PERIODIC LATTICE WITH DEFECTS

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ABSTRACT. The discrete periodic lattice of masses and springs with line and point defects is considered. The dispersion equations for propagative, guided and localised waves are obtained. The detailed analysis of example with three masses is provided.

1. Introduction

There are many papers devoted to the wave propagation through the discrete periodic lattice with different types of defects. One of the early works [M] provides explicit solution of the wave equation for the periodic lattice with two different masses. The structure with an infinite line defect embedded in an infinite square lattice has been considered in the paper [OA]. In this case the dispersion relations for localised modes can be computed in explicit form. In the paper [MS] the authors examined several classes of continuous and discrete models with various defect configurations. In the recent paper [CNJMM] the homogeneous lattice perturbed by the finite line of masses is considered with respect to analysis of eigenmodes. Also note the large number of papers devoted to periodic structures without localised defects but with the boundaries, see references in [KK1].

The motivation for the present paper is to combine perturbation of the periodic lattice by a periodic line (like in [OA]) with that by a finite defect (like in [CNJMM]) and to obtain a new dispersion equation for such configurations. The developed method can be applied for the different types of lattices with arbitrary horizontal and vertical periods. Note that this method is based on the modified Green function approach which differs from the method of [M1]. Further we plan to adapt the so-called monodromy matrix approach (see e.g. [KS]) for obtaining dispersion equations for localised modes. In particular the monodromy matrix approach should allows us to obtain localised modes in propagative and guided spectral intervals.

In the example below, we consider the homogeneous lattice with mass of particles $M = 1$ perturbed by the line defect with mass of particles $\tilde{M}$ and with one single mass $M$. The detailed analysis of the band-gap structure of propagative and guided spectra and the necessary and sufficient conditions of existing of localised modes are obtained. We note an interesting phenomenon: if the mass $\tilde{M}$ increases indefinitely then the upper limit of mass $M$ for which the localised mode exists is exactly $\frac{3}{4} - \frac{1}{2\pi}$ (somewhat unusual appearance of $\pi$).

The work is organized as follows. Section 2 contains our main results, namely, the dispersion equations for three types of defects: 1) periodic lattice without defects 2) periodic lattice with periodic strip 3) periodic lattice with periodic strip and with finite defects. In Section 3 the derivations of dispersion equations from the Section 2 are provided. In Section 4 the propagative, guided and localised spectra for the homogeneous lattice with line and single defect are analised.

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2. Dispersion equations

2.1. Periodic lattice. Consider the 2D periodic lattice (see Fig 1) without defects, i.e. $M_n = \bar{M}_n = \overline{M}_n$. The wave equation takes the following form

$$\sum_{n'} u_{n'} - 4u_n = -\omega^2 M_n u_n, \quad (2.1)$$

where $\omega$ is the frequency, $u_n$ is antiplane displacement and $n = (n_1, n_2)$ is a position of the mass $M_n$ on the square lattice (number of the nod). We suppose that all quantities in (2.1) are normalised (dimensionless). The notation $n \sim n'$ means that there exists a link between nodes with numbers $n$ and $n'$. Suppose that the function $M_n$ is periodic

$$M_{n+N_1 e_1 + N_2 e_2} = M_n, \quad \forall n \in \mathbb{Z}^2 \quad (2.2)$$

with basis vectors $e_1 = (1, 0)$, $e_2 = (0, 1)$ and periods $N_1, N_2 \geq 1$. After applying Fourier transformation (see (3.4)-(3.6)) the equation (2.1) takes the following form

$$\hat{\mathbf{L}} \hat{\mathbf{u}} = -\omega^2 \hat{\mathbf{M}} \hat{\mathbf{u}} \quad (2.3)$$

with finite matrices defined on the unit cell $\mathcal{N} = [1..N_1] \times [1..N_2]$:

$$\hat{\mathbf{M}} = (M_{n,n'}\delta_{nn'})_{n,n'\in\mathcal{N}}, \quad \hat{\mathbf{L}} = \hat{\mathbf{L}}_0 - 4\hat{\mathbf{I}}, \quad (2.4)$$

