Quantum Square Wells with Capacitive Walls: A Toy Model for Quantum Capacitors

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Abstract: This research aims to determine the energy quantization in a one-dimensional infinite square well modified by capacitive walls. The electric field inside the wall produces a linear potential. The solution to the Schrdinger equation is the Airy function for an infinite square well. Furthermore, the Wentzel-Kramers-Brillouin (WKB) approach is applied to finite wells, and the energy quantization for both cases based on this modified potential has been derived. In this paper, we also examine the quantum capacitance of the system, which is determined from the density of states and depends on dimensionality. The result of this work is a toy model that does not yet provide a complete complex picture of the quantum capacitance model. However, this model shows similarities in terms of energy dispersion relations and quantum capacitance with several types of graphene systems.

Keywords: Quantum square wells; Quantum capacitance; WKB Approximation

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I. INTRODUCTION

The infinite square well is one of the most fundamental problems in quantum mechanics, typically characterized by rigid, infinite potential barriers. It serves as an idealized model to introduce the principles of quantum confinement and energy quantization. However, its simplicity often limits its applicability to real-world systems, for example conjugated polyene [1], quantum well lasers [2], and quantum dots [3, 4]. If there is a electric field generates inside the wells, this problem lead to some what called Quantum capacitance. The quantum capacitance is required for incorporating the quantum mechanical effects, particularly in nanoscale and low-dimensional systems, for example graphene-based structures, quantum dots, nanowires, etc. Unlike classical capacitance, which depends only on the geometry and permittivity of the system, quantum capacitance arises from the finite density of states (DOS). The metals serve classical capacitance, with density of states for two-dimensional metal like electron gas (2DEG) with parabolic dispersion leads to a constant quantum capacitance [5]. This subject is studied along some number in material devices i.e metals, monolayer and bilayer graphene, carbon nanotubes [6–11].

To calculate quantum capacitance, which is directly related to the density of states and the energy dispersion of energy in the system. In a material, quantum capacitance is defined as the change in charge density relative to changes in electrochemical potential, which plays an important role in determining the electronic behavior of devices at the nanoscale. For example, in graphene, the quantum capacitance is derived from the density of states, which in the case of pure monolayer graphene shows its proportionality to energy. This certainly provides a theoretical basis for further exploring similar properties in other materials at a more advanced level [12–16]. Another very important material is supercapacitors which can act as other energy storage devices, where understanding the interaction between quantum and classical capacitance is very important to optimize their performance [17–20].

By adding an electric field in the infinite potential well, it will modify the Schrodinger equation and create a linear potential that impacts the solution of the wave function and energy eigenvalues of the particles differently from the case without a magnetic field. The solution to this equation is the Airy function, which has been found in many physical systems. The Wentzel-Kramers-Brillouin (WKB) approach can be used to analyze energy quantization in finite potentials, thereby enabling a deeper understanding of how electric fields influence quantum states for finite wells.

In this paper, the issue of energy quantization has been revisited, in which the infinite and finite potential wells have an electric field inside, and finding that the connection between quantum capacitance and materials like graphene. This paper does not intend to build a new complex and comprehensive model that matches multiple material properties and experimental findings. Our goal is to solve the Schrodinger equation for our scenario and then compare it with current models. We believe that our discoveries provide perspectives for studying nanoscale devices and materials with electronic characteristics.

