

Scattering states of a particle, with position-dependent mass, in a double heterojunction

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Abstract

In this work we obtain the exact analytical scattering solutions of a particle (electron or hole) in a semiconductor double heterojunction — potential well / barrier — where the effective mass of the particle varies with position inside the heterojunctions. It is observed that the spatial dependence of mass within the well / barrier introduces a nonlinear component in the plane wave solutions of the continuum states. Additionally, the transmission coefficient is found to increase with increasing energy, finally approaching unity, whereas the reflection coefficient follows the reverse trend and goes to zero.

Key words : Position-dependent effective mass; Double heterojunction; Scattering solution; Non linear wave; Potential well; Morse barrier; Transmission coefficient.

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I. INTRODUCTION

Recent developments in the nanofabrication of semiconductor devices have given a thrust to the study of quantum mechanical systems with position dependent effective mass. The spatial dependence on the effective mass of the particle arises due to its interaction with an ensemble of particles within the device, as the particle propagates from left to right. This so-called position-dependent effective mass (pdem) formalism becomes an essential ingredient in describing the electronic and transport properties of quantum wells and quantum dots, impurities in crystals, He-clusters, quantum liquids, semiconductor heterostructures, etc. [1–8]. When two such materials (having pdem) with different bandgaps are placed adjacent to each other to form a heterojunction, the effective mass approximation is valid within each material. If, for example, a thin layer of a narrower (wider) bandgap material is sandwiched between two layers of a wider (narrower) bandgap material, they form a double heterojunction. If the intermediate layer is sufficiently thin for quantum properties to be exhibited, then the alignment is called a single quantum well (barrier). A typical quantum well structure may be composed of a semiconductor thin film, embedded between two semi-infinite semiconductor materials, say $GaAs/Al_xGa_{1-x}As$, where x denotes the mole fraction. As the mole fraction varies along the z -axis, so does the effective mass of the charge carrier (electron or hole). To have a complete understanding of such a quantum system, quantum mechanics requires knowledge of both bound and scattering states.

Various attempts have been made over the years to study the scattering states in such position-dependent effective mass systems [9–16]. In two of the recent works [17, 18], the authors stud-

ied the effect of hard wall confinement and lateral dimensions on low temperature transport properties of long diffuse channels in $InSb/In_{1-x}Al_xSb$ heterostructures [17], and resonant inelastic x-ray scattering in $LaAlO_3/SrTiO_3$ heterostructures [18]. In another work, ballistic carrier emission was studied with $GaAs/Al_xGa_{1-x}As$ as a model system [19]. In one of the relatively earlier works, the authors considered the simple model of a square potential well, with the effective mass varying with position inside the well [13]. However, as the additional term introduced by the changing mass is small compared with the original potential V_0 and does not change the shape of the potential significantly, this term was neglected while finding the solutions.

In the present work our aim is to obtain the exact analytical solutions for the scattering states of a particle inside a single quantum well/barrier. It may be mentioned that exact analytical solutions play an important role in conceptual understanding of physics. They provide a valuable platform for checking and improving approximate models and numerical results. Herein lies the motivation for obtaining exact analytical solutions of wave equations with pdem, especially because of the wide range of applications of these solutions in various areas of material science and condensed matter [20]. In the double heterojunction considered here, we assume the intermediate layer to be a potential well / barrier of the form

$$V = \begin{cases} V(z) & , \quad a_1 < z < a_2 \\ V_{01} = V(a_1) & , \quad -\infty < z < a_1 \\ V_{02} = V(a_2) & , \quad a_2 < z < \infty \end{cases} \quad (1)$$

where a_1 and a_2 represent the heterojunctions. The mass of the charge carrier is assumed to be spatially varying inside the potential well / barrier

$a_1 < z < a_2$, but constant outside, viz,

$$m = \begin{cases} m(z) & , \quad a_1 < z < a_2 \\ m_1 = m(a_1) & , \quad -\infty < z < a_1 \\ m_2 = m(a_2) & , \quad a_2 < z < \infty \end{cases} \quad (2)$$

Thus both the potential $V(z)$ and mass $m(z)$ are real functions of the configuration space coordinates, and are taken to be continuous throughout the semiconductor device. The work done in refs. [15, 20] deserve special mention here. In ref. [15] approximate analytical solutions were derived for any arbitrary potential and arbitrary mass function, whereas in ref. [20], some special forms of the mass function were considered for oscillator, Coulomb and Morse potentials to produce exact analytical results. However, our study differs significantly from both these works — the mass functions considered in our case, as well as the approach used, are different from refs. [15] and [20]; the present article not only gives exact analytic results but also plots the transmission and reflection coefficients. More importantly, unlike [15, 20], this work deals with a double heterojunction.

