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Path Integral Formalism To The Evaluation Of The Density Of States Of A Four Dimensional Electron System In A Classically Smooth Potential

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ABSTRACT

We have defined the Green's function for the four-dimensional electron System in a classically smooth potential. Then the method of path integral formalism have been used for the evaluation of the density of states (DOS) of a four-dimensional electron system in a classically smooth potential. Finally we have calculated the time coordinate representation of the DOS, and as a conclusion of this study we have found the manner in which the DOS of the four−dimensional electron system varies with respect to the energy E of the system.

Key words *: path integral, density of states, four-dimensaional electron system, smooth potential.*

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1. Introduction

Density of states[1] refers to the number of energy states in each unit interval of energy and in each unit volume of the crystal. For the electrons[2] confined into a cube of side length L, The density of states in the absence of any external field may be written as ,

$$\rho(E) = \frac{2}{V}\sum_j \delta(E - \varepsilon_j) \qquad \text{for } \varepsilon_j = \frac{p_j^2}{2m} \text{ and } V = L^3$$

Classically smooth potential[3] means the potential whose variation with the space coordinate is small. In this paper we have defined the Green's function for the four dimensional electron system under classically smooth potential, then Path integral approach[4] is applied for the evaluation of the DOS of the four-dimensional electron system. Finally we have deduced the expression for the DOS of the four-dimensional electron system in the time- coordinate representation.

2. Method

Hamiltonian for the system under study is time independent as it is clear from its expression given below :

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + U(\vec{q}) \qquad \text{.....(1)}$$

Here $U(\vec{q})$ represents the classically smooth potential depending on the spatial coordinate $\vec{q}$ in the q-representation. Therefore for the system, Green's function[5] will satisfy the equation

$$(i\hbar\frac{\partial}{\partial t} - \hat{H})\hat{G}_t(\vec{q},\vec{q'}) = \delta(t).\delta(\vec{q} - \vec{q'}) \qquad \text{.....(2)}$$

Where $\vec{q}$ and $\vec{q'}$ are the spatial co- ordinates in the q- representation.

Solution of equation (2) may be written as $\hat{G}_t^R$ and $\hat{G}_t^A$ as follows:

$$\hat{G}_t^R = \frac{1}{i\hbar}exp(-i\hat{H}t/\hbar).\theta(t) \qquad \text{.....(3A)}$$

with the initial condition that $\hat{G}_t^R \to 0 \quad as \quad t \to \infty$; and

$$\hat{G_t^A} = \frac{1}{i\hbar} exp(-i\hat{H}t/\hbar).\theta(-t)$$ .....(3B)

with the initial condition that $\hat{G_t^A} \rightarrow \ 0 \quad as \ \ t \rightarrow \infty$.

therefore,

$$G_t^R(\vec{q},\vec{q'}) = \frac{1}{i\hbar}\theta(t) < \vec{q} \mid \ exp(-i\hat{H}t/\hbar) \mid \ \vec{q'} >$$ .....(4)

Let the intermediate times between 0 and t be represented as $t_1, t_2, t_3, ...t_{n-1}$ with the corresponding coordinates $\vec{q_1}, \vec{q_2}, \vec{q_3}, ...\vec{q}_{n-1}$ respectively,in such a way that,

$t_n = t \quad and \quad \vec{q}_n = \vec{q'}$ $\qquad t_k - t_{k-1} = \frac{t}{n} = \tau$

, for k = 2,3,4, ...n . .....(5)

With the boundary condition that as $n \rightarrow \propto \ , \ \tau \rightarrow 0 \quad and \ \ t_n = t$.

