A novel theoretical derivation for the existence of an energy band gap in a perfect solid state crystal lattice

Carsten Wochnowski, Rofanweg 1, 85757 Karlsfeld, Germany
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Abstract

In this paper a novel theory is presented in order to explain the existence of the energy band and energy band gap in a perfect solid state crystal lattice. It is assumed that the solid state crystal lattice consists of a lattice of equidistant Delta-potential equally spaced like it is the case in the Kronig-Penny-Model. But instead of solving the Schrödinger Equation for the Kronig-Penny-Model by differentiation, the Schrödinger Equation is integrated yielding the formula $|\psi(x=na)|^2 = (E - E_{kin})/zV_0$, by whose discussion the existence of the band gap is revealed and confirmed.
Although the existence of a band gap is already well-recognized, the derivation is novel and can be also applied in other field of physics in respect to totally other physical phenomena like high energy physics eventually leading to a unified field theory.

Introduction:

Since many decades the existence of an energy band gap in a solid state crystal lattice is well known. One of the most common theoretical models for the existence of an energy band gap is explained by the Kronig Penney Model assuming the solid state crystal consists of a lattice of Delta-potential equally spaced to one another. By solving the Schrödinger equation two different solutions are possible each representing another energy level revealing the existence of an energy band gap.
The existence of energy bands and energy band gaps in solid crystal matters are vastly theoretically discussed and experimentally confirmed in the last decades [1] – [4].

Theoretical contemplation:

It is assumed that the solid state crystal consists of a lattice with equally spaced Delta- potentials $V_0\delta(x=na)$ with a lattice constant a. Thus the Delta potentials stand for the positively charged atomic cores situated at the lattice positions of the solid state crystal. The electrons described by the probability distribution $|\psi(x)|^2$ are located either between two

adjacent atomic cores (or Delta potential) or at the sites of atomic core (Delta potential). For simplified reasons it is assumed that exactly one electron is located between two Delta potentials.

Thus the corresponding Schrödinger equation is as followed:

$$-\frac{\hbar^2}{2m}\Delta\psi + V_0 \sum_{n=-\infty}^{\infty} \delta(x+na)\,\psi = E\psi \qquad (1)$$

But instead of solving the Schrödinger equation by an complex exponential function leading to the dispersion relation, now the Schrödinger equation is integrated from -∞ to +∞ after having been multiplied with the complex conjugated ψ*:

$$-\frac{\hbar^2}{2m}\int \psi * \Delta\psi\, dx + V_0 \int \sum_{n=-oo}^{oo} \delta(x+na)\,\psi * \psi dx = \int E\psi * \psi dx \qquad (2)$$

In consideration of $\psi^*\psi(a) = |\psi(a)|^2$, the normalization $\int_{-\infty}^{\infty} \psi^*\psi dx = 1$, the definition of the dirac Delta distribution $f(a) = \int \delta(x-a) f(x) dx$ and the assumption that $\psi = \psi(x)$ is overall a steady and differentiable function, a short calculation yields the formula:

$$E_{kin} + V_0 \Sigma|\psi(x=na)|^2 = E \quad \text{or} \quad \Sigma|\psi(x=na)|^2 = (E - E_{kin}) / V_0 \qquad (3)$$

Now it is assumed that between every two adjacent Delta potentials exactly one electron is located. So due to $\Sigma|\psi(na)|^2 = z$ (summarization above all Delta potentials):

$$|\psi(x=na)|^2 = (E - E_{kin})/zV_0 \qquad (4)$$

This formula can be interpreted as follows: the probability density $|\psi(x=na)|^2$ of an electron at the Delta-potential δ(x=na) is maximum, if the kinetic energy is zero, while the electronic probability density $|\psi(x=na)|^2$ at the Delta-potential δ(x=na) is minimum, if the total energy E is equal to the kinetic energy E_{kin}.

