Kronig–Penney model in reciprocal lattice space

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(Received 25 January 1982; accepted for publication 25 March 1982)

While teaching the band theory of solids from Kittel's introductory text,[1] we noticed that most of the discussion is in reciprocal lattice space except the solution of the Kronig–Penney model.[2] This is given in ordinary lattice space. However, our students felt happier when the model was solved by using the central equation rather than going back to the usual techniques. In this note, we present one way of doing so.

The Schrödinger equation for a one-dimensional solid is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x), \tag{1}$$

where the potential $U(x)$ is periodic with the lattice constant a, i.e.,

$$U(x+a) = U(x). \tag{2}$$

By expanding the wave function and the potential in a Fourier series,

$$\psi_k(x) = \sum_k C(k)\exp(ikx), \tag{3}$$

$$U(x) = \sum_{G_n} U(G_n)\exp(iG_n x), \tag{4}$$

and substituting in (1), one can easily get the central equation[1]

$$(\lambda_k - E)C(k) + \sum_{G_n} U(G_n)C(k-G_n) = 0, \tag{5}$$

where

$$\lambda_k = \hbar^2 k^2/2m,$$

and

$$G_n = \pm 2\pi n/a \quad n = 0,1,2,\ldots,\infty \tag{6}$$

are the reciprocal lattice vectors for the one-dimensional solid. The Kronig–Penney model is described by the potential

$$U(x) = \sum_{l=-\infty}^{\infty} (\hbar^2 P/ma)\delta(x - la),$$

where P characterizes the strength of each delta function. The Fourier components are easily shown to be equal to $\hbar^2 P/ma^2$. So the central equation becomes

$$(\lambda_k - E)C(k) + \frac{\hbar^2 P}{ma^2}\sum_{G_n} C(k - G_n) = 0. \tag{7}$$

Denoting the sum by the symbol $f(k)$ and rearranging we get

$$C(k) = -2Pf(k)a^{-2}/(k^2 - 2mE/\hbar^2). \tag{8}$$

In this equation, we change k to $k - G_n$ and sum over G_n. The crucial point is to note that

$$f(k - G_n) = \sum_{G'_n} C(k - G_n - G'_n)$$

$$= \sum_{G''_n} C(k - G''_n) = f(k). \tag{9}$$

Using this equality and letting $E = \hbar^2 K^2/2m$ we get the central equation of this note:

$$-a^2/2P = \sum_{G_n} [(k - G_n)^2 - K^2]^{-1}. \tag{10}$$

The infinite sum in (10) is similar to the frequency sums occurring in the theory of finite temperature Green's functions.[3] To do this sum, we split each term into partial fractions and use the standard expansion[4]

$$\pi \cot x = \left(\frac{\pi}{x}\right) + 2\pi x \sum_{n=1}^{\infty} (x^2 - n^2\pi^2)^{-1}$$
$$= \sum_{n=-\infty}^{\infty} \left(\frac{n+x}{\pi}\right)^{-1}. \tag{11}$$

We get

$$\sum_{G_n} [(k - G_n)^2 - K^2]^{-1}$$
$$= \left(\frac{1}{2K}\right) \sum_{n=-\infty}^{\infty} \left[\left(\frac{k - K - 2\pi n}{a}\right)^{-1} - \left(\frac{k + K - 2\pi n}{a}\right)^{-1}\right]$$
$$= \left(\frac{a}{4K}\right)\left\{\cot\left[\frac{(ka - Ka)}{2}\right] - \cot\left[\frac{(ka + Ka)}{2}\right]\right\}$$
$$= \left(\frac{a}{2K}\right)\sin Ka/(\cos Ka - \cos ka), \tag{12}$$

where in obtaining the last line we have used standard trigonometric identities. Substitution in (10) gives the usual transcendental equation[1] of the model:

$$\cos ka = \cos Ka + (P/Ka)\sin Ka. \tag{13}$$

In summary, in this note we have shown one way of preserving continuity in the treatment of band theory by doing everything in the reciprocal lattice space.[5]

[1] C. Kittel, *Introduction to Solid State Physics*, 5th ed. (Wiley, New York, 1976), pp. 191–195.
[2] R. L. Kronig and W. G. Penney, Proc. R. Soc. London A **130**, 499 (1931).
[3] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), pp. 248–250; E. M. Lifshits and L. P. Pitaevskii, *Statistical Physics Part 2* (Pergamon, Oxford, 1980), p. 171.
[4] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972), p. 75.
[5] Similar mathematics was encountered in the *T*-matrix approach to this model, W. J. Titus, Am. J. Phys. **41**, 512 (1973).