Quantum well problem generated by the confined harmonic oscillator potential

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Azerbaijan


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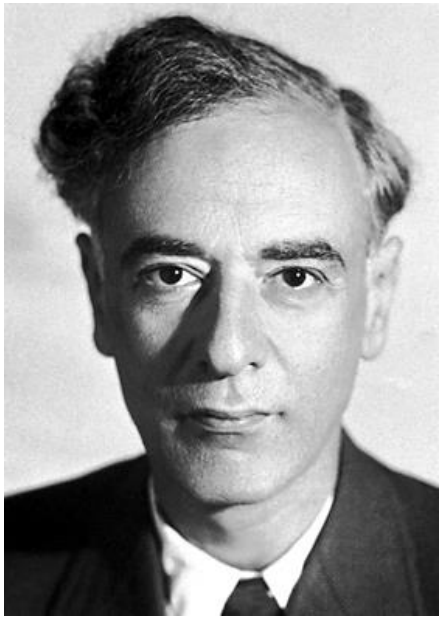
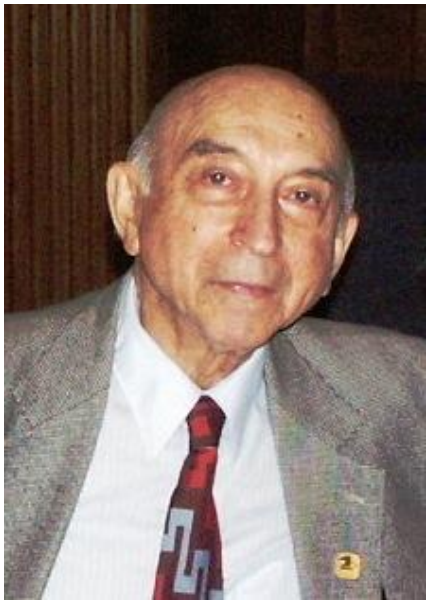
Notable Baku residents

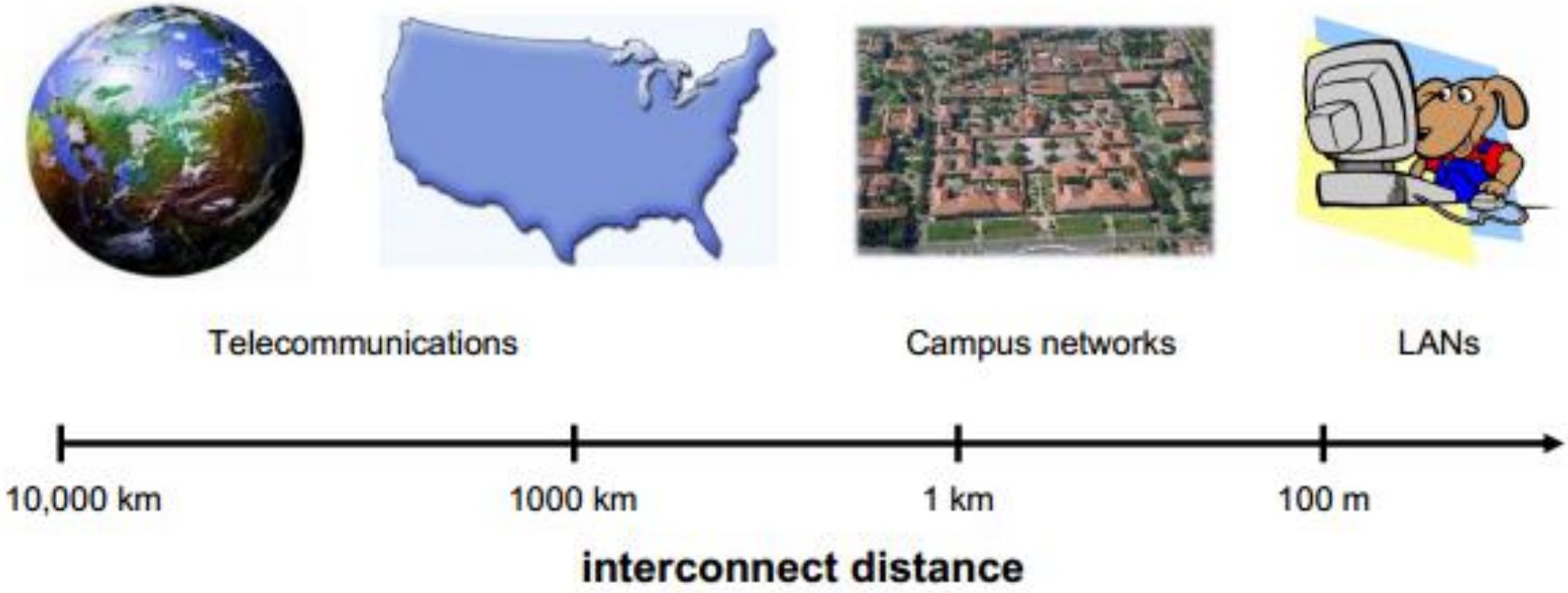


Lev Landau



Lotfi A. Zadeh

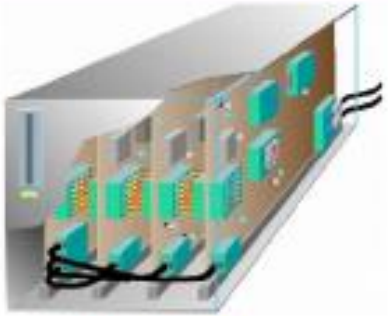
Levels of interconnection



Optics currently dominates for long distance interconnects
Increasingly, optics is used in local area network applications

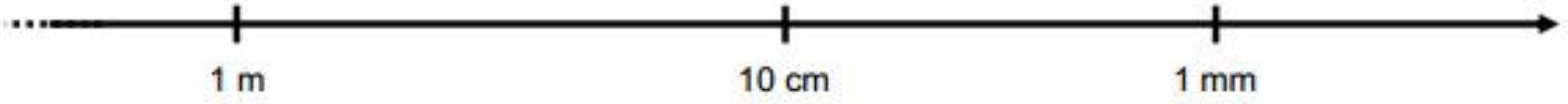
Levels of interconnection

Backplanes & board-to-board



Chip-to-chip

On-chip



interconnect distance

Electrical signaling within computers is encountering severe limitations

Quantum well problem as a base on the superconducting qubit implementation

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Jonathan R. Frie

Department of Phy
Stony Brook, New

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quantum interference device (SQUID) can be put into a superposition of two magnetic-flux states: one corresponding to a few microamperes of current flowing clockwise, the other corresponding to the same amount of current flowing anticlockwise.