Now the electronic probability density $|\psi(na)|^2$ is drawn against the kinetic energy E_{kin}, thus due to $|\psi(na, E_{kin})|^2 = (E - E_{kin})/zV_0 = E/zV_0 - E_{kin}/zV_0$ this yields a linear graph with a

negative slope $m = -1/zV_0$ and with a y-intercept $b = E/zV_0$ as shown in Fig. 1.
Thus we discuss the graph as follows: the zero point of the graph (point of intersection between the graph and x-coordinate (axis of abscissae)) is denoted as E_0, then the physically reasonable solutions are located in the area between $0 \leq E_{kin} \leq E = E_0$ between the minimal kinetic energy $E_{kin} = 0$ (the kinetic energy E_{kin} is zero) and the maximal kinetic energy $E_{kin} = E = E_0$ (kinetic energy E_{kin} is equal to the total energy E). Beyond $E_{kin} = E_0$, that means in the area of $E_{kin} > E_0$, the solutions are not reasonable, because firstly the kinetic energy E_{kin} must not be higher as the total energy E and secondly $|\psi(na)|^2$ must not become negative. On the other hand, the area $E_{kin} < 0$ is also physically forbidden, because the kinetic energy E_{kin} must not become negative either. At $E_{kin} = 0$, the probability distribution $|\psi(na)|^2$ at the Delta potential $\delta(x= na)$ becomes maximal, while at $E_{kin} = E$ (total energy E is equal to the kinetic energy E_{kin}), the probability distribution $|\psi(na)|^2$ at the Delta potential $\delta(x= na)$ becomes minimal or to be more precise, it becomes zero.

Now we can distinguish between several cases:
In the first case we assume $E = E_{kin}$, that means the total energy E is equal to the kinetic energy E_{kin}. As mentioned above, the probability distribution $|\psi(x=na)|^2$ is zero at the Delta potential x = na, that means no electron is located at the Delta potential. Consequently, the electron is located not at the positively charged lattice atomic cores, but it is located between them due to the normalisation condition $\int\psi^*\psi dx = 1$ as shown in Fig. 2. Consequently, the probability density $|\psi(0 < x < na)|^2$ betweent two adjacent Delta potentials is maximum, so the first case describes the state of lowest energy.
In the second case the kinetic energy E_{kin} is gradually reduced thus yielding $E < E_{kin} < 0$, the probability density $|\psi(x=na)|^2$ at the Delta potential x = na is increasing steadily and linearily as shown in Fig. 3. So the probability density $|\psi(x=na)|^2$ at the sites of Delta potentials x = 0, x = a and x = na is small, but not negligible any more, while the probability density $|\psi(0 < x < na)|^2$ between two adjacent Delta potential becomes smaller.
In the third case, the kinetic energy E_{kin} is further reduced, thus the probability density $|\psi(x=na)|^2$ at the Delta potential x = na is further rising, so $|\psi(x=na)|^2$ at the sites of Delta potential becomes significant, while the probability density $|\psi(0 < x < na)|^2$ between two adjacent Delta potentials is further reduced Fig. 4.
In the fourth case, the kinetic energy E_{kin} is still decreasing and the probability density $|\psi(x=na)|^2$ is still rising, until the probability density function $x: x \rightarrow |\psi(x)|^2$ becomes constant

Fig. 5. This case marks a turning point, because now the probability density $|\psi(x=na)|^2$ at the sites of Delta potential becomes larger than the probability density $|\psi(0 < x < na)|^2$ betweent two adjacent Delta potentials (fifth case, see Fig. 6).
In the sixth case E_{kin} is equal to zero and so E_{kin} attains its minimum value, consequently $|\psi(x=na)|^2$ reaches its maximum value E/zV_0, while the probability density $|\psi(0 < x < na)|^2$ between two adjacent Delta potentials becomes minimum or even zero (sixth case, see Fig. 7). That means that the probability density $|\psi(x=na)|^2$ at the sites of Delta potential is equal to E/zV_0. In this situation, the electron is located at the positively charged atomic cores of the solid lattice (the sixth case describes the state of highest energy).
Although, in the third, fourth and fifth case (Fig. 4-6) a normalisation problem occurs: because the third, fourth and fifth case does not match with the normalisation condition $\int\psi^*\psi dx = 1$. This can be very well observed in the fourth case (see Fig. 5 and 8): the probability density function x: $x \rightarrow |\psi(x)|^2$ is constant and thereby delocalisated throughout the entire lattice; that means it reaches theoretically from infinity to infinity. In order to comply with the normalisation condition, the probability density $|\psi(x)|^2$ must become almost zero as it is shown in Fig. 8. Although this is mathematically not forbidden, this does not make any physical sense. Consequently, while the first case (Fig. 2) is physically allowed and senseful (low energy) and while the sixth case (Fig 7) is also physically allowed and senseful (high energy), the fourth case is forbidden physically (medium energy), which is equivalent to the existence of an energy gap in a solid state lattice.

