THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

# Phononic crystals supporting Fermion-like Rotational modes

*Pierre A. Deymier, K. Runge, N. Swinteck and K. Muralidharan*

*School of Sustainable Engineered Systems*

*Department of Materials Science and Engineering*

*University of Arizona*

*Tucson AZ 85721*

School of Sustainable Engineered Systems

There are two types of particles: Bosons and Fermions
Fermions (e.g. electrons) behave according to the Fermi-Dirac quantum statistics
Phonons (the quanta of vibrations) have always been believed to behave as bosons (i.e. according to Bose-Einstein quantum statistics).

# The Question?

## Is it possible for phonons to behave like Fermions?

### If yes! What are the implications of fermion-like phonon behavior for technologies relying on phonon-based phenomena?

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

SSES
School of Sustainable Engineered Systems

# Phononic crystals can support rotational phonon modes

## 1. "Rigid Body"Rotational Modes in Phononic Crystals:

F. Liu, Y. Lai, X. Huang and C. T. Chan, Phys. Rev. B 84, 224113 (2011).
G. Wang, X. Wen, J. Wen, L. Shao and Y. Liu, Phys. Rev. Lett. 93, 154302 (2004).
Y. Lai, Y. Wu, P. Sheng and Z. Q. Zhang, Nat. Mater. 10, 620 (2011).
R. Sainidou, N. Stefanou and A. Modinos, Phys. Rev. B 66, 212301 (2002).
H. Zhao, Y. Liu, G. Wang, J. Wen, D. Yu, X. Han and X. Wen, Phys. Rev. B 72, 012301 (2005).
K. Maslov, V. K. Kinra and B. K. Henderson, Mech. Mater. 31, 175 (1999).
P. Peng, J. Mei and Y. Wu, Phys. Rev. B 86, 134304 (2012).

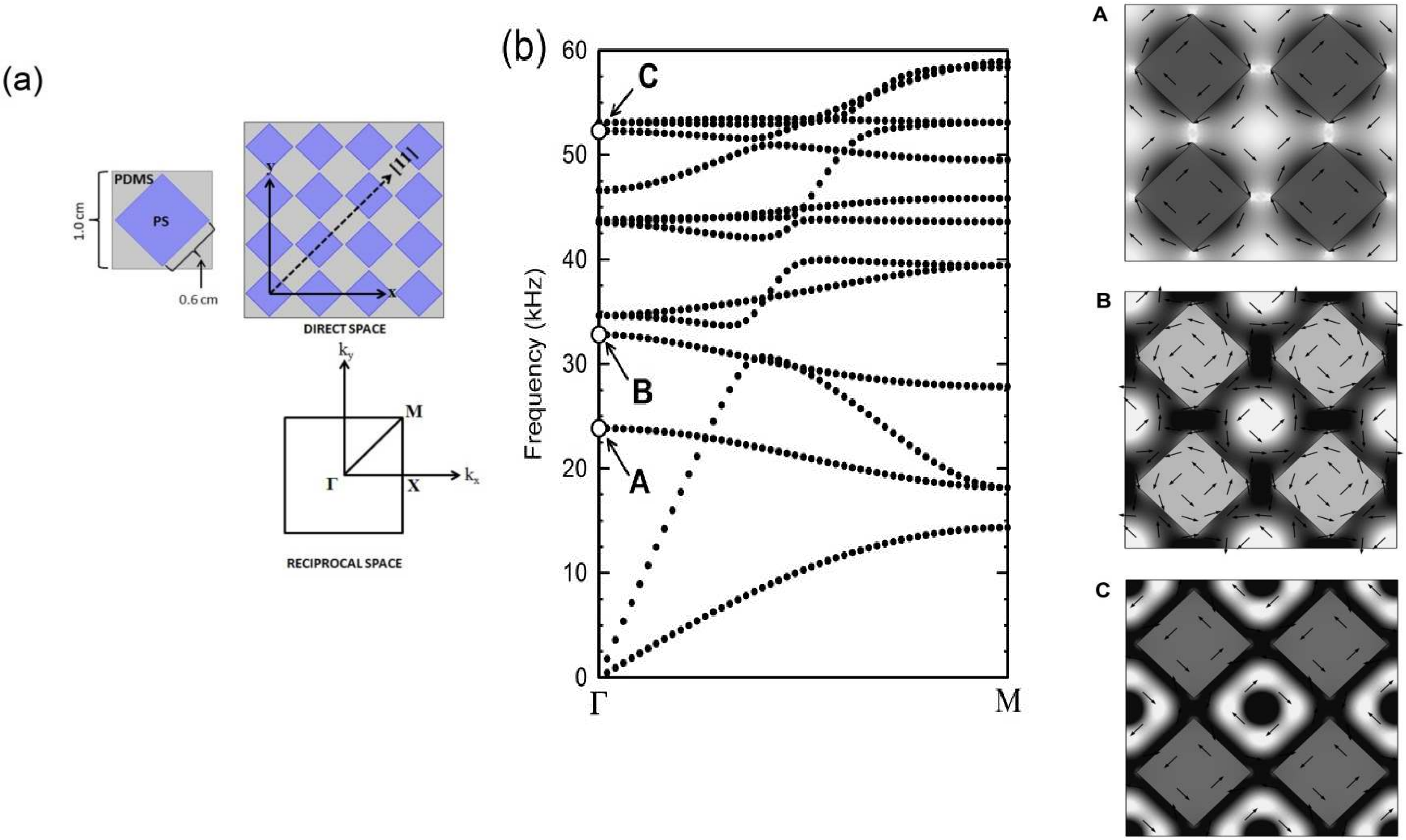
## 2. Rotational Modes in Granular Materials

