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THE NEW MECHANISM OF FOCUSING AND ENHANCING ACOUSTIC WAVES GENERATED BY METAL NANOPARTICLES WITHIN THE CRYSTAL LATTICE

We will discuss a possible mechanism for the focusing and enhancement of acoustic waves generated by metal nanoparticles embedded in a crystal lattice under ultrashort laser excitation. In contrast to continuous-medium models, the discrete lattice framework naturally gives rise to oscillatory wave tails appearing behind the propagating front. These tails arise from the breakdown of Huygens principle in even-dimensional spaces. The atomic dynamics can be interpreted as evolving within a six-dimensional configuration space, where the continuous subspace represents intra-cell displacements and the discrete indices correspond to the positions of unit cells. This effect can lead to a local enhancement of longitudinal acoustic wave amplitudes at specific lattice sites without any increase in the driving laser pulse intensity.

K e y w o r d s: nanoparticles, generating and focusing acoustic waves, Huygens principle.

1. Introduction

Metal nanoparticles embedded in dielectric crystals and excited by ultrashort laser pulses have attracted considerable attention as potential localized sources of coherent acoustic waves. The interaction of such waves with the host lattice is of interest for nanoscale energy localization, ultrafast signal processing, and the design of functional acoustic metamaterials.

In continuous media, the wave propagation in odd-dimensional spaces is usually associated with Huygens principle, whereby disturbances remain confined to a propagating front with no trailing oscillations. However, experimental and theoretical indications suggest that, in real crystals with discrete atomic structures, long-lived oscillatory wave tails may persist behind the main pulse. This points to a fundamental difference from the predictions of continuum models and suggests the need in a refined theoretical description.

One possible explanation lies in the hybrid discrete-continuous nature of crystal lattices. Atomic motion can be viewed as taking place in a configuration space of the form $\mathbb{R}^3 \times \mathbb{Z}^3$, where the continuous part represents intra-cell displacements and the discrete indices correspond to the positions of unit cells. Such a fibered description modifies propagation characteristics and can help one to account for the observed departures from Huygens principle. In this framework, the resulting oscillatory wave tails open up the possibility of focusing the acoustic energy through phase control over the multiple nanoparticle sources, potentially without increasing the laser pulse intensity.

The following sections outline a mathematical model for discrete lattice dynamics, discuss how this focusing effect may emerge, and consider implications for the energy control at the nanoscale. Connections with earlier approaches to discrete wave equations, hybrid configuration spaces, and the Bateman's formalism for oscillatory solutions are also noted.

Consider a spherical metal nanoparticle (NP) embedded in the surrounding matter (SM). A laser impulse acting on the nanoparticle (NP) can increase the electronic subsystem's temperature, and the subsystem can expand abruptly, generating sound waves in the surrounding medium (SM). The mechanism for

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generating longitudinal acoustic waves through the pressure of the hot electron gas in metal nanoparticles was proposed by P. Tomchuk [1]

$$\Delta p_e = p_0 \frac{5\pi^2}{12} \left(\frac{k_{\mathrm{B}} T_e}{\varepsilon_F}\right)^2. \tag{1}$$

As a boundary condition, the governing equation imposes equality between the additional pressure of the hot electron gas and the surface energy of the nanoparticle (NP)

$$\Delta p_e\,(t) = \frac{2\rho_s}{a^2}\xi\,(t), \tag{2}$$

The density of the nanoparticle (NP) surface energy is denoted by ρ_s, a represents the particle radius, and ξ is the radial displacement of the surface. The electronic temperature setting time is

$$\tau_e \sim 10^{-12} s. \tag{3}$$

The time required for the electron temperature to equalize with the lattice temperature in a bulk metal is

$$\tau_{e-ph} \sim 10^{-10} s. \tag{4}$$

Temporal pulsations of the nanoparticle's electronic temperature induce pressure oscillations in the surrounding dielectric, generating acoustic waves. The propagation of a longitudinal wave in the continuous approximation is described by the equation:

$$\nabla^2 \mathbf{u} - \frac{1}{s_l^2}\frac{\partial^2 \mathbf{u}}{\partial t^2} = 0, \tag{5}$$

where $\mathbf{u}$ is displacement vector. For a longitudinal wave, a scalar potential ψ can be introduced such that

$$\mathbf{u} \triangleq \nabla\psi, \tag{6}$$

where ψ is the solution of the equation

$$\nabla^2 \psi - \frac{1}{s_l^2}\frac{\partial^2 \psi}{\partial t^2} = 0, \tag{7}$$

subject to the boundary condition

$$\left.\frac{\partial \psi}{\partial r}\right|_{r=a} = \frac{a^2}{2\rho_s}\Delta p_e\,(t). \tag{8}$$

In this model of nanoparticle (NP) excitation, a longitudinal acoustic wave is generated in the matrix and oscillates at the NP's characteristic frequency. The solution to the corresponding Cauchy problem is:

$$\psi = -\frac{s_l\, a}{r}\, \exp\left\{-\frac{s_l}{a}\left[t - \frac{r-a}{s_l}\right]\right\} \times$$
$$\times \int\limits_{-\infty}^{t-\frac{r-a}{s_l}} \exp\left(s_l\, \frac{t_1}{a}\right) \xi\,(t_1)\, dt_1. \tag{9}$$

It is assumed that the oscillation begins at a specified initial time. The objective of this study is to determine the conditions under which an acoustic wave, generated by a nanoparticle (NP) in a solid matrix under the laser irradiation, can be focused and amplified. Solution (9) is inadequate for our purposes for two reasons. First, the continuum approximation must be transcended when analyzing acoustic wave propagation. Second, the excitation regime must be reconsidered from an alternative perspective – specifically, one in which excitation is driven by precisely timed femtosecond laser pulses. The justification for these conditions will be provided in subsequent sections.