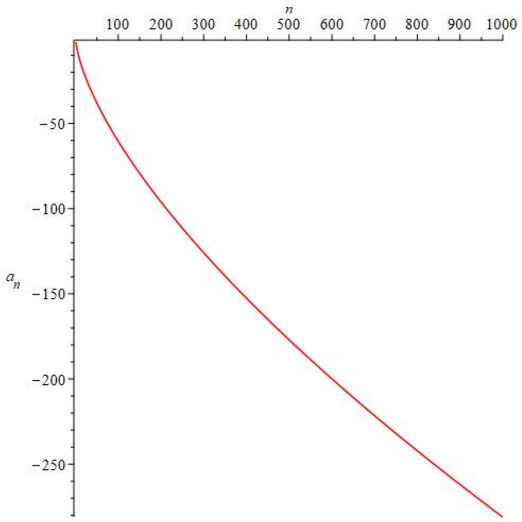

FIG. 1: Plot of Airy zeroes a_n as a function of n for $n = 1..1000$

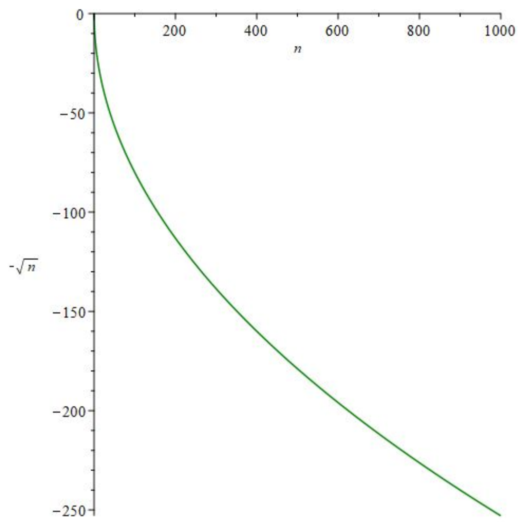

FIG. 2: Plot of $-8\sqrt{n}$ for $n = 1..1000$

II. MODIFIED INFINITE SQUARE WELL WITH CAPACITIVE WALLS

Consider a one-dimensional infinite square well of length L, in which the walls are regarded as capacitor plates at $x = 0$ and $x = L$. Inside the well is a particle with charge q. Now, the electric field E produced by the capacitive walls affects the potential inside the well. Between the capacitor plates, the uniform electric field E is produced by:

$$\mathbf{E} = \frac{\sigma}{\epsilon_\circ} \tag{1}$$

where ϵ is the permittivity of medium and σ is the surface charge density on the plates. The charged particle's potential energy $V(x)$ in the well is thus

$$V(x) = -qEx = -\frac{q\sigma x}{\epsilon_\circ} \tag{2}$$

As a result, the potential within the well varies linearly

$$V(x) = -\alpha x \tag{3}$$

where $\alpha = q\sigma/\epsilon_\circ$. Within the well, the time-independent Schrdinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \alpha x\psi(x) = E\psi(x) \tag{4}$$

Subtitute $z = \sqrt[3]{2m\alpha/\hbar^2}(x - E/\alpha)$ and the equation becomes an Airy-like function

$$\frac{d^2\phi(z)}{dx^2} - z\phi(z) = 0 \tag{5}$$

Using methods Airy-like functionswhich are the solutions to the Schrdinger equation for a linear potentialthe general solution to this differential equation can be discovered as

$$\psi(x) = C_1 \,\mathrm{Ai}\left(\sqrt[3]{\frac{2m\alpha}{\hbar^2}}\left(x - \frac{E}{\alpha}\right)\right) \tag{6}$$

By applying boundary conditions at $x = 0$, we have

$$\mathrm{Ai}\left(\sqrt[3]{\frac{2m\alpha}{\hbar^2}}\left(0 - \frac{E}{\alpha}\right)\right) = 0 \tag{7}$$

The zeros of Ai a_n with $n = 0, 1, 2, ...$ can be found in [21], then the energy quantization is

$$E_n = -\left(\frac{\alpha^2\hbar^2}{2m}\right)^{1/3} a_n \tag{8}$$

This problem is similar in principle as in gravitational potential (see Problem 8.6 in [22])

$$\psi_n(x) = C_1 \,\mathrm{Ai}\left(\sqrt[3]{\frac{2m\alpha}{\hbar^2}}\left(x - \frac{E_n}{\alpha}\right)\right) \tag{9}$$