A. Merkel, V. Tournat and V. Gusev, Phys. Rev E 82, 031305 (2010).
V. Tournat, I. Pérez-Arjona, A. Merkel, V. Sanchez-Morcillo and V. Gusev, New J. Phys. 13, 073042 (2011).
A. Merkel, V. Tournat and V. Gusev, Phys. Rev. Lett. 107, 225502 (2011).
H. Pichard, A. Duclos, J-P. Groby, and V. Tournat, Phys. Rev. B 86, 134307 (2012)

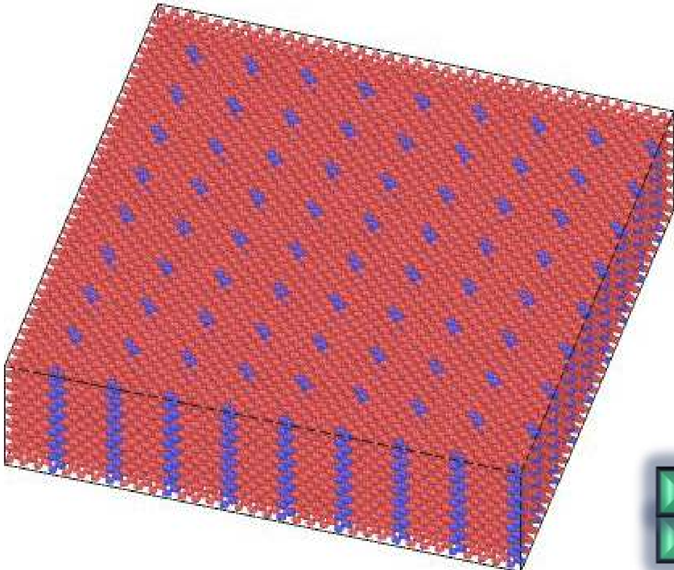
THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