The simplest SQUID (the radio frequency (r.f.) SQUID) is a superconducting loop of inductance L broken by a Josephson tunnel junction with capacitance C and critical current I_c. In equilibrium, a dissipationless supercurrent can flow around this loop, driven by the difference between the flux Φ that threads the loops and the external flux Φ_x applied to the loop. The dynamics of the SQUID

VOLUME 84, NUMBER 6 PHYSICAL REVIEW LETTERS 7 FEBRUARY 2000

Observation of Cascaded Two-Photon-Induced Transitions between Fluxoid States of a SQUID

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R. Rouse
Sun Microsystems, Sunnyvale, California 94086

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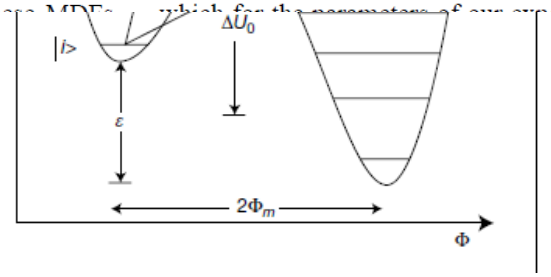
(Received 21 September 1999)

We present evidence for transitions between fluxoid wells of a SQUID due to cascaded, two-photon processes. Such transitions are evidenced by an anomalous dependence on the transition rate from the one-photon resonant level within the initial well, which cannot be explained by previously observed macroscopic resonant tunneling. These two-photon processes may be a significant source of decoherence in SQUID qubits subject to microwave radiation.

PACS numbers: 74.50.+r, 03.65.–w, 85.25.Dq

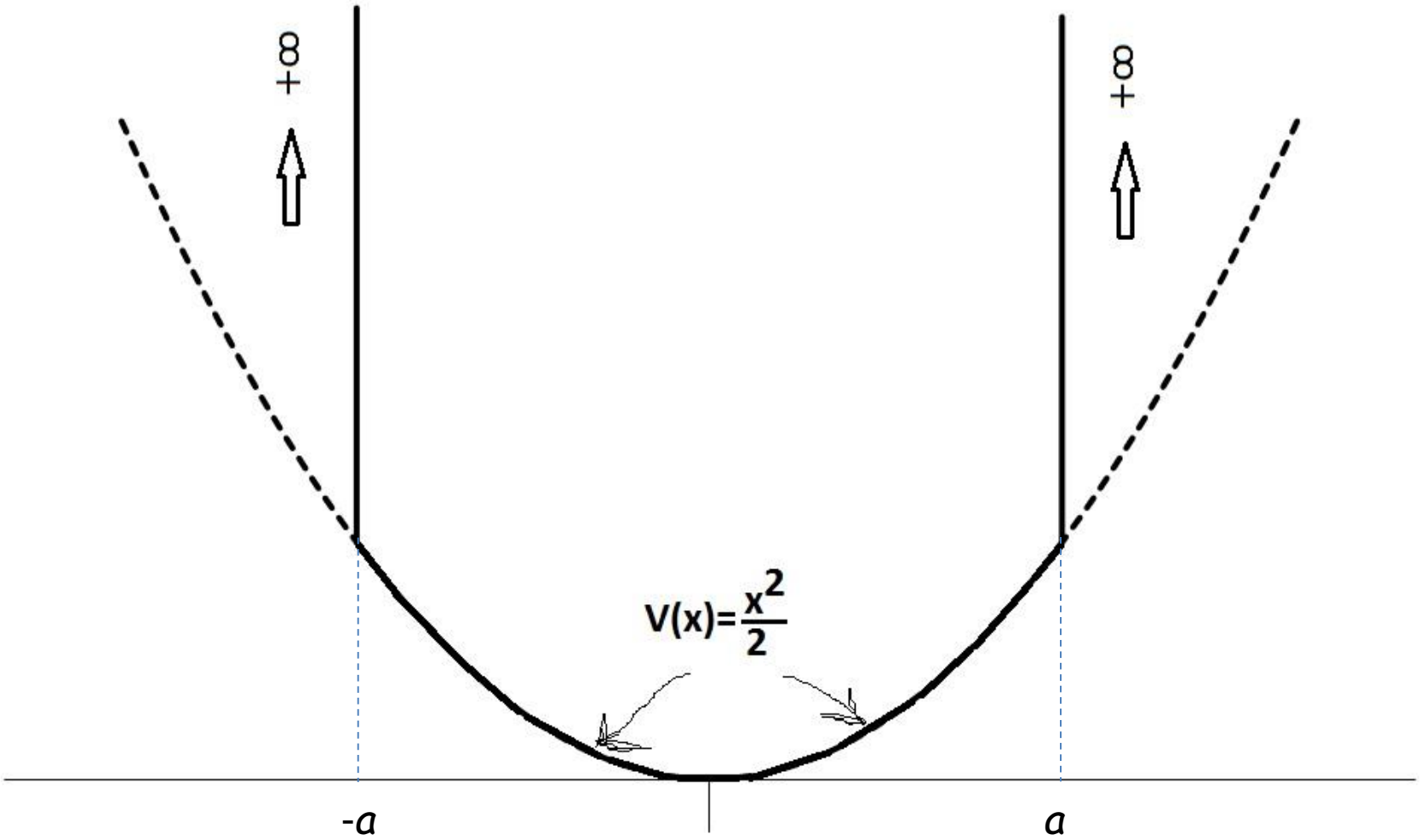
The degree to which macroscopic degrees of freedom (MDFs) obey quantum mechanics is a perennial source of

quantum Φ_0) of $\phi_x \approx \frac{1}{2}$. The two wells of the potential represent the $f = 0$ and 1 fluxoid state of the SQUID,