Conclusion:

The existence of an electronic band gap in a perfect solid state crystal lattice has been shown theoretically by another way: The Schrödinger Equation of such a perfect solid state crystal lattice (Kronig-Penny-Model) has been integrated instead of being differentiated. Thus equation Fig. 4 $|\psi(x=na)|^2 = (E - E_{kin})/zV_0$ is yielded which can be interpreted as a proof for the existence of an electronic band gap in such a solid state crystal lattice. This formula and interpretation can be supposed to be relevant also for another fields of physics like unified field theory: the string theory deals with the unbounded strings vibrating freely, while the loop quantum gravity theory is about quantized space and time. Now one can combine both theories: by putting the freely vibrating strings into a quantized elementary space unit, the strings become vibrating in a bounded state with discrete energy levels yielding the above

described formula. Now it depends on the vibration energy level if the string is a photon (light) or it forms matter.

Literature:

[1] Kittel, C.: Einführung in die Festkörperphysik, de Gruyter, Sept. 2002

[2] Ibach, H.; Lüth, H.: Festköperphysik, Springer, 2009

[3] Bonc-Bruevic, V.L.; Kalasnikov, S. G.: Halbleiterphysik, VEB Verlag, 1982

[4] Ashcroft, N. W.: Solid State Physics, Brooks Cole, 1976

Caption:

Fig. 1: The electronic probability density $|\psi(x=na, E_{kin})|^2$ is drawn against the kinetic energy E_{kin} yielding a linear graph with the slope of $-1/zV_0$ and an y-intercept of E/zV_0

Fig. 2: The electronic probability density distribution $|\psi(x, E_{kin})|^2$ inside of an array of Delta potentials (representing the positively charged atomic cores forming a perfect solid state crystal lattice) is shown; in the case of $E_{kin} = E$: the electronic probability density distribution $|\psi(x=na, E_{kin})|^2$ is zero at the site of any Delta potential $\delta(x=na)$, while the electronic probability density distribution $|\psi(0 < x < na, E_{kin})|^2$ is maximal in the space between two adjacent Delta potentials $\delta(x=na)$

Fig. 3: in the case of E_{kin} decreasing and thus a little bit smaller than E: $|\psi(x=na, E_{kin})|^2$ is small, but not zero at the sites of Delta potential, while $|\psi(0<x<na, E_{kin})|^2$ is slightly decreasing between two adjacent Delta potentials

Fig. 4: in the case of E_{kin} further decreasing: $|\psi(x=na, E_{kin})|^2$ is further increasing at the sites of Delta potential, while $|\psi(0<x<na, E_{kin})|^2$ is further decreasing between two adjacent Delta potentials

Fig. 5: in the case of E_{kin} continues to decrease: $|\psi(x=na, E_{kin})|^2$ is increasing at the sites of Delta potential, while $|\psi(0<x<na, E_{kin})|^2$ continues to decrease between two adjacent Delta potentials, until $|\psi(0<x<na, E_{kin})|^2$ is equal to $|\psi(x=na, E_{kin})|^2$ and the electronic probability density function x: x -> $|\psi(x)|^2$ becomes constant

Fig. 6: in the case of E_{kin} still continues decreasing: $|\psi(x=na, E_{kin})|^2$ continues increasing at the sites of Delta potential, while $|\psi(0<x<na, E_{kin})|^2$ continues decreasing between two adjacent Delta potentials, thus $|\psi(x=na, E_{kin})|^2$ becomes larger than $|\psi(0<x<na, E_{kin})|^2$

Fig. 7: in the case of $E_{kin} = 0$: $|\psi(x=na, E_{kin})|^2$ is equal to E/zV_0 and thus maximal, while $|\psi(0<x<na, E_{kin})|^2$ is equal to zero and thus minimal

Fig.8: In this case $1x\ (x)1^2$ is nearly equal to zero and is thus unphysical.