The article is organized as follows : For the sake of completeness, the position-dependent-mass Schrödinger equation is introduced in Section II, and the method of obtaining the solutions is discussed. A couple of explicit models are studied in Section III. To give a better insight into the physical nature of the problem, the potential and mass functions are plotted as a function of z (in Fig. 1 and Fig. 3) along with the scattering solutions (in Fig. 2 and Fig. 4). The transmission and reflection coefficients are also calculated and the same are plotted as a function of the energy of the particle, in Fig. 5 and Fig. 6 respectively. Section IV is kept for Conclusions and Discussions.

II. THEORY

We start with the basic one dimensional time independent Schrödinger equation associated with a particle endowed with pdem in the intermediate region within the heterojunctions :

$$H_{EM}(z)\psi(z) \equiv [T_{EM}(z) + V(z)]\psi(z) = E\psi(z) \quad (3)$$

where the kinetic energy term T_{EM} is given by [4, 6]

$$\begin{aligned} T_{EM} &= \frac{1}{4} (m^\alpha p m^\beta p m^\gamma + m^\gamma p m^\beta p m^\alpha) \\ &= \frac{1}{2} p \left(\frac{1}{m} \right) p \end{aligned} \quad (4)$$

with $p = -i\hbar \frac{d}{dz}$ being the momentum operator, and the ambiguity parameters α , β , γ obeying the von Roos constraint [4]

$$\alpha + \beta + \gamma = -1 \quad (5)$$

There is neither a unique nor a universal choice for the ambiguity parameters, and several suggestions exist in literature — e.g. $\alpha = \gamma = 0$, $\beta = -1$ [21], $\alpha = \gamma = -1/2$, $\beta = 0$ [22], $\alpha = \gamma = -1/4$, $\beta = -1/2$ [23], $\beta = \gamma = -1/2$, $\alpha = 0$ [24], etc. However, for continuity conditions at the abrupt interfaces, one should consider $\alpha = \gamma$, or else one gets the unphysical result of the wave function vanishing at the heterojunctions; additionally the ground state energy also diverges [25, 26]. We shall restrict ourselves to the BenDaniel-Duke choice for the ambiguity parameters, viz., $\alpha = \gamma = 0$, $\beta = -1$. Incidentally, this particular choice consistently produces the best fit to experimental results [27]. Furthermore, we shall work in units $\hbar = c = 1$, and use prime to denote differentiation w.r.t. z . Thus, inside the potential well/barrier $a_1 < z < a_2$, the Hamiltonian for the particle with pdem reduces to [28]

$$H = -\frac{1}{2m(z)} \frac{d^2}{dz^2} - \left(\frac{1}{2m(z)} \right)' \frac{d}{dz} + V(z) \quad (6)$$

whereas, outside the well/barrier, $z < a_1$ and $z > a_2$, the particle obeys the conventional Schrödinger equation :

$$\left\{ -\frac{1}{2m_{1,2}} \frac{d^2}{dz^2} + V_{01,02} \right\} \psi(z) = E\psi(z) \quad (7)$$

having plane wave solutions. In case we consider a wave incident from left, the solutions in the two regions are

$$\psi_L(z) = e^{ik_1 z} + R e^{-ik_1 z}, \quad -\infty < z < a_1 \quad (8)$$

$$\psi_R(z) = T e^{ik_2 z}, \quad a_2 < z < \infty$$

where R and T denote the reflection and transmission amplitudes, and

$$k_{1,2} = \sqrt{2m_{1,2}(E - V_{01,02})} \quad (9)$$

To find the solution in the region $a_1 < z < a_2$, we make use of the following transformations [29]

$$\psi_{in} = \{2m(z)\}^{1/4} \phi, \quad \rho = \int \sqrt{2m(z)} dz \quad (10)$$

which reduce the Schrödinger equation for position-dependent mass, to one for constant mass, viz.,

$$-\frac{d^2 \phi}{d\rho^2} + \left\{ \tilde{V}(\rho) - E \right\} \phi = 0 \quad (11)$$

with

$$\tilde{V}(\rho) = V(z) + \frac{7}{32} \frac{m'{}^2}{m^3} - \frac{m''}{8m^2} \quad (12)$$