The generation of acoustic waves by ultrashort laser pulses involves the rapid expansion of the Fermi gas within NPs on picosecond-to-femtosecond timescales. This expansion exerts pressure on the surrounding matrix atoms; consequently, the resulting sharp pressure pulse originating from the NP can be treated as an additional force acting on a free atom.

Huygens principle states that an initial state with sharply defined spatial localization later manifests at another location as an effect equally confined in space and time. Notably, this principle holds only in spaces of odd dimensionality. As will be shown, adherence to Huygens principle precludes the construction of the acoustic-wave focusing scheme proposed here.

This limitation changes fundamentally when the continuum approximation for the matrix-atom motion is abandoned. In other words, rather than using wave equation (7), which ignores the discrete nature of the atomic motion, one must revert to the equation governing the dynamics on a discrete lattice.

2. Generation of Acoustic Waves by Ultrashort Laser Pulses and the Breakdown of Huygens Principle in Lattice Systems

The generation of acoustic waves by ultrashort laser pulses involves the rapid expansion of the Fermi

electron gas within nanoparticles (NPs), occurring on femtosecond-to-picosecond timescales. This expansion generates transient electric fields that exert a pressure on the surrounding matrix atoms. The resulting sharp pressure pulse can be treated as an additional force acting on a free atom, initiating lattice vibrations and acoustic wave propagation.

To accurately describe this process, we must consider the structure and dynamics of the crystal on the atomic scale. The system of atoms in the crystal – accounting for both their discrete lattice positions and their three-dimensional displacements – is naturally described within the space

$$\mathcal{L} = \{(a,b,c) \in \mathbb{Z}^3,\ \mathbf{u}_{a,b,c} \in \mathbb{R}^3\}, \tag{10}$$

where (a,b,c) label discrete atomic sites and $\mathbf{u}_{a,b,c}$ denote the physical displacement vectors of these atoms in the ordinary Euclidean space $\mathbb{R}^3$. This space is not six-dimensional in any physical sense; rather, it is a structured representation that separates the discrete geometry of the crystal lattice from the three-dimensional kinematics of atomic motion.

Introducing the lattice–displacement space is not an approximation, but a refinement of the physical description. Unlike the continuum wave equation in R^3, which smooths out atomic discreteness and thereby enforces Huygens principle (i.e., sharp propagation of wavefronts), the discrete formulation inherently introduces dispersion and scattering effects, breaking Huygens principle. This breakdown permits propagation regimes – including controllable focusing of lattice waves – that cannot occur in a purely continuum model.

In a continuum setting, an initially localized disturbance propagates strictly on the surface of the light (or sound) cone, without internal trailing oscillations, if and only if the space dimension is odd. By contrast, in a discrete lattice, each atomic site obeys Newtonian equations of motion coupled to its neighbors, producing frequency-dependent group velocities and internal reflections. This dispersion eliminates the exact causal sharpness predicted by the continuum wave equation, thereby invalidating Huygens principle on the lattice scale.

Thus, the lattice–displacement space does not introduce artificial dimensions but instead preserves the true microscopic dynamics that the continuum approximation necessarily discards. As will be demonstrated, this discrete framework enables wave manipulation strategies – such as the acoustic focusing – that are inaccessible under the constraints imposed by Huygens principle in the continuum model.

3. The Equation of Motion of an Atom in a Three-Dimensional Crystal Lattice

Let us consider the classical equation of motion for an atom in a three-dimensional crystal lattice with regard for the interaction with the nearest atoms within the harmonic approximation [2]. For simplicity, we assume an infinite simple-cubic, isotropic, nearest-neighbor harmonic lattice. The equation of motion then reads

$$\frac{d^2\mathbf{u}(t)_{a,b,c}}{dt^2} = k^2 \cdot \Big\{\mathbf{u}(t)_{a+1,b,c} + \mathbf{u}(t)_{a-1,b,c} + \\ + \mathbf{u}(t)_{a,b+1,c} + \mathbf{u}(t)_{a,b-1,c} + \mathbf{u}(t)_{a,b,c+1} + \mathbf{u}(t)_{a,b,c-1}\Big\} - \\ - k^2 \cdot \{6 \cdot \mathbf{u}(t)_{a,b,c}\}, \tag{11}$$

where $k^2 = \frac{1}{m}\frac{d^2U(x)}{dx^2}\big|_{x=d}$, m represents the mass of the atom, $\frac{d^2U(x)}{dx^2}\big|_{x=d}$ is the second derivative of the interatomic potential evaluated at the equilibrium distance d.

