

## Problem on a particle in a periodic square well potential<sup>1</sup>

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Suppose that a particle of mass  $m$  in one dimension is subject to a potential with period  $a$ :

$$V(x) = \begin{cases} V_0 & 0 < x < ra \\ 0 & ra < x < a \end{cases}, \quad (1)$$

with  $V_0 < 0$ ,  $0 < r < 1$ , and the potential defined outside of  $0 < x < a$  by

$$V(x + a) = V(x) . \quad (2)$$

Our goal is to solve the Schrödinger equation

$$\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \quad (3)$$

with the requirement

$$\psi(x + a) = e^{-i\theta} \psi(x) . \quad (4)$$

Here we are looking for energies in the range  $-V_0 < E < 0$ . The parameter  $\theta$  is in the range  $-\pi < \theta < \pi$  and is specified. Then as  $\theta$  runs over this range,  $E$  runs over an energy “band.” We will look only for the lowest energy band.

To solve this, we can conveniently define

$$k = \sqrt{2m(E - V_0)} \quad (5)$$

and

$$\kappa = \sqrt{-2mE} \quad (6)$$

For the range  $0 < x < ra$ , I suggest taking

$$\psi(x) = \alpha \cos(kx) + \beta \sin(kx) . \quad (7)$$

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For the range  $ra < x < a$ , I suggest taking

$$\psi(x) = \sigma e^{-\kappa(x-ra)} + \tau e^{-\kappa(a-x)} . \quad (8)$$

In general, we need

$$\psi(x-a) = e^{-i\theta} \psi(x) \quad (9)$$

so

$$\psi(x) = e^{i\theta} \psi(x-a) . \quad (10)$$

Thus, for  $x$  in the range  $a < x < (1+r)a$ , we need

$$\psi(x) = \alpha' \cos(k(x-a)) + \beta' \sin(k(x-a)) . \quad (11)$$

where

$$\begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = e^{i\theta} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} . \quad (12)$$

The boundary conditions at  $x = ra$  give

$$\begin{pmatrix} \sigma \\ \tau \end{pmatrix} = R_1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} , \quad (13)$$

where  $R_1$  is a matrix that you should find. There are a lot of sines, cosines, and exponentials around. I suggest using an abbreviated notation

$$\begin{aligned} S &= \sin(kra) , \\ C &= \cos(kra) , \\ F &= \exp(\kappa(1-r)a) , \\ 1/F &= \exp(-\kappa(1-r)a) . \end{aligned} \quad (14)$$

The boundary conditions at  $x = a$  give

$$\begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = R_2 \begin{pmatrix} \sigma \\ \tau \end{pmatrix} , \quad (15)$$

where  $R_2$  is a matrix that you should find.

Then

$$\begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = R \begin{pmatrix} \alpha \\ \beta \end{pmatrix} , \quad (16)$$

where

$$R = R_2 R_1 . \quad (17)$$

We want

$$R \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = e^{i\theta} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} , \quad (18)$$

Thus  $e^{i\theta}$  is an eigenvalue of  $R$ . To calculate the eigenvalues of  $R$  you can look for the zeros of  $\det(R-\lambda)$ . Show that for a  $2 \times 2$  matrix,  $\det(R-\lambda) = \det(R) - \lambda \text{Tr}(R) + \lambda^2$ . With this, calculating the eigenvalues is straightforward. First, show that  $\det(R) = 1$ . Then you just have to calculate  $\text{Tr}(R)$ , which should be a not-so-simple function of the parameters in the problem.

For a given  $E$ , and thus a given  $k$  and  $\kappa$ , find the possible eigenvalues of  $e^{i\theta}$ . The next step would be to find  $E$  for a given  $\theta$ . However, you can omit doing this.

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