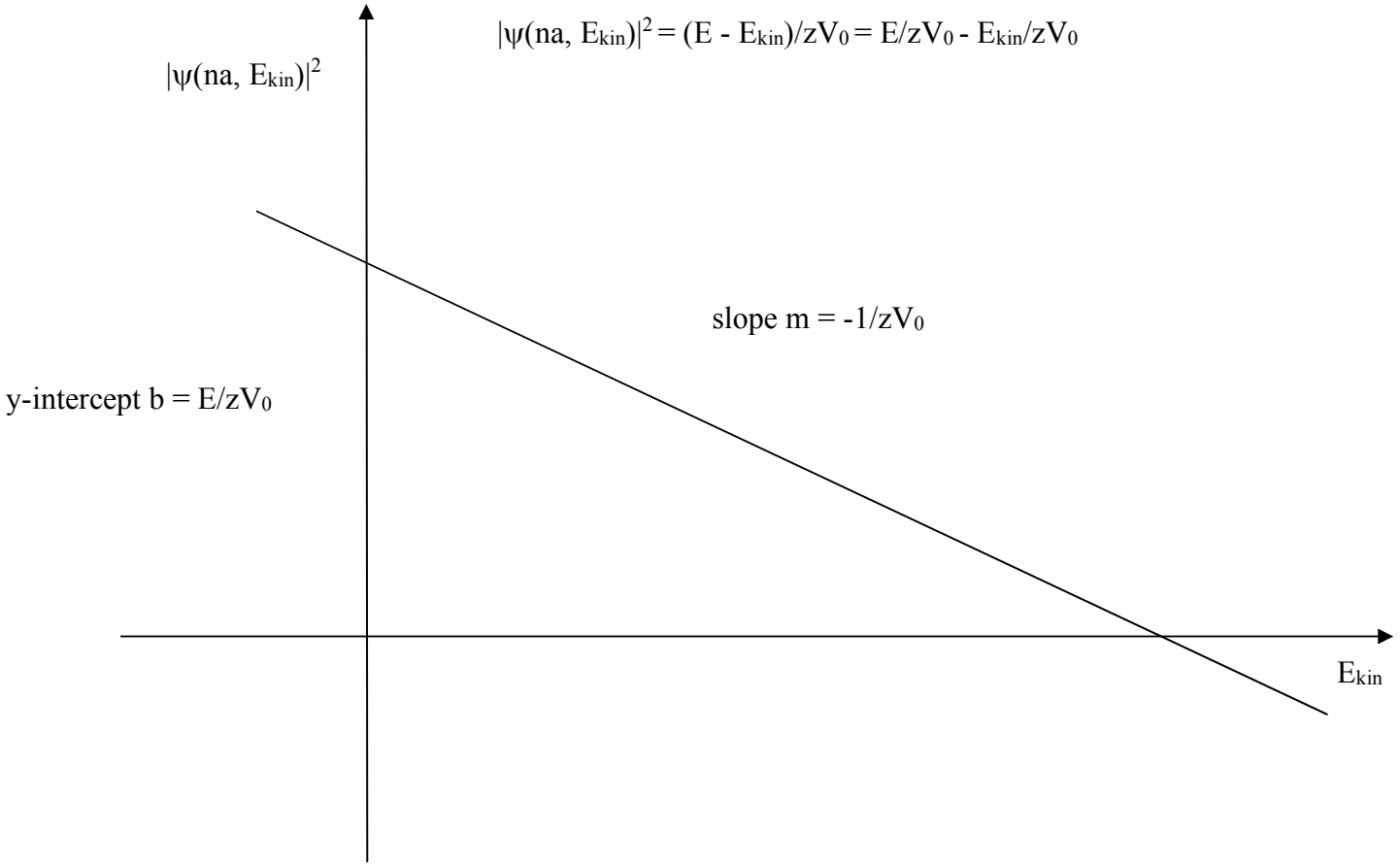
$|\psi(na, E_{kin})|^2 = (E - E_{kin})/zV_0 = E/zV_0 - E_{kin}/zV_0$
$|\psi(na, E_{kin})|^2$
slope $m = -1/zV_0$
y-intercept $b = E/zV_0$
E_{kin}