We are interested in studying the scattering states of a particle in a double heterojunction, formed by dissimilar materials, where the mass of the particle varies with position inside the well / barrier. Such heterojunctions can be described by a material potential which derives from the difference in bandgaps [6]. Crystal potential of multiple heterojunction can also be described in this manner. For this purpose, we look for some definite practical forms of $V(z)$ and $m(z)$ which will give exact analytical solutions of (11). We illustrate this with the help of a couple of explicit models in the next section.

III. EXPLICIT MODELS

A. Case 1 : Potential well with position dependent mass

The one dimensional finite square well is one of the simplest confinement potentials. In the first example, we consider the region between the abrupt heterojunctions ($-a_0 < z < a_0$) to be a symmetric potential well (more realistic than the square well) with the following ansatz (μ being some constant)

$$V(z) = \begin{cases} -\frac{\mu^2}{1+z^2}, & -a_0 < z < a_0, \\ -\frac{\mu^2}{1+a_0^2} = V_0, & -\infty < z < -a_0, a_0 < z < \infty \end{cases} \quad (13)$$

This particular model resembles the profile of a diffused quantum well, with the advantage of exact analytical solutions. In case the real situation is slightly different from this model, one can apply approximation methods like perturbation theory, etc., to obtain the solutions.

Let the mass of the particle be

$$m(z) = \begin{cases} \frac{\beta^2}{2(1+z^2)}, & -a_0 < z < a_0, \\ \frac{\beta^2}{2(1+a_0^2)} = m_0, & -\infty < z < -a_0, a_0 < z < \infty \end{cases} \quad (14)$$

where β is some constant parameter. For the spatial mass dependence given by eq. (14), eq. (10) transforms the coordinate z to

$$\rho = \beta \sinh^{-1} z \quad (15)$$

so that after some straightforward algebra $\tilde{V}(\rho)$ in eq. (12) reduces to

$$\tilde{V}(\rho) = \frac{1}{4\beta^2} - \left(\mu^2 - \frac{1}{4\beta^2} \right) \text{sech}^2 \frac{\rho}{\beta} \quad (16)$$

Thus equation (11) can be written as

$$\frac{d^2\phi}{d\rho^2} + \left\{ \kappa^2 + \lambda(\lambda-1) \text{sech}^2 \frac{\rho}{\beta} \right\} \phi = 0 \quad (17)$$

$$\text{where } \kappa^2 = E - \frac{1}{4\beta^2} \quad (18)$$

and the parameter λ depends on the constants μ and β , through the equation

$$\lambda(\lambda-1) = \mu^2 - \frac{1}{4\beta^2} \quad (19)$$

For existence of bound states $\lambda > 1$; hence, $|\mu| > \frac{1}{2\beta}$. This gives the permissible values of λ as

$$\lambda = \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4\mu^2 - \frac{1}{\beta^2}} \quad (20)$$

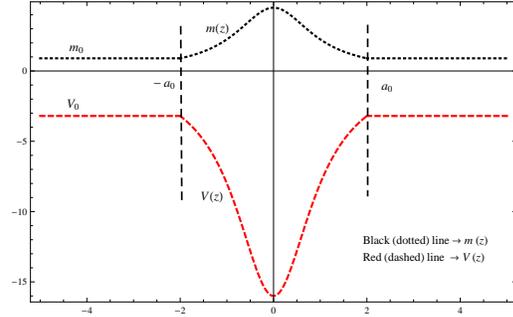


FIG. 1: Colour online : Plot showing $m(z)$ and $V(z)$ w.r.t. z

For a better understanding of the mass dependence and the potential in the semiconductor device, we plot $m(z)$ and $V(z)$ as a function of z in Fig. 1, for a suitable set of parameter values, viz., $\beta = 4$, $\mu = 3$, $a_0 = 2$.