For vortex-free atomic motion, we introduce a scalar potential such that

$$\mathbf{u} = \boldsymbol{\nabla}\varphi. \tag{12}$$

Substituting this into (11) shows that φ satisfies exactly the same discrete Laplacian form:

$$\frac{d^2\varphi(t)_{a,b,c}}{dt^2} = k^2 \cdot \Big\{\varphi(t)_{a+1,b,c} + \varphi(t)_{a-1,b,c} + \\ + \varphi(t)_{a,b+1,c} + \varphi(t)_{a,b-1,c} + \varphi(t)_{a,b,c+1} + \varphi(t)_{a,b,c-1}\Big\} - \\ - k^2 \cdot \{6 \cdot \varphi(t)_{a,b,c}\}. \tag{13}$$

Separable modes and the Cauchy solution Eq. (13) admits separable solutions of the form

$$\varphi_{p,q,r}(t) = X_{p-l}(t) \cdot Y_{q-m}(t) \cdot Z_{r-n}(t), \tag{14}$$

representing normal modes oscillating independently along each lattice axis. This captures purely axis-aligned interactions within the crystal basis. The full Cauchy problem, with arbitrary initial displacements and velocities, was solved in closed form by Bateman

[3]. The solution embeds the three- dimensional lattice into a higher – dimensional framework, producing an explicit expression

$$\varphi_{l,m,n}(t) = F(l,m,n,t;\, \varphi(0),\, \varphi'(0)), \tag{15}$$

where F is determined by this formalism. Physically, this reveals that the discrete lattice structure breaks the Huygens principle by generating persistent "wave tails". The solution of the Cauchy problem for (12), with given initial data $\varphi_{l,m,n}(0)$ and $\varphi'_{l,m,n}(0)$, can be written as

$$\varphi(t)_{p,q,r} = \sum I_{p,q,r;l,m,n}(t)\, \varphi(0)_{l,m,n} + \\ + \sum \int_0^t I_{p,q,r;l,m,n}(t_1)\, \varphi'(0)_{l,m,n} dt_1, \tag{16}$$

where the sums run over all lattice sites $(l,m,n) \in \mathbb{Z}^3$. The kernel $I_{p,q,r;l,m,n}(t)$ admits the explicit factorized representation

$$I_{p,q,r;l,m,n}(t) = \frac{1}{4\pi}\frac{d}{dt}\times \\ \times \left\{ t \int_0^{2\pi} \left[\int_0^{\pi} A(t,\theta,\alpha)_{p,q,r;l,m,n}\, \sin(\theta)\, d\theta \right] d\alpha \right\}, \tag{17}$$

with

$$A(t,\theta,\alpha)_{p,q,r;l,m,n} = J_{2\,(p-l)}(2kt\, \sin(\theta) \times \\ \times \cos(\alpha))\, J_{2\,(q-m)}(2kt\, \sin(\theta) \times \\ \times \sin(\alpha))\, J_{2(r-n)}(2kt\, \cos(\theta)) \tag{18}$$

and J_ν denoting the Bessel function of the first kind, which admits the integral representation

$$J_{2\,(p-l)}\,(2kt) = \\ = \frac{1}{\pi} \int_0^{\pi} \cos\left(2\,k\,t\, \sin\left(\phi\right) - 2(p-l)\,\phi\right) d\phi. \tag{19}$$

Thus, while the separable product form $\varphi_{p,q,r}(t) = X_{p-l}(t) Y_{q-m}(t) Z_{r-n}(t)$ represents a particular solution of Eq. (12), expression (13) with kernels (14)–(16) represents the general solution of the Cauchy problem, valid for arbitrary initial displacements and velocities on the infinite simple-cubic, isotropic, nearest-neighbor harmonic lattice.

The lattice dynamics are most naturally formulated not in the ordinary 3D space, but in a hybrid configuration space $\mathbb{R}^3 \times \mathbb{Z}^3$, where the continuous component $\mathbb{R}^3$ describes displacements of atoms within the unit cell and the discrete component $\mathbb{Z}^3$ indexes the lattice cells. This six-dimensional embedding makes separability along crystallographic axes explicit into this six-dimensional setting, making separability along crystallographic axes explicit. In even-dimensional spaces, however, Huygens principle fails: wavefronts are always followed by a dispersive oscillatory plume, even for initially localized excitations.

4. Focusing Acoustic Waves

The presence of an oscillating tail behind the sound front can be used to create devices that generate a self-focusing acoustic wave. Specifically, by generating acoustic waves in such a sequence that their extremums converge at a certain point in space simultaneously, the amplitude of oscillations at this point can be increased. Let the wavefront travels from the point of its generation to a certain point in space over the time t_0. Then, the extrema from other impulses follow with a tailored delay of Δt_i, such that they will reach the same point simultaneously. Therefore, the potential of waves at a given point in space, as given by

$$\bar{\varphi}(t_0, N)_{p,q,r,m,r,n} \equiv \sum_{i=0}^{N} \varphi(t_0 - \Delta t_i)_{p,l,q,m,r,n}, \\ \Delta t_0 = 0 \tag{20}$$

can greatly exceed the potential generated by a single impulse. The delay time before sending the next impulse is dependent on both the coordinates of the impulse generation point and the observation point. To avoid the unnecessary complexity of the formulas, we retain the notation of the time delay as presented in (20), understanding that Δt_i is a function of the indices p, l, q, m, r, n. For example, let us consider the result of a sequence of impulses generated by a single matrix atom, assuming that an external source of power acted on the atom. This sequence is selected such that the amplitude of the atom's vibration in the acoustic wave field increases over time at the chosen observation point. The graph in Fig. 1 illustrates the comparison of the potential when one generated wave is compared with four consecutive waves generated according to formula (20).