See the figure (1) . Now our task is to evaluate $G_t^R(\vec{q},\vec{q'})$, For this the method of path integral formalism is used

here.Hence from the equation (4) we may write,

$$G_t^R(\vec{q},\vec{q'}) = \frac{1}{i\hbar}\theta(t) \int d\vec{q_1} d\vec{q_2} .... d\vec{q}_{n-1}$$

$$< \vec{q_1} \mid exp(-i\hat{H}\tau/\hbar) \mid \vec{q_2} >< \vec{q_2} \mid exp(-i\hat{H}\tau/\hbar) \mid \vec{q_3} > \ .....$$

$$< \vec{q}_{n-2} \mid exp(-i\hat{H}\tau/\hbar) \mid \vec{q}_{n-1} >< \vec{q}_{n-1} \mid exp(-i\hat{H}\tau/\hbar) \mid \vec{q_n} >$$

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.....(6)

In writing the equation (6) we have used the completeness condition of quantum mechanics[6]. Now for the four-dimensional system, the matrix element of the operator $exp(-i\hat{H}\tau/\hbar)$ in the q-coordinate representation may be simplified as,

$$< \vec{q}_{k-1} \mid exp(-i\hat{H}\tau/\hbar) \mid \vec{q}_k >= \frac{m^2}{(2\pi i\hbar\tau)^2} \quad exp[\frac{im(\vec{q}_k - \vec{q}_{k-1})^2}{2\hbar\tau} - i\tau U(\vec{q}_k)/\hbar]$$

.....(7)

Therefore from the equations (6) and equation (7) ,

$$G_t^R(\vec{q},\vec{q'}) = \frac{1}{i\hbar}\lim_{\tau\to 0}\theta(t) \cdot \int d\vec{q_1}.d\vec{q_2}...d\vec{q}_{n-1}....$$

$$\frac{m^{2n}}{(2\pi i\hbar\tau)^{2n}} exp[\frac{1}{-i\hbar}\tau\sum_{k=1}^{n}(\frac{m(\vec{q}_k - \vec{q}_{k-1})^2}{2\tau^2} - U(\vec{q}_k))] .$$

$$G_t^R(\vec{q},\vec{q'}) = \frac{1}{i\hbar}\lim_{\tau\to 0}\theta(t) \cdot \int d\vec{q_1}.d\vec{q_2}...d\vec{q}_{n-1}....$$

$$\frac{m^{2n}}{(2\pi i\hbar\tau)^{2n}} exp[\frac{1}{-i\hbar}\tau\int_0^t d\tau(m\dot{\vec{q}}^2/2 - U(\vec{q}))]$$

.....(8)

Where,

$$\dot{\vec{q}} = \frac{\partial\vec{q}}{\partial\tau} .$$

If we take

$$D[\vec{q}] = \frac{m^{2n}}{(2\pi i\hbar\,\tau)^{2n}} d\vec{q_1}.d\vec{q_2}...d\vec{q}_{n-1} \quad \text{and} \quad S = \int_0^t d\tau.L(\vec{q},\dot{\vec{q}}) = Action .$$

For the classically smooth potential $U(\vec{q})$ we can explicitly write from equation (8) that,

$$G_t^R(|\ \vec{q} - \vec{q'}\ |) = \frac{1}{i\hbar}\theta(t). \int_{\vec{q}}^{\vec{q'}} D[\vec{q}].exp[\frac{m}{-2i\hbar}\int_0^t d\tau \dot{\vec{q}}^2 - \frac{ct^2}{2\hbar^2}]$$

.....(9)

Where c is a constant, which is interpreted as the correlation function for the case of classically smooth potential . Therefore density of states of the four-dimensional electrons can be written as ,

$$\rho(E) = \frac{2}{\pi\hbar} Re[\int_0^\infty d\tau exp(-iE\tau/\hbar) \oint D[\vec{q}]) exp(\frac{m}{-2i\hbar}\int_0^t d\tau(m\dot{\vec{q}}^2/2 - U(\vec{q}))]$$

.....(10)

