問題C

格子振動のモデルとして，図１に示すように，質量Mの原子Ａがばね定数Kの自然長のばねによって，１次元的に左右とも無限遠方までつながれている場合を考える．隣接した原子間の距離をaとする．この１次元格子を伝わる縦波は，第n番目の原子の平衡点からの変位をu_nとすると，

$$u_n = u\exp[i(qna - \omega t)] \qquad \text{(i)}$$

と表される．ただし，nは$-\infty \sim +\infty$の整数，uは振動振幅，ωは角振動数，tは時間，qは波数，iは虚数単位である．各原子に働く力はフックの法則に従うものとする．

(1) n番目の原子に関する運動方程式を示せ．

(2) ωとqの関係（分散関係）を求めよ．解答では，$1-\cos qa = 2\sin^2(qa/2)$を用いて式を簡単にせよ．また，この分散関係を第１ブリルアンゾーン内$(-\pi/a \le q \le \pi/a)$で図示せよ．

(3) 群速度$(d\omega/dq)$のq依存性を第１ブリルアンゾーン内で図示せよ．また，$q=\pm\pi/a$で起きている現象を説明せよ．

(4) 長さLの周期的境界条件を用いることにより，qの式を求めよ．

(5) 問(2)で得られた分散関係に対して状態密度$g(\omega)$を求め，$g(\omega)$が発散するωが存在することを示せ．

(6) 図２に示すように，図１のℓ番目の原子Ａを，質量$M/2$の原子Ｂで置き換える．このとき，式(ii)で表される原子 Ｂ から左右に減衰していく解のみの存在が許される．$|\exp(\gamma a)| > 1$のとき，$\exp(\gamma a)$の値を求めよ．ただし，γは減衰定数である．

$$u_n = u\exp(-i\omega t)\exp(-\gamma a|n-\ell|) \qquad \text{(ii)}$$

(7) 問(6)で求めた解に対応するqとωを求めよ．

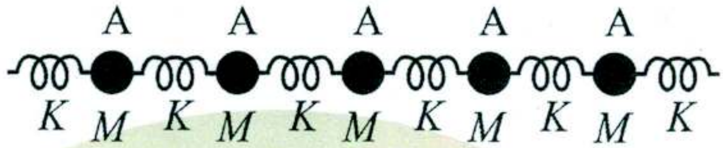

図1

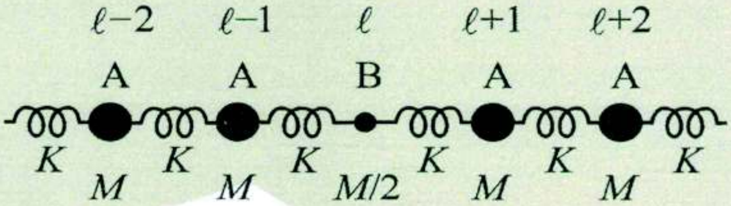

図2

Problem C

As a model of lattice vibration, consider a one-dimensional chain composed of atoms A of mass M connected with springs with a spring constant K at their natural length, as shown in Fig. 1. The chain is infinitely long in both directions. The distance between the adjacent atoms is defined as a. The longitudinal waves propagating in the one-dimensional chain are expressed by

$$u_n = u \exp[i(qna - \omega t)], \qquad \text{(i)}$$

where u_n is the deviation of the n-th atom from its equilibrium position. Here, n is an integer between $-\infty$ and $+\infty$, u is the amplitude of the oscillation, ω is the angular frequency, t is the time, q is the wave number, and i is the imaginary unit. We assume that the forces applied to each atom follow the Hooke's law.

(1) Write the equation of motion for the n-th atom.

(2) Write the relation between ω and q (dispersion relation). In the answer sheet, simplify the answer equation form by using $1-\cos qa = 2\sin^2(qa/2)$. Also, draw this dispersion relation in the first Brillouin zone ($-\pi/a \le q \le \pi/a$).

(3) Draw the q-dependence of the group velocity ($d\omega/dq$) in the first Brillouin zone. Explain the phenomenon taking place when $q = \pm\pi/a$.

(4) By using the periodic boundary conditions of length L, find an expression for q.

(5) Show the density of states $g(\omega)$ by using the dispersion relation derived in Question (2). Show that $g(\omega)$ becomes infinite at a certain value of ω.

(6) As shown in Fig. 2, we replace the ℓ-th atom A shown in Fig. 1 with an atom B of half the mass $M/2$. At this condition, only the decaying waves expressed by Eq. (ii) can exist, which propagate in the left- and right- directions from the atom B. Find the value of $\exp(\gamma a)$ when $|\exp(\gamma a)| > 1$. Here, γ is the decay constant.

$$u_n = u \exp(-i\omega t)\exp(-\gamma a|n-\ell|) \qquad \text{(ii)}$$

(7) Show q and ω corresponding to the state derived in Question (6).

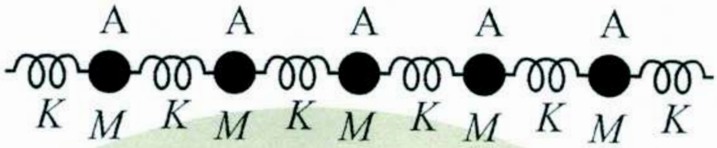

Fig. 1

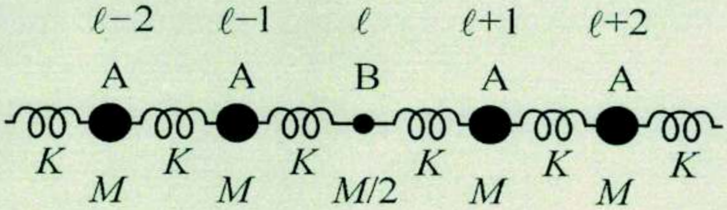

Fig. 2