partial_{x'} u(0^-, t')] = -\frac{\lambda c}{2} (u(0^+, t') + u(0^-, t')). \quad (6b)$$

Let us consider plane wave solutions to Eq. (5) in the two regions, to the left of the barrier (with amplitudes A_ω^- and B_ω^-) and to its right (with A_ω^+ and B_ω^+):

$$u_\pm(x', t') = \int d\omega e^{i\omega t'} \left(A_\omega^\pm e^{-i\omega x'/v_R} + B_\omega^\pm e^{i\omega x'/v_L} \right), \quad (7)$$

with $v_R = c - v_B$ and $v_L = c + v_B$. The boundary conditions (6a,6b) can be recast in a matrix form,

$$M_+(\omega) \begin{pmatrix} A_\omega^+ \\ B_\omega^+ \end{pmatrix} = M_-(\omega) \begin{pmatrix} A_\omega^- \\ B_\omega^- \end{pmatrix} \quad (8a)$$

where

$$M_\pm(\omega) = \begin{pmatrix} 1 & 1 \\ -i\omega v_L \mp \lambda c/2 & i\omega v_R \mp \lambda c/2 \end{pmatrix}. \quad (8b)$$

The transfer matrix $T(\omega)$ relating $\begin{pmatrix} A_\omega^+ \\ B_\omega^+ \end{pmatrix}$ to $\begin{pmatrix} A_\omega^- \\ B_\omega^- \end{pmatrix}$ is $T(\omega) = [M_+(\omega)]^{-1} M_-(\omega)$. From this transfer matrix, one obtains the needed scattering matrix:

$$S(\omega) = \begin{pmatrix} \frac{1}{1+i2\omega/\lambda} & \frac{i2\omega/\lambda}{1+i2\omega/\lambda} \\ \frac{-i2\omega/\lambda}{1+i2\omega/\lambda} & \frac{-1}{1+i2\omega/\lambda} \end{pmatrix}. \quad (9)$$

Now, to determine the heat transmission and reflection coefficients, one needs to go back to the frame of reference of laboratory (*i.e.*, that of the reservoirs). The reason is that the Bose-Einstein occupation numbers of the phonons are known in the rest frame of the reservoirs. In the laboratory frame, the solutions to Eqs. (4) away from the barrier are (to the left and right, respectively)

$$u_\pm(x, t) = \int d\omega e^{i\omega t} \left(a_\omega^\pm e^{-i\omega x/c} + b_\omega^\pm e^{i\omega x/c} \right). \quad (10)$$

These solutions can be matched to the mirror frame solutions Eq. (7) via the frequency rescalings

$$A_\omega^\pm = \left(\frac{c}{v_R} \right) a_{\omega c/v_R}^\pm, \quad B_\omega^\pm = \left(\frac{c}{v_L} \right) b_{\omega c/v_L}^\pm. \quad (11)$$

We know that the phonons leaving the reservoirs satisfy Bose-Einstein distributions at temperatures $T_{L,R}$: $\langle a_\omega^- \dagger a_\omega^- \rangle = n_L(\omega)$ and $\langle b_\omega^+ \dagger b_\omega^+ \rangle = n_R(\omega)$. Moreover, phonons incoming from different reservoirs are uncorrelated: $\langle a_\omega^- \dagger b_\omega^+ \rangle = \langle b_\omega^+ \dagger a_\omega^- \rangle = 0$. Thus, the heat current leaving the left reservoir is

$$\mathcal{J}_L^Q = I_{a^-} - I_{b^-} \quad (12)$$

where

$$I_{a^-} = \int_0^\infty d\omega \omega [n_L(\omega) + 1], \quad (13)$$

$$I_{b^-} = \int_0^\infty d\omega \omega [\langle b_\omega^- \dagger b_\omega^- \rangle + 1]. \quad (14)$$

To compute I_{b^-} we need to express $\langle b_\omega^- \dagger b_\omega^- \rangle$ in terms of the known distributions $n_{L,R}(\omega)$. Using the scattering matrix elements, after a few manipulations we can write

$$\begin{aligned} \langle b_\omega^- \dagger b_\omega^- \rangle &= \left(\frac{v_L}{v_R} \right)^2 |S_{11} \left(\frac{\omega v_L}{c} \right)|^2 n_L \left(\frac{\omega v_L}{v_R} \right) \\ &\quad + |S_{12} \left(\frac{\omega v_L}{c} \right)|^2 n_R(\omega), \end{aligned} \quad (15)$$

from which we obtain (using $|S_{11}|^2 + |S_{12}|^2 = 1$ and rescaling some integration variables)

$$\begin{aligned} \mathcal{J}_L^Q &= \int d\omega \omega |S_{12}(\omega)|^2 [n_L(\omega) - n_R(\omega)] \\ &\quad + \int d\omega \omega |S_{11}(\omega)|^2 \left\{ \left[n_L(\omega) - \left(\frac{c}{v_R} \right)^2 n_L \left(\frac{\omega c}{v_R} \right) \right] \right. \\ &\quad \left. - \left[n_R(\omega) - \left(\frac{c}{v_L} \right)^2 n_R \left(\frac{\omega c}{v_L} \right) \right] \right\}. \end{aligned} \quad (16)$$