$$\hat{\mathbf{L}}_0 = (\delta_{n-n'}\delta_{nm'})_{n,n',m',n'\in\mathcal{N}}, \quad \hat{\mathbf{I}} = (\delta_{nm'})_{n,n'\in\mathcal{N}}, \quad (2.5)$$

where $\delta_{nn'}$ is a Kronecker symbol and

$$\hat{\delta}_{n-n'} = \delta_{n-n'} + \quad (2.6)$$
\[ e^{-ik_{1}}\delta_{n-N_{1}e_{1}-n'} + e^{ik_{1}}\delta_{n+N_{1}e_{1}-n'} + e^{-ik_{2}}\delta_{n-N_{2}e_{2}-n'} + e^{ik_{2}}\delta_{n+N_{2}e_{2}-n'} \]

with \(\delta_{n-n'} = 1\) iff there exists a link between nodes \(n\) and \(n'\) and \(\delta_{n-n'} = 0\) otherwise.

The dispersion equation which determines the Floquet branches \(\omega_{p}(k)\) (dispersion curves for propagative spectrum) can be written in the form

\[ \det \hat{L}_{p}(\omega, k) = 0, \text{ where } \hat{L}_{p} \equiv \hat{L} + \omega^{2}\hat{M}. \] (2.7)

2.2. Periodic lattice with periodic strip. Here the periodic strip with masses \(\tilde{M}_{n} = M_{n} + M_{n}^{(1)}\) (see Fig. 1) is added to our lattice. In this case along with the propagative spectrum \(\omega_{p}\) there appears the guided spectrum \(\omega_{g}\). The guided spectrum corresponds to the waves which are bounded (quasiperiodic) along the added strip and decay along the direction which is perpendicular to the strip. The guided dispersion curves depend on Floquet parameter \(k_{1}\) and can be determined from the dispersion equation (see the derivation in Section 3.2)

\[ \det \hat{L}_{g}(\omega, k_{1}) = 0 \text{ where } \hat{L}_{g} \equiv \hat{1} + \omega^{2}(\hat{L}_{p}^{-1})_{2}\hat{M}_{1} \] (2.8)

and

\[ \hat{M}_{1} = (M_{n}^{(1)}\delta_{nn'})_{n,n' \in N}, \quad \langle \cdot \rangle_{j} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \cdot dk_{j}. \] (2.9)

Note that the equation (2.8) is not valid in the bands of propagative spectrum, i.e. in the sets

\[ I_{p}(k_{1}) = \omega_{p}(k_{1}, [-\pi, \pi]) \] (2.10)

which correspond to the projection of the propagative dispersion curves \(\omega_{p}(k)\) on the plane \((\omega, k_{1})\). We need this restriction because the inverse of \(L_{p}\) (see (2.8)) does not exist in the intervals \(I_{p}(k_{1})\).

2.3. Periodic lattice with periodic strip and with localised inclusions. Here the localised inclusions with masses \(\tilde{M}_{n} = M_{n} + M_{n}^{(2)}\) (see Fig. 1) are added to our periodic lattice with the strip. In this case along with propagative \(\omega_{p}\) and guided \(\omega_{g}\) spectra the localised spectrum \(\omega_{loc}\) appears. The localised spectrum corresponds to the waves which decay in any direction of our lattice. The localised spectrum \(\omega_{loc}\) can be determined from the following dispersion equation (see the derivation in Section 3.2)

\[ D_{loc}(\omega) \equiv \det(\hat{1} + \omega^{2}(\hat{L}_{g}^{-1}(\hat{L}_{p}^{-1})_{2})\hat{M}_{2}) = 0, \] (2.11)

where

\[ \hat{M}_{2} = (M_{n}^{(2)}\delta_{nn'})_{n,n' \in N}. \] (2.12)

Note that the equation (2.11) is not valid in the bands of propagative and guided spectra, i.e. in the sets

\[ I_{p} = I_{p}([-\pi, \pi]), \quad I_{g} = \omega_{g}([-\pi, \pi]) \] (2.13)

which correspond to the projection of propagative \(\omega_{p}(k)\) and guided \(\omega_{g}(k_{1})\) dispersion curves on the axis \(\omega\). We need this restriction because the inverse of \(L_{p}\) and \(L_{g}\) (see (2.11)) do not exist in the intervals \(I_{p}\) and \(I_{g}\).
3. The derivation of dispersion equations

