Mode densities of defect lines in two-dimensional Montroll-Potts lattices

1993 J. Phys.: Condens. Matter 5 33

(http://iopscience.iop.org/0953-8984/5/1/006)

J. Phys.: Condens. Matter 5 (1993) 33–56. Printed in the UK

Mode densities of defect lines in two-dimensional Montroll–Potts lattices

Max Wagner, Hilmar Dolderer and Christoff Reusch

Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, D-7000 Stuttgart 80, Federal Republic of Germany

Received 4 August 1992, in final form 29 October 1992

Abstract. The investigation addresses the problem, to what extent one-dimensional defect structures in a crystalline surrounding are able to affect the low-frequency vibrational-mode density. This problem is of importance for the thermodynamics and the energy transport properties of disordered materials, like glasses. Employing an extended Lifshitz procedure, a Green function technique is used to calculate the mode density of several prototypical linear defect structures within a two-dimensional reference lattice of Montroll–Potts type. It is shown that, depending on the softness of the chosen defect lines, even at very low frequencies the power law of the mode density may switch from the two-dimensional behaviour of the bulk ($\rho \sim \omega$) to a form which is characteristic of one-dimensional oscillatory dynamics ($\rho \sim$ constant).

1. Introduction

There is a marked difference between the specific heat and the thermal conductivity of non-crystalline dielectric solids and of crystalline ones, a fact which has been known since the seminal work of Zeller and Pohl [23] two decades ago. The measured glassy materials (SiO_2, GeO_2, etc.) display common features (T law of the specific heat, T^2 law and plateau in the heat conductivity, etc.), and a huge amount of later experimental data [3, 6, 8] hint at a universality of these features in non-metallic glasses.

In contrast to the favourable experimental situation there are still some unresolved problems in the theoretical description of these phenomena. The tunnelling model of Anderson, Varma and Halperin [1] and of Phillips [17] was very successful in explaining the power laws of the specific heat (T^1) and the thermal conductivity (T^2) in the very low temperature region, although the microscopic nature of the tunnelling centres still remains unclear.

In the temperature regime between 2 and 10 K the specific heat is enhanced by a factor of two to three compared with the pure soundwave contribution. This difference has often been referred to as an excess specific heat and has been associated with some extra modes. Such modes have indeed been found recently by Buchenau *et al* [3, 4] and by means of inelastic neutron scattering experiments they have been attributed to chains of librating SiO_4 tetrahedra. The existence of these modes results in an enhanced density of states beyond the Debye value.

On the other hand Krumhansl [7] has emphasized that non-Debye features can also be found in crystalline material of highly anisotropic nature, and he has

0953-8984/93/010033+24$07.50

given some examples. This suggests that mode densities come into effect which are characteristic of lower dimensionality than three. Since a one-dimensional crystal displays a linear temperature behaviour in the specific heat, and since the extra modes of Buchenau have been shown to be of harmonic nature, it seems desirable to investigate the question whether one-dimensional defect structures in higher-dimensional embeddings may produce a pronounced enhancement in the mode density. This has led us to choose an analytically tractable model system to study the problem.

This paper is divided into six sections. Section 2 is a short synopsis of the Green function formalism which is related to the original Lifshitz procedure [10–12] and its extension to extrinsic degrees of freedom [19, 20]. A comprehensive presentation is found in an earlier paper by Wagner and Mougios [21]. The following section describes the two-dimensional Montroll–Potts lattice which is our undisturbed reference system and specifies the symmetry vectors of linear defect structures. In section 4 detailed calculations of intrinsic defects are made whereas in section 5 the effects of an extrinsic soft linear chain coupled to the bulk are discussed. A short summary of our results is given in the last section and the possibility of calculating more complex structures is considered.

2. Preliminaries

2.1. *Density of modes*

We restrict ourselves to a specification of the basic Green function formulae which we need to carry out the calculations. A comprehensive representation of the formalism is given in an earlier paper [21], and further background information is found in books of Dederichs and Zeller [5], Böttger [2] and of Maradudin *et al* [13]. We consider a harmonic oscillatory system, characterized by the Hamiltonian

$$H = \tfrac{1}{2}\sum_{m}^{N} P_m^2 + \tfrac{1}{2}\sum_{m,n} X_m U_{mn} X_n \tag{1}$$

where X_m are mass-reduced Cartesian coordinates ($X_m = \sqrt{M_m}x_m$). Then the eigenvectors $\eta(\kappa) = [\eta_m(\kappa)]$ of the dynamical matrix U_{mn} constitute a complete orthonormal set and may be employed to define normal coordinates [13]

$$Q_\kappa = \sum_m \eta_m^*(\kappa) X_m \tag{2}$$

which diagonalize the Hamiltonian (1),

$$H = \tfrac{1}{2}\sum_{\kappa}^{N} P_\kappa P_\kappa^\dagger + \tfrac{1}{2}\sum_{\kappa} \Omega_\kappa^2 Q_\kappa Q_\kappa^\dagger. \tag{3}$$

We introduce the Zubarev Green function (GF) [24]

$$G_{mn}(E) = \frac{1}{2\pi}\sum_{\kappa}\frac{1}{E^2 - \Omega_\kappa^2}\eta_m(\kappa)\eta_n^*(\kappa) \tag{4}$$

the imaginary part of which is related to the density of states

$$\rho(\omega) = 2i\omega \sum_m [G_{mm}(\omega + i\epsilon) - G_{mm}(\omega - i\epsilon)]$$
$$= -4\omega \mathrm{Im} \sum_m G_{mm}(\omega + i\epsilon) \qquad \text{for} \quad \omega \geqslant 0. \tag{5}$$

If an oscillatory system may be conceived as a deviation from an 'undisturbed' one, the dynamics of which is known

$$H = H^{(0)} + W \tag{6}$$
$$W = \tfrac{1}{2} \sum_{mn} w_{mn} X_m X_n \tag{7}$$

such that the 'disturbance' only embodies a small number of coordinates, we may apply the Lifshitz formalism [10, 11] to calculate the disturbed GF from the undisturbed one,

$$\mathbf{G}(E) = \mathbf{G}^{(0)}(E) + 2\pi \mathbf{G}^{(0)}(E)\mathbf{w}[\mathbf{I} - 2\pi \mathbf{g}^{(0)}(E)\mathbf{w}]^{-1}\mathbf{G}^{(0)}(E). \tag{8}$$

$\mathbf{g}^{(0)}(E)$ represents that part of the undisturbed GF $\mathbf{G}^{(0)}(E)$ which pertains to the 'small space' of the matrix w_{mn}. From (5) and (8) we deduce, after some manipulation, the deviation $\Delta\rho(\omega) = \rho(\omega) - \rho^{(0)}(\omega)$ of the mode density from the undisturbed expression,

$$\Delta\rho(\omega) = 2\,\mathrm{Im}\ \mathrm{Tr}\ \left\{\mathbf{w}\left[\mathbf{I} - 2\pi \mathbf{g}^{(0)}(E)\mathbf{w}\right]^{-1} \mathrm{d}\mathbf{g}^{(0)}(E)/\mathrm{d}\omega\right\} \tag{9}$$

where $E = \omega + i\epsilon$ and

$$\mathrm{Tr}\,\{\mathbf{X}\} = \sum_m X_{mm}. \tag{10}$$

For details we refer e.g. to the book of Dederichs and Zeller [5]. For 'intrinsic' disturbances, as given by expression (7), the effective disturbance matrix w_{mn} does not depend on ω, whence expression (9) may be simplified to

$$\Delta\rho(\omega) = -(1/\pi)(\mathrm{d}/\mathrm{d}\omega)\,\mathrm{Im}\ \mathrm{Tr}\ \left\{\ln\left[\mathbf{I} - 2\pi \mathbf{g}^{(0)}(E)\mathbf{w}\right]\right\} \tag{11}$$

and by means of $\mathrm{Tr}\{\ln \mathbf{X}\} = \ln\{\det \mathbf{X}\}$ finally to

$$\Delta\rho(\omega) = -(1/\pi)(\mathrm{d}/\mathrm{d}\omega)\,\mathrm{Im}\ \ln\ \left\{\det\left[\mathbf{I} - 2\pi \mathbf{g}^{(0)}(E)\mathbf{w}\right]\right\}. \tag{12}$$

In a very similar manner we may also handle problems, in which the original reference system, characterized by the Hamiltonian $H^{(0)}$, is supplemented by additional degrees of freedom. In this case the Lifshitz procedure has to be modified somewhat [19]. We now write the Hamiltonian in the form

$$H = H^{(i)} + H^{(e)} + H^{(i,e)} \tag{13}$$

where

$$H^{(\mathrm{i})} = \tfrac{1}{2}\sum_m P_m^2 + \tfrac{1}{2}\sum_{mn} X_m U_{mn}^{(\mathrm{i})} X_n \tag{13a}$$

$$H^{(\mathrm{e})} = \tfrac{1}{2}\sum_r P_r^2 + \tfrac{1}{2}\sum_{rs} X_r U_{rs}^{(\mathrm{e})} X_s \tag{13b}$$

$$H^{(\mathrm{i,e})} = \tfrac{1}{2}\sum_{mr}(X_m K_{mr} X_r + X_r K_{rm} X_m) \qquad K_{mr} = K_{rm} \tag{13c}$$

and we introduce the convention that the indices $\{m, n\}$ are always confined to the 'intrinsic' degrees of freedom whereas $\{r, s\}$ pertain to the 'extrinsic' ones. We introduce the 'intrinsic' and 'extrinsic' GFs respectively as

$$G_{mn}^{(\mathrm{i})}(E) = (1/2\pi)\left(E^2\mathbf{I}^{(\mathrm{i})} - \mathbf{U}^{(\mathrm{i})}\right)_{mn}^{-1} \tag{14a}$$

$$G_{rs}^{(\mathrm{e})}(E) = (1/2\pi)\left(E^2\mathbf{I}^{(\mathrm{e})} - \mathbf{U}^{(\mathrm{e})}\right)_{rs}^{-1} \tag{14b}$$

where $\mathbf{I}^{(\mathrm{i})}, \mathbf{I}^{(\mathrm{e})}$ are the unit matrices in the two subspaces respectively. It should be noted that the matrix elements defined in (14*a*,*b*) are not those of the true GF in the two subspaces,

$$G_{mn}(E) \neq G_{mn}^{(\mathrm{i})}(E) \qquad G_{rs}(E) \neq G_{rs}^{(\mathrm{e})}(E). \tag{15}$$

