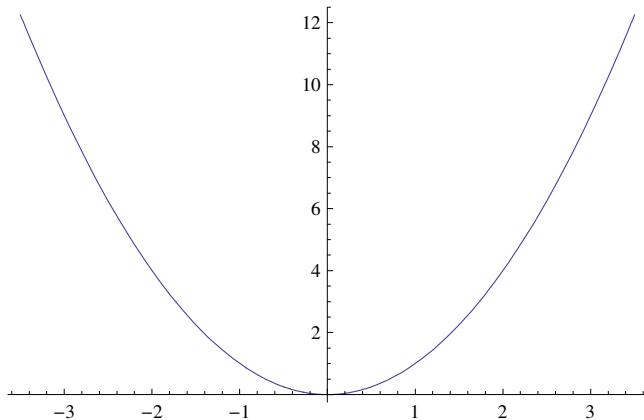


## TESTE INTERCALAR

08-11 Novembro 2013

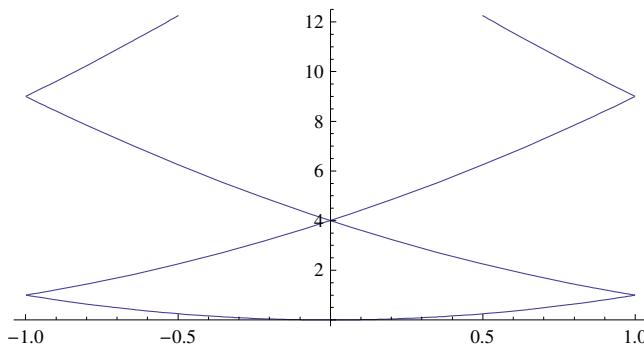
a) A relação de dispersão para a partícula livre é  $E = \hbar^2 k^2 / 2m$ , cujo gráfico em unidades reduzidas é a parábola

```
Plot[x^2, {x, -3.5, 3.5}]
```



Vejamos como se modifica esta representação se identificarmos valores de  $k$  que diferem, por exemplo, de duas unidades. A variável independente passa a tomar valores num círculo, de modo que o gráfico da função se inscreve num cilindro. A figura seguinte é a representação plana desse cilindro, e as linhas verticais de abcissas 1 e -1 devem ser vistas como estando identificadas.

```
ParametricPlot[{Mod[x, 2, -1], x^2}, {x, -3.5, 3.5}, AspectRatio -> 1/2]
```



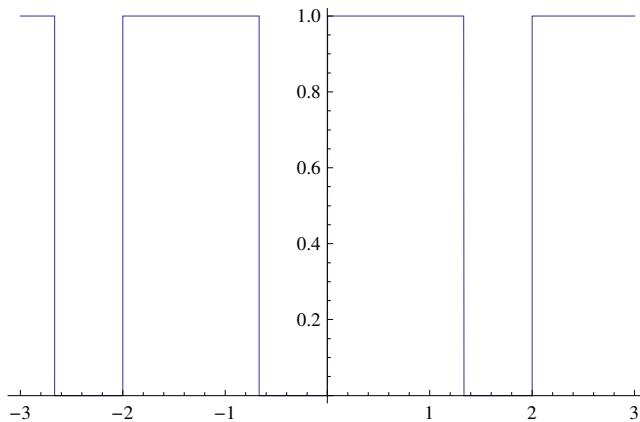
b) Consideremos então o potencial periódico de período a definido no intervalo  $[0, a]$  por

```
V[x_] := V0 /; Mod[x, a] < a - b;
V[x_] := 0 /; Mod[x, a] > a - b;
V0 =.; a =.; b =.;
?V
```

Global`V

```
V[x_] := V0 /; Mod[x, a] < a - b
V[x_] := 0 /; Mod[x, a] > a - b
```

```
V0 = 1; a = 2; b = 2 / 3; Plot[V[x], {x, -3, 3}]
```



A equação de Schrödinger independente do tempo nos poços e nas barreiras escreve-se

$$\text{ESITp} = \psi''[x] + 2mE_n/\hbar^2 \psi[x] = 0$$

$$\frac{2E_n m \psi[x]}{\hbar^2} + \psi''[x] = 0$$

$$\text{ESITb} = \psi''[x] + 2m(E_n - V_0)/\hbar^2 \psi[x] = 0$$

$$\frac{2m(E_n - V_0) \psi[x]}{\hbar^2} + \psi''[x] = 0$$

e as soluções gerais nas duas regiões são

```
solp = DSolve[ESITp, \psi, x]
```

$$\left\{ \left\{ \psi \rightarrow \text{Function}\left[\{x\}, C[1] \cos\left(\frac{\sqrt{2}\sqrt{E_n}\sqrt{m}x}{\hbar}\right) + C[2] \sin\left(\frac{\sqrt{2}\sqrt{E_n}\sqrt{m}x}{\hbar}\right) \right] \right\} \right\}$$

```
solb = DSolve[ESITb, \psi, x]
```