Let us introduce a new variable

$$y = \cosh^2 \frac{\rho}{\beta} \quad (21)$$

and write the solutions of (17) as

$$\phi = y^{\frac{\lambda}{2}} u(y) \quad (22)$$

In terms of the new variable y , equation (17) reduces to the hypergeometric equation

$$y(1-y) \frac{d^2u}{dy^2} + \left\{ \left(\lambda + \frac{1}{2} \right) - (\lambda+1)y \right\} \frac{du}{dy} - \frac{1}{4} \{ \lambda^2 + \kappa^2 \beta^2 \} u = 0 \quad (23)$$

with complete solution [30]

$$u = P {}_2F_1\left(a, b, \frac{1}{2}; 1-y\right) + Q(1-y)^{1/2} {}_2F_1\left(a + \frac{1}{2}, b + \frac{1}{2}, \frac{3}{2}; 1-y\right) \quad (24)$$

where P and Q are constants, and the parameters a and b are as defined below :

$$a = \frac{1}{2}(\lambda + i\kappa\beta) \quad , \quad b = \frac{1}{2}(\lambda - i\kappa\beta) \quad (25)$$

Thus for the even solution $Q = 0$, whereas for the odd solution $P = 0$. After some straightforward algebra, the final solution to the position-dependent mass Schrödinger equation (3), within the potential well $-a_0 < z < a_0$, is obtained as

$$\psi_{in}(z) = \left(\frac{\beta^2}{2(1+z^2)}\right)^{1/4} (1+z^2)^{\lambda/2} \left\{ P {}_2F_1\left(a, b, \frac{1}{2}; -z^2\right) + iQz {}_2F_1\left(a + \frac{1}{2}, b + \frac{1}{2}, \frac{3}{2}; -z^2\right) \right\} \quad (26)$$

whereas outside the well ($z < -a_0$, $z > a_0$), the solutions are given by eq (8), with $k_1 = k_2$.

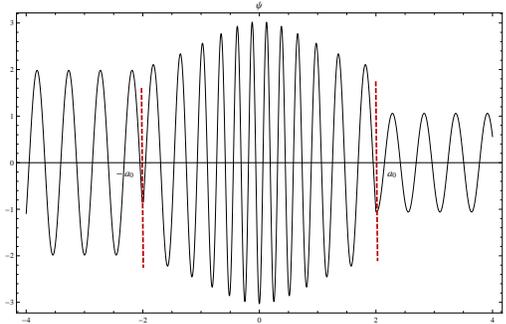


FIG. 2: Colour online : A plot of $\text{Re } \psi(z)$ vs z ; Dashed (red) lines show the abrupt heterojunctions

For scattering states, κ^2 should be positive, implying $E > \frac{1}{4\beta^2}$. Now, because of the spatial dependence of the mass function, the boundary conditions need to be modified —

the functions $\psi(z)$ and $\frac{1}{m(z)} \frac{d\psi(z)}{dz}$ should be continuous at each heterojunction $\pm a_0$ [21, 31]. These conditions enable us to evaluate the reflection and transmission amplitudes R and T respectively.

The complete solutions for the scattering states in the entire region $-\infty < z < \infty$ are plotted in Fig. 2, for the same set of parameter values as in Fig.

1, viz., $\beta = 4$, $\mu = 3$, $a_0 = 2$, $E = 40$. The solutions show a definite nonlinear character inside the well ($-a_0 < z < a_0$), where the particle mass m is a function of its position z . Thus the effect of the position-dependent mass potential well (in this particular model) is to introduce a non linear component in the otherwise plane wave solutions.

B. Case 2 : Potential barrier with position dependent mass

As the second example, we consider the region within the double heterojunction ($a_1 < z < a_2$) to be represented by an *inverted* Morse potential (barrier) [32–34] :

$$V(z) = \begin{cases} V_0 e^{\alpha z} (2 - e^{\alpha z}) & , \quad a_1 < z < a_2 \\ V_0 e^{\alpha a_1} (2 - e^{\alpha a_1}) = V_{01} & , \quad -\infty < z < a_1 \\ V_0 e^{\alpha a_2} (2 - e^{\alpha a_2}) = V_{02} & , \quad a_2 < z < \infty \end{cases} \quad (27)$$

with positive V_0 . The transmission coefficient of a potential barrier has wide applications in nuclear fission, heavy-ion fusion, tunnelling in solids [34], etc; hence we shall calculate both the transmission as well as reflection coefficients and plot them as a function of the energy of the particle. The Morse barrier potential is particularly useful in investigating the anharmonicities of the vibrational spectra in molecular and nuclear physics [33]. For the mass function of the particle, we consider

$$m(z) = \begin{cases} m_0 \alpha^2 e^{-2\alpha z} & , \quad a_1 < z < a_2 \\ m_0 \alpha^2 e^{-2\alpha a_1} = m_{01} & , \quad -\infty < z < a_1 \\ m_0 \alpha^2 e^{-2\alpha a_2} = m_{02} & , \quad a_2 < z < \infty \end{cases} \quad (28)$$

