XIIth-IIC-EMTCCM

European Master in Theoretical Chemistry and Computational Modelling

Homework on Aharonov-Bom effect

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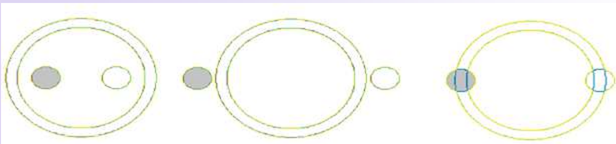
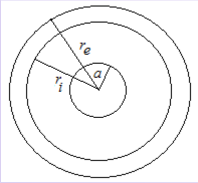
HomeWork

1. Consider two beams of magnetic field having the same strength but opposite sign. Show that only when the field pierces the ring it has an effect on the ring energy spectrum.



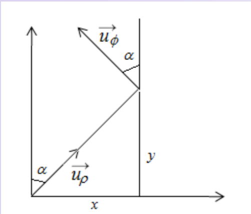
2. Consider now different strength and sign. Show that it is the total magnetic flux what matters

Potential vector yielding a beam of magnetic flux restricted to a small area inside, outside and piercing a quantum ring.



$$\begin{cases} A_1 = A(0<\rho<a) = \frac{1}{2} B_0\, \rho\, \vec{u}_\phi \\ A_2 = A(a<\rho<\infty) = \frac{1}{2\rho} B_0\, a^2\, \vec{u}_\phi \end{cases}$$

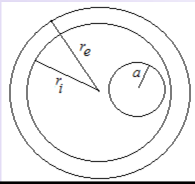
$$A_1(\rho = a) = A_2(\rho = a)$$



$$\vec{u}_\phi = \vec{\imath}\,(-\sin\alpha) + \vec{\jmath}\,(\cos\alpha) = \frac{1}{\rho}(-y, x, 0)$$

$$\begin{cases} A_1 = \frac{B_0}{2}(-y, x, 0) \;\rightarrow\; \vec{B} = \nabla \times A = B_0\; \vec{k} \\ A_2 = \frac{B_0}{2}\frac{a^2}{\rho^2}(-y, x, 0) \;\rightarrow\; \vec{B} = \nabla \times A = 0 \end{cases}$$

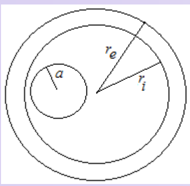
Off-centering $\quad$ x → (x-x_0)



$$\begin{cases} A_1 = \frac{B_0}{2}(-y, (x - x_0), 0) \\ A_2 = \frac{B_0}{2}\frac{a^2}{\rho^2}(-y, (x - x_0), 0) \end{cases}$$

$$\rho = \sqrt{(x - x_0)^2 + y^2}$$

Potential vector yielding a beam of a negative magnetic flux restricted to a small area centered in the opposite direction

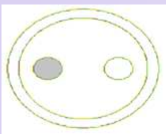


Off-centering: $\quad$ x → (x+x_0)
Negative magnetic field: –B_0

$$\begin{cases} A_1^{'} = -\frac{B_0}{2}(-y, (x + x_0), 0) \\ A_2^{'} = -\frac{B_0}{2}\frac{a^2}{\rho^2}(-y, (x + x_0), 0) \end{cases}$$

$$\rho = \sqrt{(x + x_0)^2 + y^2}$$

Potential vector yielding two opposite direction flux beams:



$$B = \nabla \times A$$
$$B' = \nabla \times A'$$

$$B_{tot} = B + B' = \nabla \times A + \nabla \times A' = \nabla \times (A + A')$$

The Hamiltonian:
a.u. and Coulomb gauge ($\nabla A = 0$)

$$H = \frac{\hat{p}^2}{2m} + \frac{(A + A') \cdot \hat{p}}{m} + \frac{(A + A')^2}{2m} + V$$

$$A \cdot p = -\boldsymbol{i}\ \frac{B_0}{2}\ f\left(-y\,\partial_x + (x - x_0)\,\partial_y\right) \begin{cases} f_1 = 1 \\ f_2 = \dfrac{a^2}{\sqrt{(x - x_0)^2 + y^2}} \end{cases}$$

$$A' \cdot p = \boldsymbol{i}\ \frac{B_0}{2}\ f\left(-y\,\partial_x + (x + x_0)\,\partial_y\right) \begin{cases} f_1 = 1 \\ f_2 = \dfrac{a^2}{\sqrt{(x + x_0)^2 + y^2}} \end{cases}$$

etc.