$$\left\{ \left\{ \psi \rightarrow \text{Function}\left[\{x\}, e^{\frac{\sqrt{2}\sqrt{-E_n+m}V_0}{\hbar}x} C[1] + e^{-\frac{\sqrt{2}\sqrt{-E_n+m}V_0}{\hbar}x} C[2] \right] \right\} \right\}$$

ou seja, temos

$$\alpha = \text{Sqrt}[2mE_n]/\hbar; \alpha = .; \psi_p = A \text{Exp}[i\alpha x] + B \text{Exp}[-i\alpha x]$$

$$B e^{-ix\alpha} + A e^{ix\alpha}$$

$$\beta = \text{Sqrt}[2m(E_n - V_0)]/\hbar; \beta = .; \psi_b = C \text{Exp}[i\beta x] + D \text{Exp}[-i\beta x]$$

$$D e^{-ix\beta} + C e^{ix\beta}$$

e para as derivadas

$$\psi'_p = D[\psi_p, x]$$

$$-i B e^{-ix\alpha} \alpha + i A e^{ix\alpha} \alpha$$

$$\psi'_b = D[\psi_b, x]$$

$$-i D e^{-ix\beta} \beta + i C e^{ix\beta} \beta$$

Impondo as condições de matching em  $x=0$ , obtemos duas equações para os coeficientes A, B, C e D:

$$\psi_p / . \quad x \rightarrow 0$$

$$A + B$$

$$\psi_b / . \quad x \rightarrow 0$$

$$C + D$$

$$m1 = A + B == C + D$$

$$A + B == C + D$$

$$\psi_p' / . \quad x \rightarrow 0$$

$$i A \alpha - i B \alpha$$

$$\psi_b' / . \quad x \rightarrow 0$$

$$i C \beta - i D \beta$$

$$m2 = \alpha (A - B) == \beta (C - D)$$

$$(A - B) \alpha == (C - D) \beta$$

c) Para uma função de onda de Bloch, ou seja, dada pelo produto de uma onda plana por uma função periódica de período  $a$ ,

$$\psi(x + a) = u_k(x + a) e^{i k(x + a)} = u_k(x) e^{i k(x + a)} = e^{i k a} \psi(x)$$

e o mesmo vale para a derivada  $\psi'(x)$  de uma função de onda de Bloch. Vamos então impor estas duas condições adicionais às soluções gerais encontradas.

$$\psi_b / . \quad x \rightarrow a - b$$

$$D e^{-i(a-b)\beta} + C e^{i(a-b)\beta}$$

$$\psi_p / . \quad x \rightarrow -b$$

$$A e^{-i b \alpha} + B e^{i b \alpha}$$

$$m3 = e^{i k a} (A e^{-b i \alpha} + B e^{b i \alpha}) == D e^{-(a-b)i\beta} + C e^{(a-b)i\beta}$$

$$e^{i a k} (A e^{-i b \alpha} + B e^{i b \alpha}) == C e^{i(a-b)\beta} + D e^{i(-a+b)\beta}$$

$$\psi_b' / . \quad x \rightarrow a - b$$

$$-i D e^{-i(a-b)\beta} \beta + i C e^{i(a-b)\beta} \beta$$

$$\psi_p' / . \quad x \rightarrow -b$$

$$i A e^{-i b \alpha} \alpha - i B e^{i b \alpha} \alpha$$

$$m4 = e^{i k a} (A e^{-b i \alpha} i \alpha - B e^{b i \alpha} i \alpha) == -D e^{-(a-b)i\beta} i \beta + C e^{(a-b)i\beta} i \beta$$

$$e^{i a k} (i A e^{-i b \alpha} \alpha - i B e^{i b \alpha} \alpha) == i C e^{i(a-b)\beta} \beta - i D e^{i(-a+b)\beta} \beta$$

$$\{m1, m2, m3, m4\}$$

$$\left\{ A + B == C + D, (A - B) \alpha == (C - D) \beta, e^{i a k} (A e^{-i b \alpha} + B e^{i b \alpha}) == C e^{i(a-b)\beta} + D e^{i(-a+b)\beta}, e^{i a k} (i A e^{-i b \alpha} \alpha - i B e^{i b \alpha} \alpha) == i C e^{i(a-b)\beta} \beta - i D e^{i(-a+b)\beta} \beta \right\}$$