School of Sustainable Engineered Systems

# Example 1: PS-PDMS PC



# Example 2:Nano-Phononic crystals

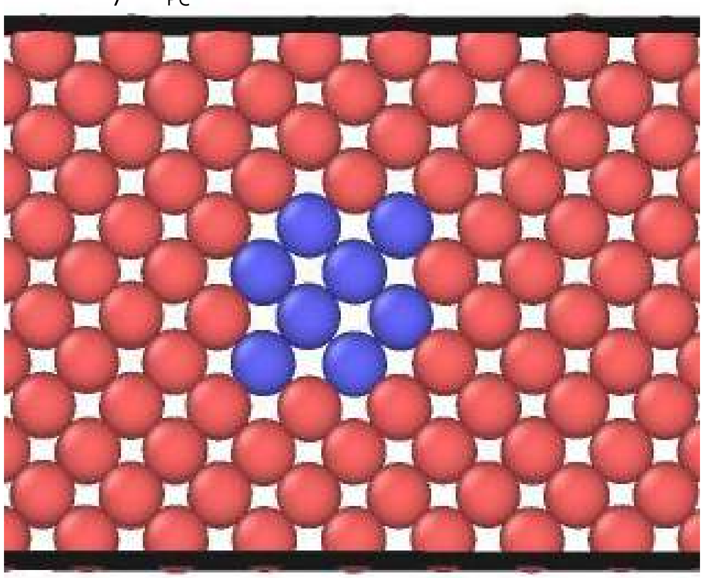


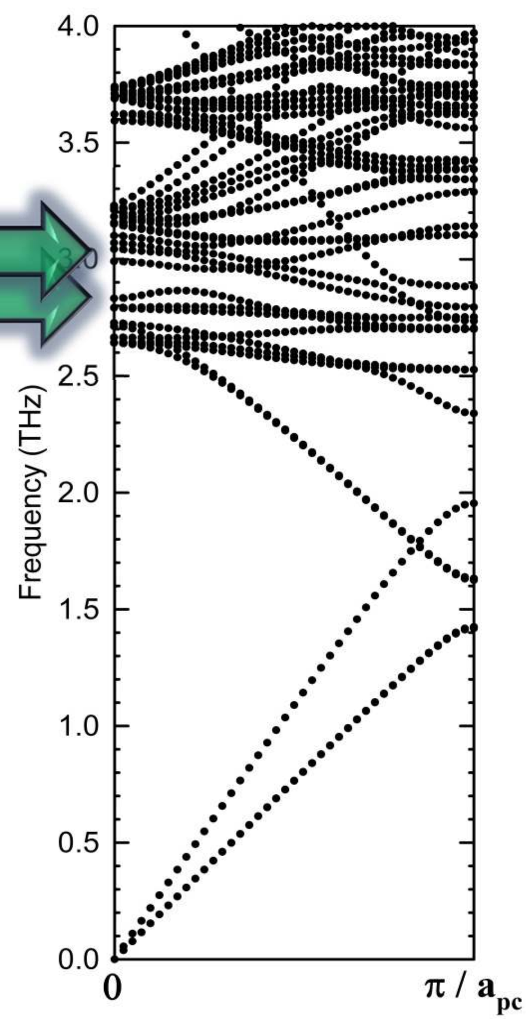
SiGe PC – Ge pillars in Si matrix (crystalline)

PC unit cell has 216 atoms (24 Ge; 192 Si)