$$H\ F(x, y) = E\ F(x, y)$$

diagonals of the sparse matrix diags_spm.m

```
%diags_spm.m

% defined in main.m ->
cons=-1/(2*m*h^2);cons2=i*bf/(4*m*h);cons2e=cons2*radbf^2;cons3=bf^2/(8*m);

d=zeros((n-2)^2,1);                                  % filling diagonals with
zeros
b=d;bet=d;a=d;alp=d;

n0=round((n-1)/2);                                   % center of the system
n1=round(n*(x0/lon));                                % centers of the magnetic disks
n2=round(n*(-x0/lon));

for ii=1:(n-2)
   for jj=1:(n-2)
      kk=(ii-1)*(n-2)+jj;
      aux=sqrt(((ii-n0-n1)^2+(jj-n0)^2))*h;          % distance node - magnetic disk
      centerd
      auxm=sqrt(((ii-n0-n2)^2+(jj-n0)^2))*h;

      if aux < radbf                                 % filling diagonals region B neq 0
         aux1=cons3*(aux^2+radbf^4/auxm^2);
         aux1=aux1-(bf^2*radbf^2/4/m)*(h^2*((jj-n0)^2+(ii-n0-n1)*(ii-n0-n2))/auxm^2);

        d(kk)=-4*cons+aux1+pote(ii,jj);
        b(kk)=cons-cons2*(ii-n0-n1)*h+cons2e*(ii-n0-n2)*h/auxm^2;
        bet(kk)=cons+cons2*(ii-n0-n1)*h-cons2e*(ii-n0-n2)*h/auxm^2;
        a(kk)=cons+cons2*(jj-n0)*h-cons2e*(jj-n0)*h/auxm^2;
        alp(kk)=cons-cons2*(jj-n0)*h+cons2e*(jj-n0)*h/auxm^2;

     elseif auxm < radbf
         aux1=cons3*(auxm^2+radbf^4/aux^2);
         aux1=aux1-(bf^2*radbf^2/4/m)*(h^2*((jj-n0)^2+(ii-n0-n1)*(ii-n0-n2))/aux^2);
        d(kk)=-4*cons+aux1+pote(ii,jj);
        b(kk)=cons+cons2*(ii-n0-n2)*h-cons2e*(ii-n0-n1)*h/aux^2;
        bet(kk)=cons-cons2*(ii-n0-n2)*h+cons2e*(ii-n0-n1)*h/aux^2;
        a(kk)=cons-cons2*(jj-n0)*h+cons2e*(jj-n0)*h/aux^2;
        alp(kk)=cons+cons2*(jj-n0)*h-cons2e*(jj-n0)*h/aux^2;

        else                                         % filling diagonals region B = 0

         aux1=cons3*((radbf^4/aux^2)+(radbf^4/auxm^2));
         aux1=aux1-(bf^2*radbf^4/4/m)*h^2*((jj-n0)^2+(ii-n0-n1)*(ii-n0-n2))/aux^2/auxm^2;
        d(kk)=-4*cons+aux1+pote(ii,jj);
        b(kk)=cons-cons2e*(ii-n0-n1)*h/aux^2+cons2e*(ii-n0-n2)*h/auxm^2;
        bet(kk)=cons+cons2e*(ii-n0-n1)*h/aux^2-cons2e*(ii-n0-n2)*h/auxm^2;
        a(kk)=cons+cons2e*(jj-n0)*h/aux^2-cons2e*(jj-n0)*h/auxm^2;
        alp(kk)=cons-cons2e*(jj-n0)*h/aux^2+cons2e*(jj-n0)*h/auxm^2;
      end
   end
end
```

```
%diags_spm.m

% defined in main.m ->  cons=-1/(2*m*h^2);cons2=i*bf/(4*m*h);cons2e=cons2*radbf^2;cons3=bf^2/(8*m);

d=zeros((n-2)^2,1);                                     % filling diagonals with zeros
b=d;bet=d;a=d;alp=d;

n0=round((n-1)/2);                                      % center of the system