Lastly, potentials (20) enable the calculation of wave displacement. For example, if we introduce a

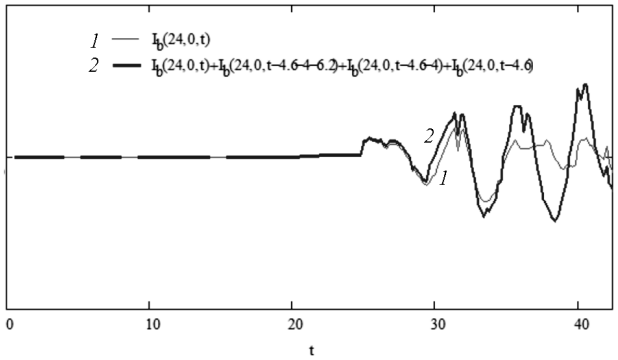

Fig. 1. The line (*1*) represents a change in the wave potential over time for a single generated wave, while the line (*2*) depicts a change in the wave potential over time for four generated waves, as described in formula (20)

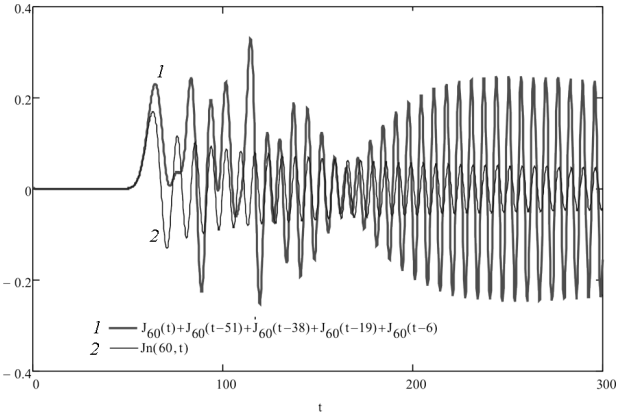

Fig. 2. Compares the graphs of waves generated by five consecutive impulses of the same initial amplitude with a single impulse of equivalent amplitude. The smallest distance between atoms is defined as the unit of length, and the time it takes for the wave front to pass through the distance between the two nearest atoms in the dielectric matrix is defined as the unit of time measurement unit

displacement component along one of the lattice's basis vectors, as shown in the equation

$$v\,(t,a)_{p,l,q,m,r,n} = \frac{\varphi(t)_{p+a,l,q,p,l,q} - \varphi(t)_{p-a,l,q,p,l,q}}{2a} \approx$$
$$\approx \frac{1}{2a}\frac{\partial\left(\varphi(t)_{p+a,l,q,p,l,q} - \varphi(t)_{p-a,l,q,p,l,q}\right)}{\partial a} +$$
$$+ \ldots \xrightarrow{a\to 0} v\,(t,p,l,q)_c\,, \qquad (21)$$

where a denotes the lattice constant and c signifies the continuous approximation applied within the crystal lattice framework This conceptualization of wave displacement within the lattice is consistent with the expression of wave displacement in a continuum, as

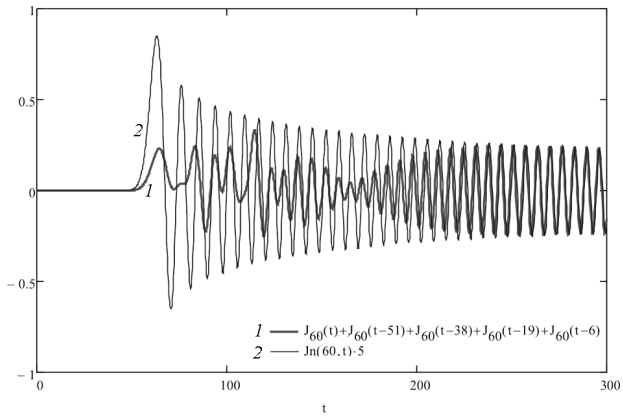

Fig. 3. The line (*2*) represents a series of five impulses, while the line (*1*) depicts a single impulse with an amplitude that is five times greater than that of each impulse in the series

demonstrated in this equation, where the variable p can be considered a continuous variable. The principal difference in determining the displacement of movement of an atom in the lattice using Eq. (13) compared to Eq. (21) is that the former accounts for the displacement of an individual atom, while the latter considers the difference in the displacement of neighboring atoms. Imagine a scenario, where all atoms move at the same displacement. There would be no wave in this case; instead, there would be a process equivalent to transitioning to a coordinate system moving with displacement **u**. In the latter case, $v\,(t,a)_{p,l,q,m,r,n} = 0$, since all atoms share the same potential and, consequently, the same displacement.

5. One-Dimensional Case

Let the wave travel along the crystalline axis of a cubic crystal with a primitive basis consisting of a single atom. Since all atomic planes are shifted in a co-phased manner, it suffices to consider a one-dimensional chain of atoms. This model was utilized by Havelock [2] to study the propagation of a periodic wave in the crystal and to determine the dispersion relations. The equation describing the motion of an atom along the base vector, in a harmonic approximation with the initial condition of non-zero displacement for that atom, is

$$\frac{d^2u_p}{dt^2} = k^2(u_{p-1} - 2u_p + u_{p+1}), \quad p \geq 2,$$
$$u_{p=0}(0) \neq 0, \quad u_{p>0}(0) = 0. \qquad (22)$$

The solution to this problem is a known function [3]

$$u(t)_{p-l} = J_{2(p-l)}(2kt). \qquad (23)$$

Similarly to the three-dimensional phenomenon, it is possible to increase the amplitude of vibrations at a specific point by generating acoustic waves in such a sequence that their peaks arrive at the same point in space simultaneously. Consider this sequence of impulses: the first impulse contributes to the movement of the impulse front initiated with a delay $t_0 - \Delta t_N$, and the subsequent impulses are associated with the action of the waves following the front. It is essential that all values at a given point reach their peak and trough simultaneously. This mechanism inherently leads to an increase in the amplitude of the vibration. The cumulative effect of a set of N impulses results in the amplification of the resultant signal by nearly N-fold

$$\bar{J}(t_0, N)_{p-l} \equiv \sum_{i=0}^{N} J_{2(p-l)}\left(2k\left(t_0 - \Delta t_i\right)\right), \quad \Delta t_0 = 0. \tag{24}$$

Figure 2 shows a comparison of a sequence of 5 impulses, all with the same initial amplitude, to a single impulse.