Defining the decomposition

$$U_{mn}^{(\mathrm{i})} = U_{mn}^{(0,\mathrm{i})} + w_{mn}^{(\mathrm{i})} \tag{16}$$

it is found (see [21]) that an effective intrinsic disturbance may be introduced,

$$w_{mn}^{(\mathrm{eff})} = w_{mn}^{(\mathrm{i})} + 2\pi \sum_{rs} K_{mr} G_{rs}^{(\mathrm{e})}(E) K_{sn} \tag{17}$$

such that again the GF pertaining to the intrinsic degrees of freedom may be written in the Lifshitz form (8)

$$G_{mn}(E) = G_{mn}^{(0,\mathrm{i})}(E) + 2\pi\left\{\mathbf{G}^{(0,\mathrm{i})}(E)\mathbf{w}^{(\mathrm{eff})}\left[\mathbf{I}^{(\mathrm{i})} - 2\pi\mathbf{g}^{(0,\mathrm{i})}(E)\mathbf{w}^{(\mathrm{eff})}\right]^{-1}\mathbf{G}^{(0,\mathrm{i})}(E)\right\}_{mn} \tag{18}$$

where

$$G_{mn}^{(0,\mathrm{i})}(E) = (1/2\pi)\left(E^2\mathbf{I}^{(\mathrm{i})} - \mathbf{U}^{(0,\mathrm{i})}\right)_{mn}^{-1}. \tag{19}$$

The extrinsic elements $G_{rs}(E)$ of the true GF are found as

$$G_{rs}(E) = (1/2\pi)\left\{E^2\mathbf{I}^{(\mathrm{e})} - \left[\mathbf{U}^{(\mathrm{e})} + 2\pi\mathbf{K}\,\mathbf{G}^{(\mathrm{i})}(E)\,\mathbf{K}\right]\right\}_{rs}^{-1} \tag{20}$$

where $\mathbf{G}^{(i)}(E)$ is defined in (14*a*) and, in view of the decomposition (16) the intrinsic GF $\mathbf{G}^{(i)}(E)$ may also be written in the Lifshitz form (8)

$$G^{(i)}_{mn}(E) = G^{(0,i)}_{mn}(E) + 2\pi \left\{ \mathbf{G}^{(0,i)}(E)\mathbf{w}^{(i)} \left[\mathbf{I}^{(i)} - 2\pi \mathbf{g}^{(0,i)}(E)\mathbf{w}^{(i)}\right]^{-1} \mathbf{G}^{(0,i)}(E) \right\}_{mn} . \tag{21}$$

The total mode density is given by means of

$$\rho(\omega) = \rho^{(0,i)}(\omega) + \Delta\rho^{(i)}(\omega) + \rho^{(e)}(\omega) \tag{22}$$

where $\rho^{(0,i)}(\omega)$ stands for the undisturbed intrinsic density and

$$\begin{aligned}\Delta\rho^{(i)}(\omega) &= -4\omega \operatorname{Im} \sum_m G_{mm}(E) - G^{(0,i)}_{mm}(E) \\ &= 2 \operatorname{Im} \operatorname{Tr} \left\{ \mathbf{w}^{(\mathrm{eff})}(E) \left[\mathbf{I}^{(i)} - 2\pi \mathbf{g}^{(0,i)}(E)\mathbf{w}^{(\mathrm{eff})}(E)\right]^{-1} \frac{\mathrm{d}\mathbf{g}^{(0,i)}(E)}{\mathrm{d}\omega} \right\}\end{aligned} \tag{23}$$

$$\rho^{(e)}(\omega) = -4\omega \operatorname{Im} \sum_r G_{rr}(E) \tag{24}$$

2.2. *Collective disturbance coordinates*

The small 'space' of coordinates which characterizes the deviation of the disturbed Hamiltonian H from the undisturbed reference Hamiltonian $H^{(0)}$ does not necessarily involve only a small number of Cartesian coordinates. Rather we assume that it is small in the sense that it can be described by a small number Γ of generalized orthonormal coordinates $\{S(\gamma)\}$,

$$S(\gamma) = \sum_m \sigma_m(\gamma)^* X_m \qquad \gamma = 1, 2, \ldots, \Gamma \tag{25}$$

$$\sum_m^N \sigma_m(\gamma)^* \sigma_m(\gamma') = \delta_{\gamma\gamma'} \tag{26}$$

such that the disturbance (7) displays the form

$$W = \tfrac{1}{2} \sum_{\gamma\gamma'}^{\Gamma} \tilde{w}_{\gamma\gamma'} S(\gamma)^* S(\gamma') \tag{27}$$

where $\tilde{\mathbf{w}}$ is the projection of the disturbance matrix $\mathbf{w}$ onto the vector set $\{\sigma_m(\gamma), \gamma = 1, \ldots \Gamma\}$,

$$\tilde{w}_{\gamma\gamma'} = \sum_{mn} \sigma_m(\gamma)^* w_{mn} \sigma_n(\gamma'). \tag{28}$$

We emphasize that the number of Cartesian coordinates involved may be much larger than the number Γ of effective 'disturbance coordinates' $S(\gamma)$. In a similar manner the GF $\mathbf{G}^{(0)}(E)$ may be projected onto this set [21],

$$\tilde{G}^{(0)}_{\gamma\gamma'}(E) = \frac{1}{2\pi}\sum_{\kappa}\frac{1}{E^2-\Omega_\kappa^2}\left(\sum_m^N \sigma_m(\gamma)^*\,\eta_m^{(0)}(\kappa)\right)\left(\sum_n^N \eta_n^{(0)}(\kappa)^*\,\sigma_n(\gamma')\right) \tag{29}$$

The Lifshitz expression (8) then can be shown to reduce to the form

$$\tilde{\mathbf{G}}(E) = \tilde{\mathbf{G}}^{(0)}(E) + 2\pi\tilde{\mathbf{G}}^{(0)}(E)\tilde{\mathbf{w}}\left[\mathbf{I} - 2\pi\tilde{\mathbf{g}}^{(0)}(E)\tilde{\mathbf{w}}\right]^{-1}\tilde{\mathbf{G}}^{(0)}(E) \tag{30}$$

where

$$\tilde{g}^{(0)}_{\gamma\gamma'}(E) = \sum_{mn}\sigma_m(\gamma)^*\,g^{(0)}_{mn}(E)\,\sigma_n(\gamma'). \tag{31}$$

The deviation $\Delta\rho(\omega)$ of the intrinsic mode density (12) from the undisturbed value now reads

$$\Delta\rho(\omega) = -(1/\pi)\,(\mathrm{d}/\mathrm{d}\omega)\,\mathrm{Im}\,\ln\,\left\{\det\,\left[\tilde{\mathbf{I}} - 2\pi\tilde{\mathbf{g}}^{(0)}(E)\tilde{\mathbf{w}}\right]\right\}. \tag{32}$$

In the case of extrinsic disturbances we also may introduce appropriate collective coordinates for the extrinsic degrees of freedom $\{X_r(\mathrm{e})\}$, as shown in section 5. For further details about the derivation of the preceding formulae we refer to an earlier paper [21].

3. Linear defect structures embedded in the two-dimensional Montroll–Potts lattice

3.1. Montroll–Potts lattice

This lattice is useful in model calculations and was introduced by Montroll and Potts [14–16]. In the MPL only nearest-neighbour interaction is taken account of and is described by longitudinal and transversal spring constants f. The Hamiltonian reads

$$H^{(0)} = \tfrac{1}{2}\sum_{m,\mu}P^2_{m,\mu} + \frac{f}{4M}\sum_{m,\mu}\sum_{\delta}\left(X_{m+\delta,\mu} - X_{m,\mu}\right)^2 \tag{33}$$

where $m = m_x e_x + m_y e_y$; $m_x, m_y = 0, \pm 1, \ldots \pm N/2$. e_x, e_y are Cartesian unit vectors and $\delta = \pm e_x, \pm e_y$. The index μ covers the space directions x, y. The eigenvectors read

$$\eta^{(0)}_{m\mu}(k_\lambda) = [2(N+1)^2]^{-1/2}\,\mathrm{e}^{\mathrm{i}k\cdot m}\,\delta_{\mu\lambda} \tag{34}$$

with eigenfrequencies

$$\Omega^{(0)}(k_x,k_y,\lambda)^2 = \tfrac{1}{2}\Omega_{\mathrm{D}}^2\left\{1 - \tfrac{1}{2}(\cos k_x + \cos k_y)\right\} = \Omega^{(0)}(k_x)^2 + \Omega^{(0)}(k_y)^2 \tag{35}$$

$$\Omega_{\mathrm{D}}^2 = 8f/M \qquad \Omega^{(0)}(k_x)^2 = 4(f/M)\sin^2(k_x/2)$$

$$\Omega^{(0)}(k_y)^2 = 4(f/M)\sin^2(k_y/2) \tag{36}$$

where λ denotes the two frequency branches, Ω_D the Debye frequency, and

$$k_x = [2\pi/(N+1)]\, n_x \qquad n_x = 0, \pm 1, \ldots, \pm N/2 \tag{37}$$

$$k_y = [2\pi/(N+1)]\, n_y \qquad n_y = 0, \pm 1, \ldots, \pm N/2. \tag{38}$$

The two frequency branches λ are degenerate. A van Hove singularity occurs at $\Omega_{vH} = \Omega_D/\sqrt{2}$.