Theoretical computations

Confined quantum oscillator vs. infinite potential well



1D Schrödinger equation – infinite potential well

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x),$$

we have to solve the following second order differential equation:

$$\frac{d^2\psi}{dx^2}+\kappa^2\psi=0,$$

where, $\kappa=\sqrt{\frac{2mE}{\hbar^2}}>0.$

explicit expressions of the wavefunction $\psi_n(x)$ of the stationary states and the discrete energy spectrum E_n as follows:

$$\psi_n(x)=\frac{1}{\sqrt{a}}\cos\left(\frac{\pi}{2a}nx\right),$$

$$E_n=\frac{\pi^2\hbar^2n^2}{4ma}, \qquad n=1,2,3,\ldots .$$

1D Schrödinger equation – harmonic oscillator within the canonical approach

$$\left[\frac{\hat{p}_x^2}{2m} + V(x)\right]\psi(x) = E\psi(x) \qquad \hat{p}_x = -i\hbar\frac{d}{dx} \qquad V(x) = \frac{m\omega^2 x^2}{2}$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{m\omega^2 x^2}{2}\right)\psi = 0$$

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right), \qquad n = 0, 1, 2, \ldots$$

Confined harmonic oscillator

ENERGY LEVELS OF AN ARTIFICIALLY BOUNDED LINEAR OSCILLATOR.

By F. C. AULUCK, *Dyal Singh College, Lahore.*

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DYNAMICAL FRICTION

II. THE RATE OF ESCAPE OF STARS FROM CLUSTERS AND THE EVIDENCE FOR THE OPERATION OF DYNAMICAL FRICTION

S. CHANDRASEKHAR
Yerkes Observatory
Received January 7, 1943

ABSTRACT

In this paper a general method is described for determining the rate of escape of stars from galactic and globular clusters which is based on certain general statistical principles. Essentially the method consists in reducing the problem to a boundary-value problem in partial differential equations and in making use of the interpretation of the stochastic process in the velocity space as a diffusion process of a rather general type.

The rate of escape has been evaluated, first, ignoring dynamical friction, and, second, making due allowance for it. It appears that the rate of escape of stars predicted on the first basis is too rapid to be compatible with a life for galactic clusters even of the order of 5×10^8 years. However, the rates of escape are drastically reduced when dynamical friction is allowed for and permits a time scale of the order of 3×10^9 years. It is concluded that in the very existence of galactic clusters like the Pleiades we can look for direct evidence for the operation of dynamical friction which was predicted on theoretical grounds in the preceding paper.

1. *Introduction.*—In the preceding paper[1] we have shown that stars must experience dynamical friction during their motion. This conclusion, first reached on the basis of certain very general considerations, was later confirmed by a more direct analysis of the

Hypergeometric function

$$ {}_rF_s\left(\left.\begin{matrix}a_1,\dots,a_r\\ b_1,\dots,b_s\end{matrix}\right| z\right) := \sum_{k=0}^{\infty} \frac{(a_1,\dots,a_r)_k}{(b_1,\dots,b_s)_k}\frac{z^k}{k!}, $$

$$ (a_1,\dots,a_r)_k := (a_1)_k \cdots (a_r)_k. $$

Pochhammer symbol

$$ (a)_k := a(a+1)(a+2)\cdots(a+k-1),\ k = 1,2,3,\dots. $$

$$ (a)_0 := 1 $$

The Polynomial

If $a_i := -n$

Then

$$(-n)_k := -n\cdot(-n+1)(-n+2)\cdots(-n+k-1),\ k=1,2,3,\ldots.$$

With a definition

$$ {}_rF_s\left(\left.\begin{matrix}\overbrace{-n}^{}\\ a_1,\ldots,a_r\\ b_1,\ldots,b_s\end{matrix}\right| z\right) := \sum_{k=0}^{\cancel{n}\ -n} \frac{(a_1,\ldots,a_r)_k}{(b_1,\ldots,b_s)_k}\frac{z^k}{k!}$$

Orthogonal Polynomials: Basic Properties

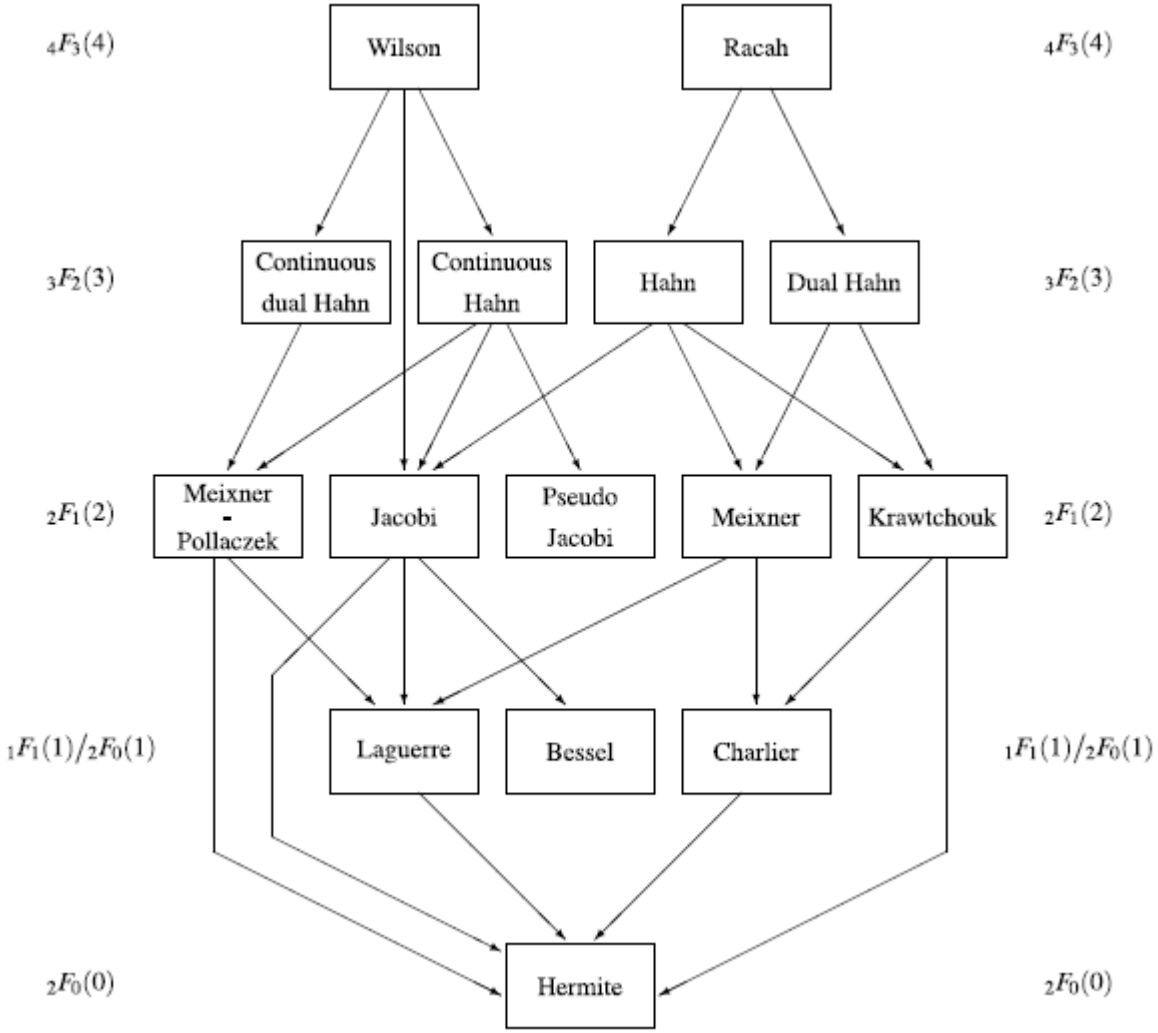
- Definition in terms of the hypergeometric function
- Orthogonality (continuous or discrete, finite or infinite measure)
- How kind of recurrence relations it satisfies
- It is a solution of some equation
- Shift operators for it (Forward & Backward)
- Rodrigues-type formula
- Possible generating functions (including bilinear generating ones)

