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NUMERICAL COMPUTATION OF THE PSEUDO-GAUSSIAN QUANTUM WELL LEVELS

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Abstract
The potential in a pseudo-Gaussian quantum well behaves asymptotically as Gaussian, but approaches harmonic oscillator (HO) potential near to the origin. A whole family of such potentials can be defined. The quantum problem of finding discrete levels into the pseudo-Gaussian well cannot be solved analytically. First, the generating functional is constructed using symbolic computations. Then, numerical values for the model parameters are allocated and numerical procedures follow to calculate matrix elements of the Hamiltonian operator in the energy basis of HO. Solving these models can be useful for designing new quantum electronic devices.
Keywords: Pseudo-Gaussian well; Generating functional method; Discrete levels in quantum heterostructures

1. Introduction

Advances in technology allowing for deposing ultra thin layers have opened a domain for semiconductor devices where charge carriers exhibit quantum behavior and discrete energy levels. We use a new class of potentials with a Gaussian asymptotic behavior [1] but approaching to the potential of the harmonic oscillator when $x \to 0$. It is shown [2] that, in the energy basis of the harmonic oscillator, the matrix elements of the Hamiltonian operators of these new models can be derived from generating functionals.

The progress in algebraic and numerical computation offers new possibilities of analyzing new classical or quantum systems that cannot be analytically solved. We aim to define a large family of models whose potentials have a Gaussian asymptotic behavior but behave like the HO potential near $x \square 0$.

2. Method and Calculations

The one-dimensional HO of mass m and frequency ω has the well-known Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2 x^2}{2} + V_0 \qquad (1)$$

where V_0 is an arbitrary ground energy. The energy is measured in units of $\varepsilon = \hbar\omega$ so that we can write

$$H_0 = \frac{\varepsilon}{2} N_0, \quad N_0 = -\frac{d^2}{d\xi^2} + \xi^2 + \lambda, \tag{2}$$

using the dimensionless coordinate $\xi = x / a$ measured in units of $a = \hbar / \sqrt{m\varepsilon}$, and denoting $\lambda = 2V_0 / \varepsilon$. The number operator N_0 has the eigenvalues $2n + \lambda + 1$ where $n = 0, 1, 2...$ is the quantum number of the discrete energy levels $E_n = \varepsilon[n + \frac{1}{2}(\lambda + 1)]$.

We propose a Gaussian generalization of HO, defining pseudo-Gaussian models (PGM) with new number operators

$$N = -\frac{d^2}{d\xi^2} + W(\xi), \tag{3}$$

in which we use dimensionless potentials

$$W(\xi) = \left(\lambda + \sum_{k=1}^{r} C_k \xi^{2k} \right) \exp(-\mu\xi^2). \tag{4}$$

In this way we constructed a family of models, denoted from now by $(\lambda, \mu)^r$, depending on dimensionless parameters, $\lambda \in R$ and $\mu > 0$, and the integer number $r = 1, 2, ...$ which is called the *order* of PGM. The genuine Gaussian potential is of the order $r = 0$. For $\lambda \geq 0$ the potentials (4) are positively defined representing pseudo-Gaussian barriers but when $\lambda < 0$ we have pseudo-Gaussian wells of different profiles (Fig. 1).

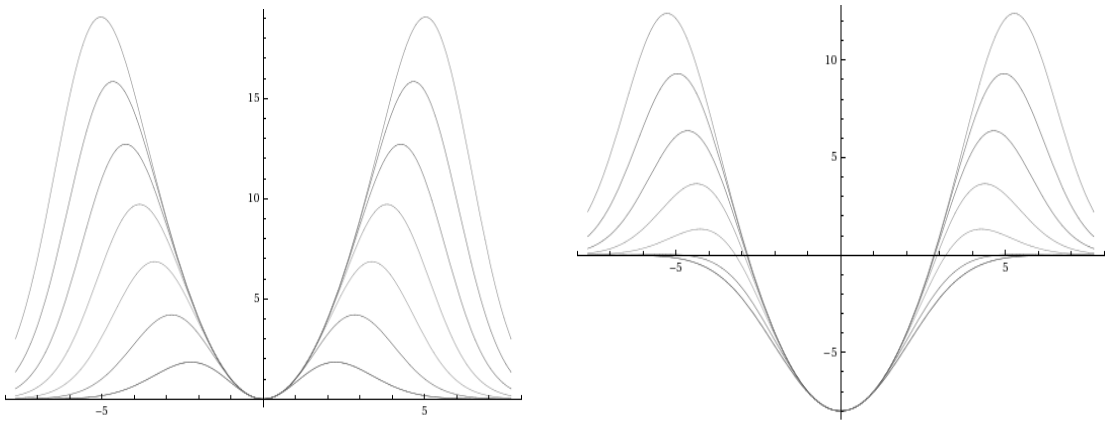

Figure 1. Pseudo-Gaussian barriers ($\lambda = 0$, $\mu = 0.2$) and wells ($\lambda = -8$, $\mu = 0.2$) for r = 1,2,3,4,5,6 7.