The undisturbed Green function for the MP Hamiltonian is of the form (see equation (4))

$$G^{(0)}_{m\mu,n\nu}(E) = \frac{1}{2\pi}\frac{1}{(N+1)^2}\sum_{k}\frac{e^{ik\cdot(m-n)}}{E^2 - \Omega^{(0)}(k)^2}\,\delta_{\mu\nu} \tag{39}$$

and the (undisturbed) mode density reads (see equation (5))

$$\rho^{(0)}(\omega) = [8(N+1)^2/\pi^2\Omega_D^2]\,\omega K(\sqrt{1-(s/2)^2}) \tag{40}$$

with abbreviation

$$s = 2 - 4(\omega/\Omega_D)^2 \tag{41}$$

where

$$K(z) = \int_0^{\pi/2} d\Theta\, \frac{1}{\sqrt{1 - z^2 \sin^2\Theta}}. \tag{42}$$

For low frequencies we find

$$\rho^{(0)}(\omega) = [4(N+1)^2/\pi\Omega_D]\left\{1 + (\omega/\Omega_D)^2\right\}\omega/\Omega_D \qquad \omega \ll \Omega_D. \tag{43}$$

3.2. Intrinsic defect arrays and symmetry vectors

We consider defect lines along the x-axis, such that translational invariance is not broken in this direction, whereas it is broken in the y-direction. By way of this symmetry breaking the wavevector component k_x remains a legitimate characterization of the irreducible group representation, whereas k_y does not.

We assume the spring constants to be disturbed in such a way that only x displacements of a single or a few neighbouring chains are involved and that the deviation from the ideal MPL is given by the Hamiltonian

$$W = \sum_j W^j \tag{44}$$

$$W^j = -\alpha^j \frac{f}{2M}\sum_{m_x}\left\{X_{m_x,m_y^j} - X_{m_x+\delta_x^j,m_y+\delta_y^j}\right\}^2 \tag{45}$$

$$\alpha^j = (f - f^j)/f. \tag{46}$$

In the examples given below the defect structure will always be chosen in such a way that there is mirror symmetry in the y-direction, so that the index γ, introduced in equation (25) to characterize the degrees of freedom involved in the defect, may be specified as

$$\gamma \rightarrow (k_x, p, r) \qquad p = \mathrm{u, g} \qquad r = 1, \ldots R_p$$

where p is the parity with regard to reflection symmetry in the y-direction, and r is the multiplicity index of the respective representation. The vectors $\sigma_m(\gamma)$ (see equation (25)) then may be written in a factorized form,

$$\sigma_{m_x m_y, x} = \sigma_{m_x}(k_x)\, \sigma_{m_y}(p, r) \tag{47}$$

$$\sigma_{m_x m_y, y} = 0. \tag{48}$$

We use the definition

$$\sigma_{m_x}(k_x) = (1/\sqrt{N+1})\, \mathrm{e}^{\mathrm{i}k_x m_x} \tag{49}$$

where k_x is defined in (37). Inserting expressions (47) and (49) in equation (28) with substitutions $m \rightarrow m_\mu$, $\gamma \rightarrow \{k_x, p, r\}$ we find from (45)

$$\widetilde{w}_{rr'}(k_x, p) = -\frac{f}{M} \sum_j \alpha^j \left[\mathrm{e}^{\mathrm{i}\delta_x^j k_x} \sigma_{m_y^j + \delta_y^j}(p, r) - \sigma_{m_y^j}(p, r)\right]^* \times \left[\mathrm{e}^{\mathrm{i}\delta_x^j k_x} \sigma_{m_y^j + \delta_y^j}(p, r') - \sigma_{m_y^j}(p, r')\right] \tag{50}$$

and the corresponding projected GF (31) in the 'small' space is given by

$$\bar{g}^{(0)}_{rr'}(k_x, p; E) = \frac{1}{2\pi} \frac{1}{N+1} \sum_{\substack{k_y \\ m_y, n_y}} \frac{\left(\sigma_{m_y}(p, r)^* \mathrm{e}^{\mathrm{i}k_y m_y}\right) \left(\mathrm{e}^{-\mathrm{i}k_y n_y} \sigma_{n_y}(p, r')\right)}{E^2 - \Omega^{(0)}(k_x, k_y)^2} \tag{51}$$

which may be written as

$$\bar{g}^{(0)}_{rr'}(k_x, p; E) = \sum_{m_y, n_y} \sigma_{m_y}(p, r)^*\, G^{(0)}_{m_y n_y}(\bar{E})\, \sigma_{n_y}(p, r') \tag{52}$$

where

$$G^{(0)}_{m_y n_y}(\bar{E}) = \frac{1}{2\pi} \frac{1}{N+1} \sum_{k_y} \frac{\mathrm{e}^{\mathrm{i}k_y(m_y - n_y)}}{\bar{E}^2 - \Omega^{(0)}(k_y)^2} = G^{(0)}_{n_y m_y}(\bar{E}) \tag{53}$$

$$\bar{E}^2 = E^2 - \Omega^{(0)}(k_x)^2 \qquad E = \omega + \mathrm{i}\epsilon \tag{54}$$

and where $\Omega^{(0)}(k_y)^2, \Omega^{(0)}(k_x)^2$ are given by equation (36). In view of equations (50) and (51) we note that the effective rank of the computational problem is given by the multiplicity R_p of the coordinates pertaining to a given parity p. We further observe that the only GF involved in our calculation will be that of the linear chain (see equation (53)). This GF has been studied intensively by many workers [13, 22]. Specifically one finds

$$G_{00}^{(0)}(\bar{E}) = \frac{1}{2\pi}\frac{1}{N+1}\sum_{k_y}\frac{1}{\bar{E}^2 - \Omega^{(0)}(k_y)^2} = -\frac{2}{\pi^2\Omega_{\mathrm{D}}^2}\int_0^{\pi} \mathrm{d}k_y \frac{1}{s - \mathrm{i}\epsilon - \cos k_y}$$

$$= \frac{2}{\pi\Omega_{\mathrm{D}}^2}\begin{cases} 1/\sqrt{s^2-1} & \text{for } s < -1 \\ -\mathrm{i}/\sqrt{1-s^2} & \text{for } -1 < s < 1 \\ -1/\sqrt{s^2-1} & \text{for } s > 1 \end{cases} \qquad (55a)$$

where

$$s = 2 - 4(\omega/\Omega_{\mathrm{D}})^2 - \cos k_x. \qquad (56)$$

For our calculations we also need the equations

$$G_{10}^{(0)}(\bar{E}) = \frac{2}{\pi\Omega_{\mathrm{D}}^2}\begin{cases} 1 + s/\sqrt{s^2-1} & \text{for } s < -1 \\ 1 - \mathrm{i}s/\sqrt{1-s^2} & \text{for } -1 < s < 1 \\ 1 - s/\sqrt{s^2-1} & \text{for } s > 1 \end{cases} \qquad (55b)$$

$$G_{20}^{(0)}(\bar{E}) = \frac{2}{\pi\Omega_{\mathrm{D}}^2}\begin{cases} 2s + (2s^2-1)/\sqrt{s^2-1} & \text{for } s < -1 \\ 2s + \mathrm{i}(1-2s^2)/\sqrt{1-s^2} & \text{for } -1 < s < 1 \\ 2s - (2s^2-1)/\sqrt{s^2-1} & \text{for } s > 1 \end{cases} \qquad (55c)$$

Employing (47) and (48) we deduce from equation (32) the partial deviations $\Delta\rho(k_x, p; \omega)$ from the undisturbed mode density,

$$\Delta\rho(k_x, p; \omega) = -(1/\pi)\frac{\mathrm{d}}{\mathrm{d}\omega}\,\mathrm{Im}\,\ln\,\det\left[\bar{\mathrm{I}} - 2\pi\bar{\mathrm{g}}^{(0)}(k_x, p; E)\bar{\mathrm{w}}(k_x, p)\right] \qquad (57)$$

and the total deviation reads

$$\Delta\rho(\omega) = \sum_{k_x,p}\Delta\rho(k_x, p; \omega) = \sum_p \frac{N+1}{\pi}\int_{-\pi}^{\pi}\mathrm{d}k_x\,\Delta\rho(k_x, p; \omega). \qquad (58)$$

It is practical in obtaining an overview of the behaviour of $\Delta\rho(k_x, p; \omega)$ to discuss also the function $F(k_x, p; \omega)$ given as

$$F(k_x, p; \omega) = -(1/\pi)\,\mathrm{Im}\,\ln\,\det\left[\bar{\mathrm{I}} - 2\pi\bar{\mathrm{g}}^{(0)}(k_x, p; E)\bar{\mathrm{w}}(k_x, p)\right] \qquad (59)$$

which by means of equation (57) is the 'parental function' of $\Delta\rho(k_x, p; \omega)$,

$$\Delta\rho(k_x, p; \omega) = (\mathrm{d}/\mathrm{d}\omega)F(k_x, p; \omega). \qquad (60)$$

For a given k_x-value the band of undisturbed modes lies between the limits

$$\Omega_{\min}(k_x) = \tfrac{1}{2}\Omega_{\mathrm{D}}\sqrt{1 - \cos k_x} \qquad (61)$$

$$\Omega_{\max}(k_x) = \tfrac{1}{2}\Omega_{\mathrm{D}}\sqrt{3 - \cos k_x}. \qquad (62)$$

Therefore, according to the theorem of Ledermann [9], the disturbed modes also lie in this region with the exception of a few singular (i.e. 'localized') modes, the number of which is not larger than two times the rank of the effective disturbance. These singular modes are found via the Lifshitz equation [10–12]

$$\det\left[\bar{\mathrm{I}} - 2\pi\bar{\mathrm{g}}^{(0)}(k_x, p; E)\bar{\mathrm{w}}(k_x, p)\right] = 0 \qquad (63)$$

for $\omega > \Omega_{\max}(k_x)$ or $\omega < \Omega_{\min}(k_x)$.