Figure 3 differs from the previous one in that the initial amplitude of a single impulse (represented by the line (*2*)) is five times greater than the amplitude of each individual impulse (represented by the line (*1*)) in a series of five impulses.

6. Conclusions

It is shown that such a system can generate longitudinal acoustic waves in a dielectric lattice, whose amplitude can be enhanced at a specific matrix point without increasing the intensity of the laser impulses. This effect arises from two key factors:

(i) the mathematical violation of Huygens principle due to the discrete-continuous coupling, and

(ii) the unique physical properties of metal nanoparticles.

The mathematical factor involves the breakdown of Huygens principle within a fibered space formed by the direct product of three-dimensional physical space and a discrete lattice index space. In this extended framework, the wavefront is followed by an oscillatory tail due to the coupling between continuous and discrete coordinates. By carefully timing the generation of each acoustic impulse so that their extremums converge both spatially and temporally at a chosen point, constructive interference can significantly amplify the total oscillation amplitude.

The second factor pertains to the unique properties of metal nanoparticles. Exciting the electronic subsystem of these particles can result in effects such as the emission of electrons at temperatures higher than 8000 K, as well as the radiation of light by hot electrons at frequencies an order of magnitude higher than those of the incident laser beam [1].

As demonstrated in the publications [2, 5–8], the electron-phonon interaction constants of hot electrons in metal nanoparticles cause a phenomenal decrease by an order of magnitude compared to bulk metal. As a result, an electron-phonon system can remain in a stationary, non-equilibrium state for $10^3 \sim 10^4$ hours without the nanoparticles melting or being destroyed, provided there is constant external maintenance of the non-equilibrium state. Without this support, the thermodynamic equilibrium of the electron-phonon system is achieved within a dozen femtoseconds.

Recall that the temperature of the electronic gas can reach thousands of degrees in NP. This situation is not observed in bulk metal, where the electron-phonon system achieves equilibrium within 10^{-10} second. That is, it is possible to achieve the desired intensity of acoustic activity at a given crystal point by irradiating a system of metal nanoparticles with a sequence of ultra-short laser impulses. These impulses must have sufficient power for generation but less than the power that would destroy the nanoparticles. Additionally, there needs to be an interval between impulses to allow for the cooling of the nanoparticles. This provides a reason to consider a system of metal nanoparticles as a suitable instrument for generating the sequence of acoustic waves discussed in this article.

It should be noted that if the exposure time of the impulse from the hot electronic gas of nanoparticles on the atoms of the dielectric matrix is much shorter than the time it takes for the atoms to be displaced by the integrated range, then Eq. (16) can be expressed as follows:

$$\varphi(t)_{p,q,r} \cong \sum \varphi'(0)_{l,m,n} \int_0^t I_{p,q,r;l,m,n}(t_1) dt_1, \tag{25}$$

and for

$$\varphi'(t)_{p,q,r} \cong \sum \varphi'(0)_{l,m,n} I_{p,q,r;l,m,n}(t) \tag{26}$$

[1] The new mechanism of focusing and enhancing acoustic waves generated by metal nanoparticles within the crystal lattice.

the calculations provided above for the potential displacement are applicable.

The proposed mechanism of focusing and enhancing acoustic waves provides a novel route to controlling the energy localization in structured media. By simultaneously concentrating and amplifying wave energy, it enables improved manipulation of wave propagation for both fundamental studies and applied technologies.

Note on Addenda and Notation

To enhance both the physical clarity and broader applicability of our model, we include three supplementary appendices. These additions provide extended context and technical depth on topics not fully elaborated in the main text. Specifically, they address:

(i) the justification for modelling acoustic waves via scalar potentials in cubic crystals (Appendix A);

(ii) the semi-discrete formulation of the wave operator on a 3D lattice (Appendix B);

(iii) the potential for extending the current linear analysis to weakly nonlinear regimes via perturbative methods (Appendix C).

From a physical standpoint, a crystal lattice has a discrete symmetry group, distinct from the continuous symmetry of empty space. Because of this discrete translational symmetry, only shifts by integer multiples of the lattice basis vectors are permitted, reflecting a fundamentally different structure than systems with continuous symmetry. The transition to a fibered space that couples three-dimensional physical coordinates with discrete lattice indices is therefore not a heuristic approximation, but a mathematically consistent and physically motivated step. The resulting six-dimensional space should not be seen as an extension of Euclidean space, but rather as a hybrid configuration space. This is directly analogous to classical phase space, which unites position and momentum coordinates: in the same way, our 6D space unites spatial coordinates with lattice indices to capture the full wave dynamics in a crystal.

This approach reflects the same embedding principles and reflects the intrinsic nature of wave phenomena in crystalline structures, where the interplay between continuous and discrete variables fundamentally alters propagation dynamics.