The matrix elements of an operator X can be derived from the corresponding generating functional,

$$Z_{\sigma,\tau}[X] = \int d\xi F_\sigma(\xi)[XF_\tau](\xi), \tag{5}$$

according to the rule

$$\langle m \mid X \mid n \rangle = \frac{1}{\sqrt{m!n!2^{m+n}}} \partial_\sigma{}^m \partial_\tau{}^n Z_{\sigma,\tau}[X] \Big|_{\sigma=\tau=0}. \tag{6}$$

In the simplest case of HO we obtain the functional

$$Z_{\sigma,\tau}[N_0] = (1 + \lambda + 4\sigma\tau)\exp(2\sigma\tau) \tag{7}$$

giving rise to the diagonal matrix elements $\langle m \mid N_0 \mid n \rangle = (2n + \lambda + 1)\delta_{nm}$.

The generating functional of an arbitrary model $(\lambda, \mu)^r$,

$$Z_{\sigma,\tau}[N] = Z_{\sigma,\tau}\left[-\tfrac{d^2}{d\xi^2}\right] + Z_{\sigma,\tau}\left[W(\xi)\right], \tag{8}$$

can be also calculated in terms of Gaussian integrals. We obtain the final result (for more details see [2]):

$$Z_{\sigma,\tau}[N] = \tilde{Z}_{\sigma,\tau}[N]\exp(2\sigma\tau). \tag{9}$$

where

$$\tilde{Z}_{\sigma,\tau}[N] = \frac{1}{2} - (\sigma - \tau)^2$$

$$+\left[\lambda + \sum_{k=1}^{r} (-1)^k C_k \partial_\mu^k\right]\left\{\frac{1}{\sqrt{\mu+1}}\exp\left[-\frac{\mu}{\mu+1}(\sigma+\tau)^2\right]\right\}.$$

3. Results

The *Mathematica* code written for calculating energy levels has two distinct parts. First, the potential (Eq. 4) and the generating functional (Eq. 9) is analytically calculated, then it follows a numeric evaluation in which matrix element computation (Eq. 6) and diagonalization for obtaining energy eigenvalues (levels) is numerically performed.

In Figure 2 we depict our results in form of energy levels: bound states for negative energies, resonances for positive, for $\lambda = 8$, $\mu = 0.2$, r = 4. We used a matrix [m,n] up to 30x30, for larger ones the computations are becoming prohibitive (because of the higher order derivatives).

For positive energy levels, a subsequent computation (to be published) using the transfer matrix method applied to the barriers [3] using the potential as in Figure 2b, proved that the resonances are genuine and they are not an artifact of the method.

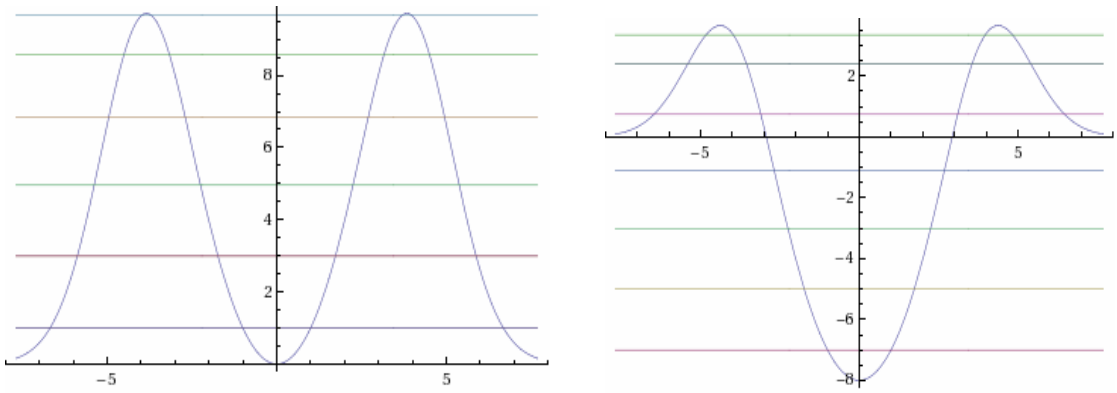

Figure 2. Calculated energy levels in Pseudo-Gaussian barriers ($\lambda = 0$, $\mu = 0.2$) and wells ($\lambda = -8$, $\mu = 0.2$) for r = 4.

4. Conclusions

We calculated energy levels and resonances for PGO potential and obtained the same results using two very different methods. Energy level computations for a given potential may prove to be an essential new method for designing nanometer electronic devices with new properties.

Acknowledgements

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