4. Examples

4.1. Longitudinal defect line

We first consider the specific case where the longitudinal springs in the line $m_y = 0$ of a MPL are disturbed, as depicted in figure 1(a),

$$W = -\alpha \frac{f}{2M} \sum_{m_x} \left\{ X_{(m_x,0)} - X_{(m_x+1,0)} \right\}^2 \tag{64}$$

where

$$\alpha = (f - f')/f. \tag{65}$$

Then the defect line itself is the mirrorline for the coordinates involved in the disturbance, whence there is only parity p = g, which has multiplicity $R_g = 1$. Therefore the 'symmetry vector' $\sigma_{m_y}(p,r)$ introduced in (47) now reads

$$\sigma_{m_y}(\mathrm{g},r) = \begin{cases} 1 & \text{for } m_y = 0 \\ 0 & \text{otherwise} \end{cases} \tag{66}$$

such that (see equations (50) etc.)

$$\tilde{w}(k_x) \equiv \tilde{w}_{11}(k_x,\mathrm{g}) = -4\alpha(f/M)\left(\sin\tfrac{1}{2}k_x\right)^2 \tag{67}$$

$$\bar{g}^{(0)}(k_x;E) \equiv \bar{g}^{(0)}_{11}(k_x,\mathrm{g};E) = G^{(0)}_{00}(\bar{E}) \tag{68}$$

where $G^{(0)}_{00}(\bar{E})$ is given by (55a) and $\bar{E}^2 = E^2 - \Omega^{(0)}(k_x)^2$, $E = \omega + \mathrm{i}\epsilon$. The Lifshitz equation (63) yields a single localized mode which appears below the band for a 'soft' disturbance, $\alpha > 0 (f' < f)$, and above the band for a 'hard' disturbance, $\alpha < 0 (f' > f)$:

$$\omega_{\mathrm{loc}}(k_x) = \tfrac{1}{2}\Omega_{\mathrm{D}}\sqrt{2 - \cos k_x \pm \sqrt{1 + \alpha^2(1-\cos k_x)^2}} \qquad \text{for} \quad f' \gtrless f. \tag{69}$$

The solution of this equation is shown in figure 2. Inserting equations (67) and (68) in equation (57) we find

$$\begin{aligned} \Delta\rho(k_x;\omega) = &-(1/\pi\Omega_{\mathrm{D}})\,(8\alpha(1-\cos k_x)\,x\,s) \\ &\times \left\{\sqrt{1-s^2}\,[1 - s^2 + \alpha^2(1-\cos k_x)^2]\right\}^{-1} \\ &- \tfrac{1}{2}\delta\,[\omega - \Omega_{\min}(k_x)] - \tfrac{1}{2}\delta\,[\omega - \Omega_{\max}(k_x)] + \delta\,[\omega - \omega_{\mathrm{loc}}(k_x)] \end{aligned} \tag{70}$$

where

$$x = \omega/\Omega_{\mathrm{D}} \qquad \alpha = 1 - (f'/f) \qquad s = 2 - 4\,(\omega/\Omega_{\mathrm{D}})^2 - \cos k_x. \tag{71}$$

Figure 3 shows both the parental function $F(k_x;\omega)$ of $\Delta\rho(k_x;\omega)$ (see equations (59) and (60)) and $\Delta\rho(k_x;\omega)$ itself. The global change of the mode density (58) is depicted in figure 4. In this particular case study it does not display peculiar structural features. For low frequencies it may be approximated by

$$\Delta\rho(\omega) = [2(N+1)/\pi\Omega_{\mathrm{D}}]\,\alpha(\omega/\Omega_{\mathrm{D}}) \qquad \omega \ll \Omega_{\mathrm{D}} \tag{72}$$

and this has the same power-law behaviour in ω as the undisturbed mode density.

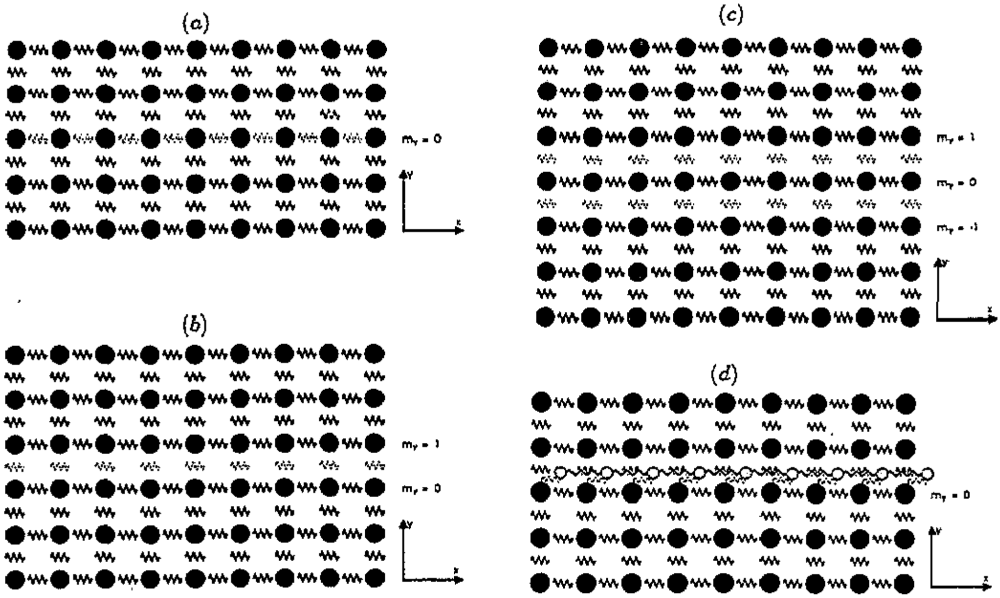

Figure 1. *(a)* Linear defect structure in the two-dimensional Montroll–Potts lattice (f, M). The longitudinal spring constants along the x axis are changed to f'. *(b)* Linear chain of transversal spring defects in the MPL. The coupling constants between the atoms $(m_x, 0)$ and $(m_x, 1)$ are altered to f'. *(c)* Two neighbouring chains of transversal spring defects with modified spring constant f' between atoms $(m_x, 1), (m_x, 0)$ and $(m_x, 0), (m_x, -1)$ in the two-dimensional MPL. *(d)* Extrinsic linear chain (spring constant f_e, masses M_e) coupled to an intrinsic chain of the MPL (f, M). Extrinsic atom at site m_x is coupled to intrinsic atom $(m_x, 0)$ with transversal springs g in x direction.

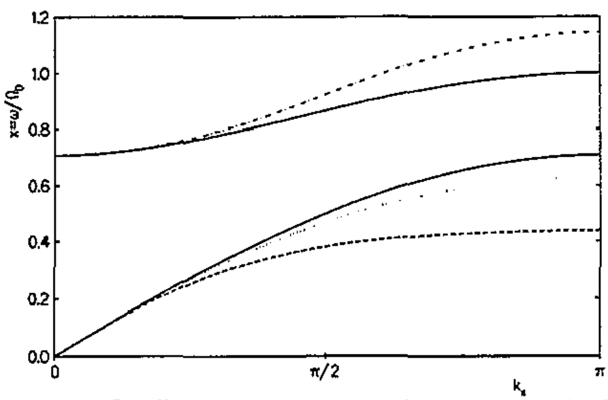

Figure 2. Localized bands due to a defect line of longitudinal springs in the two-dimensional Montroll–Potts lattice. The full lines encase the continuum of band frequencies. Dashed line: $f' = 0$, dotted line: $f' = 0.5\,f$, dashed-dotted line: $f' = 2\,f$.

4.2. Transversal defect line

We now consider the case of a defect line of the transversal springs between the atoms $m_y = 0$ and $m_y = 1$ (see figure 1(*b*)), which initiates a defect Hamiltonian

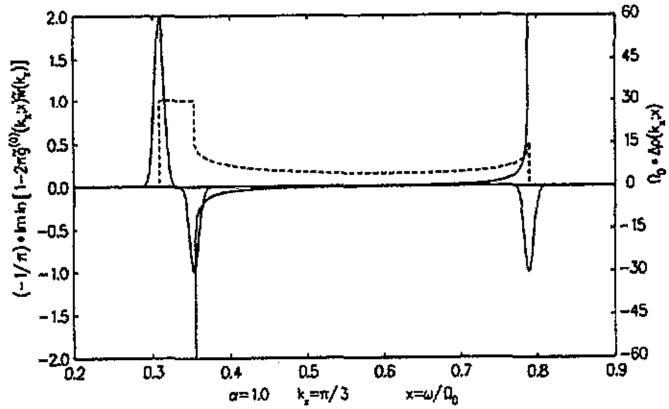

Figure 3. Change of the partial mode density, $\Delta\rho(k_x;\omega)$, and parental function $F(k_x;\omega)$ caused by the softening of the longitudinal springs for a representative value of $k_x\,(=\pi/3)$. Maximal disturbance $\alpha = 1 \leftrightarrow f' = 0$ means springs are completely cut.

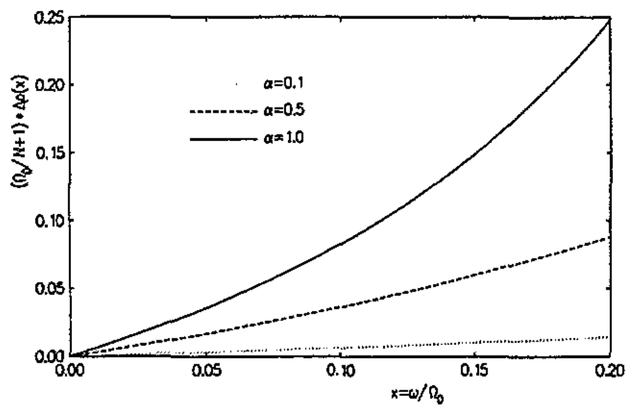

Figure 4. Low-frequency behaviour of the excess density of modes of the two-dimensional Montroll–Potts lattice due to a defect line of longitudinal springs. Full line: $f' = 0$, dashed line: $f' = 0.5f$, dotted line: $f' = 0.9f$.

$$W = -\alpha \frac{f}{2M} \sum_{m_x=-N/2}^{N/2} \left(X_{(m_x,0)} - X_{(m_x,1)} \right)^2 \tag{73}$$

and $\alpha = (f - f')/f$. Now the number of coordinates involved in the disturbance is twice as large as in 4.1. There is a mirror line along the disturbed springs and each pair of coordinates $\{X_{(m_x,0)}, X_{(m_x,1)}\}$ constitutes both an even and an odd representation of the mirror-symmetry group ($R_g = 1, R_u = 1$). Therefore we may choose the symmetry vectors

$$\sigma_{m_y}(\mathrm{g}, 1) = \begin{cases} 1/\sqrt{2} & \text{for } m_y = 0, 1 \\ 0 & \text{otherwise} \end{cases} \tag{74}$$

and

$$\sigma_{m_y}(\mathrm{u}, 1) = \begin{cases} \pm 1/\sqrt{2} & \text{for } m_y = 0, 1 \\ 0 & \text{otherwise} \end{cases} \tag{75}$$