d) Para que existam soluções não triviais o determinante deste sistema linear tem que se anular.

```

Simplify[  

Det[{ {1, 1, -1, -1}, {α, -α, -β, β}, {e^a i k e^-b i α, e^a i k e^b i α, -e^(a-b) i β, -e^(-a+b) i β},  

{α e^a i k e^-b i α, -α e^a i k e^b i α, -β e^(a-b) i β, β e^(-a+b) i β} } ]]  

e^-i (b (α-β)+a β) (e^i (a k+2 b α) (α-β)^2 + e^i (-2 b β+a (k+2 β)) (α-β)^2 +  

4 e^i (b (α-β)+a β) α β + 4 e^i (b (α-β)+a (2 k+β)) α β - e^i a k (α+β)^2 - e^i (2 b (α-β)+a (k+2 β)) (α+β)^2 )  

Collect[  

e^-i a k e^-i b α e^-i (a-b) β Expand[e^i (a k+2 b α) (α-β)^2 + e^i (-2 b β+a (k+2 β)) (α-β)^2 + 4 e^i (b (α-β)+a β) α β +  

4 e^i (b (α-β)+a (2 k+β)) α β - e^i a k (α+β)^2 - e^i (2 b (α-β)+a (k+2 β)) (α+β)^2 ], {α, β}, Simplify]  

- e^-i (a β+b (α+β)) (-1 + e^2 i b α) (e^2 i a β - e^2 i b β) α^2 - 2 e^-i (a (k+β)+b (α+β))  

(e^i a (k+2 β) + e^i (a k+2 b β) - 2 e^i (a β+b (α+β)) - 2 e^i (a (2 k+β)+b (α+β)) + e^i (a k+2 b (α+β)) + e^i (2 b α+a (k+2 β))) α β -  

e^-i (a β+b (α+β)) (-1 + e^2 i b α) (e^2 i a β - e^2 i b β) β^2  

FullSimplify[-e^-i (a β+b (α+β)) (-1 + e^2 i b α) (e^2 i a β - e^2 i b β)]  

4 Sin[b α] Sin[(a-b) β]  

FullSimplify[-2 e^-i (a (k+β)+b (α+β))  

( e^i a (k+2 β) + e^i (a k+2 b β) - 2 e^i (a β+b (α+β)) - 2 e^i (a (2 k+β)+b (α+β)) + e^i (a k+2 b (α+β)) + e^i (2 b α+a (k+2 β))) ]  

8 (Cos[a k] - Cos[b α] Cos[(a-b) β])

```

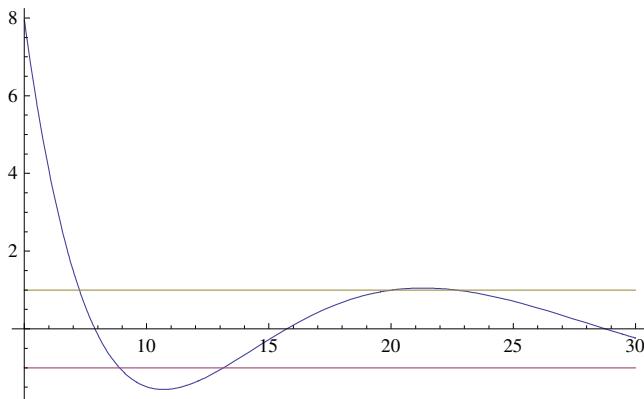
A existência de soluções depende então da condição

$$\begin{aligned}
\text{eq} = \cos[a k] &= \cos[b \alpha] \cos[(a-b) \beta] - \sin[b \alpha] \sin[(a-b) \beta] (\alpha^2 + \beta^2) / (2 \alpha \beta) \\
\cos[a k] &= \cos[b \alpha] \cos[(a-b) \beta] - \frac{(\alpha^2 + \beta^2) \sin[b \alpha] \sin[(a-b) \beta]}{2 \alpha \beta} \\
\cos[b \alpha] \cos[(a-b) \beta] &- \frac{(\alpha^2 + \beta^2) \sin[b \alpha] \sin[(a-b) \beta]}{2 \alpha \beta} / . \\
\{\beta \rightarrow \text{Sqrt}[\mu (\text{En} - \text{V0})], \alpha \rightarrow \text{Sqrt}[\mu \text{En}]\} \\
\cos[b \sqrt{\text{En} \mu}] \cos[(a-b) \sqrt{(\text{En} - \text{V0}) \mu}] &- \\
\frac{(\text{En} \mu + (\text{En} - \text{V0}) \mu) \sin[b \sqrt{\text{En} \mu}] \sin[(a-b) \sqrt{(\text{En} - \text{V0}) \mu}]}{2 \sqrt{\text{En} \mu} \sqrt{(\text{En} - \text{V0}) \mu}}
\end{aligned}$$

