Note on the exact solutions of Kronig-Penney model

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In an introduction to the band theory of solids, there is used the Kronig-Penney model which is a one-dimensional solvable system of an electron interacting via delta-function potentials with particles at crystal lattices arrayed in a circle. As has been pointed out[1] for Kittel's text[2], however, the eigen-value problem of the model is solved in ordinary space, while the band theory is discussed in reciprocal lattice space. It is then instructive to show an introductory and consistent treatment for the band theory in reciprocal lattice space. In this short note, we present such a treatment in the field theoretical framework.

The Hamiltonian of our one-dimensional system with a coupling constant g, a lattice length L, and the number of lattice points $N$is given by

$$H = H_0 + H_{\text{int}} = \sum_p \frac{p^2}{2m} a_p^* a_p + \sum_q \sum_{G,G'} \frac{Ng}{L} a_{q+G}^* a_{q+G'} \quad , \tag{1}$$

in terms of creation and annihilation operators a_p^* and a_p of an electron of mass m with a momentum $p \equiv 2\pi\hbar n/L\,(n = 0,\pm1,\pm2,\cdots,)$, which are obeyed by the usual anti-commutation relations

$$a_p\, a_{p'}^* + a_{p'}^* a_p = \delta_{p',p} \quad , \tag{2}$$

where $\delta_{p',p}$ means Kronecker's delta, and the spin indices are saved briefly for the present one-particle case. In (1), G denotes a reciprocal lattice momentum, $G \equiv 2\pi\hbar n/a\,(n = 0,\pm1,\pm2,\cdots,)$, where a is the lattice constant and then the lattice length is given by $L = Na$. Furthermore q indicates $2\pi\hbar j/L\,(j = 0,\pm1,\pm2,\cdots,\pm(N-1)/2)$, where the number $N$is assumed to be odd for convenience' sake.

The one-particle eigen-state for the above Hamiltonian is given by the following form

$$\left|\Psi_{q_1}\right\rangle = N_{q_1} \sum_{G_1} \frac{1}{{p_1}^2 - {k_1}^2} a_{p_1}^* |0) \quad , \tag{3}$$

in which $p_1 = q_1 + G_1$, where q_1 is our quantum number and the eigen-energy E is given by $E = {k_1}^2/(2m)$. In (3), N_{q_1} denotes the normalization constant and $|0)$ indicates the vacuum state.

The straightforward calculation gives the following equations

$$\frac{mg}{\hbar k_1} \sin\left(\frac{k_1 a}{\hbar}\right) + \cos\left(\frac{k_1 a}{\hbar}\right) = \cos\left(\frac{k_1 a}{\hbar}\right) \tag{4}$$

under which the above one-particle state in (3) satisfies the exact eigen-value equation,

$$(H_0 + H_{\text{int}})\left|\Psi_{q_1}\right\rangle = E\left|\Psi_{q_1}\right\rangle \quad . \tag{5}$$

For a given quantum number q_1 (q_1 : $-\pi\hbar(N-1)/L, -\pi\hbar(N-3)/L, \cdots, 0, \cdots, \pi\hbar(N-3)/L, \pi\hbar(N-1)/L$), the equation (4) yields the many eigen-values which are classified by a function $k_1(q_1, n_B)$ of one another band quantum number n_B (n_B :0,1, 2,$\cdots$). This is easily confirmed through the numerical calculation of the left hand side in (4), of which the result is plotted by a oscillating curve in Fig.1, where $x \equiv k_1 a/\hbar$,

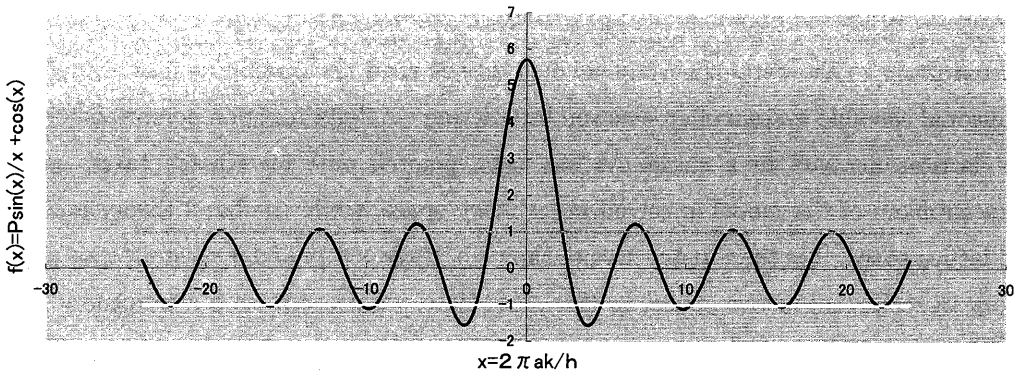

Fig.1

and the dimensionless coefficient, $P \equiv mga/\hbar^2$, is taken to be $3\pi/2$ according as in the case of Kronig-Penney paper. The region, $-\pi \le q_1 a/\hbar \le \pi$, (which is called the first Brillouin zone) for $q_1 a/\hbar$ in the limit of an infinite N, yields a value lying between -1 and +1 for $\cos(q_1 a/\hbar)$ which is given by a straight line parallel to the x-axis. The eigen-values mentioned above are given by intersections between the parallel line and the oscillating curve.

By omitting a factor $(\hbar^2/2ma^2)$ from the eigen-energy, the dimensionless quantity $[k(y, n_B)a/\hbar]^2$ is plotted in Fig.2, where the crystal momentum, defined as $y \equiv q_1 a/\hbar$, has been introduced instead of q_1.

The above treatment for the band theory of solid is natural from the field theoretical point of view, and is instructive one as an introduction to the band theory of solid.

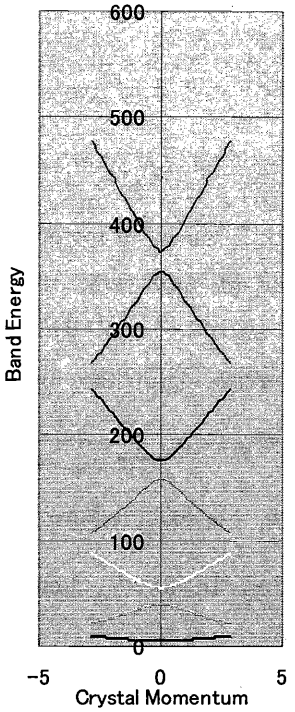

Fig.2

1) S. Singh, Am. J. 51(2), February 1983, p.179.
2) C. Kittel, Introduction to Solid State Physics, 5th ed. (Wiley, New York, 1976), pp.191-195.

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