Fig. 1

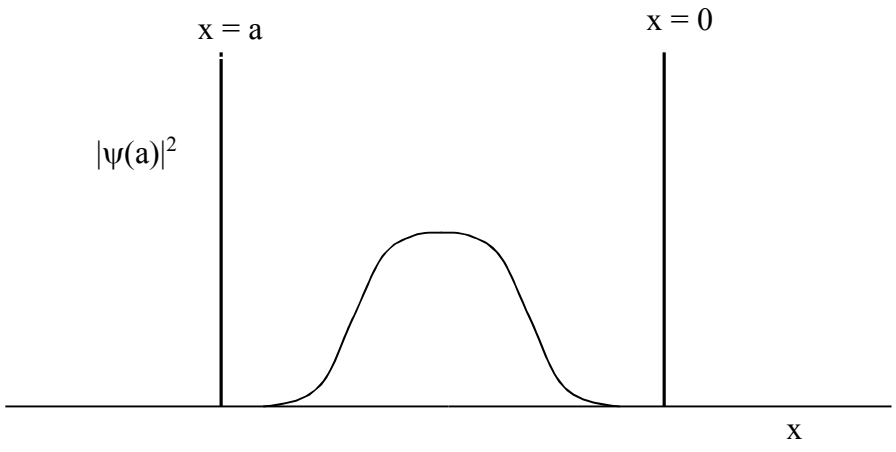
x = a
x = 0
$|\psi(a)|^2$
x

Fig. 2

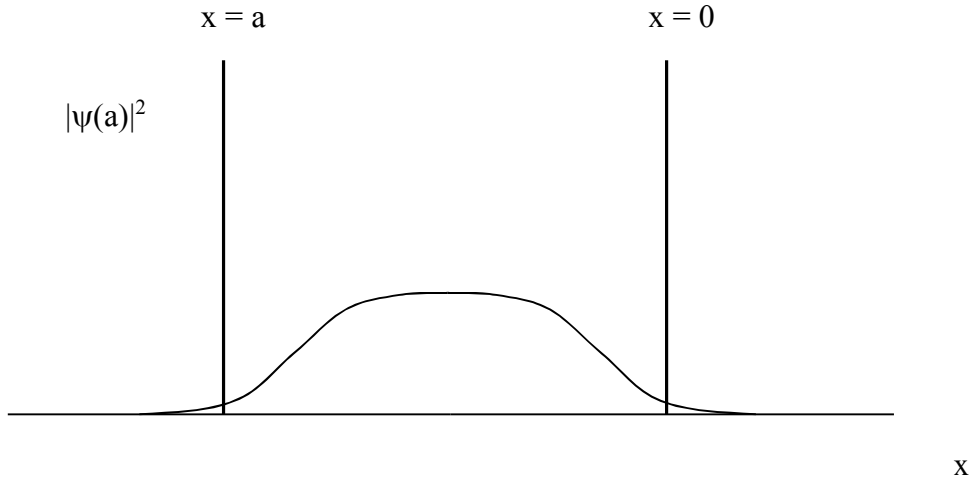