Moreover, the passage of a wavefront through a lattice node is accompanied by a phase jump: the configuration of force interactions changes as new atoms begin to move. This kind of dynamics requires the apparatus of generalized functions, although that topic lies beyond the scope of the present work.

APPENDIX A
Negligible Transverse Contribution in Quasi-Longitudinal Waves

Definition. *A quasi-longitudinal wave is an acoustic eigenmode in which the polarization vector* $\mathbf{u}$ *is predominantly aligned with the propagation direction* $\mathbf{n}$*, though not exactly parallel due to elastic anisotropy.*

In modelling lattice dynamics and acoustic wave propagation in cubic crystals, we adopt the approximation that the displacement field $\mathbf{u}$ can be derived from a scalar potential ϕ via $\mathbf{u} = \nabla\phi$. This implies that the wave motion is essentially longitudinal – a well-supported approximation based on experimental evidence.

In anisotropic elastic media such as cubic crystals, eigenmodes of the Christoffel equation are not strictly longitudinal or transverse except along high-symmetry directions. However, for quasi-longitudinal modes, the transverse component is consistently small. Supporting evidence includes:

1. Brillouin scattering studies in silicon and germanium show that quasi-longitudinal modes contain less than 5% transverse polarization in most directions.

2. Phonon imaging in alkali metals (e.g., Li, Na, K) indicates that quasi-longitudinal waves remain predominantly longitudinal. While quasi-transverse modes can show longitudinal admixture up to 15%, the reverse is negligible.

3. Theoretical analysis of the Christoffel tensor for cubic symmetry confirms that the polarization vector of quasi-longitudinal modes remains nearly aligned with $\mathbf{k}$ throughout the Brillouin zone, except at isolated degenerate directions [9]. Therefore, representing the acoustic displacement field in terms of a scalar potential is a valid and experimentally justified simplification for modelling quasi-spherical wavefronts in cubic lattices.

APPENDIX B

We distinguish between the physical space where acoustic disturbances propagate and the mathematical space where the problem is formulated. Physically, waves evolve in a three-dimensional Euclidean lattice. Mathematically, however, the governing equations for the discrete atomic displacement field naturally lead to a fibered configuration space – the product of the physical continuum $\mathbb{R}^3$ and a discrete index space $\mathbb{Z}^3$ labeling the lattice nodes.

In this extended space, wave behavior is shaped not only by physical geometry but also by the additional discrete structure. The emergence of oscillatory "tails" behind the wavefront and the breakdown of Huygens principle follows directly from this discrete-continuous coupling, rather than from spatial geome-

try alone. Our calculations identify the conditions for acoustic-wave focusing for both spherical and planar waveforms.

Direct experimental verification of these six-dimensional effects is not yet available, but analogous phenomena appear in related contexts:

• Bessel beams (optical and acoustic), governed by Bessel functions, exhibit characteristic tails and concentric ring structures; their self-healing behavior – beam regeneration after obstruction – provides clear physical evidence of the underlying wave structure.

• Diffraction phenomena, studied since Lord Rayleigh, likewise reveal lattice-like configurations that produce similar tail effects, even if not explicitly described in terms of Huygens principle.

Thus, while direct measurements in the modeled six-dimensional setting are lacking, experimental studies of Bessel-function wave systems strongly support the existence of such features. The distinction between physical and extended spaces corresponds to the formal lifting discussed in Section Continuous vs. Lattice Dynamics, where admissibility constraints and the representation of the displacement field on $\mathbb{R}^3 \times \mathbb{Z}^3$ provide the mathematical foundation for oscillatory tails and Violation of Huygens principle as natural outcomes of the hybrid lattice model.

The insights above motivate a more rigorous treatment of the hybrid lattice–continuum structure. In the following sections, we formalize the distinction between continuous and discrete dynamics by introducing the Admissibility Condition in Discrete Lattice Dynamics, detailing the associated admissibility constraints, and analyzing the behavior of the Generalized Discrete Laplacian. These tools enable the consistent lifting of the displacement field to the indexed configuration space $\mathbb{R}^3 \times \mathbb{Z}^3$, establishing the mathematical foundation for the tails, violation of Huygens principle, and focusing effects discussed above.

Continuous vs. Lattice Dynamics: Poisson Formula and Admissibility Constraints

Definition.
Poisson solution to the 3D wave equation

Let $u : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$ solve the standard wave equation:

$$\Box u(x,t) := \frac{\partial^2 u}{\partial t^2}(x,t) - k^2 \Delta u(x,t) = 0, \tag{B.1}$$

with initial conditions

$$u(x,0) = f(x), \quad \frac{\partial u}{\partial t}(x,0) = g(x), \quad x \in \mathbb{R}^3, \tag{B.2}$$

where $f \in C^2(\mathbb{R}^3)$ and $g \in C^1(\mathbb{R}^3)$. The solution is given by the Poisson formula:

$$u(x,t) = \frac{\partial}{\partial t}\left[\frac{1}{4\pi ct} \int\limits_{|y-x|=ct} f(y) dS_y\right] + \frac{1}{4\pi ct} \int\limits_{|y-x|=ct} g(y) dS_y, \tag{B.3}$$

where dS_y denotes surface measure on the sphere of radius $c \cdot t$ centred at x.

Minimal regularity

The Poisson formula requires only:

1. $f \in C^2(\mathbb{R}^3)$,
2. $g \in C^1(\mathbb{R}^3)$.

In contrast, discrete lattice systems impose stricter compatibility constraints on initial data.