Since the Airy function cannot be normalized use C_1, which can be determined by applying the Airy delta-dirac properties:

$$\int_{-\infty}^{+\infty} dx \mathrm{Ai}(y - x)\mathrm{Ai}(y' - x) = \delta(y' - y) \tag{10}$$

The normalized wave function can be written as

$$\psi_n(x) = \sqrt[6]{2m\alpha/\hbar^2}\mathrm{Ai}\left(\sqrt[3]{\frac{2m\alpha}{\hbar^2}}\left(x - \frac{E_n}{\alpha}\right)\right) \tag{11}$$

Now, we will find a dispersion relation for our energy quantization. The plot of the first 1,000 airy zeros is shown in Fig.1. We also plotted $-\gamma\sqrt{n}$, with $\gamma = 8$, which is approximately close to a_n. Then, we use the zeros of the Airy function, which is proportional to $\sqrt{n}$ in the energy dispersion relation (see Fig.1 and Fig.2).

III. FINITE WELL AND WKB APPROXIMATION

The potential energy V(x) inside the well now becomes

$$V(x) = \begin{cases} -\alpha x \text{ for } 0 \leq x \leq L \\ V_\circ \text{ for } x < 0 \,\text{or}\, x > L \end{cases} \tag{12}$$

To investigate energy quantization in a modified finite square well with capacitive walls and a placed charge using WKB (Wentzel-Kramers-Brillouin) approximations, we examine how the capacitive walls' potential influences the energy levels of the particle inside the well. The WKB approximation is ideal for this problem because it can handle the slowly varying potential within the finite well.

The WKB approximation is applicable in regions where the potential changes slowly concerning the de Broglie wavelength of the particle. Inside the well, the potential is linear and smooth, which satisfies the slow variation condition, i.e., V(x) changes gradually over the width of the well. In particular, since potential outside the well is constant $V_\circ$, the turning points can be accurately treated, and the WKB solution is straightforward to match at the boundaries. The general WKB solution for the wavefunction $\psi(x)$ in a potential is given by

$$\psi(x) \approx \frac{C}{\sqrt{k(x)}} \exp\left(\pm i \int_{x_0}^{x} k(x')dx'\right) \tag{13}$$

where the $k(x) = \sqrt{2m(E - V(x))/\hbar^2}$

In the WKB approximation, the quantization condition for bound states is expressed by the Bohr-Sommerfeld rule:

$$\int_{x_1}^{x_2} k(x)dx = \left(n + \frac{1}{2}\right)\pi\hbar \tag{14}$$

where x_1 and x_2 are the classical turning points, which are determined by $E = V(x)$. The classical turning points x_1 and x_2 correspond to the locations where the energy $E = V(x)$

$$E = -\alpha x_1 + V_\circ; E = -\alpha x_2 + V_\circ \tag{15}$$

Solving these for x_1 and x_2 gives:

$$x_1 = \frac{V_\circ - E}{\alpha}; \;\; x_2 = \frac{V_\circ - E}{\alpha} + \frac{2E}{\alpha} \tag{16}$$

The integral for the WKB quantization condition is then

$$\int_{x_0}^{x} k(x)dx = \left(n + \frac{1}{2}\right)\pi\hbar \tag{17}$$

where the $k(x) = \sqrt{2m(E + \alpha x - V_\circ)/\hbar^2}$. We substitute $k(x)$ into the quantization condition and evaluate the integral

$$\int_{x_0}^{x} k(x)dx = \sqrt{2m(E + \alpha x - V_\circ)/\hbar^2} \tag{18}$$

Changing the variable $u = E + \alpha x - V_\circ$ the integral then becomes

$$\begin{aligned} \int_{E-V_\circ}^{E-V_\circ+\alpha L} u^{1/2}\frac{du}{\alpha} &= \frac{2}{3\alpha}u^{3/2}\Bigg| \begin{matrix} E - V_\circ \\ E - V_\circ + \alpha L \end{matrix} \\ &= \frac{2}{3\alpha}\Big[(E - V_\circ + \alpha L)^{3/2} \\ &\quad -(E - V_\circ)^{3/2}\Big] \end{aligned} \tag{19}$$

