NOTES AND DISCUSSIONS

Kronig–Penney model with the tail-cancellation method

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The Kronig–Penney model of an electron moving in a periodic potential is solved by the so-called tail-cancellation method. The problem also serves as a simple illustration of the tail-cancellation method itself.
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The Kronig–Penney model serves to illustrate the formation of energy bands in a periodic solid and appears as a pedagogical example in many textbooks in elementary solid state physics. The model is generally solved either by matching the boundary conditions for the wave functions at the cell boundaries,[1] by a plane-wave expansion of the wave function in the reciprocal lattice space,[2] or even by the somewhat more involved T-matrix method.[3]

In this note, we point out that perhaps the simplest way of solving the problem is by using the tail-cancellation condition, which has been used extensively in the solution of the band structure problem in realistic solids.[4] The solution therefore serves as a simple illustration of the tail-cancellation method as well.

The Schrödinger equation for a one-dimensional solid is

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

where the potential is periodic with lattice constant a:

$$U(x)=\sum_{n=-\infty}^{\infty} V(x-na). \tag{2}$$

Consider first a single potential well, where the potential is $V(x)$ in the central cell, $-a/2\leqslant x\leqslant a/2$, and zero elsewhere. Once we find a solution $\phi(x)$ to this potential for a given energy E, the wave function for the solid $\Psi(x)$ may be constructed by taking a linear superposition of such functions centered in different cells, with the coefficients given by the Bloch theorem, i.e.,

$$\Psi(x)=\sum_n e^{ikna}\phi(x-na), \tag{3}$$

where k is the Bloch momentum. Now, since $\phi(x)$ already is a solution of the Schrödinger equation in the central cell, the ''tails'' of the functions $\phi(x-na)$ coming from other cells must interfere destructively inside the central cell (and hence inside any other cell). Thus we have the condition

$$\sum_{n\neq 0} e^{ikna}\phi(x-na)=0 \tag{4}$$

for all values of x in the central cell. This is the so-called ''tail-cancellation'' condition. The problem therefore boils down to finding the solution $\phi(x)$ for a given energy for a single potential well and then applying the tail-cancellation condition. If the condition can be satisfied then we have a solution for that energy, otherwise not.

We now apply the method to the Kronig–Penney model. For a single potential well, the most general solution of the Schrödinger equation for the energy E is given by

$$\phi(x)=A\phi_1(x)+B\phi_2(x), \tag{5}$$

where ϕ_1 and ϕ_2 are the two independent solutions with energy E. These solutions extend in all space and for the case of the one-dimensional potential may be written in terms of the transmission and reflection coefficients:

$$\begin{aligned}\phi_1(x)&=e^{iKx}+re^{-iKx}, \quad x\leqslant -a/2\\ &=te^{iKx}, \quad x\geqslant a/2\end{aligned} \tag{6}$$

and

$$\begin{aligned}\phi_2(x)&=te^{-iKx}, \quad x\leqslant -a/2\\ &=e^{-iKx}+re^{iKx}, \quad x\geqslant a/2,\end{aligned} \tag{7}$$

where $\hbar^2K^2/2m=E$. Notice that the above wave functions are simply the ''tails''—we don't really care at this point how the wave function looks inside the cell itself, i.e., for $|x|\leqslant a/2$. Once the energy is obtained, the wave function inside the cell (and hence everywhere) may be obtained by integrating the Schrödinger equation.

Substituting the expression for $\phi(x)$ from Eqs. (5) to (7) in the tail-cancellation condition Eq. (4), equating the coefficients of $e^{\pm iKx}$ to zero, and eliminating A and B, we obtain the following condition:

$$(r^2-t^2)f_+f_- - t(f_+f_-^* + f_+^*f_-) - f_+^*f_-^*=0, \tag{8}$$

where $f_\pm \equiv f(K\pm k)$ and $f(\kappa)=\Sigma_{n=1}^{\infty} e^{i\kappa na}$.

The last sum is over a series of oscillating terms. The oscillation can be traced to the fact that the plane-wave-like tails in Eqs. (6) and (7) continue undamped to infinity. If we keep a finite number of terms N in the summation, then the second term in the numerator of the result $f(\kappa)=(e^{i\kappa a}-e^{i\kappa(N+1)a})/(1-e^{i\kappa a})$ oscillates rapidly between -1 and $+1$ as $N\rightarrow\infty$ with the average value zero. It turns out that taking this average value yields the correct answer for the problem at hand.