Askey Scheme of Hypergeometric Orthogonal Polynomials - 1

J. LABELLE, Tableau d'Askey. In: Polynomes Orthogonaux et Applications, (eds. C. Brezinski et al.). Lecture Notes in Mathematics 1171, Springer-Verlag, New York, 1985, xxxvi-xxxvii

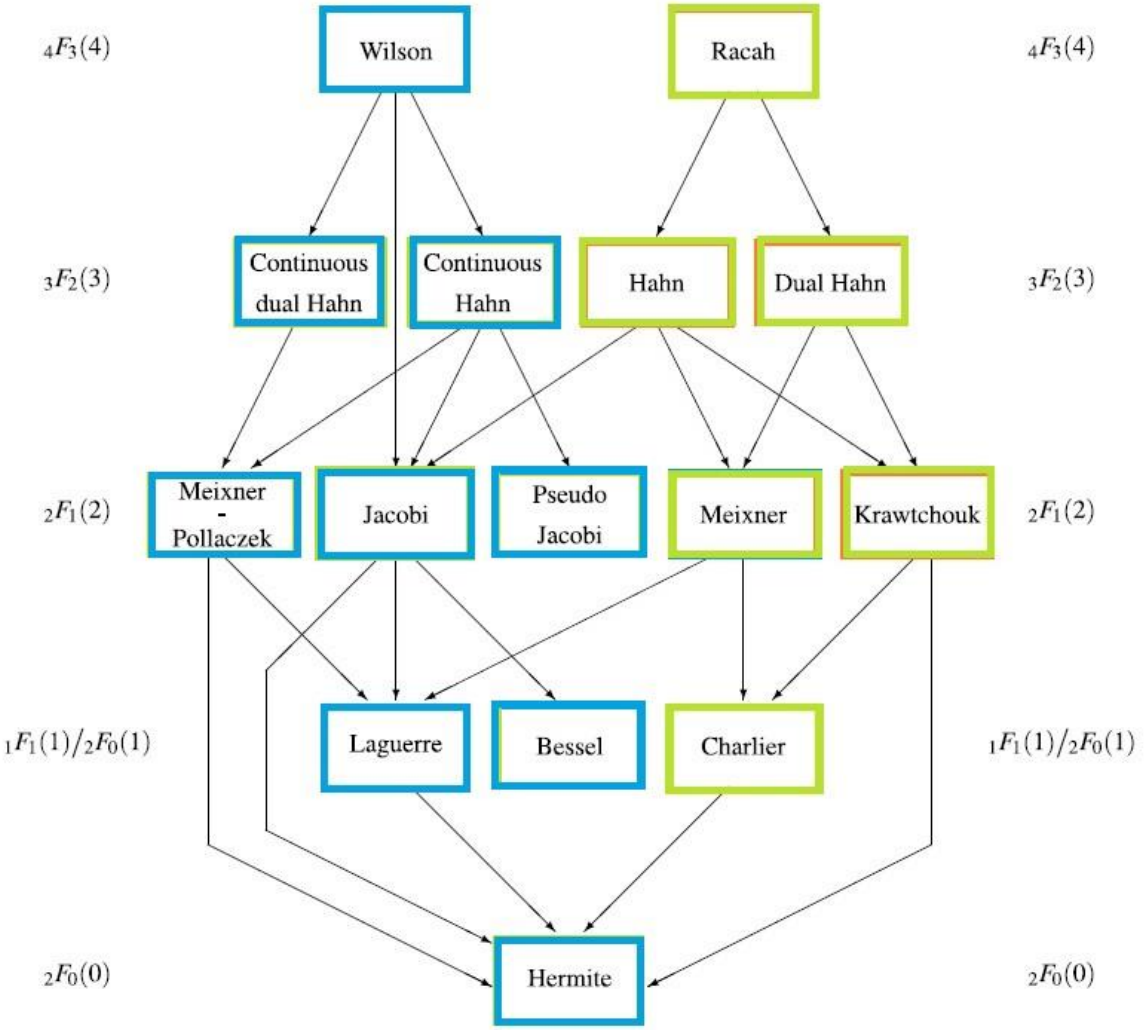
R. ASKEY and J.A. WILSON, Some basic hypergeometric orthogonal polynomials that generalize Jacobi polynomials. Memoirs of the American Mathematical Society 319, Providence, Rhode Island, 1985