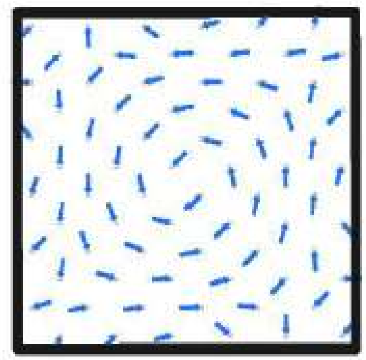
**Si-Ge**

PC periodicity = $a_{PC}$

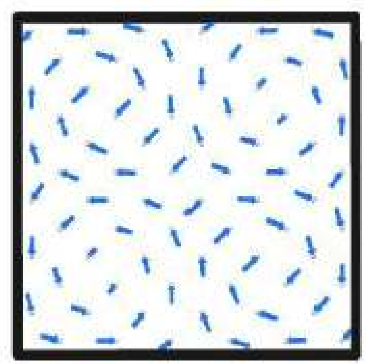





Eigenmodes at Gamma Point
quasiharmonic approx. (T = 300K) GULP



2.79 THz

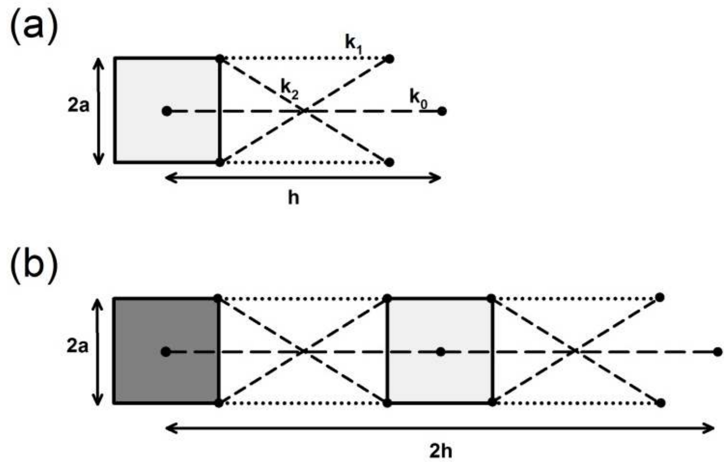


3.06 THz

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

# 1D Discrete Model that supports rotational phonon modes

# Mass Spring Phononic Structure

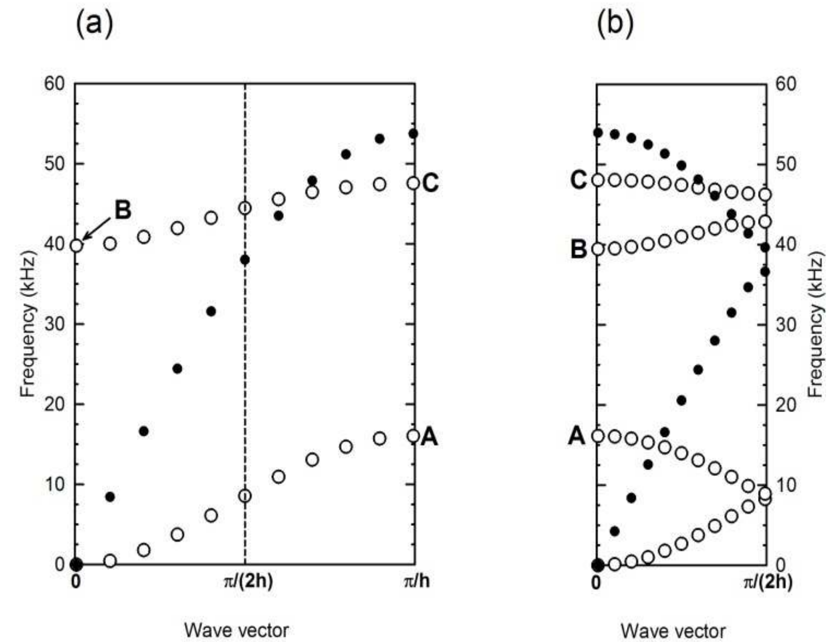



$$E_{n,n+1} = \frac{1}{2}K_0(u_{n+1} - u_n)^2 + \frac{1}{2}K_1\left[(v_{n+1} - v_n) + \frac{h}{2}(\varphi_{n+1} + \varphi_n)\right]^2 + \frac{1}{2}K_2(\varphi_{n+1} - \varphi_n)^2$$

where $K_0 = \left(\frac{k_0}{h^2} + \frac{2k_1}{l^2} + \frac{2k_2 l^2}{l_d{}^4}\right)$, $K_1 = \left(\frac{2k_2(2a)^2}{l_d{}^4}\right)$, $K_2 = \left(\frac{2a^2k_1}{l^2}\right)$, $l = h - (2a)$, $l_d = \sqrt{(l^2 + (2a)^2)}$.


A. Vasiliev, A. Miroshnichenko and M. Ruzzene, Mech. Res. Comm. **37**, 225-229 (2010)

A. Vasiliev, A. Miroshnichenko and M. Ruzzene, Jour. Mech. Mater. **3**, 1365-1382 (2008)

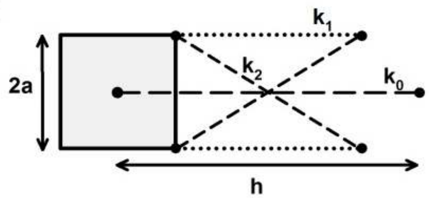

$$m\frac{d^2u_n}{dt^2} = K_0(u_{n+1} - 2u_n + u_{n-1})$$

$$m\frac{d^2v_n}{dt^2} = K_1(v_{n+1} - 2v_n + v_{n-1}) + \frac{hK_1}{2}(\varphi_{n+1} - \varphi_{n-1})$$

$$I\frac{d^2\varphi_n}{dt^2} = K_2(\varphi_{n+1} - 2\varphi_n + \varphi_{n-1}) + \frac{hK_1}{2}(v_{n-1} - v_{n+1}) - \frac{h^2K_1}{4}(\varphi_{n+1} + 2\varphi_n + \varphi_{n-1})$$