Substituting into WKB quantization condition yields

$$\begin{aligned} (E_n - V_\circ + \alpha L)^{3/2} &- (E_n - V_\circ)^{3/2} \\ &= \frac{3\pi\alpha\hbar}{2}\left(n + \frac{1}{2}\right) \\ (E_n - V_\circ)^{3/2} &\left[\left(1 + \frac{\alpha L}{E_n - V_\circ}\right)^{3/2} - 1\right] \\ &= \frac{3\pi\alpha\hbar}{2}\left(n + \frac{1}{2}\right) \end{aligned} \tag{20}$$

For $E_n - V_\circ \gg \alpha L$, we use the Taylor expansion of $(1+x)^n \approx 1 + nx$, which gives

$$\begin{aligned} (E_n - V_\circ)^{3/2}\frac{3}{2}\frac{\alpha L}{E_n - V_\circ} &= \frac{3\pi\alpha\hbar}{2}\left(n + \frac{1}{2}\right) \\ E_n &= V_\circ + \frac{\pi^2\hbar^2}{L^2}\left(n + \frac{1}{2}\right)^2 \end{aligned} \tag{21}$$

We can see that the α, which contains the electric field information, is cancelled out. The energy dispersion relation $E_n \sim n^2$, which is similar to 2DFG or parabolic dispersion relation. This equation is implicit and generally requires numerical methods to solve for E_n. The energy levels are thus quantized according to this modified WKB condition, reflecting the influence of the capacitive walls on the potential within the finite well.

IV. THE QUANTUM CAPACITANCE

The old method to calculate quantum capacitance from density of states, i.e., the energy relation. The quantum capacitance C_Q is given by

$$C_Q = e^2 g(E) \tag{22}$$

where e and $g(E)$ are electron charge and density of states. The density of states is determined from the dispersion relation. In d-dimensional systems, the number of states up to k is proportional to the volume of a d-dimensional sphere of radius k

$$N(k)_d = C_d k^d \tag{23}$$

where C_d is a constant depending on the dimensionality and the system size. For $d = 1, 2, 3$ the $N(k)$ are

$$N(k)_1 = \left(\frac{L}{2\pi}\right)2k \tag{24}$$

$$N(k)_2 = \left(\frac{A}{(2\pi)^2}\right)\pi k^2 \tag{25}$$

$$N(k)_3 = \left(\frac{V}{(2\pi)^3}\right)\frac{4}{3}\pi k^3 \tag{26}$$

The density of states can be calculated as

$$g(E) = \frac{dN(k)}{dk}\frac{dk}{dE} \tag{27}$$

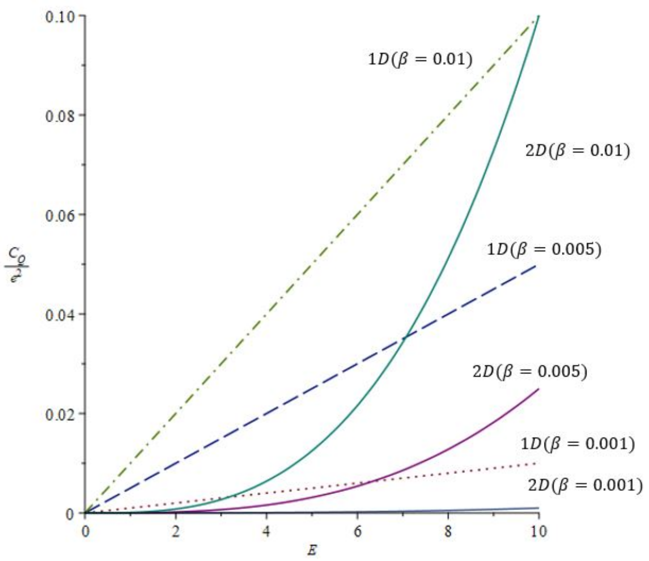

FIG. 3: Plot of quantum capacitance in modified infinite square wells for various strengths ($\beta = 10^{-3}, 5 \times 10^{-3}, 10^{-2}$). The solid line indicating a one-dimensional case, while the dot, dashed, and dotdashed line is for a two-dimensional case.