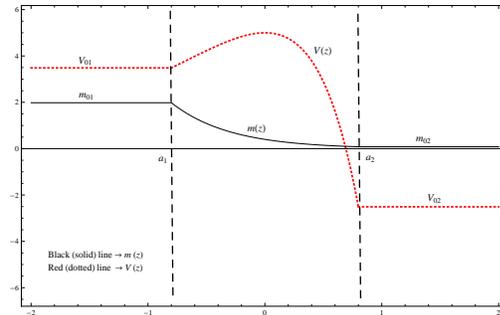


FIG. 3: Colour online : Plot showing $m(z)$ and $V(z)$ w.r.t. z ; The dashed lines show the abrupt heterojunctions

In Fig. 3, we show the plot of $m(z)$ and $V(z)$ for this particular model, for a suitable set of parameter values, viz., $m_0 = 0.4$, $V_0 = 5$, $E = 33$, with the heterojunctions at $a_1 = -0.8$, $a_2 = 0.8$.

For the spatial mass dependence given by eq. (28), eq. (10) transforms the coordinate z to

$$\rho = -\sqrt{2m_0}e^{-\alpha z} \quad (29)$$

so that after some straightforward algebra $\tilde{V}(\rho)$ in eq. (12) reduces to the simple form

$$\tilde{V}_\rho = -\frac{2V_0\sqrt{2m_0}}{\rho} - \frac{2m_0V_0 - 3/4}{\rho^2} \quad (30)$$

Thus the Schrödinger equation for constant mass (11) takes the final form

$$\frac{d^2\phi}{d\rho^2} + \left\{ \kappa^2 + \frac{2m_0V_0 - 3/4}{\rho^2} + \frac{2V_0\sqrt{2m_0}}{\rho} \right\} \phi = 0 \quad (31)$$

with $\kappa^2 = E$. To solve equation (31) given above, let us introduce a new variable

$$y = -2i\kappa\rho = i\kappa 2\sqrt{2m_0}e^{-\alpha z} \quad (32)$$

in terms of which equation (31) gets simplified to the form of a Whittaker differential equation [35]

$$\frac{d^2\phi}{dy^2} + \left\{ -\frac{1}{4} + \frac{\lambda_1^2 + 1/4}{y^2} + \frac{i\lambda_2}{y} \right\} \phi = 0 \quad (33)$$

with

$$\lambda_1^2 = 2m_0V_0 - 1 \quad , \quad \lambda_2 = \frac{V_0\sqrt{2m_0}}{\kappa} \quad (34)$$

The solutions of eq (33) are given as [35]

$$\phi = e^{\pm y/2} y^{\pm i\lambda_1} M(a^\pm, b^\pm; y) \quad (35)$$

where $M(a^\pm, b^\pm; y)$ are the Whittaker functions and

$$a^\pm = \frac{1}{2} \pm i\lambda_1 - i\lambda_2 \quad , \quad b^\pm = 1 \pm 2i\lambda_1 \quad (36)$$

Thus for the entire semiconductor device, the complete solution for the scattering states in the different regions are given by

$$\begin{aligned} \psi_L &= e^{ik_1z} + R e^{-ik_1z} \quad , \quad -\infty < z < a_1 \\ \psi_{in} &= (2m_0)^{1/4} \sqrt{\alpha} e^{-\frac{\alpha z}{2}} \left\{ P_1 e^{\frac{y}{2}} y^{i\lambda_1} M(a^+, b^+; y) \right. \\ &\quad \left. + P_2 e^{-\frac{y}{2}} y^{-i\lambda_1} M(a^-, b^-; y) \right\} \quad , \quad a_1 < z < a_2 \\ \psi_R &= T e^{ik_2z} \quad , \quad a_2 < z < \infty \end{aligned} \quad (37)$$

where the constants P_1, P_2 and the reflection and transmission amplitudes R and T respectively, are determined by matching the boundary conditions (for pdem systems) at the heterojunctions, and y and ρ are as defined above.

