Solution of the quantum mechanical potential barrier

Boundary conditions for

$\psi_A(x) = e^{i k x} + a\, e^{-i k x}$

$\psi_B(x) = \text{b1}\, e^{i\, \text{k1}\, x} + \text{b2}\, e^{-i\, \text{k1}\, x}$

$\psi_C(x) = c\, e^{i k x}$

In[1]:=

```
eqs = Solve[{
    1 + a == b1 + b2,
    k (1 - a) == k1 (b1 - b2),
    b1 ⅇ^(ⅈ k1 L) + b2 ⅇ^(-ⅈ k1 L) == c ⅇ^(ⅈ k L),
    k1 (b1 ⅇ^(ⅈ k1 L) - b2 ⅇ^(-ⅈ k1 L)) == k c ⅇ^(ⅈ k L)
  }, {a, b1, b2, c}]
```

Out[1]=

$$\left\{\left\{a \to -\frac{\left(-1+e^{2 i\, \text{k1}\, L}\right)\left(-k^2+\text{k1}^2\right)}{-k^2+e^{2 i\, \text{k1}\, L} k^2-2 k\, \text{k1}-2 e^{2 i\, \text{k1}\, L} k\, \text{k1}-\text{k1}^2+e^{2 i\, \text{k1}\, L}\, \text{k1}^2},\right.\right.$$

$$\text{b1} \to -\frac{2 k (k+\text{k1})}{-k^2+e^{2 i\, \text{k1}\, L} k^2-2 k\, \text{k1}-2 e^{2 i\, \text{k1}\, L} k\, \text{k1}-\text{k1}^2+e^{2 i\, \text{k1}\, L}\, \text{k1}^2},$$

$$\text{b2} \to \frac{2 e^{2 i\, \text{k1}\, L} k (k-\text{k1})}{-k^2+e^{2 i\, \text{k1}\, L} k^2-2 k\, \text{k1}-2 e^{2 i\, \text{k1}\, L} k\, \text{k1}-\text{k1}^2+e^{2 i\, \text{k1}\, L}\, \text{k1}^2},$$

$$\left.\left.c \to -\frac{4 e^{-i k L+i\, \text{k1}\, L} k\, \text{k1}}{-k^2+e^{2 i\, \text{k1}\, L} k^2-2 k\, \text{k1}-2 e^{2 i\, \text{k1}\, L} k\, \text{k1}-\text{k1}^2+e^{2 i\, \text{k1}\, L}\, \text{k1}^2}\right\}\right\}$$

```
sol = FullSimplify[eqs]
```

Out[2]=

$$\left\{\left\{a \to \frac{(k-\text{k1})(k+\text{k1}) \operatorname{Sin}[\text{k1}\, L]}{2 i k\, \text{k1} \operatorname{Cos}[\text{k1}\, L]+\left(k^2+\text{k1}^2\right) \operatorname{Sin}[\text{k1}\, L]},\ \text{b1} \to -\frac{2 k (k+\text{k1})}{e^{2 i\, \text{k1}\, L}(k-\text{k1})^2-(k+\text{k1})^2},\right.\right.$$

$$\left.\left.\text{b2} \to \frac{2 e^{2 i\, \text{k1}\, L} k (k-\text{k1})}{e^{2 i\, \text{k1}\, L}(k-\text{k1})^2-(k+\text{k1})^2},\ c \to -\frac{4 e^{-i (k-\text{k1}) L} k\, \text{k1}}{e^{2 i\, \text{k1}\, L}(k-\text{k1})^2-(k+\text{k1})^2}\right\}\right\}$$

The reflection coefficient is $R = |a|^2 = a^* a$.

Notice how we have to use assumptions in order to tell *Mathematica* that k, k1 and L are reals.

(Complex conjugation is typed as a* →a[Esc]conj[Esc]) or one can use a* a=Conjugate[a] a)

In[3]:=

```
R = Assuming[k ∈ Reals && k1 ∈ Reals && L ∈ Reals, FullSimplify[(a* a) /. sol[[1]]]]
```

Out[3]=

$$\frac{\left(k^2-\text{k1}^2\right)^2 \operatorname{Sin}[\text{k1}\, L]^2}{4 k^2\, \text{k1}^2 \operatorname{Cos}[\text{k1}\, L]^2+\left(k^2+\text{k1}^2\right)^2 \operatorname{Sin}[\text{k1}\, L]^2}$$

To massage Expression we use $\text{Expand}\left[k^4+6 k^2\, \text{k1}^2+\text{k1}^4-\left(k^2-\text{k1}^2\right)^2\right] = 8 k^2\, \text{k1}^2$

In[41]:=
```
cc = Simplify[
  Assuming[k ∈ Reals && k1 ∈ Reals && L ∈ Reals, FullSimplify[((c* c)) /. sol[[1]]]] /.
    Cos[2 k1 L] → 1 - 2 Sin[k1 L]^2 /. k^4 + 6 k^2 k1^2 + k1^4 -> (k^2 - k1^2)^2 + 8 k^2 k1^2]
```

Out[41]=
$$\frac{4\,k^2\,k1^2}{4\,k^2\,k1^2+\left(k^2-k1^2\right)^2\,\mathrm{Sin}[k1\,L]^2}$$

In[45]:=
```
aa = Simplify[Assuming[k ∈ Reals && k1 ∈ Reals && L ∈ Reals,
    FullSimplify[((a* a)) /. sol[[1]]]] /. Cos[k1 L]^2 → 1 - Sin[k1 L]^2]
```

Out[45]=
$$\frac{\left(k^2-k1^2\right)^2\,\mathrm{Sin}[k1\,L]^2}{4\,k^2\,k1^2+\left(k^2-k1^2\right)^2\,\mathrm{Sin}[k1\,L]^2}$$

Here we express $|a|^2$ and $|c|^2$ in terms of $\epsilon = k^2$ and $\mathrm{k1}^2 = \epsilon - U$

In[42]:=
```
cc1 = FullSimplify[cc /. {k^2 → ϵ, k1^2 → ϵ - U, k^4 → ϵ^2, k1^4 → (ϵ - U)^4}] /.
  Cos[2 k1 L] → 1 - 2 Sin[k1 L]^2
```

Out[42]=
$$\frac{1}{1+\frac{U^2\,\mathrm{Sin}[k1\,L]^2}{-4\,U\,\epsilon+4\,\epsilon^2}}$$

In[46]:=
```
aa1 = FullSimplify[aa /. {k^2 → ϵ, k1^2 → ϵ - U}] /. Cos[2 k1 L] → 1 - 2 Sin[k1 L]^2
```

Out[46]=
$$\frac{1}{1+\frac{4\,\epsilon\,(-U+\epsilon)\,\mathrm{Csc}[k1\,L]^2}{U^2}}$$

The transmission coefficient $T = |c|^2$

In[43]:=
```
T = cc1
```

Out[43]=
$$\frac{1}{1+\frac{U^2\,\mathrm{Sin}[k1\,L]^2}{-4\,U\,\epsilon+4\,\epsilon^2}}$$

The reflection coefficient $R = |a|^2$

In[47]:=
```
R = aa1
```

Out[47]=
$$\frac{1}{1+\frac{4\,\epsilon\,(-U+\epsilon)\,\mathrm{Csc}[k1\,L]^2}{U^2}}$$

We finally check the expected relation $R + T = 1$

In[50]:=
```
FullSimplify[R + T]
```

Out[50]=
```
1
```