Definition.
Admissibility condition in discrete lattice dynamics

Let $\varphi_{a,b,c}(t)$ denote the displacement field at lattice site $(a,b,c) \in \mathbb{Z}^3$ and time $t \in \mathbb{R}$, governed by the discrete wave equation on a cubic lattice:

$$\Box^3_{\text{lattice}} \varphi_{a,b,c}(t) = 0, \tag{B.4}$$

where $\Box^3_{\text{lattice}}$ is the discrete analogue of the d'Alembertian operator, typically defined via finite differences in both space and time. The initial conditions are given by the field configuration $\varphi_{a,b,c}(0)$ and its time derivative $\partial_t \varphi_{a,b,c}(0)$.

To ensure consistency with the discrete evolution, the following admissibility condition must be satisfied:

$$\partial_t^2 \varphi_{a,b,c}(t)\big|_{t=0} = k^2 \cdot \Delta_{\mathbb{Z}^3} \varphi_{a,b,c}(0), \tag{B.5}$$

where k is a coupling constant characterizing the interaction strength between neighboring lattice sites, and $\Delta_{\mathbb{Z}^3}$ denotes the discrete Laplacian on the three-dimensional integer lattice. Explicitly, the discrete Laplacian is defined as:

$$\Delta_{\mathbb{Z}^3} \varphi_{a,b,c} = \sum_{\substack{(i,j,k) \in \mathbb{Z}^3 \\ \|(i,j,k)-(a,b,c)\|_1 = 1}} (\varphi_{i,j,k} - \varphi_{a,b,c}), \tag{B.6}$$

which sums over the six nearest neighbors of the site (a,b,c). Unlike the continuous wave equation, where field amplitudes are unrestricted, the discrete lattice model imposes a natural bound on atomic displacements: the initial displacement at each site must not exceed the interatomic spacing. This constraint reflects the physical limits of atomic motion and ensures that the model remains within the harmonic regime of lattice dynamics.

Generalized discrete Laplacian behavior

In many physical settings, lattice interactions extend beyond the six nearest neighbors or differ along crystallographic axes. This motivates replacing the operator (B.6) by a generalized discrete Laplacian

$$\Delta^{(w)}_{\mathbb{Z}^3} \varphi_{l,m,n} := \sum_{(p,q,r) \in \mathcal{N}} w_{pqr} (\varphi_{l+p,m+q,n+r} - \varphi_{l,m,n}), \tag{B.7}$$

where $\mathcal{N} \subset \mathbb{Z}^3 \setminus \{(0,0,0)\}$ is a finite neighborhood of interactions and w_{pqr} are real symmetric weights ($w_{pqr} = w_{-p,-q,-r}$). The discrete standard Laplacian corresponds to $w_{\pm 1,0,0} = w_{0,\pm 1,0} = w_{0,0,\pm 1} = 1$ and all other weights zero.

This generalization allows the modeling:

• of anisotropic lattices,

• long-range forces,

• frequency-dependent corrections to the dispersion relation.

Remark. ***Physical Interpretation – Lifting to a Fibered 6D Space***

Discrete lattice wave equations can be naturally lifted to a six-dimensional fibered space, wherein each lattice node is endowed with a local continuous displacement field. This framework exhibits a dual character: it simultaneously captures local vibrational dynamics and nonlocal interactions dictated by the lattice topology. Crucially, this lifting is not merely formal – discrete translational symmetry induces couplings that cannot be faithfully represented within purely three-dimensional models. Embedding the problem in this higher-dimensional space preserves physical fidelity while enabling analytical tractability.

The classical Poisson formula yields a closed-form solution under minimal regularity assumptions, inherently bypassing the need for additional admissibility conditions. By contrast, discrete-lattice systems – particularly those modeled via numerical schemes – must impose explicit admissibility constraints to ensure consistency with the discrete evolution equation. The analytical framework, grounded in Bateman's approach, constructs solutions that satisfy these constraints intrinsically.

Extending the formulation to a six-dimensional configuration space enables the derivation and solution of a discrete-continuous hybrid equation that accurately reflects lattice systems coupled to continuous displacement fields. This extension naturally induces a fibered structure over physical space. A key consequence of this discrete-continuous interplay is the breakdown of strict Huygens principle, manifesting as oscillatory wave tails trailing the primary wavefront – a phenomenon that can be exploited for spatiotemporal wave focusing via constructive interference.

Shift operators via exponential differential form

Proposition

Shift operators

$$(T_x f)(x) = f(x+1) = \left(e^{\partial_x} f\right)(x), \tag{B.8}$$

where

$$e^{\partial_x} = \sum_{n=0}^{\infty} \frac{1}{n!} \partial_x^n \tag{B9}$$

In several variables, shifts along lattice directions are generated by:

$$e^{\pm\partial_x}, \quad e^{\pm\partial_y}, \qquad e^{\pm\partial_z}. \tag{B10}$$

□

The discrete Laplacian appearing in (13) can be compactly written as:

$$\Delta_d = (e^{\partial_x} + e^{-\partial_x} + e^{\partial_y} + e^{-\partial_y} + e^{\partial_z} + e^{-\partial_z} - 6), \tag{B.11}$$

acting on

$$\varphi_{a,b,c}(t) = \varphi(x = a,\, y = b,\, z = c,\, t), \tag{B12}$$

as in the nearest-neighbor lattice model.

Remark. ***Functional calculus and generalized shift dynamics***

For a smooth function f, define $T_h := e^{h\partial_x}$, giving:

$$(T_h f)(x) = f(x+h), \tag{B.13}$$

with $h \in \mathbb{R}$ for the continuous case and $h \in \mathbb{Z}$ for discrete lattice translations.