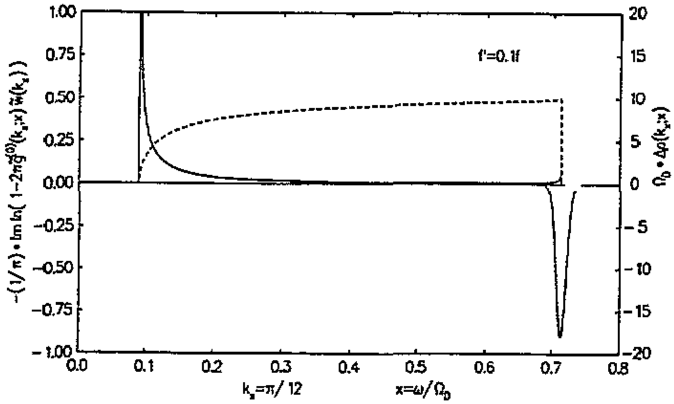

Figure 5. Change of the partial mode density, $\Delta\rho(k_x;\omega)$, and parental function $F(k_x;\omega)$ due to a linear chain of softened transversal springs for a representative value of $k_x\,(=\pi/12)$. Disturbed spring constant $f' = 0.1f$.

Inserting these in (50) and (51) we immediately observe that the even-parity motion ($p = \mathrm{g}$) does not produce a change in mode density. We thus only have the odd-mode contribution, for which we find the projections (see equations (50)–(52))

$$\tilde{w}(k_x) \equiv \tilde{w}_{11}(k_x,\mathrm{u}) = -\tfrac{1}{4}\alpha\Omega_{\mathrm{D}}^2 \tag{76}$$

$$\bar{g}^{(0)}(k_x;E) \equiv \bar{g}_{11}^{(0)}(k_x,\mathrm{u};E) = G_{00}^{(0)}(\bar{E}) - G_{10}^{(0)}(\bar{E}) \tag{77}$$

or, using equations (55*a*) and (55*b*)

$$2\pi\bar{g}^{(0)}(k_x;E) = -\frac{4}{\Omega_{\mathrm{D}}^2}\begin{cases} 1-\sqrt{(s-1)/(s+1)} & s<-1 \\ 1+\mathrm{i}\sqrt{(1-s)/(1+s)} & -1<s<1 \\ 1-\sqrt{(s-1)/(s+1)} & s>1 \end{cases} \tag{78}$$

where s is given by (56). In this case the Lifshitz equation (63) only yields a localized mode for a 'hard' disturbance, i.e. for $\alpha < 0$ ($f' > f$),

$$\omega_{\mathrm{loc}}(k_x) = \tfrac{1}{2}\Omega_{\mathrm{D}}\sqrt{2-\cos k_x - (2\alpha^2-2\alpha+1)/(2\alpha-1)}. \tag{79}$$

Inserting equations (76) and (78) in equation (57) we have

$$\Delta\rho(k_x;\omega) = \frac{1}{\sqrt{2}\pi\Omega_{\mathrm{D}}}\,\frac{\alpha(1-\alpha)x}{\sqrt{1-s}\,\left[(1-\alpha)^2+\frac{1}{2}\alpha^2(1-s)\right]}$$
$$-\tfrac{1}{2}\delta[\omega-\Omega_{\max}(k_x)] + \begin{cases} \delta[\omega-\omega_{\mathrm{loc}}(k_x)] & \text{for } \alpha<0 \\ 0 & \text{for } 0<\alpha<1 \\ \frac{1}{2}\delta\left[\omega-\Omega_{\min}(k_x)\right] & \text{for } \alpha=1 \end{cases} \tag{80}$$

where x, α and s are given in (71).

Figure 5 shows the behaviour of the partial mode density deviation (80) and its parental function $F(k_x;\omega)$ (see definition (59)) for a 'soft' disturbance line, $f' < f$. As physically expected the low frequency mode density increases, whereas at the upper band edge there is a decrease. Nevertheless, also in this defect arrangement the deviation of the global mode density (see definition (58)) does not display a qualitative change in the power law of ω: we still have $\Delta\rho(\omega) \sim \omega$, or more specifically

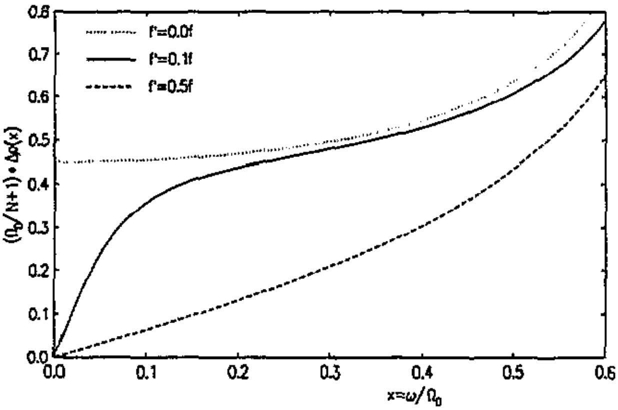

Figure 6. Low-frequency behaviour of the excess density of modes of the MPL due to an intrinsic defect line of transversal springs. Dotted line: $f' = 0$, full line: $f' = 0.1f$, dashed line: $f' = 0.5f$.

$$\Delta\rho(\omega) = \begin{cases} [2(N+1)/\pi\Omega_D]\,[\alpha/(1-\alpha)]\omega/\Omega_D & \text{for } \alpha < 1 \\ \sqrt{2}(N+1)/\pi\Omega_D & \text{for } \alpha = 1\,. \end{cases} \tag{81}$$

The full behaviour of $\Delta\rho(\omega)$ is shown in figure 6. It is worth noting that for small α-values (i.e. for $f' \to 0$) the prefactor of ω in (81) turns very big and the power-law behaviour even at low frequencies switches from $\Delta\rho \sim \omega$ to $\Delta\rho \sim$ constant, which is indicative of one-dimensional harmonic dynamics.

4.3. Double transversal defect line

The defect arrangement depicted in figure 1(*c*) is of particular interest, since it partially separates a full chain of atoms from the surroundings. The Hamiltonian alteration now reads

$$W = -\alpha\frac{f}{2M}\sum_{m_x=-N/2}^{N/2}\left\{\left(X_{(m_x,0)} - X_{(m_x,1)}\right)^2 + \left(X_{(m_x,0)} - X_{(m_x,-1)}\right)^2\right\} \tag{82}$$

and $\alpha = (f - f')/f$. The number of coordinates involved this time is $3(N+1)$ and there is a mirror line along the chain $m_y = 0$ of atoms. Each triplet of atoms $\{X_{(m_x,-1)}, X_{(m_x,0)}, X_{(m_x,1)}\}$ constitutes respectively one odd-parity and two even-parity representations of the mirror symmetry group. But one of the even-parity representations is not effective in the dynamics, whence we have to consider only the two symmetry vectors

$$\sigma_{m_y}(\mathrm{u},1) = \begin{cases} \pm 1/\sqrt{2} & \text{for } m_y = \pm 1 \\ 0 & \text{for } m_y = 0 \end{cases} \tag{83}$$

$$\sigma_{m_y}(\mathrm{g},1) = \begin{cases} 1/\sqrt{6} & \text{for } m_y = \pm 1 \\ -2/\sqrt{6} & \text{for } m_y = 0 \end{cases} \tag{84}$$

which generate the projections (see equations (50)–(52))

$$\widetilde{w}(k_x,\mathrm{u}) = \widetilde{w}_{11}(k_x,\mathrm{u}) = -\tfrac{1}{8}\alpha\Omega_\mathrm{D}^2 \tag{85}$$

$$2\pi\bar{g}(k_x,\mathrm{u};E) = -\frac{8}{\Omega_\mathrm{D}^2}\begin{cases} s+\sqrt{s^2-1} & \text{for} \quad s<-1 \\ s+\mathrm{i}\sqrt{1-s^2} & \text{for} \ -1<s<1 \\ s-\sqrt{s^2-1} & \text{for} \quad s>1 \end{cases} \tag{86}$$

and

$$\widetilde{w}(k_x,\mathrm{g}) = \widetilde{w}_{11}(k_x,g) = -\tfrac{3}{8}\alpha\Omega_\mathrm{D}^2 \tag{87}$$

$$2\pi\bar{g}(k_x,\mathrm{g};E) = -(8/3\Omega_\mathrm{D}^2) \times \begin{cases} 2-s+(s-1)\sqrt{(s-1)/(s+1)} & \text{for } s<-1 \\ 2-s-\mathrm{i}(s-1)\sqrt{(1-s)/(1+s)} & \text{for } -1<s<1 \\ 2-s+(s-1)\sqrt{(s-1)/(s+1)} & \text{for } s>1 \end{cases} \tag{88}$$

where s is given by (56). The Lifshitz equation (63) yields the odd-parity localized mode

$$s_\mathrm{loc}^{(u)} = 2-4\left(\omega_\mathrm{loc}^{(u)}(k_x)/\Omega_\mathrm{D}\right)^2 - \cos(k_x) = (1+\alpha)/2\alpha \tag{89}$$

which only exists for $\alpha<0$ ($f'>f$) and then appears above the quasi-continuous band of modes ($s<-1$). There is also an even-parity localized mode for $\alpha<0$ above the band

$$s_\mathrm{loc}^{(g)} = 2-4\left(\omega_\mathrm{loc}^{(g)}(k_x)/\Omega_\mathrm{D}\right)^2 - \cos(k_x) = (1/4\alpha)\left\{3\alpha^2+2\alpha-1+\sqrt{(3\alpha^2+2\alpha-1)^2-8\alpha(1-4\alpha+5\alpha^2)}\right\}. \tag{90}$$