Fig. 3

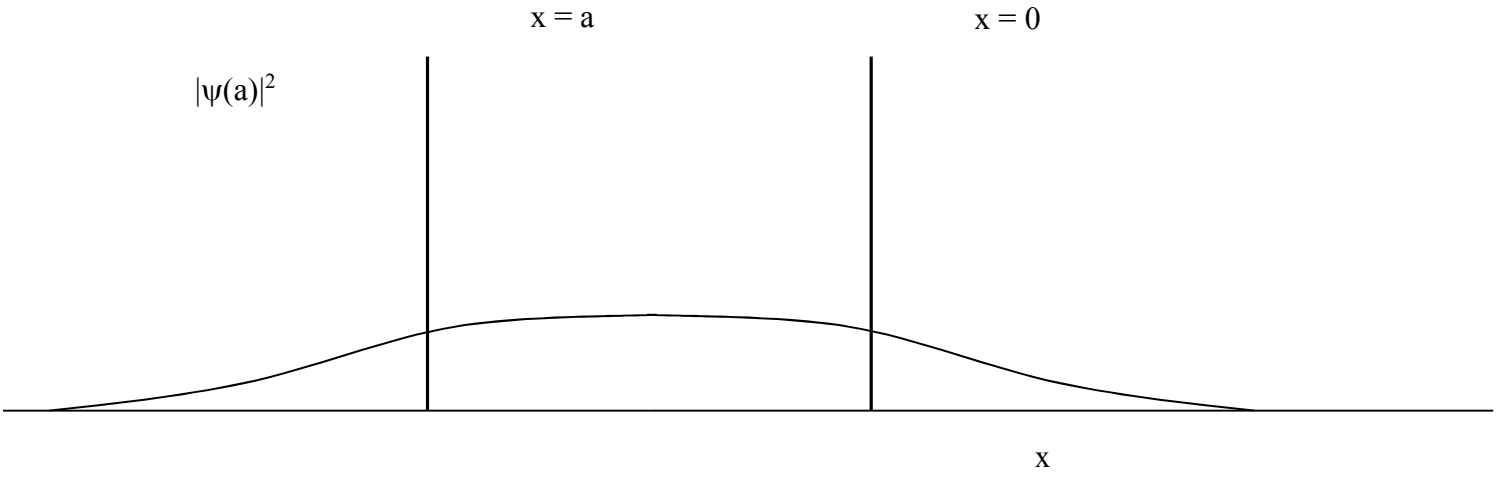

Fig. 4

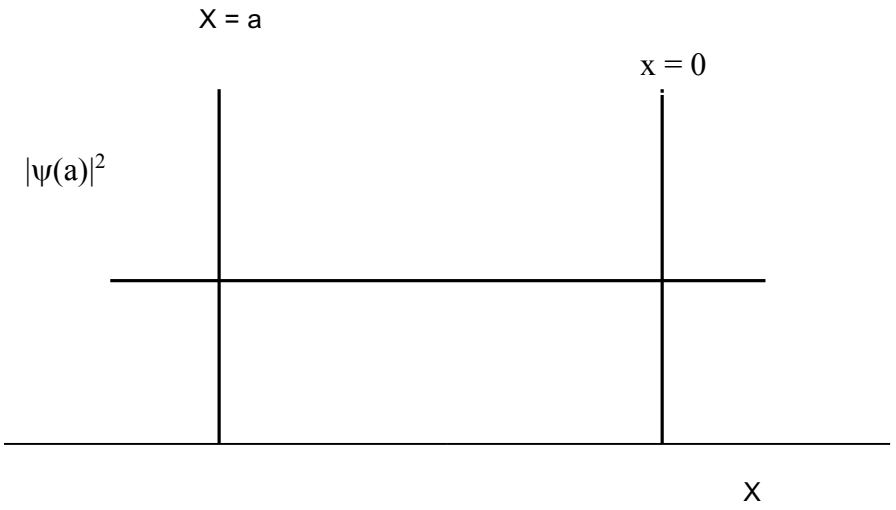

Fig. 5