Using time-coordinate representation we simplify the equation (10) as,

$$\rho(E) = \lim_{\xi\to 0+} \frac{m^2}{4\pi^3\hbar^3}\int_{-\infty}^{\infty} \frac{d\tau\ .exp(-c\tau^2/2\hbar^2\ + iE\tau/\hbar)}{(\xi + i\tau)^2}$$

.....(11)

3. Results and Discussion

After simplifying the equation (11) we get,

$$\rho(E) = \frac{m^2}{4\pi^3\hbar^3}[E + \sqrt{\frac{2c}{\pi}}.F(1,1,\frac{2E^2}{\sqrt{2\pi c}}) + \frac{2E^2}{\sqrt{2\pi c}}.F(1/2,3/2,-E^2/2c)]$$

Where $F(1,1,2E^2/\sqrt{2\pi c})$ and $F(1/2,3/2,-E^2/2c)]$ are confluent hypergeometric function[7] . We have plotted the graph of μE versus $\rho(E)$ by assuming that $\mu = \frac{4\pi^3\hbar^3}{m^2}$. For simplicity we have drawn the graph for two different values of c namely , c=1/2 $(Joule)^2$, and c=1 $(Joule)^2$, See the figure (2) and figure(3) . From the graph for c=1/2 $(Joule)^2$, and c=1 $(Joule)^2$, it is evident that the density of states (DOS) of four-dimensional electron system increases by increasing E, in the manner which is shown in the graph.

4.Conclusion

we have studied the four-dimensional electron system in which we have evaluated the density of states of the four-dimensional electron system, from which it is clear that the density of states (DOS) increases by increasing the energy E of the system and the rate of increase of the density of states also increases by increasing E for small positive values of E.

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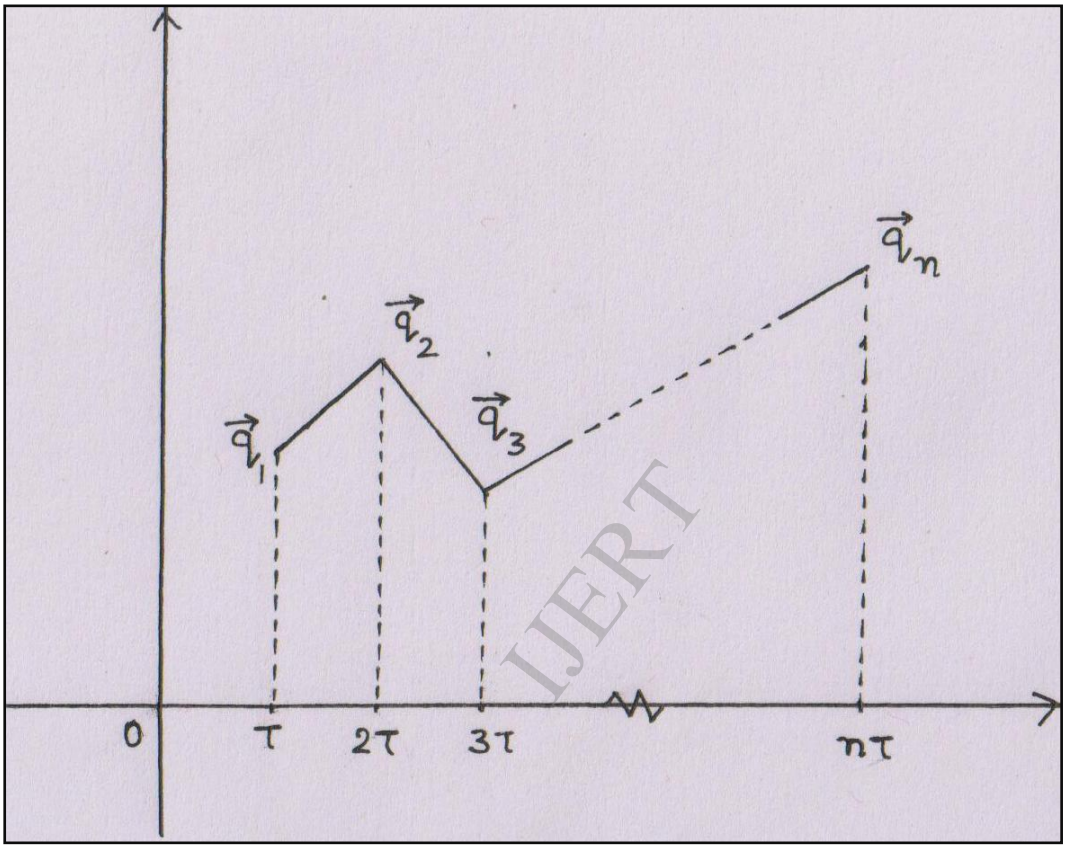
Caption:

Figure 1 : Representation of the coordinates $\vec{q}_k$ at different times $k\tau$ for $k = 1, 2, 3, ..., n.$

Figure 2 : Graph of μE versus $\rho(E)$ for c=1/2 $(Joule)^2$.

Figure 3 : Graph of μE versus $\rho(E)$ for c=1 $(Joule)^2$.



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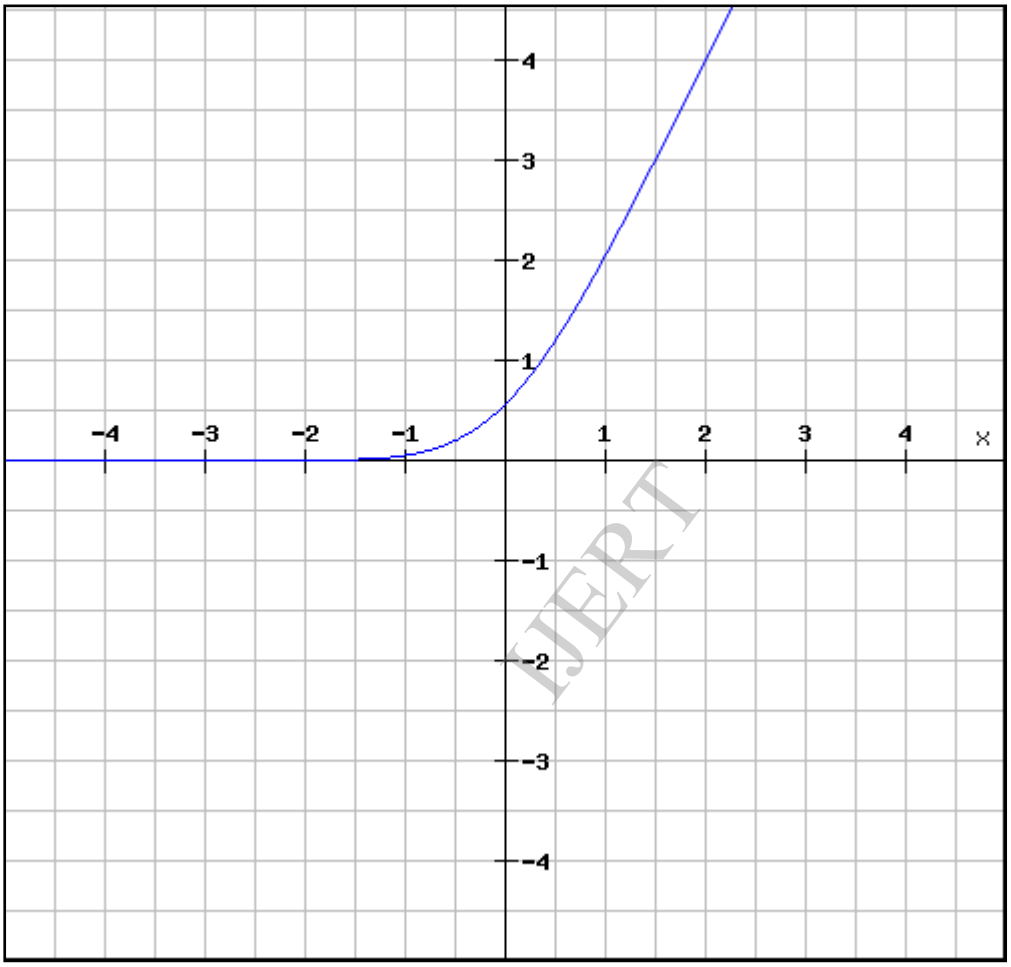

Figure 2 : Graph of μE versus $\rho(E)$ for c=1/2 $(Joule)^2$.