Inserting respectively equations (85) and (86) and equations (87) and (88) in equation (57) we have

$$\Delta\rho(k_x,\mathrm{u};\omega) = -\frac{8x}{\pi\Omega_\mathrm{D}}\frac{\alpha(\alpha-s)}{\sqrt{1-s^2}\left[(1-\alpha s)^2+\alpha^2(1-s^2)\right]} + \begin{cases} \delta\left[\omega-\omega_\mathrm{loc}(k_x)\right] & \text{for } \alpha<0 \\ 0 & \text{for } 0<\alpha<1 \\ \tfrac{1}{2}\delta\left[\omega-\Omega_\mathrm{min}(k_x)\right] & \text{for } \alpha=1 \end{cases} \tag{91}$$

$$\Delta\rho(k_x,\mathrm{g};\omega) = \frac{8x}{\pi\Omega_\mathrm{D}}\frac{\alpha\sqrt{1-s}\left\{[1-\alpha-\alpha(1-s)]+(1-\alpha)(1+s)\right\}}{\sqrt{1+s}\left\{[1-\alpha-\alpha(1-s)]^2(1+s)+\alpha^2(1-s)^3\right\}} - \tfrac{1}{2}\delta\left[\omega-\Omega_\mathrm{max}(k_x)\right] + \begin{cases} \delta\left[\omega-\omega_\mathrm{loc}(k_x)\right] & \text{for } \alpha<0 \\ 0 & \text{for } 0<\alpha<1 \\ \delta\left[\omega-\Omega_\mathrm{min}(k_x)\right] & \text{for } \alpha=1 \end{cases} \tag{92}$$

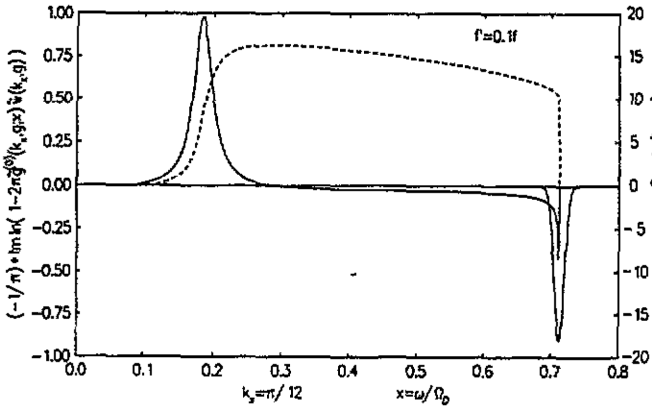

Figure 7. Change of the partial even-mode density, $\Delta\rho(k_x, g; \omega)$, and parental function $F(k_x, g; \omega)$ due to a linear double chain of softened transversal springs for a representative value of k_x $(= \pi/12)$. Disturbed spring constant $f' = 0.1f$.

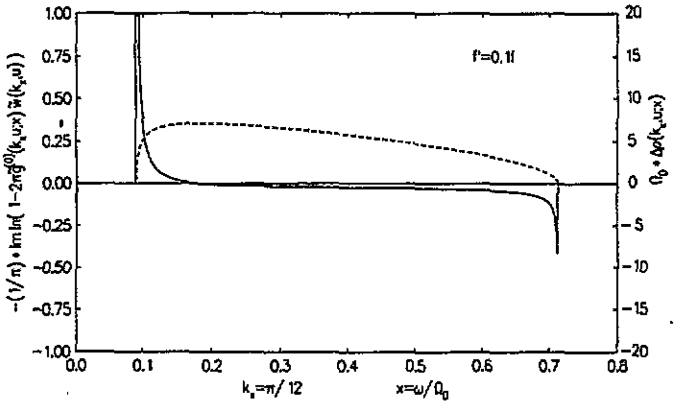

Figure 8. Same as figure 7 but for odd-mode density $\Delta\rho(k_x, u; \omega)$ and parental function $F(k_x, u; \omega)$.

where x, α and s are given in (71).

Figures 7 and 8 show the behaviour of the partial mode density deviation (91) and (92) and the respective parental function $F(k_x; \omega)$ (see definition (59)) for a 'soft' disturbance. Again, as physically expected, the low-frequency mode density increases in both parity cases, but the effect is considerably more pronounced in the odd-parity case (figure 8). For the global mode density (see definition (58)), as depicted in figures 9 and 10, the very low-frequency behaviour is given by

$$\Delta\rho(u;\omega) = \begin{cases} \dfrac{N+1}{\pi\Omega_D}\dfrac{4\alpha}{1-\alpha}\dfrac{\omega}{\Omega_D} & \text{for } \alpha < 1 \\ \dfrac{N+1}{\pi\Omega_D}\left[\sqrt{2} - 2\dfrac{\omega}{\Omega_D}\right] & \text{for } \alpha = 1 \end{cases} \qquad \omega \ll \Omega_D \tag{93}$$

$$\Delta\rho(g;\omega) = \begin{cases} \dfrac{N+1}{\pi\Omega_D}\dfrac{12\alpha}{1-\alpha}\left(\dfrac{\omega}{\Omega_D}\right)^3 & \text{for } \alpha < 1 \\ \dfrac{N+1}{\pi\Omega_D}\left[2\sqrt{2}-\dfrac{\omega}{\Omega_D}\right] & \text{for } \alpha = 1 \end{cases} \qquad \omega \ll \Omega_D \tag{94}$$

and for $\alpha \neq 1$ neither parity case displays a reduction in the power of ω against the undisturbed mode density. However, as most distinctly seen in figure 10, for small values of f' there is a jumplike approach of $\Delta\rho(\omega)$ to a behaviour which is indicative of a *one-dimensional subdynamics*.

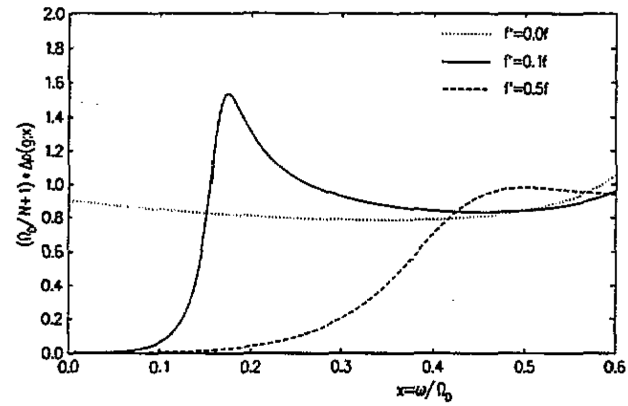

Figure 9. Low-frequency behaviour of the even-parity excess density of modes of two neighbouring chains of transversal spring defects. Dotted line: $f' = 0$, full line: $f' = 0.1f$, dashed line: $f' = 0.5f$.

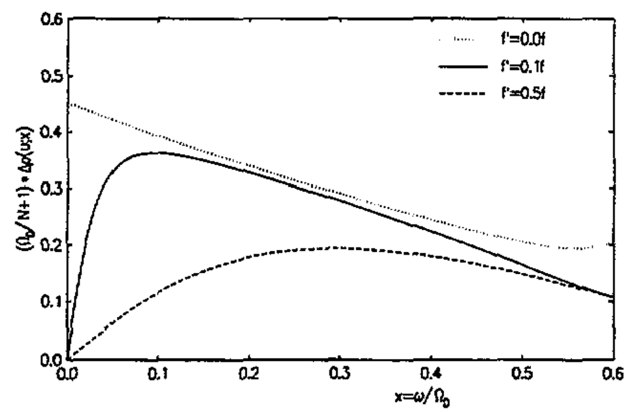

Figure 10. Same as figure 9 but for odd-parity modes.

5. Extrinsic chain

We now consider an extrinsic harmonic chain of atoms (NN springs f_e, masses M_e), which is coupled to the intrinsic line of atoms $\{m_x, m_y = 0\}$ by transversal springs g, as illustrated in figure 1(d). We decompose the total Hamiltonian in the form

$$H = H^{(i)} + H^{(e)} + H^{(i,e)} \qquad H^{(i)} = H^{(0)} + W^{(i)} \tag{95}$$

where $H^{(0)}$ is given by equation (33). Since $K_{mr} \sim \delta_{m_x r}\, \delta_{m_y 0}$, which means that atom number m_x of the extrinsic chain is coupled to atom $(m_x, m_y = 0)$ of the MPL, we may replace the indices $\{r, s\}$ in equations (13b,c) by $\{m_x, n_x\}$ and write for the several components of the Hamiltonian

$$H^{(e)} = \tfrac{1}{2} \sum_{m_x=-N/2}^{N/2} P_{m_x}^{(e)\,2} + \tfrac{1}{2} \frac{f_e}{M_e} \sum_{m_x=-N/2}^{N/2} \left(X_{m_x}^{(e)} - X_{m_x+1}^{(e)} \right)^2 + \tfrac{1}{2} \frac{g}{M_e} \sum_{m_x=-N/2}^{N/2} X_{m_x}^{(e)\,2} \tag{96}$$

$$W^{(i)} = \frac{1}{2} \frac{g}{M} \sum_{m_x=N/2}^{N/2} X_{(m_x,0)}^2 \tag{97}$$

$$H^{(i,e)} = -\frac{g}{\sqrt{M M_e}} \sum_{m_x=N/2}^{N/2} X_{m_x}^{(e)} X_{(m_x,0)}. \tag{98}$$

$X_{m_x}^{(e)}, P_{m_x}^{(e)}$ denote the extrinsic coordinates and momenta. We introduce the intrinsic symmetry vectors (see (47) and (48))

$$\sigma_{(m_x,m_y)}(k_x) = \sigma_{m_x}(k_x)\, \delta_{m_y,0} \qquad \sigma_{m_x}(k_x) = (1/\sqrt{N+1}) e^{ik_x m_x} \tag{99}$$

and the extrinsic ones

$$\sigma_{m_x}^{(e)}(k_x) = (1/\sqrt{N+1})\, e^{ik_x m_x} = \sigma_{m_x}(k_x) \tag{100}$$

which define the intrinsic symmetry coordinates (see equation (25))

$$S(k_x) = \sum_{m_x} \sigma_{m_x}^*(k_x)\, X_{(m_x,0)} \tag{101}$$

and the extrinsic ones

$$Q_e(k_x) = \sum_{m_x} \sigma_{m_x}^{(e)}(k_x)^*\, X_{m_x}^{(e)} \qquad P_e(k_x) = \sum_{m_x} \sigma_{m_x}^{(e)}(k_x)^*\, P_{m_x}^{(e)}. \tag{102}$$