Askey Scheme of Hypergeometric Orthogonal Polynomials - 2



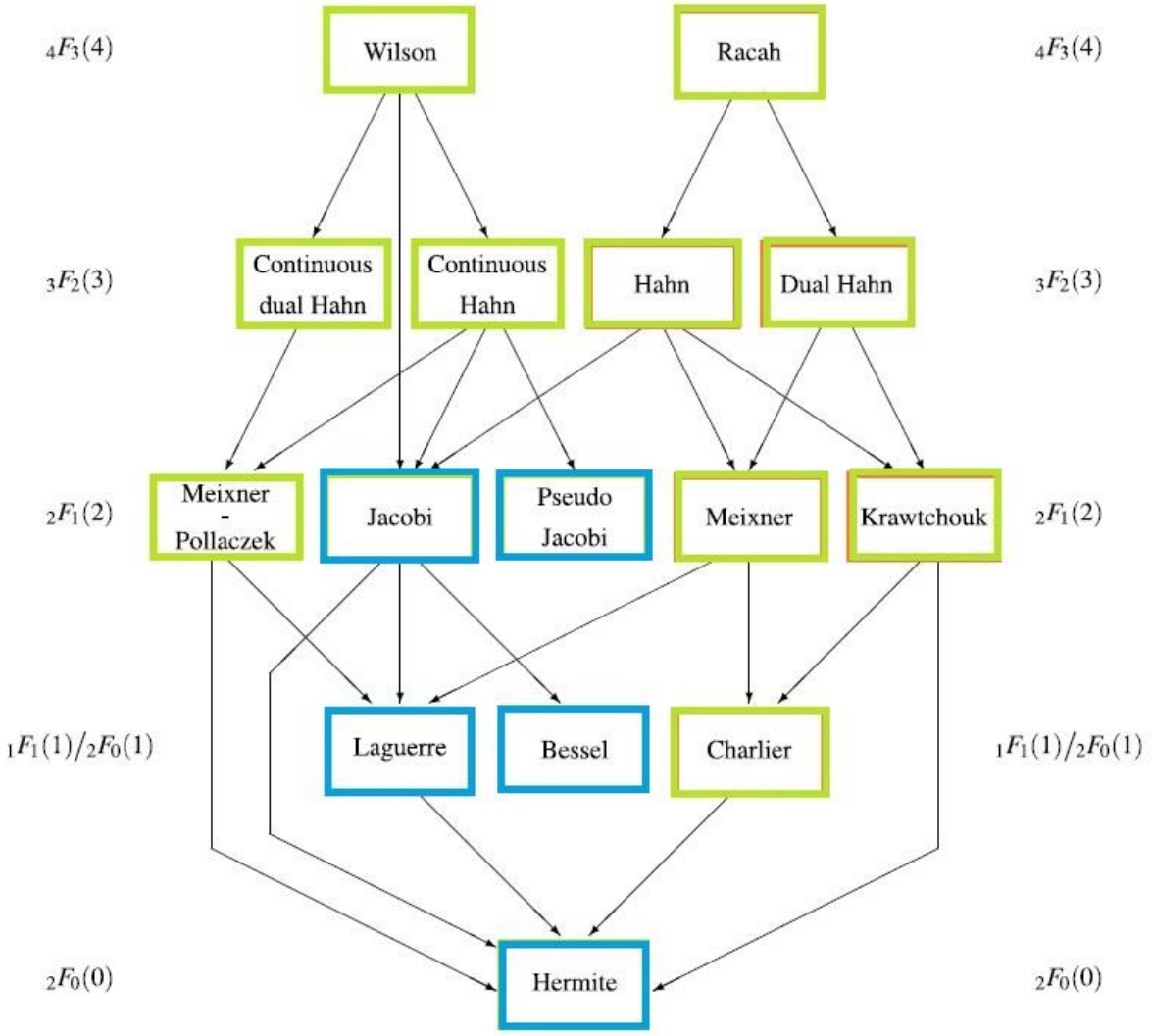
Askey scheme of orthogonal polynomials

continuous or discrete



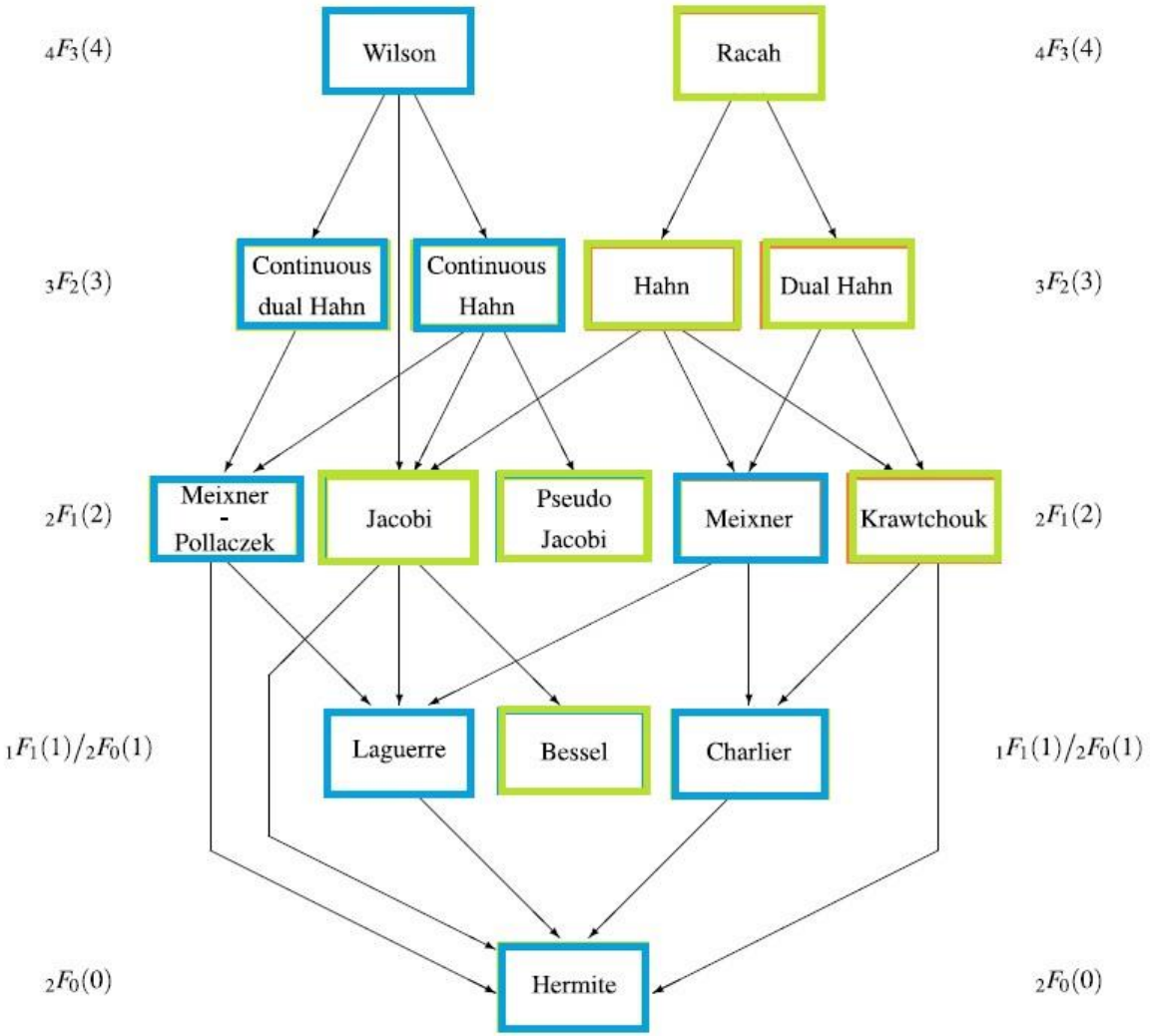
Askey scheme of orthogonal polynomials

explicit solutions of differential or difference equations



Askey scheme of orthogonal polynomials

finite or infinite



Hermite polynomials

$$H_n(x) = (2x)^n \, {}_2F_0\left(\begin{matrix} -n/2, -(n-1)/2 \\ - \end{matrix} ; -\frac{1}{x^2} \right)$$

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} H_m(x) H_n(x) \, dx = 2^n n! \, \delta_{mn}$$

$$y''(x) - 2xy'(x) + 2ny(x) = 0, \quad y(x) = H_n(x)$$

Jacobi polynomials

$$P_n^{(\alpha,\beta)}(x) = \frac{(\alpha+1)_n}{n!}\, {}_2F_1\left(\begin{matrix}-n, n+\alpha+\beta+1 \\ \alpha+1\end{matrix}; \frac{1-x}{2}\right)$$

For $\alpha > -1$ and $\beta > -1$ we have

$$\int_{-1}^{1} (1-x)^\alpha (1+x)^\beta P_m^{(\alpha,\beta)}(x) P_n^{(\alpha,\beta)}(x)\, dx$$
