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Quantum energy wave function Equation and harmonic oscillator

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ABSTRACT: The physics of conduction by hopping in superconductivity is not yet well established. This work is concerned with trying to throw light on conduction by hopping in superconductivity. It uses Schrödinger equation for energy wave function which time and spatial dependent or spatial dependent only. It is found that the wave function is highly localized in most cases which means that electrons conduct through hopping to adjacent atoms only. One solution shows the possibility to electron travelling which agrees with cooper model. The critical temperature is shown to depend on binding energy.

KEYWORDS: Quantum energy, wave function; Harmonic oscillator.

I. INTRODUCTION

The history of quantum mechanics dates from the discovery of plank that light behaves like particles[1].Later on De Broglie proposed that particles like electrons behaves as waves[2].This confirms the dual nature of atomic and sub atomic particles[3,4].This encourages Schrödinger and Heisenberg to formulate a quantum equation that describes atomic world[5]. Heisenberg representation was developed by so called matrix representation, which represents quantum systems in different space [6].These includes energy, momentum and coordinate space. As far as the energy of atoms and electrons are important, it is there for important to study quantum Schrödinger equation in the energy space [6]. This is since the energy wave function gives the probability of electrons transition [7].This energy representation is used by the so called Hubbard model to describe superconductivity behavior [8].This model is complex and cannot directly explain why the resistance vanishes beyond some critical temperature [9].How ever some attempts were model to do this [9].But this model is mathematically complex. Thus there is a need for simple model. This is done in this work.

Section 2 is concerned with energy wave function equation for spatially and time dependent case. Harmonic oscillator solution is in section 3. Section 4 is devoted for spatial dependent wave function and particle in a box solution discontinuity and can clear in section 5 and 6 respectively.

II.QUANTUM ENERGY WAVE FUNCTION

It is very investing to see how the energy wave function can evolve with time and coordinates .

ThusC_k Is a function of x and t:

$|\Psi>= \sum c_{k|}u_k>$(1)

Where :

$C_{k=}\, c_k(\,x\,,t\,)$ (2)

In this case Schrödinger equation becomes:

$i\hbar = \frac{\partial|\Psi>}{\partial t} = \hat{H}|\Psi>$(3)

$i\hbar\frac{\partial}{\partial t}\sum_k c_k|u_k> = \sum_k \hat{H}c_k|u_k>$

$i\hbar\frac{\partial}{\partial t}\sum c_k u_k = \sum_k \hat{H}c_k u_k = \sum_k (H_{0+}V_1)c_k u_k$

Where the perturbed Hamiltonian:

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$$\hat{H} = H_0 + V_1$$

Thus:

$\sum \left[i\hbar \left(\frac{\partial c_k}{\partial t}\right) u_k + i\hbar c_k \left(\frac{\partial u_k}{\partial t}\right] = \sum_k \hat{H}\, c_k u_k$ (4)

But for non perturbed system [see equation (1)]:

$i\hbar \frac{\partial u_k}{\partial t} = E_k u_k = \hat{H}_0 u_k = \left(-\frac{\hbar^2}{2m}\nabla^2 u_k + V_0 u_k\right)$ (5)

Thus:

$\sum_k \left[i\hbar \left(\frac{\partial c_k}{\partial t}\right) u_k + c_k E_k u_k \right] = \sum_k \hat{H} c_k u_k + \nabla^2 (c_k u_k) \sum_k -\frac{\hbar^2}{2m} =$

$V_0 c_K u_k + V_1 c_k u_k$ (6)

But the second term in the right hand side of(6) is given by:

$$\nabla^2 (c_k u_k) + V c_k u_k = \sum_k -\frac{\hbar^2}{2m} [u_k \nabla^2 c_k + c_k \nabla^2 u_k + 2\nabla u_k \nabla c_k] \sum_k -\frac{\hbar^2}{2m} + V_0 c_k u_k + V_1 c_k u_k$$

$\sum_k V_1 u_k c_k + \sum_k \left[-\frac{\hbar^2}{2m}\nabla^2 u_k + V_0 u_k\right] c_k + \sum_k -\frac{\hbar^2}{2m} [u_k \nabla^2 c_k + 2\nabla u_k \nabla c_k]$

From(5):

$$= \sum_k E_k u_k c_k + \sum_k -\frac{\hbar^2}{2m} [u_k \nabla^2 c_{k+} 2\nabla u_k \nabla c_k] + \sum_k V_1 u_k c_k \quad (7)$$

Thus from(6):

$\sum_k \left[i\hbar \frac{\partial c_k}{\partial t} + \frac{\hbar^2}{2m}\nabla^2 c_k \right] u_k = -\frac{\hbar^2}{m} \sum_k \nabla u_k \nabla c_k + \sum_k V_1 u_k c_k$ (8)

Setting:

$\nabla c_k \Psi =$

And using the hermiticity of$\hat{p}$:

$$\int \overline{\hat{p}\bar{u}}_k \Psi dr = \int \overline{\overline{u_k}\hat{p}}\, \Psi dr$$

$$\frac{-\hbar}{i} \int \nabla \overline{\overline{u_k}} \Psi dr = -\frac{\hbar}{i} \int \overline{\overline{u_k}}\, \nabla \Psi dr$$

$\int \nabla u_k \nabla c_k dr = \int u_k \nabla^2 c_k dr$-(9)

Thus:

$\nabla u_k \nabla c_k = -u_k \nabla^2 c_k$ (10)

Substituting (10)in(8) yields:

$$\sum_k \left[i\hbar \frac{\partial c_k}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 c_k \right] u_k = \sum_k V_1 u_k c_k \quad (11)$$

$$\sum_k \left[i\hbar \frac{\partial c_k}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 c_k - V_1 c_k \right] u_k = 0$$

Can be solving by selecting, this:

$i\hbar \frac{\partial c_k}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 c_k - V_1 c_k = 0$ (12)

III. Harmonic oscillator

Consider equation (12) :

$i\hbar \frac{\partial c_k}{\partial t} = \frac{\hbar^2}{2m}\nabla^2 c_k + V_1 c_k$ (13)

For time independent potential, let:

$c_k = e^{+i/\hbar E_k t} u_k$ (14)

To get:

$E_k u_k = \frac{\hbar^2}{2m}\nabla^2 u_k + V_1 u_k$ (15)

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For harmonic oscillator perturbation by electromagnetic field :

$V_1 = ½ kx^2 = c_1 x^2$ (16)

Thus:

$\frac{\hbar^2}{2m}\nabla^2 u_k + c_1 x^2 = -E_k c_k$ (17)

Substituting:

$u_k = A e^{-\alpha x^2}$ (18)

$\nabla u_k = -2\alpha x e^{-\alpha x^2} = -2\alpha x u_k$

$\nabla^2 u_k = -2\alpha u_k - 2\alpha x \nabla u_k = -2\alpha u_k + 4\alpha^2 x^2 u_k$ (19)

$\frac{\hbar^2}{2m}[-2\alpha + 4\alpha^2 x^2 + c_1 x^2]u_k = -E_k u_k$ (20)

$E_k = \frac{\hbar^2}{m}\alpha ; 4\alpha^2 = -c_1$ (23)

$\alpha = ½\sqrt{-k/2} = \frac{i}{\sqrt{2}} k = \frac{i\sqrt{m}}{2\sqrt{2}}\omega$

Thus from (14) and (18) beside (23):

$c_k = A e^{+\frac{iE_k T}{\hbar}} e^{\frac{ik}{2\sqrt{2}}x^2}$ (24)

Which represents non localized travelling wave?

However for particles affected by additional perturbing potentials like applying sound wave with frequency ω_s and electron magnetic wave with frequencyω_e , such that the two forces apposes each other; in this case :

$-\nabla V = F = m\ddot{x} = F_e - F_s = -k_e x + k_s x$

$-\frac{\partial V}{\partial X} = -m\omega_e x + m\omega_s x$

Thus :

$V = ½ m\omega_s^2 x^2 - ½ m\omega_e^2 x^2$

$= ½ m(\omega_s^2 - \omega_e^2) x^2$

$= 1/2m(\omega_s + \omega_e)(\omega_s - \omega_e)x^2$

$= -½ \mathbf{k} x^2$

$K = m(\omega_s + \omega_e)(\omega_e - \omega_s) = C_1$ (25)

When :

$\omega_s > \omega_e$

In this case :

$C_2 = -C_1 = m(\omega_s + \omega_e)(\omega_s - \omega_e) > 0$ (26)

Thus equation (23) gives :

$\alpha = ½\sqrt{c_2}$ (27)

Due to the periodicity of C_k in (14) :

$C_k (t + T) = C_k (t)$

Thus :

$e^{\frac{+i}{\hbar}E_k T} = 1$

$\cos\frac{E_k T}{\hbar} = 1 ; \sin\frac{E_k T}{\hbar} = 0$ (28)

Hence :

$\frac{T E_k}{\hbar} = 2n\pi$

$E_k = n\hbar(\frac{2\pi}{T}) = n\hbar\omega$

Thus from equation (23) :

$\alpha = \frac{m}{\hbar^2}E_k = \frac{n m\omega}{\hbar}$ (29)

From equation(18):

$u_k = A e^{-\alpha x^2}$

Thus the energy is quantized, and is mighty localized thus move by hopping.