The first line of Eq. (16) is the thermal heat current I_{thermal} from left to right in the presence of a non-moving barrier. The second line, which we name I_{pump} , results from the barrier motion and it is clearly zero when $v_B \rightarrow 0$ ($v_L = v_R = c$). In the limit when the barrier

amplitude is high, $\lambda \gg T_{R,L}$, we obtain for the total heat current

$$\mathcal{J}_L^Q \approx \frac{4\pi^4}{15} \frac{1}{\lambda^2 c^2} (T_L^4 v_R^2 - T_R^4 v_L^2). \quad (17)$$

Notice that this current is always negative if $T_L < T_R$ and $v_B > 0$ (with $v_R > v_L$), thus, as expected, we are fighting this heat flux with the energy flux of Eq. (3). A net flux of energy is indeed possible if we satisfy $\mathcal{J}_L^E + \mathcal{J}_L^Q > 0$, which requires

$$T_L^2 > \frac{8\pi^3}{5} \frac{1}{\lambda^2 c v_B (1 + \gamma)} (T_R^4 v_L^2 - T_L^4 v_R^2). \quad (18)$$

As mentioned earlier, for a fully reflective barrier ($\lambda \rightarrow \infty$), cooling can be obtained for any temperature gradient. For a semi-reflective barrier, to leading order in v_B/c , cooling requires $T_L > T_{\min}$, where T_{\min} is given by Eq. (1) with $T_H = T_R$. Notice that when $T_L = T_R = T$, the proposed mechanism also allows one to transfer heat between reservoirs provided that $T/\lambda < (1/4\pi)\sqrt{5(1+\gamma)}/2\pi$, independently of the barrier speed.

A few remarks are in order. First, even though the inequality (18) is weakly dependent on γ , anharmonicity is crucial for the operation of the cooling mechanism. Without anharmonicity, there would be no equilibration and thermalization with the left and right reservoirs as the barrier moves and heat transverse the barrier. A lower bound on the value of the Grüneisen parameter that can lead to refrigeration can be established by imposing that the phonon relaxation time is much shorter than the time required to move the barrier at speed v_B between reservoirs. Second, work is inevitably done when the barriers are activated and deactivated during the $B \rightarrow C$ and $C \rightarrow A'$ processes. However, during a fixed cycle, this work does not scale with the length of the cavity connecting the two reservoirs, while the amount of energy extracted from the cold reservoirs does. Therefore, the contribution of this work to the energy balance of the cooling process can be made very small for a sufficiently long cavity and we neglected it. Finally, although Eq. (16) has been derived assuming coherent heat transport, Eq. (3) does not rely on quantum coherence. Therefore, coherence is not an essential ingredient of the present heat pump.

For a practical implementation of this cooling mechanism, one has to produce a local and propagating pinning potential which couples to the atomic vibrational motion, or alternatively a propagating variation of the sound velocity of the medium. In fact, it is likely unavoidable that both effects occur simultaneously and what is most important is that the combined effect consists of creating a propagating barrier for phonons. An effective way of generating a moving pinning potential is by using some sort of electromechanical coupling (for instance by back gating), which is preferred to a purely mechanical one because

it allows for faster switching times. Following this reasoning, strongly electrostrictive materials at the nanoscale, in which local changes in the phonon couplings arise from anharmonic effects, should be the most attractive active media for realizing our heat pump. In particular, carbon or boron nitride nanotubes appear to be a promising class of materials for several reasons: (1) Measurements of nanoscale heat transport in nanotubes, although challenging, have already been performed by several groups [12–14]; (2) There are theoretical predictions of giant electrostrictive effects for both carbon [15] and boron nitride [16]; (3) Current technology and engineering of nanotube electromechanical devices are at an advanced level, as exemplified by development of carbon-nanotube nonvolatile electromechanical memories [17]. Another promising class of materials are strongly electrostrictive polymers such as poly-vinylidene fluoride (PVDF), in which giant electrostriction has been observed [18]. Recent theoretical predictions show that electric fields can virtually block the torsion modes contribution to heat transmission in PVDF [19], which would be equivalent to introducing an infinite barrier for such phonons in our scheme. Graphene is also an attractive possibility, since it has been experimentally demonstrated that substrate interactions (which can be tuned by gating) can strongly modulate the contribution of the ZA flexural modes to the thermal conductance of this material [20]. These modes, which have quadratic dispersion (zero sound velocity) for an unperturbed graphene sheet, can become linearly dispersive in strained graphene, therefore leading to substantial variations in the phonon propagation for these modes.

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