This allows generalizing dynamics via "functional calculus" on the generator ∂_x.

Extensions and applications

1. *Fractional shifts.*

Introducing the operator $T_\alpha = e^{\alpha\partial_x}$, with $\alpha \in \mathbb{R}$, defines fractional lattice shifts – a generalization of discrete translations to non-integer displacements.

Physical example:

Within the framework of anomalous transport models, atoms or excited states can undergo displacements that are fractional multiples of the lattice vector $\mathbf{a}$, i.e., $\mathbf{r} = \alpha\mathbf{a}$, where $\alpha \in \mathbb{R}$, $0 < \alpha < 1$. This enables the description of dynamics that interpolate between ballistic transport to nearest neighbors and nonlocal Lévy-type jumps. Such an approach captures intermediate transport regimes that are neither purely local nor fully nonlocal, and is particularly relevant for systems with fractal structures or scale-invariant behavior.

2. *Discrete dispersion relations.*

The Fourier symbol of the 1D discrete Laplacian:

$$\widehat{\Delta_d}(\xi) = 2\cos\xi - 2 \tag{B.14}$$

and in 3D:

$$\widehat{\Delta_d}(\xi_x, \xi_y, \xi_z) = 2(\cos\xi_x + \cos\xi_y + \cos\xi_z) - 6. \tag{B.15}$$

Physical example:

These relations characterize phonon dispersion in a simple cubic lattice, where the propagation speeds are identical along all crystallographic axes.

3. *Anisotropic operators.*

Allowing different coupling strengths:

$$\Delta_{d,\text{anis}} = \alpha_x(e^{\partial_x} + e^{-\partial_x} - 2) + \alpha_y(e^{\partial_y} + e^{-\partial_y} - 2) + \\ + \alpha_z(e^{\partial_z} + e^{-\partial_z} - 2), \tag{B.16}$$

where $\alpha_x, \alpha_y, \alpha_z$ reflect anisotropic coupling.

Physical example:

Layered or fibrous crystals where atomic bonds are stronger in one direction (e.g., graphite planes or optical waveguide arrays).

4. *Integral transforms via shift semigroups.*

More general convolution-type evolutions:

$$(K^* f)(x) = \int_{\mathbb{R}} K(h)(T_h f)(x)dh, \tag{B.17}$$

where K encodes spectral or temporal modulation.

Physical example:

In tight-binding electron models, kernels describe effective hopping amplitudes to non-nearest neighbors, or time-dependent modulation of lattice couplings (Floquet engineering).

Conclusion of Appendix B

The ascent to a fibered 6D wave space should be understood as a mathematically justified modeling necessity rather than a metaphysical claim.

The discrete translational symmetry of the lattice induces nonlocal couplings that cannot be adequately described within a purely 3D formulation. By embedding the problem in a higher-dimensional configuration space, we retain physical fidelity while gaining analytical tractability.

Expressing discrete operators through shift–exponential calculus (viewing shifts as exponentials of differential operators) offers a unified framework to:

• connect discrete lattice dynamics with their continuous differential counterparts,

• extend nearest-neighbor models to fractional, anisotropic, or long-range couplings,

• interpret lattice dispersions and generalized propagators in physically meaningful terms.

Within this framework, the familiar Bessel-function factorization appears merely as one special instance of a broader class of shift-generated operator dynamics.

APPENDIX C
Linear Approximation and Perturbative Extensions

The present work is conducted within the framework of linear elasticity theory, wherein wave propagation is governed by harmonic response and displacement fields satisfy the principle of superposition. This approach ensures broad applicability across a wide range of materials without requiring knowledge of higher-order elastic constants.

However, nonlinear effects may become relevant in certain regimes, including:

1. High-amplitude excitation,
2. Strong phonon–phonon interactions,
3. Temperature-induced softening of the lattice.

To account for such phenomena, a material-specific nonlinear elasticity model would be required, incorporating higher-order stress-strain tensors. A natural approach is to apply perturbative methods, treating nonlinear contributions as small corrections to the linear solution.

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НОВИЙ МЕХАНІЗМ ФОКУСУВАННЯ ТА ПІДСИЛЕННЯ АКУСТИЧНИХ ХВИЛЬ, ЩО ГЕНЕРУЮТЬСЯ МЕТАЛЕВИМИ НАНОЧАСТИНКАМИ В КРИСТАЛІЧНІЙ ҐРАТЦІ

Ми обговорюємо можливий механізм фокусування та підсилення акустичних хвиль, які генеруються металевими наночастинками, вбудованими у кристалічну ґратку, під дією ультракороткого лазерного збудження. На відміну від моделей неперервного середовища, дискретна ґраткова структура зумовлює появу осциляційних хвостів хвиль, які виникають позаду фронту поширення внаслідок порушення принципу Гюйгенса у просторах парної розмірності. Атомна динаміка може розглядатися як еволюція у шестивимірному просторі конфігурацій, де неперервна компонента фізичного простору описує внутрішньокоміркові зміщення, а дискретні індекси визначають положення елементарних комірок. Цей ефект може призводити до локального підсилення амплітуди поздовжніх акустичних хвиль у вибраних вузлах кристалічної ґратки без збільшення інтенсивності збуджувального лазерного імпульсу.

Ключові слова: наночастинки, генерування та фокусування акустичних хвиль, принцип Гюйгенса.