# Focusing on the Rotational Waves

(a)




$$I\frac{\partial^2\varphi_n}{\partial t^2} = K_1'(\varphi_{n+1} - 2\varphi_n + \varphi_{n-1}) - K_2'\varphi_n$$

$K_1' = K_2 - \frac{h^2K_1}{4}$, and $K_2' = h^2K_1$ . Dividing the equation by $I$ yields our rotational wave equation:

$$\frac{\partial^2\varphi_n}{\partial t^2} - \beta^2(\varphi_{n+1} - 2\varphi_n + \varphi_{n-1}) + \alpha^2\varphi_n = 0$$

with $\beta^2 = \frac{K_1'}{I}$ and $\alpha^2 = \frac{K_2'}{I}$.

**Relativistic quantum mechanics**
**Klein-Gordon Equation**

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

SSES School of Sustainable Engineered Systems

# Rotational Phonons are Solutions of Dirac-like Equation

## Relativistic quantum mechanics
## Klein-Gordon Equation

$$\frac{\partial^2 \varphi_n}{\partial t^2} - \beta^2(\varphi_{n+1} - 2\varphi_n + \varphi_{n-1}) + \alpha^2 \varphi_n = 0$$

" $\sqrt{\ }$ "

$$\left[\boldsymbol{\sigma_x} \otimes \boldsymbol{I} \frac{\partial}{\partial t} + i\beta \boldsymbol{\sigma_y} \otimes \{\boldsymbol{e_1}\Delta^+ + \boldsymbol{e_2}\Delta^-\} \pm i\alpha \boldsymbol{I} \otimes \boldsymbol{I}\right] \psi = 0$$

## Dirac Equation

where $\boldsymbol{\sigma_x}$ and $\boldsymbol{\sigma_y}$ are the 2x2 Pauli matrices:

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\Delta\varphi_n = D(D\varphi_n)$ $\quad$ $D = \boldsymbol{e_1}\Delta^+ + \boldsymbol{e_2}\Delta^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\Delta^+ + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\Delta^-$

$\Delta^+\varphi_n = \varphi_{n+1} - \varphi_n$ and $\Delta^-\varphi_n = \varphi_n - \varphi_{n-1}$

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

sses
School of Sustainable Engineered Systems

# Long Wavelength limit

$$\left[\boldsymbol{\sigma_x}\otimes\boldsymbol{I}\frac{\partial}{\partial t} + i\beta\boldsymbol{\sigma_y}\otimes\{\boldsymbol{e_1}\Delta^+ + \boldsymbol{e_2}\Delta^-\} \pm i\alpha\boldsymbol{I}\otimes\boldsymbol{I}\right]\psi = 0$$

$$\left[\boldsymbol{\sigma_x}\frac{\partial}{\partial t} + i\beta\boldsymbol{\sigma_y}\frac{\partial}{\partial x} \pm i\alpha\boldsymbol{I}\right]\psi = 0$$

**Eigen vector solutions: plane wave solutions**

**Four spinor**

$$\psi = \begin{pmatrix}\psi_{1n}\\ \psi_{2n}\\ \psi_{3n}\\ \psi_{4n}\end{pmatrix}$$