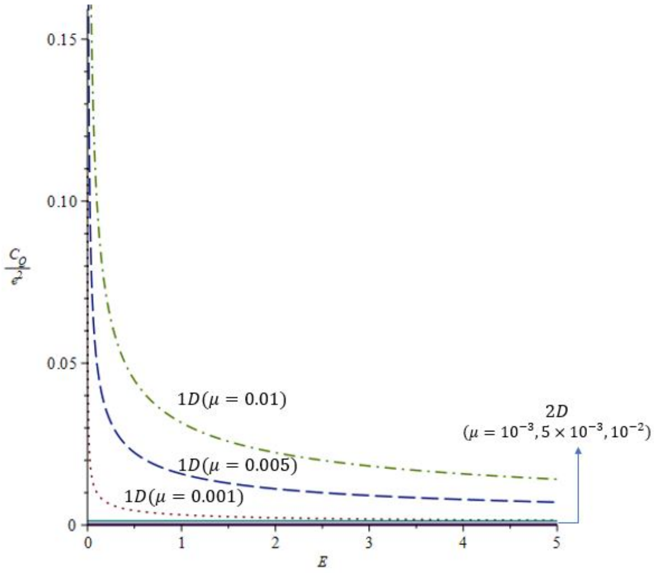

FIG. 4: Plot of quantum capacitance in modified finite square wells with WKB approximation for various strengths ($\mu = 10^{-3}, 5 \times 10^{-3}, 10^{-2}$). The solid line indicating for a one-dimensional case, while dot, dashed, and dotdashed line is for a two-dimensional case.

A. Infinite square well

Recall the energy relation in equation (8). For continuum states, the zeros of the Airy function for large n can be approximated as $\gamma n^{1/2}$, for some constant γ. Changing variable $k = n\pi/L$, then the k as a function of E is given by

$$k = \frac{\pi}{L}\left[\frac{2m}{\hbar^2\alpha^2\gamma^3}\right]^{2/3}|E|^2 \quad (28)$$

Therefore, we can calculate the density of states for one-dimensional square well, which gives

$$g(E) = \left[\frac{2m}{\hbar^2\alpha^2\gamma^3}\right]^{2/3} E \quad (29)$$

Thus, the quantum capacitance is given by

$$C_{1D} = e^2\left[\frac{2m}{\hbar^2\alpha^2\gamma^3}\right]^{2/3}|E| \equiv e^2\beta|E| \quad (30)$$

where β is defined as field strength. We can see that the quantum capacitance is proportional to E which is related to pure and perfect monolayer graphene quantum capacitance. The perfect monolayer graphene quantum capacitance formula is given by [7]

$$C_{MLG} = \frac{g_s g_\nu m*}{\pi\hbar^2\gamma_\ell}|E| \quad (31)$$

where g_s, g_ν, $m*$, and γ_ℓ are spin degeneracy, valley degeneracy, effective mass, and interlayer coupling. That two formulas of quantum capacitances are the same shape up to constant proportionality. For a two-dimensional square well, the quantum capacitance becomes

$$C_{2D} = e^2\left[\frac{2m}{\alpha^2\hbar^2\gamma^3}\right]^{4/3}|E|^3 = e^2\beta^2|E|^3 \quad (32)$$

The plot of the quantum capacitance of one and two dimensional infinite square wells shows in Fig.3.