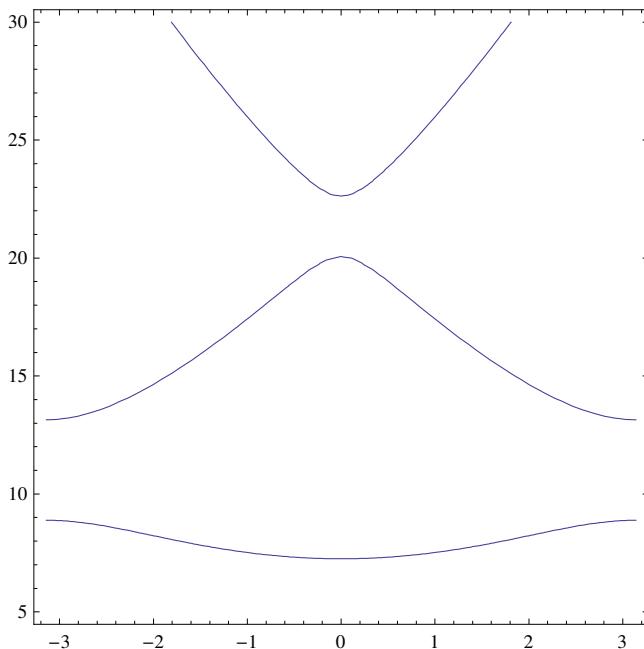
e) Definimos uma função para representar o segundo membro da equação eq como função da energia:

$$\begin{aligned}
F[\text{En}_-, \text{a}_-, \text{v0}_-, \text{b}_-, \mu_-] := \cos[b \sqrt{\text{En} \mu}] \cos[(a-b) \sqrt{(\text{En} - \text{V0}) \mu}] - \\
\frac{(\text{En} \mu + (\text{En} - \text{V0}) \mu) \sin[b \sqrt{\text{En} \mu}] \sin[(a-b) \sqrt{(\text{En} - \text{V0}) \mu}]}{2 \sqrt{\text{En} \mu} \sqrt{(\text{En} - \text{V0}) \mu}}
\end{aligned}$$

```
Plot[{F[x, 1, 10, 0.2, 3], -1, 1}, {x, 5, 30}, PlotRange -> All]
```

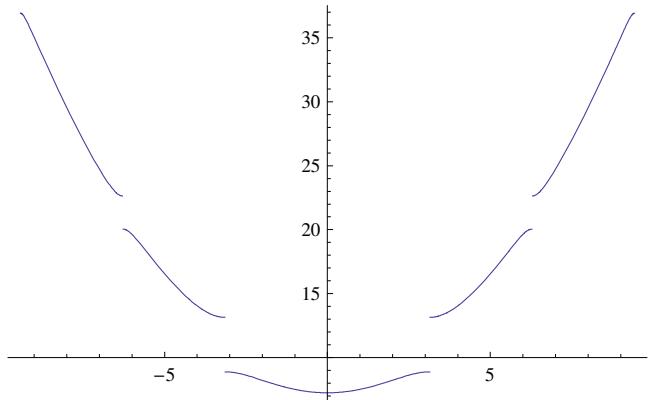


```
ContourPlot[Cos[k] == F[En, 1, 10, 0.2, 3], {k, -Pi, Pi}, {En, 5, 30}]
```



```
disp1[k_] := Re[x /. FindRoot[Cos[k] == F[x, 1, 10, 0.2, 3], {x, 1}]]
disp2[k_] := Re[x /. FindRoot[Cos[k] == F[x, 1, 10, 0.2, 3], {x, 15}]]
disp3[k_] := Re[x /. FindRoot[Cos[k] == F[x, 1, 10, 0.2, 3], {x, 30}]]
disp[k_] := disp1[k] /; Abs[k] < Pi; disp[k_] := disp2[k] /; Pi < Abs[k] < 2 Pi;
disp[k_] := disp3[k] /; 2 Pi < Abs[k] < 3 Pi
```

```
Plot[disp[k], {k, -3 Pi, 3 Pi}, Exclusions → {Sin[k] == 0}]
```



f)

```
Solve[k N a == 2 n Pi, k]
```

$$\left\{ \left\{ k \rightarrow \frac{2 n \pi}{a N} \right\} \right\}$$

```
disp1[k_] := Re[x /. FindRoot[Cos[k] == F[x, 1, 10, 0.2, 3], {x, 1}]]
```

```
disp2[k_] := Re[x /. FindRoot[Cos[k] == F[x, 1, 10, 0.2, 3], {x, 15}]]
```

```
disp3[k_] := Re[x /. FindRoot[Cos[k] == F[x, 1, 10, 0.2, 3], {x, 30}]]
```

```
NN = 10; b1 = Table[disp1[2 j Pi / NN], {j, -NN / 2, NN / 2}];
```