$$= \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)n!} \delta_{mn}$$

$$(1-x^2)y''(x) + [\beta - \alpha - (\alpha+\beta+2)x]\, y'(x)$$
$$+ n(n+\alpha+\beta+1)y(x) = 0, \quad y(x) = P_n^{(\alpha,\beta)}(x)$$

Gegenbauer polynomials

The Gegenbauer (or ultraspherical) polynomials are Jacobi polynomials with $\alpha = \beta = \lambda - \frac{1}{2}$ and another normalization:

$$C_n^{(\lambda)}(x) = \frac{(2\lambda)_n}{(\lambda+\frac{1}{2})_n} P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x)$$

$$= \frac{(2\lambda)_n}{n!}\, {}_2F_1\left(\begin{matrix}-n, n+2\lambda \\ \lambda+\frac{1}{2}\end{matrix}; \frac{1-x}{2}\right), \quad \lambda \neq 0$$

$$\int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} C_m^{(\lambda)}(x) C_n^{(\lambda)}(x)\, dx$$

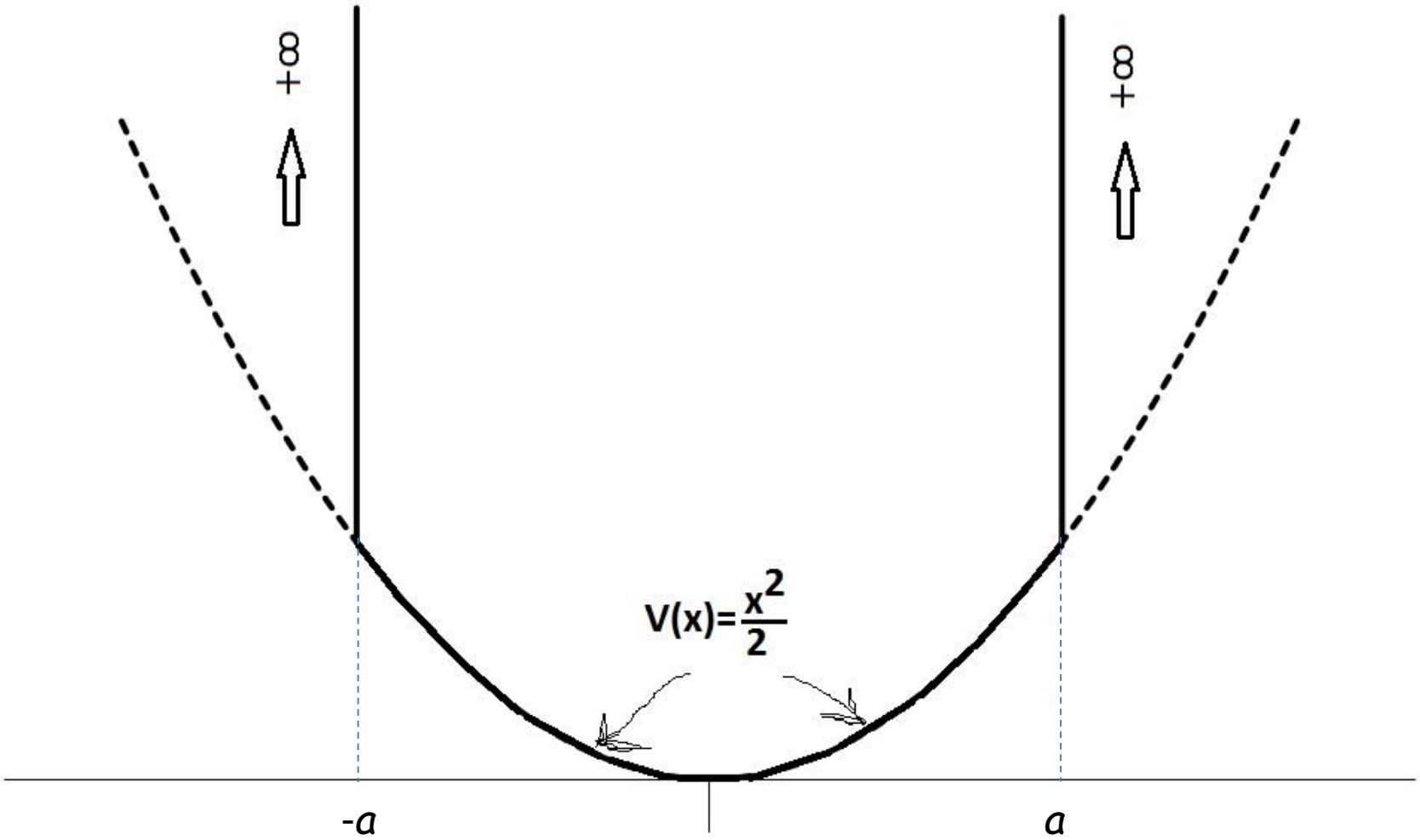
$$= \frac{\pi\Gamma(n+2\lambda)2^{1-2\lambda}}{\{\Gamma(\lambda)\}^2 (n+\lambda)n!}\, \delta_{mn}, \quad \lambda > -\frac{1}{2} \quad \text{and} \quad \lambda \neq 0.$$