The complete solutions for the entire region $-\infty < z < \infty$ are plotted in Fig. 4, for a suitable set of parameter values, viz., $m_0 = 0.4$, $V_0 = 5$, $E = 33$, $a_1 = -1.5$, $a_2 = 1.5$. The solutions show a definite nonlinear character inside the barrier ($a_1 < z < a_2$), where the particle mass is dependent on its position. Thus the effect of the position-dependent mass barrier (similar to that of the position dependent potential well in the previous example) is to introduce a non linear component in the plane wave solutions.

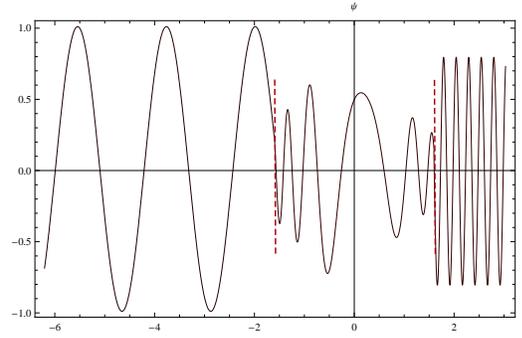


FIG. 4: Colour online : A plot of $\text{Re } \psi(z)$ vs z ; Dashed (red) lines show the abrupt heterojunctions

IV. CONCLUSIONS AND DISCUSSIONS

To conclude, we obtained the exact analytical solutions for the scattering states of a particle (electron or hole) inside a semiconductor device with a double heterojunction, when the mass of the particle is assumed to be dependent on its position inside the heterojunctions, but constant outside. We studied two explicit models in this work — one a pdem diffused potential well, the other a pdem potential barrier (Morse barrier). In each case it is observed that the effect of the spatial dependence on the particle mass is to introduce a non linear component in the otherwise plane wave solutions.

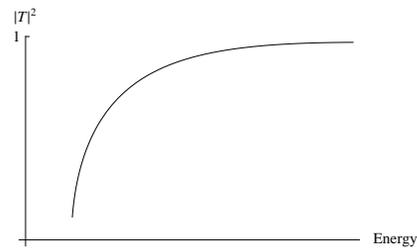


FIG. 5: Plot of $|T|^2$ vs E

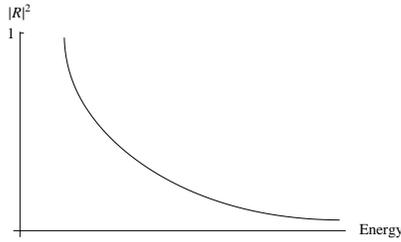


FIG. 6: Plot of $|R|^2$ vs E

We also calculated the transmission and reflection coefficients, $|T|^2$ and $|R|^2$ respectively, for the potentials studied here. These are plotted in Fig. 5 and Fig. 6 respectively, as a function of the energy E for the pdem particle in a Morse barrier. As the energy increases, the transmission coefficient also increases, finally reaching unity, whereas the reflection coefficient follows the reverse trend and goes to zero. This observation is similar to that in ref. [36], where the authors show that the transmission coefficient for the one-dimensional scattering problem with pdem normally tends to unity as energy goes to infinity, provided the mass is a continuous function of position.

This simple, yet straightforward approach is just a way of understanding basic physics of the electronic properties of a semiconductor device,

comprising of a double heterojunction, where the intermediate layer is sufficiently thin for quantum properties to be exhibited. It is expected that the observations made in this work will provide some useful insight in studies related to electron transport in semiconductor heterostructures, i.e. in the physical properties of such materials. Actual materials are made up of a large number of atomic potentials. Nevertheless, the crystal potential may be approximated by a single potential — the global average of the individual potentials, and this approach would still be valid. However, for extremely thin intermediate layer, the individual potentials may become significant enough for this approximation to break down. This calls for a more rigorous approach, and we propose to take up its study in the near future.

V. ACKNOWLEDGEMENT

The author thanks P. Roy for some very fruitful discussions. Financial assistance for the work was provided for by the Dept. of Science and Technology, Govt. of India, through its grant SR/WOS-A/PS-06/2008. Thanks are also due to the unknown referee for some useful comments.

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