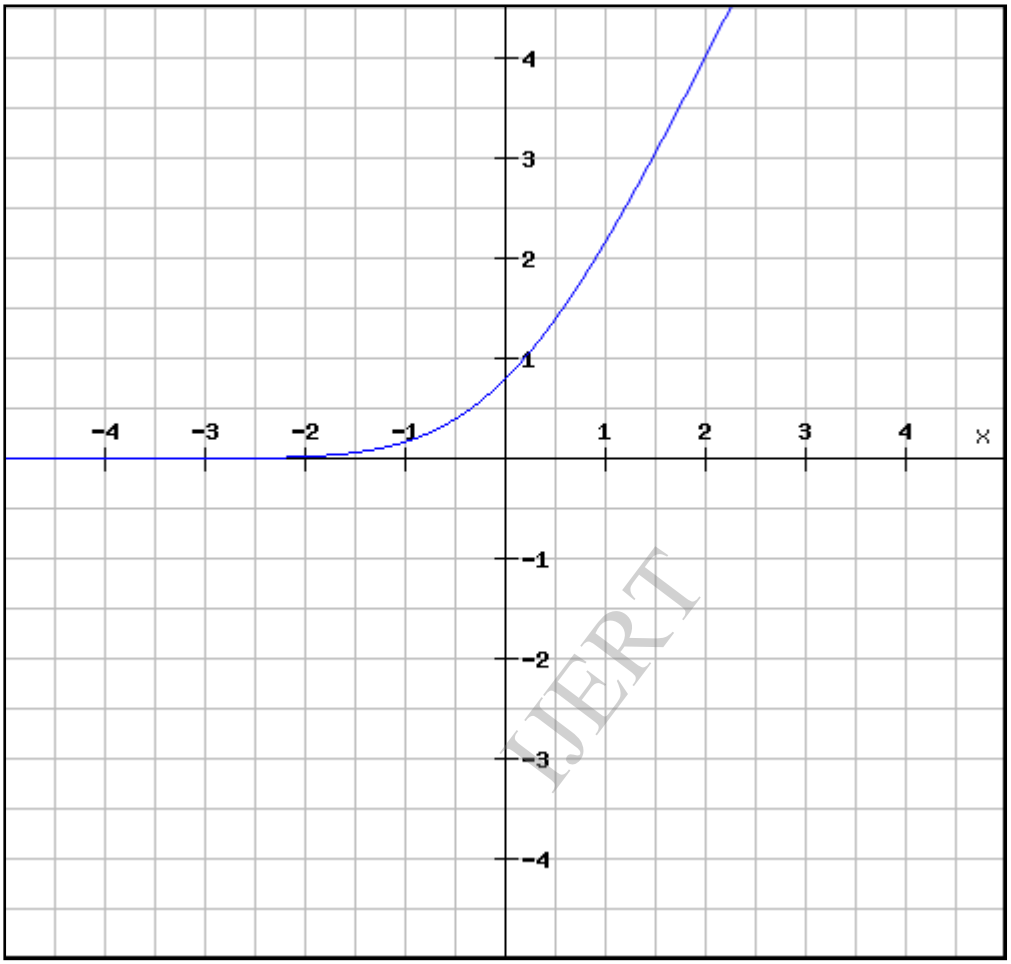

Figure 3 : Graph of μE versus $\rho(E)$ for c=1 $(Joule)^2$