3.1. Periodic lattice. The set of linear equations (2.1) can be represented in the form of infinite matrices

\[ Lu = -\omega^2 Mu, \quad \text{where} \quad u = (u_n)_{n \in \mathbb{Z}^2} \quad (3.1) \]

and

\[ M = (M_n \delta_{nn'})_{n,n' \in \mathbb{Z}^2}, \quad L = L_0 - 4I, \quad (3.2) \]

\[ L_0 = (\delta_{n-n'})_{n,n' \in \mathbb{Z}^2}, \quad I = (\delta_{nn'})_{n,n' \in \mathbb{Z}^2}. \quad (3.3) \]

The infinite system (3.1) can be rewritten in the Fourier space as a finite system. For this we introduce the operator

\[ F : \ell^2(\mathbb{Z}^2) \rightarrow L^2_N([\pi, \pi]^2), \quad F(u) = \hat{u}(k), \quad (3.4) \]

where

\[ \hat{u}(k) = (\hat{u}_n(k))_{n \in \mathbb{N}}, \quad \hat{u}_n(k) = \sum_{r \in \mathbb{Z}^2} u_{n+r_1N_1r_2N_2} e^{i(r \cdot k)}. \quad (3.5) \]

Under the action of the operator \( F \) any sequence \( u \) from \( \ell^2(\mathbb{Z}^2) \) becomes the vector-function \( \hat{u}(k) \) with \( N_1N_2 \) components, any component is a function from \( L^2([\pi, \pi]^2) \). Then the wave equation (3.1) can be rewritten in the form

\[ FLF^{-1} \hat{u} = -\omega^2 FMF^{-1} \hat{u} \quad (3.6) \]

which coincide with (2.3) because \( FLF^{-1} = \hat{L} \) and \( FMF^{-1} = \hat{M} \).

3.2. Periodic lattice with periodic strip. In this case the wave equation (2.3) becomes

\[ \hat{L}\hat{u} = -\omega^2(\hat{M}\hat{u} + \hat{M}_1 \langle \hat{u} \rangle_2) \quad (3.7) \]

with \( \hat{M}_1 \) defined in (2.9). From the equation (3.7) we obtain that

\[ \hat{u} = -\omega^2\hat{L}_p^{-1}\hat{M}_1 \langle \hat{u} \rangle_2 \quad (3.8) \]

with \( \hat{L}_p \) defined in (2.7). Integrating with respect to \( k_2 \) we get

\[ \langle \hat{u} \rangle_2 = -\omega^2\langle \hat{L}_p^{-1}\hat{M}_1 \hat{u} \rangle_2 \quad (3.9) \]

or (see definition of \( \hat{L}_g \) in (2.8))

\[ \hat{L}_g \langle \hat{u} \rangle_2 = 0. \quad (3.10) \]

From (3.10) we obtain the condition of existence of guided waves (2.8).

For our purpose we need the following fact. Consider the equation

\[ \hat{L}\hat{u} + \omega^2 \hat{M}\hat{u} + \omega^2 \hat{M}_1 \langle \hat{u} \rangle_2 = \hat{f} \quad (3.11) \]

with some vector-function \( \hat{f} \) from \( L^2_N([\pi, \pi]^2) \). Then the solution of this equation takes the following form