B. Finite square well

Take the continuum states in equation (21), the $k = n\pi/L$ as a function of E can be written as

$$k = -\frac{\pi}{2L} + \frac{1}{\hbar}\sqrt{E - V_\circ} \quad (33)$$

Thus, the quantum capacitance for one and two-dimensional finite square wells is given by

$$C_{1D} = \frac{L}{4\pi\hbar}\left(E - V_\circ)\right)^{-1/2} \equiv \mu\left(E - V_\circ)\right)^{-1/2} \quad (34)$$

$$C_{2D} = \frac{L^2}{4\pi\hbar}\left(\frac{1}{\hbar} - \frac{1}{2\sqrt{E - V_\circ}})\right) \simeq \frac{L^2}{4\pi\hbar^2} = 4\pi\mu^2 \quad (35)$$

In case 2D finite square well, the quantum capacitance is a constant value, which is similar to bilayer graphene near dirac-point or parabolic dispersion with 2DFG: $C_Q = g_\nu m e^2/\pi\hbar^2$ [5, 7]. The plot of the above quantum capacitance is shown in Fig.4.

C. Comparisson and future improvements

There is a difference in the approach used between solving cases of infinite potential wells and finite potential wells. In the case of an infinite potential well, the solution to the Schrodinger equation is an exact solution, whereas in the case of a finite potential well, we use the WKB approach. Fig. 1 and Fig. 2 show energy quantization in an infinite square well with capacitive walls. The energy eigenvalues are proportional to $n^{1/2}$, in contrast to the original infinite square well. This behavior highlights the significance of the linear potential of the electric field. On the other hand, the WKB approximation shows a more complex relationship between the energy levels and the well depth, $V_\circ$, in the finite well (Fig. 3). However, Fig. 3 is for limit $E - V_\circ \gg \alpha L$, the quantization condition simplifies, surprisingly, independent from the electric field strength. The more general results can be solved numerically from the equation (20) and the electric field dependency is restored.

The improvements of this model, for example, applied a uniform magnetic field applied perpendicular to the plane of the quantum well. This modifies the Hamiltonian through the vector potential $\mathbf{A}$ using minimal substitution and then applying the Landau gauge. The resulting guest is discrete Landau levels, which cause oscillations in quantum capacitance. This scenario allowed us to have precise control over electronic properties. This tunability is essential for magnetic field-sensitive electronics such as quantum dots and nanoscale energy storage systems. Another improvement is incorporating spin-dependent effects via electric field and spin coupling. This coupling modifies the Hamiltonian. In a 2D system with structural inversion asymmetry, this effect is called the Rashba SOC (spin-orbit coupling) effect. In the capacitive quantum well, this leads to spin-split subbands. The SOC modifies the density of states by introducing spin-dependent energy levels, which can be exploited for spintronic devices. Specifically, the quantum capacitance becomes a function of the Rashba parameter, which allows for control via external electric fields. This extension enables spin-resolved transport features required for spintronic devices.

V. DISCUSSION AND CONCLUSION

The consequence of introducing capacitive walls is that it results in significant deviations from traditional infinite square well behavior. Our analysis shows the energy levels proportional to the square root of quantum number n when we analyze the zeroes of airy functions. This relation is deviating from parabolic dispersion in typical quantum wells. The resulting quantum capacitance shows dimensional dependence: proportional to E in one-dimensional systems, which is similar to a perfect monolayer graphene system, and E^3 in two-dimensional systems.

For finite wells, the WKB approximation provides a framework for quantifying the influence of electric fields. In case $E - V_\circ \gg \alpha L$, the quantization condition is surprisingly independent of the applied electric field. The quantum capacitance is proportional to the square root of the energy for one dimension, while for two dimensions it results in a constant value that is similar to the 2DEG model or bilayer graphene near the dirac point.

This paper relies on the infinite and finite square well model by incorporating capacitive walls, a homogeneous electric field, and a linear potential. We used Airy functions and the WKB approximation to calculate the energy dispersion relation and quantum capacitance values. The observed results support the dimension dependence of quantum capacitance and exhibit parallels to graphene-like structures.

Future research could look into interactions with magnetic fields, spin-orbit coupling, and multilayer topologies to improve the model's applicability to nanoscale materials science.

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