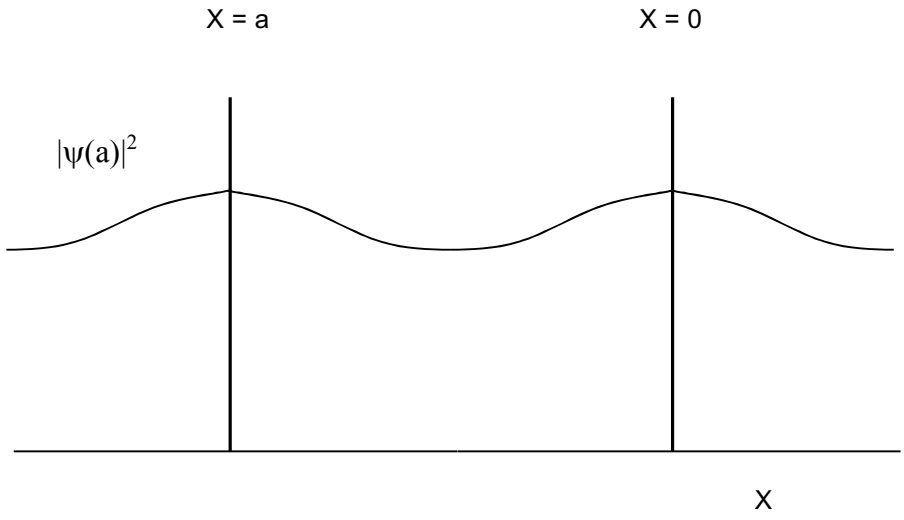

Fig. 6

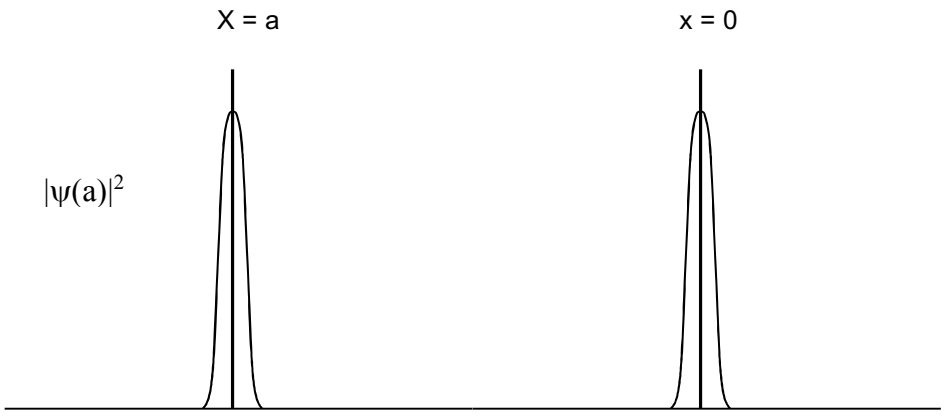

Fig. 7

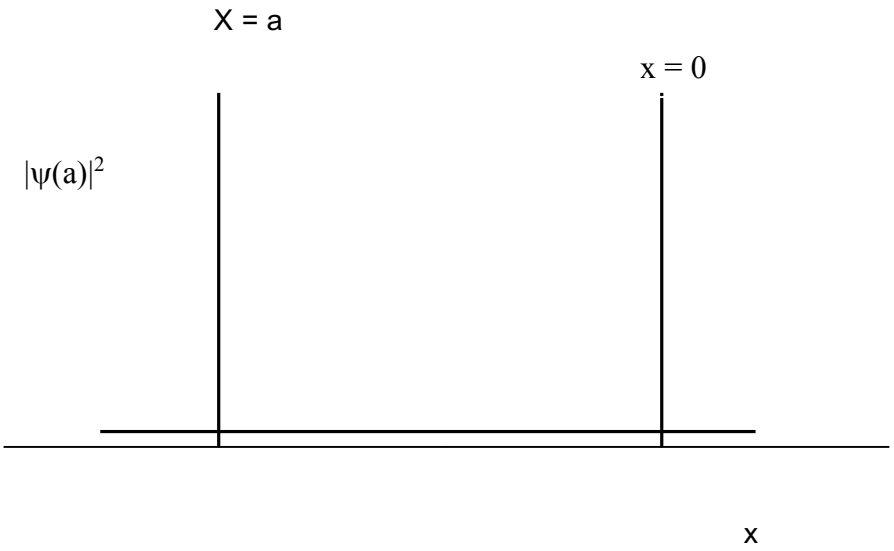

Fig. 8