In[]:=
```
ClearAll["Global`*"]
```

Solve With Trial Wave Functions

In[]:=
```
λ = 1; (*set to 1 for incident electron -1 for incident hole*)
```

```
rCoeffs = {roe, roh, ωoe, ωoh};
tCoeffs = {toe, toh, ωoe, ωoh};
consts = {c1, c1, c2, c2};
kvalues = {ke, kh, ke, kh};

If[λ == 1,
 wfsD1 = {Exp[I * k * x] + roe * Exp[-I * k * x], toe * Exp[I * k * x]};
 wfsB1 = {roh * Exp[I * k * x], toh * Exp[-I * k * x]};
 wfsD2 = {ωoe * Exp[-I * k * x], ωoe * Exp[I * k * x]};
 wfsB2 = {ωoh * Exp[I * k * x], ωoh * Exp[-I * k * x]};,
 If[λ == -1,
  wfsD1 = {roe * Exp[-I * k * x], toe * Exp[I * k * x]};
  wfsB1 = {Exp[-I * k * x] + roh * Exp[I * k * x], toh * Exp[-I * k * x]};
  wfsD2 = {ωoe * Exp[-I * k * x], ωoe * Exp[I * k * x]};
  wfsB2 = {ωoh * Exp[I * k * x], ωoh * Exp[-I * k * x]};,
  {Print["error: λ must be ±1"], Abort[]},
  {Print["error: λ must be ±1"], Abort[]}],
 {Print["error: λ must be ±1"], Abort[]}]

listOfWfs = {wfsD1, wfsB1, wfsD2, wfsB2};
diffEqFunction[ϕ_] := D[ϕ, {x, 2}] + k^2 * ϕ + c1 * DiracDelta[x]
testFunction[ϕLis_] := Table[
  If[FullSimplify[
    diffEqFunction[ϕLis[[i]]] == 0,
    If[i == 1, x > 0, x < 0]],
   Nothing,
   Print["error: wfs do not solf diffeq"],
   Print["error: wfs do not solf diffeq"]],
  {i, 1, Length[ϕLis]}]
If[
 ParallelMap[testFunction, listOfWfs] == Table[{Nothing},
   {Length[listOfWfs]}],
 Null,
 {Print[ParallelMap[testFunction, listOfWfs]], Abort[]}]
(*check that wfs solve diffeq*)

zValuePaper = enM^2 - (en + I * (t1^2/ve + t1^2/vh)) * (en + I * (t2^2/ve + t2^2/vh));
(*form of Z given in Paper*)
c1Paper = λ * t1 * (en + I * (t2^2/ve + t2^2/vh)) / zValuePaper;  (*form of c1 given in Paper*)
c2Paper = λ * (I * enM * t1) / zValuePaper;  (*form of c2 given in Paper*)
```

■ Match wfs for first BC

```
boundaryConds1 = Flatten[Table[
   Solve[FullSimplify[listOfWfs[[i, 1]] == listOfWfs[[i, 2]], x == 0], tCoeffs[[i]]],
   {i, Length[listOfWfs]}], 1]
```

- **Second BC derivatives have discontinuity due to bound state**

$\partial_x \phi_+ \,|_{x=\epsilon} - \partial_x \phi_- \,|_{x=-\epsilon} + c_1\, t_1 = 0$

```
In[•]:= probsInit = Flatten[Table[
   Solve[Limit[(D[listOfWfs[[i, 2]], x] /. x -> ϵ) -
         (D[listOfWfs[[i, 1]], x] /. x -> ϵ), ϵ → 0] + consts[[i]] == 0 /.
      boundaryConds1[[i]] /. k -> kvalues[[i]], rCoeffs[[i]]],
   {i, 1, Length[listOfWfs]}]]

In[•]:= tunProbs = Table[probsInit[[i, 2]], {i, 1, 4}];
```

- **Solve for c1 and c2 by combining other two equations**

```
In[•]:= paperConsts = FullSimplify[Solve[
       {t1 * Limit[listOfWfs[[2, 2]] - listOfWfs[[1, 2]], x → 0] -
          I * enM * const2 - en * const1 == 0,
        t2 * Limit[listOfWfs[[4, 2]] - listOfWfs[[3, 2]], x → 0] +
          I * enM * const1 - en * const2 == 0},
       {const1, const2}] /. boundaryConds1[[1]] /. boundaryConds1[[2]]];

In[•]:= constsPaperForm =
  FullSimplify[Solve[{Evaluate[paperConsts[[1, 1, 2]] /. probsInit] == β * c1/t1,
      Evaluate[paperConsts[[1, 2, 2]] /. probsInit] == β * c2/t2},
     {c1, c2}] /. {ke -> ve/(2 * β), kh -> vh/(2 * β)}];

If[
 And[Reduce[FullSimplify[β/t1 * constsPaperForm[[1, 1, 2]] == c1Paper]],
  FullSimplify[β/t2 * constsPaperForm[[1, 2, 2]] == c2Paper]],
 Print["Math is Correct"]]
```

```
Math is Correct
```

$$\left\{\text{roe} \to \frac{i\, c1}{2\, ke},\ \text{roh} \to -\frac{i\, c1}{2\, kh},\ \omega oe \to \frac{i\, c2}{2\, ke},\ \omega oh \to -\frac{i\, c2}{2\, kh}\right\};$$

$$\left\{\text{roe} \to \frac{i\, c1}{2\, ke},\ \text{roh} \to -\frac{i\, c1}{2\, kh},\ \omega oe \to \frac{i\, c2}{2\, ke},\ \omega oh \to -\frac{i\, c2}{2\, kh}\right\};$$