$$(1-x^2)y''(x) - (2\lambda+1)xy'(x) + n(n+2\lambda)y(x) = 0, \quad y(x) = C_n^{(\lambda)}(x)$$

Gegenbauer - > Hermite

$$\lim_{\alpha \to \infty} \alpha^{-\frac{1}{2}n} C_n^{(\alpha+\frac{1}{2})}(\alpha^{-\frac{1}{2}}x) = \frac{H_n(x)}{n!}$$

Confined quantum oscillator vs. infinite potential well



Confined quantum oscillator potential with the position-dependent effective mass

$$V(x) = \begin{cases} \dfrac{M(x)\omega^2 x^2}{2}, & -a < x < a, \\ \infty, & x = \pm a. \end{cases}$$

Definition of the position-dependent effective mass

- position-dependent effective mass $M(x)$ should be equal to constant mass m at origin of position $x = 0$;
- position-dependent effective mass $M(x)$ should recover correct constant mass m under the limit $a \to \infty$;
- thanks to definition of the position-dependent effective mass $M(x)$ confinement effect at values of position $x = \pm a$ should be achieved;
- stationary Schrödinger equation for the position-dependent mass Hamiltonians should be explicitly solvable and its solutions should recover so-called Hermite oscillator solutions under the limit $a \to \infty$.

Electron Tunneling in Superconductors

VOLUME 5, NUMBER 4 PHYSICAL REVIEW LETTERS AUGUST 15, 1960

ENERGY GAP I

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PHYSICAL REVIEW VOLUME 123, NUMBER 1 JULY 1, 1961

Tunneling from an Independent-Particle Point of View

WALTER A. HARRISON
General Electric Research Laboratory, Schenectady, New York
(Received February 20, 1961)

A method is developed for calculating wave functions through regions of varying band structure. This method is applied to tunneling problems using the transition-probability approach of Bardeen. It is found that the experiments of Giaever involving tunneling into superconductors cannot be understood strictly in terms of an independent quasi-particle model of the superconductor. The observed proportionality of the tunneling probability to the density of states depends upon the matrix elements being constant which, in turn, depends upon a many-particle feature of the problem. This feature does not carry over to fluctuations in the density of states arising from band structure, and contributions to the current are not expected to be proportional to the density of states in that case. Instead, a projection in wave-number space of the appropriate constant-energy surface enters. Tunneling systems are discussed which involve semiconductors, semimetals, and transition metals as well as simple metals. Finally, alterations in the properties arising from alterations in the nature of the boundary regions are discussed.

I. INTRODUCTION

BARDEEN[1] has discussed tunneling from a many-particle point of view. He did not, however, discuss systems in which the band structure varies with position. In the following treatment we restrict ourselves to an independent-particle approximation, but extend the work to allow for variations in the local band structure.

We proceed by first developing a method for construction of one-particle wave functions, taking particular care that these conserve current locally. Matrix

Sec. VI. This cannot be an exact eigenfunction for general band structure since we are required to match the wave functions on the entire plane $x=0$, but have only the coefficients of four waves at our disposal.

The problem of constructing wave functions is now reduced to the problem of obtaining two matching conditions upon the wave function; these, in conjunction with normalization and external boundary conditions, will uniquely determine the eigenstates. It will be a great mathematical simplification to assume reflection

BenDaniel-Duke kinetic energy operator

PHYSICAL REVIEW VOLUME 152, NUMBER 2 9 DECEMBER 1966

Space-Charge Effects on Electron Tunneling

D. J. BENDANIEL AND C. B. DUKE
General Electric Research and Development Center, Schenectady, New York
(Received 2 June 1966)

The one-electron (Bethe-Sommerfeld) model of electron tunneling is formulated to describe tunneling when the curvature (electron mass) and centroid of the one-electron constant-energy surfaces vary across the junction. The conductance for an abrupt GaAs *p-n* tunnel diode is calculated and shown to exhibit minima near zero bias for highly asymmetrical doping ratios. The conductance of metal-oxide-semimetal (M-O-SM) tunnel junctions is evaluated both with and without the inclusion of space-charge effects and of surface states. All calculations are performed using solvable models for which the WKBJ approximation is not imposed. Neither the removal of the WKBJ approximation nor the space-charge effects give rise to maxima in the conductance of the M-O-SM junctions near a band edge.

I. INTRODUCTION

ALTHOUGH electron tunneling in metal-insulator-metal (M-I-M) junctions has been extensively studied,[1] junctions in which one or more of the components is a semimetal[2] or degenerate semiconductor have been systematically examined primarily within the context of *p-n* junctions.[3] In this paper we consider the modifications of the tunneling current in semimetal and *p-n* junctions caused by the dependence of the shape of the space-charge-induced barrier on the applied bias. We construct sufficiently simple models

has developed an effective-mass theory of tunneling in *p-n* junctions. However, he limited his attention to symmetric diodes and used the WKBJ approximation.