\[ \hat{u} = \hat{L}_p^{-1}(\hat{f} - \omega^2 \hat{M}_1 \hat{L}_g^{-1}(\hat{L}_p^{-1}\hat{f})_2). \quad (3.12) \]
3.3. Periodic lattice and strip with localised inclusion. In this case the wave equation (3.7) becomes
\[
\hat{L}\hat{u} = -\omega^2(\hat{M}\hat{u} + M_1\langle \hat{u} \rangle_2 + \hat{M}_2\langle \hat{u} \rangle_2) \tag{3.13}
\]
with \(\langle \cdot \rangle \equiv \langle \langle \cdot \rangle_1 \rangle_2\). The equation (3.13) is equivalent to
\[
\hat{L}\hat{u} + \omega^2\hat{M}\hat{u} + \omega^2\hat{M}_1\langle \hat{u} \rangle_2 = -\omega^2\hat{M}_2\langle \hat{u} \rangle_2. \tag{3.14}
\]
Applying (3.11)-(3.12) to (3.14) with \(\hat{f} = -\omega^2\hat{M}_2\langle \hat{u} \rangle_2\) leads to
\[
\hat{u} = \hat{L}^{-1}_p(\hat{I} - \omega^2\hat{M}_1\hat{L}_g^{-1}(\hat{L}^{-1}_p)_2)(-\omega^2\hat{M}_2\langle \hat{u} \rangle_2) \tag{3.15}
\]
and then
\[
\langle \hat{u} \rangle = \left(\langle \hat{L}^{-1}_p \rangle_2(\hat{I} - \omega^2\hat{M}_1\hat{L}_g^{-1}(\hat{L}^{-1}_p)_2)\right)_1(-\omega^2\hat{M}_2\langle \hat{u} \rangle_2) \tag{3.16}
\]
which can be rewritten in the form of
\[
(\hat{I} + \omega^2\langle \hat{L}^{-1}_g(\hat{L}^{-1}_p)_2\rangle_1\hat{M}_2)(\hat{u}) = 0. \tag{3.17}
\]
The equation (3.17) gives us the condition of existence of localised modes (2.11).

4. Example

![Figure 2](image_url)

**Figure 2.** a) Homogeneous lattice with mass \(M = 1\), b) perturbed by periodic strip with mass \(\hat{M} = M + M^{(1)}\), c) perturbed by single mass \(\bar{M} = M + M^{(1)} + M^{(2)}\).

4.1. Uniform lattice. We start from homogeneous square lattice with mass \(M = 1\), see Fig. 2a). The wave equation for this structure takes the following form (see (2.3))
\[
(2\cos k_1 + 2\cos k_2 - 4)u = -\omega^2u. \tag{4.1}
\]
The operator \(\hat{L}_p\) and Floquet branches are (see (2.7))
\[
\hat{L}_p = \omega^2 - 4 + 2\cos k_1 - 2\cos k_2, \tag{4.2}
\]
\[
\omega_p(k) = \sqrt{4 - 2\cos k_1 - 2\cos k_2}. \tag{4.3}
\]
4.2. **Uniform lattice with uniform line.** Now we add the periodic line with mass \( M + M^{(1)} \) (recall that \( M = 1 \), see Fig. 2b). In this case

\[
\langle \hat{L}^{-1} \rangle_2 = \begin{cases} 
\sqrt{(2 \cos k_1 - 4 + \omega^2)^2 - 4}, & \text{if } \omega^2 < 2 - 2 \cos k_1, \\
1, & \text{if } \omega^2 > 6 - 2 \cos k_1.
\end{cases}
\] (4.4)

Due to (2.8) the guided spectrum \( \omega_g(k_1) \) is determined by

\[
(\det \hat{L}_g =) \begin{cases} 
1 - \frac{\omega^2 M^{(1)}}{\sqrt{(2 \cos k_1 - 4 + \omega^2)^2 - 4}}, & \text{if } \omega^2 < 2 - 2 \cos k_1, \\
1 + \frac{\omega^2 M^{(1)}}{\sqrt{(2 \cos k_1 - 4 + \omega^2)^2 - 4}}, & \text{if } \omega^2 > 6 - 2 \cos k_1.
\end{cases}
\] (4.5)

These equations can be solved directly

\[
\omega_g^2(k_1) = \begin{cases} 
2 \cos k_1 - 4 - 2 \sqrt{(M^{(1)})^2 (\cos k_1 - 2)^2 - (M^{(1)})^2 + 1}, & \text{if } -1 < M^{(1)} < 0, \\
2 \cos k_1 - 4 + 2 \sqrt{(M^{(1)})^2 (\cos k_1 - 2)^2 - (M^{(1)})^2 + 1}, & \text{if } M^{(1)} > 0.
\end{cases}
\] (4.6)

The projection of the propagative spectrum \( \omega_p(k) \) (4.3) on the plane \((\omega, k_1)\) (see (2.10)) is

\[
I_p(k_1) = \left[ \sqrt{2 - 2 \cos k_1}, \sqrt{6 - 2 \cos k_1} \right].
\] (4.7)

![Figure 3](image-url)  
**Figure 3.** Projection of the Floquet spectrum \( I_p(k_1) \) (4.7) on the plane \((\omega, k_1)\) (red area) and the guided spectrum (green line) \( \omega_g(k_1) \) (4.6) for homogeneous square lattice (mass \( M = 1 \)) with perturbed line (mass \( \tilde{M} = M + M^{(1)} \), see Fig. 2b).