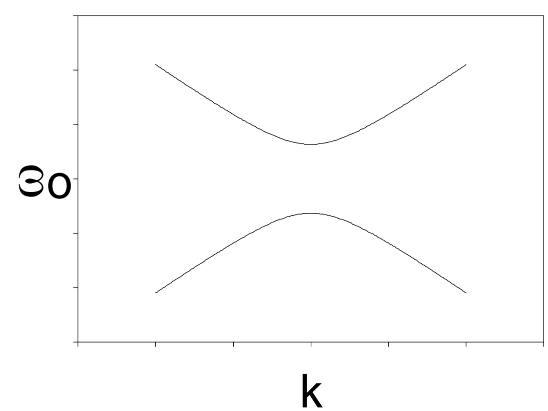
**Two spinor**

$$\psi = \begin{pmatrix}\psi_{a,n}\\ \psi_{b,n}\end{pmatrix}$$

**Eigen values-Dispersion relations**

$$\omega = \pm\sqrt{\alpha^2 + 4\beta^2 si^{n_2}\frac{kh}{2}}$$

$$\omega = \pm\sqrt{\alpha^2 + \beta^2(kh)^2}$$



THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

sses
School of Sustainable Engineered Systems

# Lagrangian representation

$$L_1\left(\psi,\frac{\partial\psi}{\partial t},\frac{\partial\psi}{\partial x}\right)=\psi^*\boldsymbol{\sigma}_{\mathbf{x}}\frac{\partial\psi}{\partial t}+i\beta\psi^*\boldsymbol{\sigma}_{\boldsymbol{y}}\frac{\partial\psi}{\partial x}-i\alpha\psi^*\boldsymbol{I}\psi$$

**Lagrange equation for fields**

$$\frac{\partial}{\partial t}\left(\frac{\partial L_{1,2}}{\partial(\partial_t\psi^{(*)})}\right)+\frac{\partial}{\partial x}\left(\frac{\partial L_{1,2}}{\partial(\partial_x\psi^{(*)})}\right)-\frac{\partial L_{1,2}}{\partial(\psi^{(*)})}=0$$

$$L_2\left(\psi^*,\frac{\partial\psi^*}{\partial t},\frac{\partial\psi^*}{\partial x}\right)=\frac{\partial\psi^*}{\partial t}\boldsymbol{\sigma}_{\mathbf{x}}\psi+i\beta\frac{\partial\psi^*}{\partial x}\boldsymbol{\sigma}_{\boldsymbol{y}}\psi+i\alpha\psi^*\boldsymbol{I}\psi$$

$$\left[\frac{\partial}{\partial t}\boldsymbol{\sigma}_{\boldsymbol{x}}+i\beta\frac{\partial}{\partial x}\boldsymbol{\sigma}_{\boldsymbol{y}}+i\alpha\boldsymbol{I}\right]\psi^*=0$$

$$\left[\boldsymbol{\sigma}_{\boldsymbol{x}}\frac{\partial}{\partial t}+i\beta\boldsymbol{\sigma}_{\boldsymbol{y}}\frac{\partial}{\partial x}-i\alpha\boldsymbol{I}\right]\psi=0$$

**Dirac Equations**

$\psi$ and $\psi$ * are not self-dual and represent different objects ("particle" and "antiparticle")

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

# Solutions

SSES School of Sustainable Engineered Systems

$$\psi_k = \psi(k,\omega_k) = \xi_k(k,\omega_k)e^{(\pm)i\omega_k t}e^{(\pm)ik^x} \qquad \psi_k^* = \psi^*(k,\omega_k) = \xi_k^*(k,\omega_k)e^{(\pm)i\omega_k t}e^{(\pm)ik^x}$$

$\xi_k$ and $\xi_k^*$ are two by one spinors

| | $e^{+i\omega_k t}e^{+ik^x}$ | $e^{+i\omega_k t}e^{-ik^x}$ | $e^{-i\omega_k t}e^{+ik^x}$ | $e^{-i\omega_k t}e^{-ik^x}$ |
|---|---|---|---|---|
| $\xi_k$ | $\begin{pmatrix}\sqrt{\omega+\beta k^{\hbar}}\\ \sqrt{\omega-\beta k^{\hbar}}\end{pmatrix}$ | $\begin{pmatrix}\sqrt{\omega-\beta k^{\hbar}}\\ \sqrt{\omega+\beta k^{\hbar}}\end{pmatrix}$ | $\begin{pmatrix}-\sqrt{\omega-\beta k^{\hbar}}\\ \sqrt{\omega+\beta k^{\hbar}}\end{pmatrix}$ | $\begin{pmatrix}-\sqrt{\omega+\beta k^{\hbar}}\\ \sqrt{\omega-\beta k^{\hbar}}\end{pmatrix}$ |
| $\xi_k^*$ | $\begin{pmatrix}\sqrt{\omega-\beta k^{\hbar}}\\ \sqrt{\omega+\beta k^{\hbar}}\end{pmatrix}$ | $\begin{pmatrix}\sqrt{\omega+\beta k^{\hbar}}\\ \sqrt{\omega-\beta k^{\hbar}}\end{pmatrix}$ | $\begin{pmatrix}\sqrt{\omega+\beta k^{\hbar}}\\ -\sqrt{\omega-\beta k^{\hbar}}\end{pmatrix}$ | $\begin{pmatrix}\sqrt{\omega-\beta k^{\hbar}}\\ -\sqrt{\omega+\beta k^{\hbar}}\end{pmatrix}$ |