A more careful way of evaluating the sum is to take the limit

$$f(\kappa)=\lim_{N\to\infty,\mu\to 0}\sum_{n=1}^{N} e^{(i\kappa-\mu)na}=\frac{e^{i\kappa a}}{1-e^{i\kappa a}}, \tag{9}$$

where the limit has been taken in such a way that $\mu a \ll 1$ and $\mu Na \gg 1$. Physically this corresponds to a small damping term $e^{-\mu|x|}$ in the two basis functions Eqs. (6) and (7) such that the amplitudes of the plane-wave tails damp out at infinity but do not change appreciably over the length of a unit cell.

We now write the transmission coefficient in terms of the phase-shift η, $t=|t|e^{i\eta}$, so that the reflection coefficient has the well-known general form $r=\pm i|r|e^{i\eta}$. Substituting Eq. (9) into Eq. (8) we get the desired result

$$\frac{\cos(Ka+\eta)}{|t|}=\cos ka. \tag{10}$$

This is the standard transcendental equation for the model,[5] which we derived here from the tail-cancellation condition.

For a periodic array of δ functions $V(x)=g\,\delta(x)$, Eq. (10) takes the form

$$\left(\frac{P}{Ka}\right)\sin Ka+\cos Ka=\cos ka, \tag{11}$$

where the well-known result, $|t|=\cos\eta$ and $\tan\eta=-mg/\hbar^2 k$, for the transmission coefficient of the delta-function potential has been used and $P\equiv mag/\hbar^2$.

In summary, we have shown how the tail-cancellation condition can be applied to the solution of the Kronig–Penney model.

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[2]S. Singh, ''Kronig–Penney Model in Reciprocal Lattice Space,'' Am. J. Phys. **51**, 179 (1983).
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Comment on ''A simple demonstration of the Alford–Gold effect using a diode laser and optical fibers,'' by L. Basano and P. Ottonello [Am. J. Phys. 68 (4), 325–328 (2000)]

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An experimental demonstration[1] has been presented in this journal[2] using a diode laser, two optical fibers, a photodiode, and a wave analyzer. This demonstration is very simple and has the didactic value of clearly presenting important optical concepts. In this note I propose a simplification of the experimental apparatus that, as a further advantage, should allow the observation of the Alford–Gold effect in a more interesting way.

In their experimental demonstration, L. Basano and P. Ottonello use *two* optical fibers although the same can be achieved with just *one* optical fiber, as is schematically shown in Fig. 1. In this case, one of the beams goes directly to the photodiode and the other, extracted with the beam splitter BS1, is retarded in an optical fiber before being directed, with a beam splitter BS2, to the photodiode (I have omitted in the drawing possible positioning of lenses). In the space between the two beam splitters, additional beam splitters, or a partially reflecting mirror, can be placed if it is desired to compensate for the transmission losses of the other beam. This setup amounts to a slight simplification of the apparatus but is essentially the same experiment. A real improvement of the experiment is obtained with a further modification of the setup. For this, we can eliminate the second beam splitter (BS2) and place the end of the optical fiber at the *top side* of (BS1) in order to feed the reflected part into the photodiode. Notice, however, that the *transmitted* part can make (with proper alignment) a second turn along the optic fiber with the corresponding time delay 2τ. This would cause second-order dips in the spectral analysis, separated by half of the separation of the first-order dips. Perhaps higher order dips can also be observed.

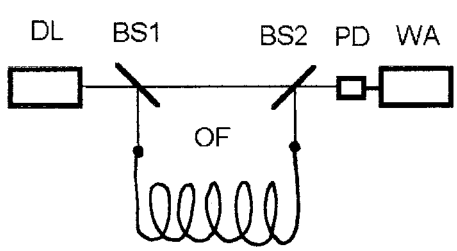

Fig. 1. Experimental setup. DL=diode laser; BS1, BS2=beam splitters; PD=photodiode; WA=wave analyzer; OF=optic fiber.

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[2]L. Basano and P. Ottonello, ''A simple demonstration of the Alford–Gold effect using a diode laser and optical fibers,'' Am. J. Phys. **68**, 325–328 (2000).