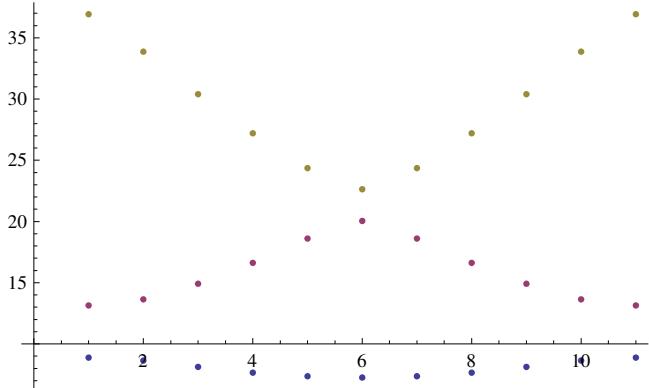
```
b2 = Table[disp2[2 j Pi / NN], {j, -NN / 2, NN / 2}];
```

```
b3 = Table[disp3[2 j Pi / NN], {j, -NN / 2, NN / 2}];
```

```
b1
```

```
{8.8853, 8.63683, 8.13284, 7.66499, 7.35644,
 7.25005, 7.35644, 7.66499, 8.13284, 8.63683, 8.8853}
```

```
ListPlot[{b1, b2, b3}]
```

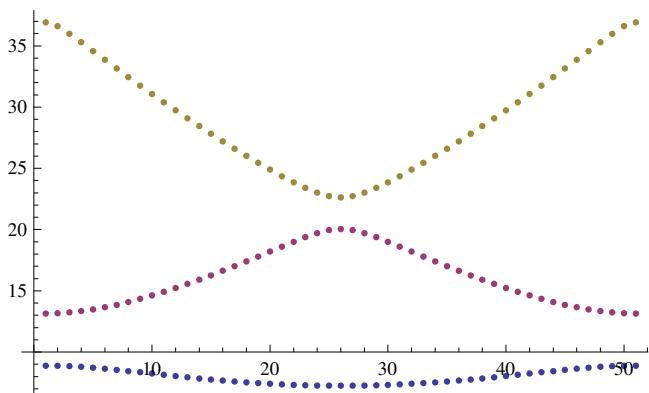


```
NN = 50; b1 = Table[disp1[2 j Pi / NN], {j, -NN / 2, NN / 2}];
```

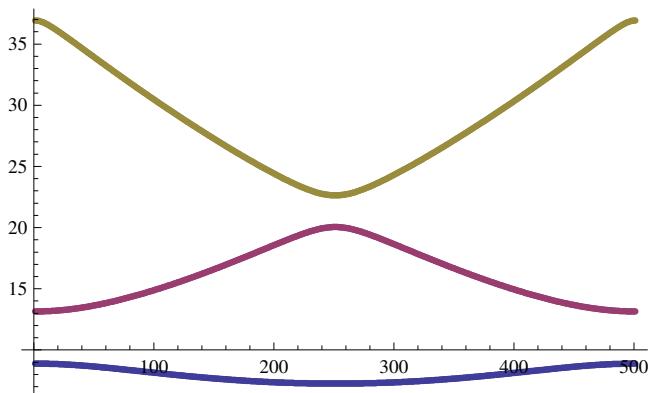
```
b2 = Table[disp2[2 j Pi / NN], {j, -NN / 2, NN / 2}];
```

```
b3 = Table[disp3[2 j Pi / NN], {j, -NN / 2, NN / 2}];
```

```
ListPlot[{b1, b2, b3}]
```



```
NN = 500; b1 = Table[disp1[2 j Pi / NN], {j, -NN/2, NN/2}];  
b2 = Table[disp2[2 j Pi / NN], {j, -NN/2, NN/2}];  
b3 = Table[disp3[2 j Pi / NN], {j, -NN/2, NN/2}];  
  
ListPlot[{b1, b2, b3}]
```



g) e h) Ver notas indicadas na alínea h).

i) Ver notas indicadas nesta alínea.