These transmute the disturbances into the diagonalized form

$$W^{(i)} = \frac{g}{2M} \sum_{k_x} S(k_x)\, S(k_x)^* \tag{103}$$

$$H^{(i,e)} = -\frac{g}{\sqrt{M M_e}} \sum_{k_x} Q_e(k_x)\, S(k_x)^* \tag{104}$$

and also diagonalize the extrinsic Hamiltonian

$$H^{(e)} = \tfrac{1}{2}\sum_{k_x}\left[P_e(k_x)\,P_e(k_x)^\dagger + [\Omega^{(e)}(k_x)]^2\,Q_e(k_x)\,Q_e(k_x)^\dagger\right] \quad (105)$$

where

$$\Omega^{(e)}(k_x)^2 = \Omega^{(0,e)}(k_x)^2 + g/M_e \quad (106a)$$

$$\Omega^{0,e}(k_x)^2 = 4(f_e/M_e)\sin^2(K_x/2) \quad (106b)$$

The extrinsic GF then reads (see (14*b*) and (4))

$$G^{(e)}_{m_x,n_x}(E) = \frac{1}{2\pi}\sum_{k_x}\frac{1}{E^2-\Omega^{(e)}(k_x)^2}\,\sigma^{(e)}_{m_x}(k_x)\,\sigma^{(e)}_{n_x}(k_x)^* \quad (107)$$

by means of which, exploiting equation (17), the effective projected intrinsic disturbance is found to be

$$\begin{aligned}\tilde{w}^{\text{eff}}(k_x;E) &= \sum_{m_x,n_x}\sigma_{m_x}(k_x)^*\,w^{(\text{eff})}_{m_x n_x}\,\sigma_{n_x}(k_x)\\ &= (g/M)\,[E^2-\Omega^{(0,e)}(k_x)^2]/[E^2-\Omega^{(e)}(k_x)^2]\\ &= \tfrac{1}{8}\alpha\Omega_D^2[(E/\Omega_D)^2-\tfrac{1}{2}\beta\mu\sin^2(k_x/2)]/\\ &\quad[(E/\Omega_D)^2-\tfrac{1}{2}\beta\mu\sin^2(k_x/2)-\alpha\mu/8]\end{aligned} \quad (108)$$

with abbreviations:

$$\alpha = g/f \qquad \beta = f_e/f \qquad \mu = M/M_e \qquad \Omega_D^2 = 8f/M. \quad (109)$$

Inserting equation (108) in (23) we find for the alteration of the intrinsic mode density

$$\Delta\rho^{(i)}(\omega) = \sum_{k_x}\Delta\rho^{(i)}(k_x;\omega) \quad (110)$$

$$\begin{aligned}\Delta\rho^{(i)}(k_x;\omega) &= 2\,\mathrm{Im}\,\tilde{w}^{(\text{eff})}(k_x;E)\left[1-2\pi\tilde{g}^{(0,i)}(k_x;E)\tilde{w}^{(\text{eff})}(k_x;E)\right]^{-1}\\ &\quad\times\frac{\mathrm{d}\tilde{g}^{(0,i)}(k_x;E)}{\mathrm{d}\omega}\\ &= 2\,(g/M)\,\mathrm{Im}\,\left(\left\{[E^2-\Omega^{(0,e)}(k_x)^2](\mathrm{d}/\mathrm{d}\omega)\tilde{g}^{(0,i)}(k_x;E)\right\}\right.\\ &\quad\left.\times\left\{[E^2-\Omega^{(0,e)}(k_x)^2]\left[1-2\pi(g/M)\tilde{g}^{(0,i)}(k_x;E)\right]-g/M_e\right\}^{-1}\right)\end{aligned} \quad (111)$$

where $\tilde{g}^{(0,i)}(k_x;E) = \tilde{g}^{(0)}(k_x;E)$ is given by equation (68). For the modified extrinsic mode density (see (23)) we may write

$$\rho^{(e)}(\omega) = \sum_{k_x}\rho^{(e)}(k_x;\omega)$$

$$\rho^{(e)}(k_x;\omega) = -4\omega\,\mathrm{Im}\,\tilde{G}_e(k_x;E) \quad (112)$$

where $\widetilde{G}_e(k_x;E)$ follows from the projection of equation (20)

$$\widetilde{G}_e(k_x;E) = \frac{1}{2\pi}\sum_{m_x,n_x}\sigma_{m_x}(k_x)^* \times \left\{E^2 \mathsf{I}^{(e)} - \left[\mathsf{U}^{(e)} + 2\pi\,\mathsf{K}\,\mathsf{G}^{(i)}(E)\,\mathsf{K}\right]\right\}^{-1}_{m_x n_x}\sigma_{n_x}(k_x)$$
$$= (1/2\pi)\left\{E^2 - \left[\Omega^{(e)}(k_x)^2 + 2\pi(g^2/MM_e)\bar{g}^{(i)}(k_x;E)\right]\right\}^{-1}. \quad (113)$$

From the projection of (21) we get

$$\bar{g}^{(i)}(k_x;E) = \bar{g}^{(0,i)}(k_x;E) \times \left[1 + (2\pi g/M)\left(1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)\right)^{-1}\bar{g}^{(0,i)}(k_x;E)\right]$$
$$= \bar{g}^{(0,i)}(k_x;E)/[1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)] \quad (114)$$

which we insert in (113)

$$\widetilde{G}_e(k_x;E) = (1/2\pi)\left[E^2 - \Omega^{(e)}(k_x)^2 - 2\pi(g^2/MM_e)\bar{g}^{(0,i)}(k_x;E) \times [1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)]^{-1}\right]^{-1}$$
$$= (1/2\pi)[1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)] \times \left\{[E^2 - \Omega^{(0,e)}(k_x)^2][1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)] - g/M_e\right\}^{-1}. \quad (115)$$

This yields for $\rho^{(e)}(k_x;\omega)$, if inserted in (112)

$$\rho^{(e)}(k_x;\omega) = -(2\omega/\pi)\,\mathrm{Im}\left[\!\left[[1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)] \left\{[E^2 - \Omega^{(0,e)}(k_x)^2][1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)] - g/M_e\right\}^{-1}\right]\!\right]. \quad (116)$$

Considering equations (111) and (116) we observe that they display the same denominator. In point of fact we may combine the two formulae to give the single equation

$$\Delta\rho^{(i)}(k_x;\omega) + \rho^{(e)}(k_x;\omega) \equiv \Delta\rho(k_x;\omega)$$
$$= -(1/\pi)(\mathrm{d}/\mathrm{d}\omega)\,\mathrm{Im}\,\ln\left\{\left(E^2 - \Omega^{(0,e)}(k_x)^2\right) \times \left(1 - 2\pi(g/M)\bar{g}^{(0,i)}(k_x;E)\right) - (g/M_e)\right\} \quad (117)$$

where $\Delta\rho(k_x;\omega)$ is to be understood as the deviation of the mode density from that of the ideal intrinsic MPL. In this manner we have also succeeded in expressing the solution of the extrinsic coupling problem by means of a parental function (see equation (12)).

Again singular 'localized' modes occur outside the intrinsic band, which we found by searching the real poles of equation (115),

$$\left(\omega^2 - \Omega^{(0,e)}(k_x)^2\right)\left(1 - 2\pi(g/M)\tilde{g}^{(0,i)}(k_x;\omega)\right) - (g/M_e) = 0. \quad (118)$$

Inserting equation (68) for $2\pi\tilde{g}^{(0,i)}(k_x;\omega) = 2\pi\tilde{g}^{(0)}(k_x;\omega)$ we finally arrive at

$$\begin{aligned}\Delta\rho^{(i)}(k_x;\omega) + \rho^{(e)}(k_x;\omega) &\equiv \Delta\rho(k_x;\omega)\\ &= (1/\pi\Omega_D)\frac{\frac{1}{2}\alpha^2\mu x(1-s^2) + 16\alpha x s\left[x^2 - x^{(0)}(k_x)^2\right]\left[x^2 - x^{(e)}(k_x)^2\right]}{\sqrt{1-s^2}\left[\alpha^2\left(x^2 - x^{(0)}(k_x)^2\right)^2 + 4(1-s^2)\left(x^2 - x^{(e)}(k_x)^2\right)^2\right]}\\ &\quad - \tfrac{1}{2}\delta\left[\omega - \Omega_{\min}(k_x)\right] - \tfrac{1}{2}\delta\left[\omega - \Omega_{\max}(k_x)\right] + \delta\left[\omega - \omega_{\mathrm{loc1}}(k_x)\right]\\ &\quad \{+\delta\left[\omega - \omega_{\mathrm{loc2}}(k_x)\right]\}\end{aligned} \quad (119)$$

where $x = \omega/\Omega_D$. The curved brackets around the δ function of the second localized mode are a reminder of the fact, that this mode only exists if the frequency of the extrinsic chain for k_x is not degenerate in the band modes. Figure 11 shows the bands of localized modes due to a soft extrinsic chain for several coupling strengths. Soft in this case means that for all values of k_x the frequency of the chain is below the continuum of the undisturbed MPL. The partial change of the mode density $\Delta\rho(k_x;\omega)$ and its parental function $F(k_x,\omega)$ are depicted in figure 12 for an extrinsic chain with spring constant $f_e = 0.5f$ and masses $M_e = M$.