n1=round(n*(x0/lon));                                   % centers of the magnetic disks
n2=round(n*(-x0/lon));
```

```
for ii=1:(n-2)
   for jj=1:(n-2)
      kk=(ii-1)*(n-2)+jj;
      aux=sqrt(((ii-n0-n1)^2+(jj-n0)^2))*h;                  % distance node - magnetic disk center
      auxm=sqrt(((ii-n0-n2)^2+(jj-n0)^2))*h;

      if aux < radbf                                         % filling diagonals region B neq 0
         aux1=cons3*(aux^2+radbf^4/auxm^2);
         aux1=aux1-(bf^2*radbf^2/4/m)*(h^2*((jj-n0)^2+(ii-n0-n1)*(ii-n0-n2))/auxm^2);

        d(kk)=-4*cons+aux1+pote(ii,jj);
        b(kk)=cons-cons2*(ii-n0-n1)*h+cons2e*(ii-n0-n2)*h/auxm^2;
        bet(kk)=cons+cons2*(ii-n0-n1)*h-cons2e*(ii-n0-n2)*h/auxm^2;
        a(kk)=cons+cons2*(jj-n0)*h-cons2e*(jj-n0)*h/auxm^2;
        alp(kk)=cons-cons2*(jj-n0)*h+cons2e*(jj-n0)*h/auxm^2;

     elseif auxm < radbf
         aux1=cons3*(auxm^2+radbf^4/aux^2);
         aux1=aux1-(bf^2*radbf^2/4/m)*(h^2*((jj-n0)^2+(ii-n0-n1)*(ii-n0-n2))/aux^2);
        d(kk)=-4*cons+aux1+pote(ii,jj);
        b(kk)=cons+cons2*(ii-n0-n2)*h-cons2e*(ii-n0-n1)*h/aux^2;
        bet(kk)=cons-cons2*(ii-n0-n2)*h+cons2e*(ii-n0-n1)*h/aux^2;
        a(kk)=cons-cons2*(jj-n0)*h+cons2e*(jj-n0)*h/aux^2;
        alp(kk)=cons+cons2*(jj-n0)*h-cons2e*(jj-n0)*h/aux^2;

        else                                                 % filling diagonals region B = 0

         aux1=cons3*((radbf^4/aux^2)+(radbf^4/auxm^2));
         aux1=aux1-(bf^2*radbf^4/4/m)*h^2*((jj-n0)^2+(ii-n0-n1)*(ii-n0-n2))/aux^2/auxm^2;
        d(kk)=-4*cons+aux1+pote(ii,jj);
        b(kk)=cons-cons2e*(ii-n0-n1)*h/aux^2+cons2e*(ii-n0-n2)*h/auxm^2;
        bet(kk)=cons+cons2e*(ii-n0-n1)*h/aux^2-cons2e*(ii-n0-n2)*h/auxm^2;
        a(kk)=cons+cons2e*(jj-n0)*h/aux^2-cons2e*(jj-n0)*h/auxm^2;
        alp(kk)=cons-cons2e*(jj-n0)*h/aux^2+cons2e*(jj-n0)*h/auxm^2;
      end
   end
end
```

```
for k=1:(n-2):(n-2)^2                          % filling with zeros
    b(k)=0;                                    % upper diagonal [0,values]
end

for k=(n-2):(n-2):(n-2)^2                      % filling with zeros
    bet(k)=0;                                  % lower diagonal [values,0]
end

for k=1:(n-2)                                  % filling with zeros
    a(k)=0;                                    % upper diagonal [0,values]
end

for k=(n-2)*(n-2)+1:(n-2)^2                    % filling with zeros
    alp(k)=0;                                  % lower diagonal [values,0]
end

%BCs : F = 0 at the grid borders
```

HomeWork results:

Two beams of magnetic field having the same strength but opposite sign.