4.3. **Uniform lattice and line with localised inclusion.** Now we add one perturbed mass \( \tilde{M} = M + M^{(2)} \). The condition on \( \omega_{\text{loc}} \) (see (2.11)) takes the following form

\[
D_{\text{loc}}(\omega) \equiv 1 + \frac{\omega^2 M^{(2)}}{2\pi} \int_{-\pi}^{\pi} \frac{dk_1}{\omega^2 M^{(1)} + (2 \cos k_1 - 4 + \omega^2)^2 - 4} = 0.
\] (4.8)
The projection of the propagative and guided spectrum on the axis $\omega$ (see (2.13)) is

$$I_p = [0, 2\sqrt{2}],$$

$$I_g = \begin{cases} 
\frac{2}{\sqrt{1-(M^{(1)})^2}} & \text{if } -1 < M^{(1)} < 0, \\
\sqrt{\frac{6+2\sqrt{8(M^{(1)})^2+1}}{(M^{(1)})^2-1}} & \text{if } M^{(1)} > 0.
\end{cases}$$

Figure 4. Function $D_{\text{loc}}(\omega)$ (4.8) (blue curve) and its zeroes $\omega_{\text{loc}}$ (localised spectrum) with the projection of propagative $I_p$ (4.9) (red bold line) and guided $I_g$ (4.9) (green thin line) spectra on the axe $\omega$.

4.4. Existence of the localised waves (states). The equation (4.8) can be rewritten in the form

$$D_{\text{loc}}(\omega) = 1 + M^{(2)}D_1(\omega) = 0$$

with

$$D_1(\omega) \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\omega^2 dk_1}{\omega^2 M^{(1)} + \sqrt{(2 \cos k_1 - 4 + \omega^2)^2 - 4}}.$$  

The integrand function in (4.12) is strictly decreasing in $\omega \in \mathbb{R}_+ \setminus (I_p \cup I_g)$ for any $k_1$. Then $D_1(\omega)$ is strictly decreasing function in $\omega \in \mathbb{R}_+ \setminus (I_p \cup I_g)$. So knowing the values of $D_1(\omega)$ at the edges of $I_p$ and/or $I_g$ and using (4.11) with monotonicity of $D_1(\omega)$ we can predict the existence of localised modes in the corresponding gap. It is convenient to consider different cases (recall that $1 + M^{(1)} > 0$ and $1 + M^{(1)} + M^{(2)} > 0$ because these are the masses of inclusions):
4.4.1. The case $M^{(1)} \in (-1, -1/\sqrt{2})$. Due to (4.9) we have two disjoint gaps $\mathcal{G}_1$ and $\mathcal{G}_2$ in the propagative and guided spectrum, i.e.
\[
\mathbb{R}_+ \setminus (I_p \cup I_g) = \mathcal{G}_1 \cup \mathcal{G}_2,
\]
where
\[
\mathcal{G}_1 = \left(2\sqrt{2}, \frac{2}{\sqrt{1 - (M^{(1)})^2}}\right), \quad \mathcal{G}_2 = \left(\frac{\sqrt{6 + 2\sqrt{8(M^{(1)})^2 + 1}}}{\sqrt{1 - (M^{(1)})^2}}, +\infty\right).
\]
The values of $D_1$ at the edges of gaps are
\[
D_1(2\sqrt{2}) = \frac{4}{\pi} \int_0^\pi \frac{dk_1}{4M^{(1)} + \sqrt{(\cos k_1 + 2)^2 - 1}} < 0,
\]
\[
D_1\left(\frac{2}{\sqrt{1 - (M^{(1)})^2}}\right) = -\infty, \quad D_1\left(\frac{\sqrt{6 + 2\sqrt{8(M^{(1)})^2 + 1}}}{\sqrt{1 - (M^{(1)})^2}}\right) = +\infty,
\]
\[
D_1(+) = \frac{1}{1 + M^{(1)}} > 0.
\]
Using (4.15)-(4.17), (4.11) with monotonicity of $D_1$ we conclude that:
\begin{itemize}
  \item[a)] If $M^{(2)} < 0$ then there are no localised states in $\mathcal{G}_1$ and there is only one localised state in $\mathcal{G}_2$.
  \item[b)] If $M^{(2)} = 0$ then there are no localised states in $\mathcal{G}_1$ and in $\mathcal{G}_2$.
  \item[c)] If $M^{(2)} \in (0, -1/D_1(2\sqrt{2}))$ then there is only one localised state in $\mathcal{G}_1$ and no localised states in $\mathcal{G}_2$.
  \item[d)] If $M^{(2)} \geq -1/D_1(2\sqrt{2})$ then there are no localised states in $\mathcal{G}_1$ and $\mathcal{G}_2$.
\end{itemize}