**Table** : Spinor part of solutions for the different plane wave forms.

**We note that the $\xi_k^*$ are Hermitian conjugates of $\xi_k$.**

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

sses
School of Sustainable Engineered Systems

# Hamiltonian

$$H_1 = \Pi \frac{\partial \psi}{\partial t} - L_1$$

momentum conjugate $\Pi = \frac{-\partial L_1}{\partial \left( {}^{\partial \psi}/_{\partial t} \right)} = \psi^* \boldsymbol{\sigma_x}$

Hamiltonian density $H_1 = \psi^* \boldsymbol{\sigma_x} \frac{\partial \psi}{\partial t}$

Energy $E = \int dx H_1$

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

sses
School of Sustainable Engineered Systems

# Replace wave function by field operator

$$\psi^*(x) = \sum_k \frac{1}{\sqrt{2\omega}}\left[a_k^* \xi_k^* e^{-ik^x} e^{i\omega^t} + \bar{a}_k^* \bar{\xi}_k^* e^{ik^x} e^{-i\omega^t}\right]$$

$$\psi(x) = \sum_k \frac{1}{\sqrt{2\omega}}\left[a_k \xi_k e^{ik^x} e^{-i\omega^t} + \bar{a}_k \bar{\xi}_k e^{-ik^x} e^{i\omega^t}\right]$$

**The quantities: $a_k^*$,$\bar{a}_k^*$, $a_k$, and $\bar{a}_k$ are creation and annihilation operators.**

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

sses
School of Sustainable Engineered Systems

# Anticommutation rules

$$E = \int dx H_1$$

Using spinor properties

$\xi_k^* \boldsymbol{\sigma_x} \xi_k = \bar{\xi}_k^* \boldsymbol{\sigma_x} \bar{\xi}_k = 2\omega$ and $\xi_k^* \boldsymbol{\sigma_x} \bar{\xi}_k = \bar{\xi}_k^* \boldsymbol{\sigma_x} \xi_k = 0$

$$E = \sum_k \omega \left( a_k^* a_k - \bar{a}_k^* \bar{a}_k \right)$$

Energy is positive

**Need to introduce anticommutation rules**

$$\{a_k, a_{k'}\} = a_k^* a_{k'} + a_k a_{k'}^* = \delta_{k,k'}$$

$$E - E_0 = \sum_k \omega \left( a_k^* a_k + \bar{a}_k \bar{a}_k^* \right)$$

**Fermion-like phonons!**

# Number operator is invariant

$$N = \int dx\, \psi^* \sigma_x \psi$$

Reformulate the fields

$$\psi(x) = \sum_k \frac{1}{\sqrt{2\omega}} \left[ a_k \xi_k e^{ikx} e^{-i\omega t} + \bar{a}_{-k} \bar{\xi}_{-k} e^{ikx} e^{i\omega t} \right] = \sum_k \frac{1}{\sqrt{2\omega}} \left[ a_k \xi_k e^{ikx} e^{-i\omega t} + b_k \eta_k e^{ikx} e^{i\omega t} \right]$$

$$\psi^*(x) = \sum_k \frac{1}{\sqrt{2\omega}} \left[ a_k^* \xi_k^* e^{-ikx} e^{i\omega t} + \bar{a}_{-k}^* \bar{\xi}_{-k}^* e^{-ikx} e^{-i\omega t} \right] =$$
$$\sum_k \frac{1}{\sqrt{2\omega}} \left[ a_k^* \xi_k^* e^{-ikx} e^{i\omega t} + b_k^* \eta_k^* e^{-ikx} e^{-i\omega t} \right]$$

$$N = \sum_k \frac{1}{2\omega} \left( a_k^* a_k \xi_k^* \boldsymbol{\sigma_x} \xi_k + b_k^* b_k \eta_k^* \boldsymbol{\sigma_x} \eta_k \right)$$