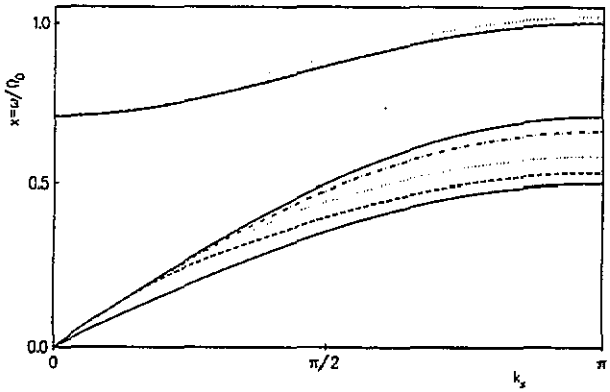

Figure 11. Location of the singular bands due to a soft extrinsic linear chain ($f_e = 0.5\,f$, $M_e = M$) coupled by g to the two-dimensional Montroll–Potts lattice. The full lines indicate the edges of the continuum of band frequencies and the dispersion curve of the free extrinsic chain. Dashed lines: $g = 0.1f$ dotted lines: $g = 0.5f$, dashed-dotted line: $g \to \infty$.

The global change $\Delta\rho(\omega)$ which is given by definition (58) again shows a linear dependence in the very low-frequency region

$$\Delta\rho(\omega) = [(N+1)/\Omega_D][2(2-\beta\mu)/\pi\mu]\,(\omega/\Omega_D) \qquad \omega \ll \Omega_D. \quad (120)$$

The total behaviour of $\Delta\rho(\omega)$ is displayed in figure 13 for several coupling constants g and in figure 14 for several external masses M_e. Although for very low frequencies the change of the mode density is given by equation (120), we see that there is a transition to one-dimensional behaviour ($\Delta\rho(\omega) \sim$ constant) which is shifted to very low frequencies with decreasing coupling constant g (or increasing masses M_e).

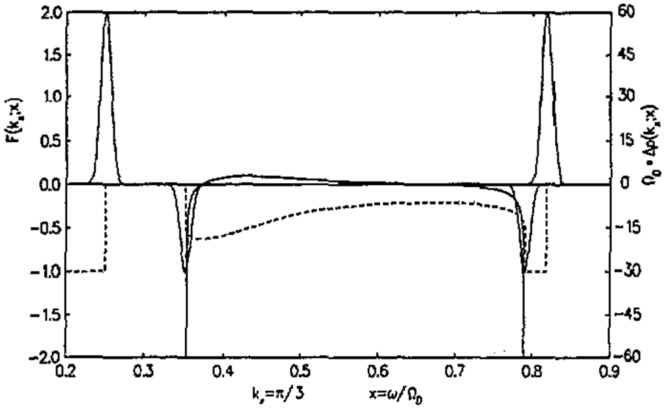

Figure 12. Change of the partial mode density, $\Delta\rho(k_x;\omega)$, and parental function $F(k_x;\omega)$ due to a soft extrinsic chain ($f_e = 0.5f$, $M_e = M$) for a representative value of k_x ($= \pi/3$). Coupling constant $g = f$.

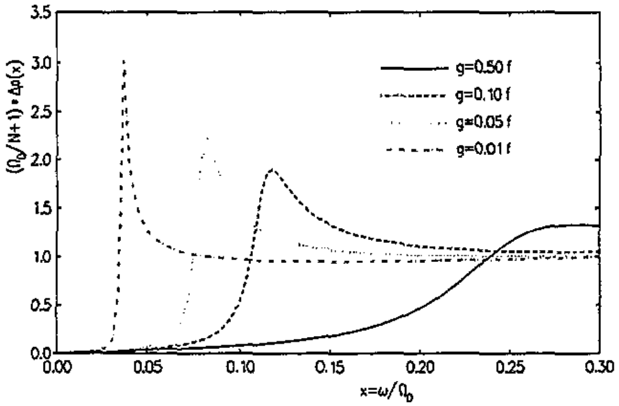

Figure 13. Low-frequency behaviour of the excess density of modes of the two-dimensional Montroll–Potts lattice due to an extrinsic linear chain ($f_e = f$, $M_e = M$) for several coupling strengths. Full line: $g = 0.5f$, dashed line: $g = 0.1f$, dotted line: $g = 0.05f$, dashed–dotted line: $g = 0.01f$.

6. Summary and further perspectives

The present investigation addresses the problem to what extent linear defect structures in crystalline systems are able to affect the low-frequency power law of the vibrational mode density. This question seems suggestive, since purely one-dimensional vibrational systems exhibit a constant mode density at $\omega \to 0$, and thus the low-temperature specific heat would increase linearly with T. Glassy systems (SiO_2, GeO_2) also display such a behaviour, although it is not clear whether one-dimensional substructures in the material are responsible for it. For these systems there is also neutron scattering evidence that the low-frequency mode density is strongly increased. Inspired by these findings we have calculated in detail the effects of linear defect structures softly embedded in a two-dimensional lattice.

A Green function formalism is presented which is a kind of generalization of the original Lifshitz formalism. Whereas the Lifshitz procedure is restricted to a few

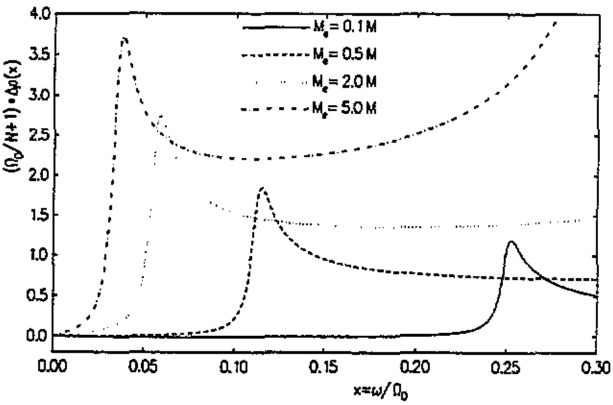

Figure 14. Low frequency behaviour of the excess density of modes of the two-dimensional Montroll–Potts lattice due to an extrinsic linear chain ($f_e = f$) coupled with springs $g = 0.1f$ to the MPL. Full line: $M_e = 0.1M$, dashed line: $M_e = 0.5M$, dotted line: $M_e = 2.0M$, dashed–dotted line: $M_e = 5.0M$

Cartesian disturbance coordinates, in our calculation new 'mesoscopic' coordinates and a new orthonormal basis are introduced in such a way that only a few of these mesoscopic coordinates are involved in the disturbance. By means of group theory the problems are reduced to low-rank subproblems. The formalism is extended to cases in which foreign degrees of freedom are coupled to the lattice.

Archetypical models of line defects with translational symmetry in x-direction in the two-dimensional Montroll–Potts lattice (MPL) are discussed. For soft defects ($f' < f$) it is found that all these structures generate a mode density, $\Delta\rho(\omega) \sim \omega$, in the very-low-frequency region which equals the power law of the reference system (MPL). However, as most clearly seen in the last two examples, there are new features. If there exists a softly coupled linear chain which may be intrinsic (by softening of transversal springs to neighbouring chains) or extrinsic (coupling with springs g to a chain of the MPL), a transition of the additional density to one-dimensional behaviour, $\Delta\rho(\omega) \sim$ constant, takes place. The frequency at which this transition occurs is shifted to lower and lower frequencies as the coupling becomes softer.

We have not presented similar calculations for linear defect embeddings in three-dimensional lattices, although our formalism also applies there. These calculations require much more numerical effort and will be given later. Also the case of softly embedded librational chains will be given elsewhere. This latter case is of particular interest, since it represents a simulation of modes which are suggested by neutron scattering experiments [3]. A highly desirable future extension of the present work is the investigation of thermal transport properties in the presence of one-dimensional defect structures, since from such investigations one may expect new insight with respect to the measured particular features in glassy material.

References

[1] Anderson P W, Halperin B I and Varma C M 1972 *Phil. Mag.* **25** 1

[2] Böttger H 1984 *Principles in the Theory of Lattice Dynamics* (Weinheim: Physik)

[3] Buchenau U 1987 *Phys. Scr.* T **19** 350

[4] Buchenau U, Zhou H M, N. Nücker, Gilroy K S and Phillips W A 1988 *Phys. Rev. Lett.* **60** 1318

[5] Dederichs P H and Zeller R 1980 *Point Defects in Metalls II (Springer Tracts in Modern Physics 87)* (Berlin: Springer)
[6] Hunklinger S and Arnold W 1976 *Physical Acoustics* vol 12, ed W P Mason and R N Thurston (New York: Academic) p 155
[7] Krumhansl J A 1986 *Phys. Rev. Lett.* 56 2696
[8] Lasjaunias J C, Ravex A, Vandorpe M, Hunklinger S 1975 *Solid State Commun.* 17 1045
[9] Ledermann W 1943 *Proc. R. Soc.* **182a** 362
[10] Lifshitz I M, 1947 *JETP* **17** 1017
[11] Lifshitz I M 1956 *Nuovo Cimento Suppl. 10* **3** 716
[12] Lifshitz I M and Kosevich A M 1966 *Rep. Prog. Phys.* **29** I, 217
[13] Maradudin A A, Montroll E W, Weiss G H and Ipatova I P, 1971 *Theory of Lattice Dynamics in the Harmonic Approximation* Suppl. 3 2nd ed (New York: Academic)
[14] Montroll E W 1947 *J. Chem. Phys.* **15** 575
[15] Montroll E W and Potts R B 1955 *Phys. Rev.* **100** 525
[16] Montroll E W 1956 *Proc. Third Berkeley Symp. on Math. Stat. Prob.* vol 3 ed J Neuman (Berkeley: University of California Press) p 209
[17] Phillips W A 1972 *J. Low Temp. Phys.* 7 351
[18] Phillips W A (ed) 1981 *Amorphous Solids, Low Temperature Properties* (Berlin: Springer)
[19] Wagner M 1963 *Phys. Rev.* **131** 2520
[20] Wagner M 1964 *Phys. Rev.* A **133** 750
[21] Wagner M and Mougios T 1990 *Physica* A **166** 229
[22] Wallis R F and Maradudin A A 1960 *Prog. Theor. Phys. (Japan)* 24 1055
[23] Zeller R C and Pohl R O 1971 *Phys. Rev.* B **4** 2029
[24] Zubarev D N 1960 *Sov. Phys. Usp.* **3** 320