4.4.2. The case $M^{(1)} \in [-1/\sqrt{2}, 0]$. Due to (4.9) we have only one gap $\mathcal{G}_2$ in the propagative and guided spectrum, i.e.
\[
\mathbb{R}_+ \setminus (I_p \cup I_g) = \mathcal{G}_2 = \left(\frac{\sqrt{6 + 2\sqrt{8(M^{(1)})^2 + 1}}}{\sqrt{1 - (M^{(1)})^2}}, +\infty\right).
\]
Applying the same arguments as in the previous case we deduce that:
\begin{itemize}
  \item[a)] If $M^{(2)} < 0$ then there is only one localised state in $\mathcal{G}_2$.
  \item[b)] If $M^{(2)} \geq 0$ then there are no localised states in $\mathcal{G}_2$.
\end{itemize}

4.4.3. The case $M^{(1)} > 0$. Due to (4.9) we have only one gap $\mathcal{G}$ in the propagative and guided spectrum, i.e.
\[
\mathbb{R}_+ \setminus (I_p \cup I_g) = \mathcal{G} = (2\sqrt{2}, +\infty).
\]
Applying the same arguments as in the previous cases we deduce that:
\begin{itemize}
  \item[a)] If $M^{(2)} < -1/D_1(2\sqrt{2})$ then there is only one localised state in $\mathcal{G}$.
  \item[b)] If $M^{(2)} \geq -1/D_1(2\sqrt{2})$ then there are no localised states in $\mathcal{G}$.
\end{itemize}
Note that in this case $D_1(2\sqrt{2}) > 0$ (compare with (4.15)).

4.4.4. Summation. Now we summarize above statements.
1) For the strip "I" there are two spectral gaps, first gap is located between propagative and guided spectra, the second is above the guided spectrum (Fig. 3a). For the brown area the localised mode is in the first gap (Figs. 4b,c), for the purple one is in the second (Fig. 4a).

2) For the strip "II" there is one spectral gap above the guided spectrum. Guided and propagative spectra intersect (Fig. 3b). For the purple area there is one localised mode in the gap (Fig. 4e).

3) For the quadrant "III" there is one gap above the propagative spectrum. Guided spectrum lies inside the propagative (Figs. 3c,d). For the purple area there is one localised mode in the gap (Fig. 4g).

For the white area we have no localised modes in the spectral gaps (Figs. 4d,f,h).

Figure 5. The regions of emergence of localised modes for different masses $\tilde{M}, \overline{M}$ in the lattice Fig. 2c). The boundary of these regions consist of curves $\overline{M} = \tilde{M} - \frac{1}{D_1(2\sqrt{2})}$ (see (4.15) for $D_1$) and $\overline{M} = \tilde{M}$. The maximal mass $\overline{M}$ for which the localised mode exists tends to 1 (with $\tilde{M} \rightarrow 1$). After increasing of mass $\tilde{M} \geq 1$ we see at the beginning the rapid fall of mass $\overline{M}$, which reach the limit $\frac{3}{4} - \frac{1}{2\pi}$ for $\tilde{M} \rightarrow +\infty$.

5. Conclusion.

The dispersion equations for the propagative, guided and localised waves in the discrete periodic lattice with the strip and with localised inclusions are obtained. For the uniform lattice with the line and with one single inclusion the existence of localised modes and its position is analysed.

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