$$N = \sum_k \left( a_k^* a_k + b_k^* b_k \right)$$

# Direction occupancy operator

$$N = \sum_k \frac{1}{2\omega}\left(a_k^* a_k \xi_k^* \boldsymbol{\sigma_x} \xi_k + b_k^* b_k \eta_k^* \boldsymbol{\sigma_x} \eta_k\right)$$

$$N_k = \frac{1}{2\omega} a_k^* a_k \xi_k^* \boldsymbol{\sigma_x} \xi_k$$

direction switching operators $\boldsymbol{S}_+ = \frac{1}{2}(\boldsymbol{\sigma_x} + i\boldsymbol{\sigma_y}) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $\boldsymbol{S}_- = \frac{1}{2}(\boldsymbol{\sigma_x} - i\boldsymbol{\sigma_y}) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$$N_k = \frac{1}{2\omega} a_k^* a_k \xi_k^* \boldsymbol{I} \boldsymbol{\sigma_x} \xi_k = a_k^* a_k \xi_k^* \left(\frac{1}{2\omega} S_+ S_- \sigma_x + \frac{1}{2\omega} S_- S_+ \sigma_x\right) \xi_k$$

$$n_k^+ = \xi_k^* \frac{1}{2\omega} S_+ S_- \sigma_x \xi_k = \frac{\omega + \beta k^h}{2\omega}$$

$$n_k^- = \xi_k^* \frac{1}{2\omega} S_- S_+ \sigma_x \xi_k = \frac{\omega - \beta k^h}{2\omega}$$

**Eigen values**

$$\frac{1}{2\omega} S_+ S_- \sigma_x$$

$$\frac{1}{2\omega} S_- S_+ \sigma_x$$

**Direction occupancy operators**

$\boldsymbol{S}_-$ $\boldsymbol{S}_+$ **anticommute**

# Standing vs traveling waves

$$\omega = +\sqrt{\alpha^2 + \beta^2 (kh)^2}$$

$$n_k^+ = \xi_k^* \frac{1}{2\omega} S_+ S_- \sigma_x \xi_k = \frac{\omega + \beta k^h}{2\omega} \qquad n_k^- = \xi_k^* \frac{1}{2\omega} S_- S_+ \sigma_x \xi_k = \frac{\omega - \beta k^h}{2\omega}$$

$$n_k^{\pm} = \frac{1}{2} \pm \frac{\beta k^h/\alpha}{2\sqrt{1+\left(\frac{\beta k^h}{\alpha}\right)^2}}$$

$k$=o, and $n_k^+ = n_k^-$=1/2 $\quad k \to \infty, n_k^+ = 1$ and $n_k^- = 0$

**Standing wave** **Traveling wave**

# Phase Control of Fermion-like Phonons

## Dirac Field

$$\Psi_k = b_k \xi_k e^{ik^{x}} e^{-i\omega^{t}}$$

$b_k$ anticommutes

## with Spinor

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \pm\sqrt{\omega \pm \beta k^{h}} \\ \mp\sqrt{\omega \mp \beta k^{h}} \end{pmatrix}$$

$\pm$, $\mp$ depend on sign of k and $\omega$

## Define the basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

## It is a "Qubit" with controllable phase

$$\xi_k = a(k)|0\rangle + b(k)|1\rangle$$

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

sses
School of Sustainable Engineered Systems

# Potential impact

1. Physical platform for Phase-based computing and information processing (Phonon-based "Qubit")
2. New functionalities of phonon-based telecommunication and imaging devices
3. Extension of idea to nanoscale can lead to potential control of thermal phonons (e.g. thermal transport)
4. Technologies involving interactions between phonon and electrons (electronics, thermoelectrics), photons (spectroscopy, imaging), etc. will be impacted.

# Conclusions

1. The concept of fermion-like phonons is radical.
2. We have discovered a physical platform supporting fermion-like phonons.
3. Phase control of phonons through fermionic behavior is novel.
4. New selection rules for the interaction between fermion-like phonons and other elementary excitations (electrons, photons, magnons, plasmons, etc.) will lead to entirely new physical properties of matter.

THE UNIVERSITY OF ARIZONA
COLLEGE OF ENGINEERING
Department of Materials Science and Engineering

School of Sustainable Engineered Systems

# Questions ?