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IV. Spatial dependent energy wave function and particles in a box

Schrödinger equation which i s based on Newtonian energy relation is gives by :

$i\hbar = \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$ (30)

To make use of equation (30) consider:

$c_k = c_k$ (E , x) (31)

i.e , the energy wave function depends on E and x only , where :

$u_k = u_k$(E , t) = A $e^{i E_k t / \hbar}$ (32)

substituting equation (31) in (30) yields :

$i\hbar\sum_k c_k \frac{\partial u_k}{\partial t} = \frac{-\hbar^2}{2m}\sum \nabla^2 c_k u_u + \sum_k V u_k C_k$ (33)

$\sum_k c_k \frac{\partial u_k}{\partial t} = \frac{-\hbar^2}{2m}\sum \nabla^2 C_k u_k + \sum_k V u_k C_k$ (34)

In view of equation :

$i\hbar\frac{\partial u_k}{\partial t} = E_k u_k$

Thus :

$\sum_k E_k C_k u_k = \frac{-\hbar^2}{2m}\sum_k u_k \nabla^2 c_k + \sum_k V u_k c_k$ (35)

Multiply equation (35) by $\overline{u_n}$, then integrating , yields :

$\sum_k E_k c_k \int u_k \overline{u_n}$ .dr = $\frac{-\hbar}{2m}\sum_k (\int u_k \overline{u_n}$ .dr) $\nabla^2 c_k + \sum_k c_k \int \overline{u_n} V u_k dr$

$\sum_k E_k c_k \delta_{nk} = \frac{-\hbar}{2m}\sum_k (\nabla^2 c_k) \delta_{nk} + \sum_k c_k V_{nk}$

$\delta_{nk} = \delta_{nn} = 1$ (n =k)

Thus schordinger equation for energy wave function is give by :

$c_n E_n = \frac{-\hbar^2}{2m}\nabla^2 c_n + \sum_k c_k V_{nk}$ (36)

For constant potential V_0 equation (36) reduces to :

$c_n E_n = \frac{-\hbar^2}{2m}\nabla^2 c_n + \sum_k c_k V_0 \delta_{kn}$

Thus :

$\frac{-\hbar^2}{2m}\nabla^2 c_n = (E_n - V_0)\, c_n$ (37)

To solve this equation consider the solution of equation(37) to be :

c_n= A e^{ikx} (38)

Thus :

K = $\sqrt{2m(E_n - V_0)}$ (39)

For highly localized electrons :

$E_n < V_0$ (40)

In this case :

K = i$\alpha = i\sqrt{2m(V_0 - E_n)}$(41)

Thus :

c_n= A $e^{i 2\alpha x}$ = A $e^{-\alpha x}$ (42)

Thus the probability of existence of electrons in level n :

$|c_n|^2$ = A^2 $c^{-2\alpha x}$ (43)

This probability highly decays a sx→∞.Thus the electron is highly localized at x = 0, when :

$E_n < V_0$ (44)

If one considers energy to be thermal, then:

$$E_n = KT$$

Thus:

kT $< V_0$ (45)

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T $<\frac{V_0}{K}$ (46)
The critical temperature beyond which the electron s are highly localized is :
Tc = $\frac{V_0}{K}$ (47)
Thus :
T < Tc (48)
The fact that electrons are highly localized indicates that electron current does not result from electron motion in the whole super conductivity . This localization confirms the fact that electron conduction mechanism in super conductivity is by hopping of electrons from atom to adjacent one .
This forces the next atom to eject another electron to hope to third one .
Another solution is of the form :
c_n = A sin α x (49)
Substituting equation (49) in equation (37) yields :
+ $\frac{\hbar^2}{2m}\alpha^2 = (E_n - V_0)$
α = $\frac{\sqrt{2m\ (E_n - V_0)}}{\hbar}$ (50)
Where:
$E_n < V_0$
Thus the electrons are bound to adjacent atoms.
Only for particle in a box which , indicates that electrons in super conductivity does not move freely but hope just to the adjacent atom ,
$|C_n\ (x = d)|^2 = 0$ (51)
Hence from (49) :
Sinαd = 0 (52)
Therefore:
α d = 2n π
α = $\frac{2\,n\,\pi}{d}$ (53)
Thus from equation (50) and (53) :
$E_n = \frac{h^2}{2md} n^2 + V_0$ (54)
This means that the energy is quantized in a superconductivity temperature material.

V. DISCUSSION

According to equation (12) the energy wave function is affected by perturbed potential only. This is similar to that happens for time dependent perturbation ordinary equation. The harmonic oscillator solution in section (3).shows according to equation (24) that electrons travel in the whole superconductivity. This agrees with cooper pair model. However when the atoms vibrate due to effect of two sources the electrons are localized and move by hopping to adjacent atoms only.
For spatial dependent energy wave function and by considering electrons hope only to adjacent atoms, one can consider electrons as particle in a box. The solution (42) indicates that the electrons are highly localized thus hope only to adjacent atoms. The critical temperature T_c
Is found in equation (47) to dependent on binding energy V_0
However equation (49) predicts standing wave solution. Thus the particles are localized at:

$$x = \frac{(n + \frac{1}{2})}{\propto}$$

The energy is shown to be quantized (see equation (54)).Since one assumes that:

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$$C_n(x = a) = 0$$

This confirms that the electrons are localized and hope only to adjacent atoms.

VI.CONCLUSION

The solution of Schrödinger equation by using energy approach suggests that the electrons in most cases conduct by hopping mechanism. There is a critical temperature for hopping process is dependent on binding energy.

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