The theoretical discussion of metal-oxide-semimetal (M-O-SM) junctions given herein is, to the authors' knowledge, the first that has been presented. A treatment of metal-semiconductor contacts has been given by one of us elsewhere.[7] Although our models of the junctions are not as refined as those customarily used in metal-oxide-metal junctions,[1] they exhibit the advantage that the entire calculation of the tunneling probability can be performed in closed form. As the

BenDaniel-Duke kinetic energy operator – explicitly

$$\hat{H}^{BD} = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx} + V(x)$$

BenDaniel-Duke kinetic energy operator – solution

$$-\frac{1}{2}\frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx} = -\frac{1}{2M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx}\right]$$

$$\frac{d^2\psi}{dx^2} - \frac{M'}{M}\frac{d\psi}{dx} + \frac{2M}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0$$

BenDaniel-Duke kinetic energy operator – solution

$$\frac{d^2\psi}{dx^2} - \frac{M'}{M}\frac{d\psi}{dx} + \left(\frac{2ME}{\hbar^2} - \frac{M^2\omega^2x^2}{\hbar^2}\right)\psi = 0$$

BenDaniel-Duke kinetic energy operator – PDEM ***M(x)***

$$M(x) = \frac{a^2 m}{a^2 - x^2}$$

$$\lim_{a \to \infty} \frac{a^2 m}{a^2 - x^2} = m$$

$$V(-a) = V(a) = \infty.$$

Schrödinger equation with the BenDaniel-Duke kinetic energy operator – solution

$$\left[\partial_\xi^2 + \frac{\tilde{\tau}(\xi)}{\sigma(\xi)}\partial_\xi + \frac{\tilde{\sigma}(\xi)}{\sigma^2(\xi)}\right]\psi = 0,$$

$$\xi = x/a,\ \tilde{\tau} = -2\xi,\ \sigma = 1-\xi^2,\ \tilde{\sigma} = c_0 - c_2\xi^2,$$

$$c_0 = \frac{2ma^2E}{\hbar^2} \text{ and } c_2 = c_0 + \lambda_0^4 a^4.$$

$$\lambda_0 = \sqrt{\frac{m\omega}{\hbar}}$$

Nikiforov-Uvarov method

$$\psi = \varphi(\xi)\, y, \quad \varphi(\xi) = e^{\int \frac{\pi(\xi)}{\sigma(\xi)} d\xi}.$$

$\pi(\xi)$ is a first degree polynomial

Nikiforov-Uvarov method – polynomial solution

$$y'' + \frac{\tau(\xi)}{\sigma(\xi)} y' + \frac{\bar{\sigma}(\xi)}{\sigma^2(\xi)} y = 0,$$

$$\tau(\xi) = 2\pi(\xi) + \tilde{\tau}(\xi),$$

$$\bar{\sigma}(\xi) = \tilde{\sigma}(\xi) + \pi^2(\xi) + \pi(\xi)\left[\tilde{\tau}(\xi) - \sigma'(\xi)\right] + \pi'(\xi)\sigma(\xi).$$

$$\bar{\sigma}(\xi) = \lambda\sigma(\xi), \quad \lambda = const.$$

Nikiforov-Uvarov method – polynomial solution-2

$$\sigma(\xi)y'' + \tau(\xi)y' + \lambda y = 0.$$

$$\pi^2(\xi) + \left[\tilde{\tau}(\xi) - \sigma'(\xi)\right]\pi(\xi) + \tilde{\sigma}(\xi) - \mu\sigma(\xi) = 0$$

$$\mu = \lambda - \pi'(\xi)$$

Nikiforov-Uvarov method – polynomial solution-3

$$\pi(\xi) = \frac{\sigma' - \tilde{\tau}}{2} + e\sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 + \mu\sigma - \tilde{\sigma}}, \quad e = \pm 1$$

in our case $\sigma' - \tilde{\tau} = 0$

$$\mathscr{D} = -4(c_2 - \mu)(\mu - c_0) = 0.$$

Nikiforov-Uvarov method – polynomial solution-4

$$\pi(\xi) = \begin{cases} e\lambda_0^2 a^2 \xi, & \mu = c_0, \\ e\lambda_0^2 a^2, & \mu = c_2. \end{cases}$$

$$\varphi(\xi) = \left(1 - \xi^2\right)^{-\frac{1}{2} e\lambda_0^2 a^2} \quad \text{for case } \mu = c_0$$

$$\varphi(\xi) = \left(\frac{1+\xi}{1-\xi}\right)^{\frac{1}{2} e\lambda_0^2 a^2} \quad \text{for case } \mu = c_2$$

Nikiforov-Uvarov method – polynomial solution-5

From considerations of the finiteness of the wavefunction at points $\xi = \pm 1$ (or $x = \pm a$), one observes the condition $e = -1$ should be satisfied, and the case $\mu = c_0$ should be chosen for $\varphi(\xi)$, i.e.

$$\pi(\xi) = -\lambda_0^2 a^2 \xi, \quad \varphi(\xi) = \left(1 - \xi^2\right)^{\frac{1}{2}\lambda_0^2 a^2}$$

Nikiforov-Uvarov method – polynomial solution-6

$$\lambda = c_0 - \lambda_0^2 a^2, \quad \tau(\xi) = -2\left(\lambda_0^2 a^2 + 1\right)\xi$$

$$\sigma(\xi)\, y'' + \tau(\xi)\, y' + \lambda y = 0.$$

equation for the Gegenbauer polynomials $\bar{y} = C_n^{(\nu)}(x)$

$$\left(1 - x^2\right)\bar{y}'' - (2\nu + 1)\, x\bar{y}' + n(n + 2\nu)\,\bar{y} = 0$$

we obtain that $\nu = \lambda_0^2 a^2 + 1/2$

Wavefunction

$$\psi_n^{BD}(x) = c_n^{BD}\left(1-\frac{x^2}{a^2}\right)^{\frac{\lambda_0^2 a^2}{2}} C_n^{\left(\lambda_0^2 a^2+\frac{1}{2}\right)}\left(\frac{x}{a}\right)$$

$$c_n^{BD} = 2^{\lambda_0^2 a^2}\Gamma\left(\lambda_0^2 a^2+\frac{1}{2}\right)\sqrt{\frac{\left(n+\lambda_0^2 a^2+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+2\lambda_0^2 a^2+1\right)}}$$

$$\int_{-a}^{a}\left[\psi_m^{BD}(x)\right]^*\psi_n^{BD}(x)dx = \delta_{m,n}.$$

Energy spectrum

$$E_n^{BD} = \hbar\omega\left(n + \tfrac{1}{2} + \frac{n(n+1)}{2\lambda_0^2 a^2}\right), \quad n = 0, 1, 2, \ldots$$

Li-Kuhn kinetic energy operator

PHYSICAL REVIEW B VOLUME 47, NUMBER 19 15 MAY 1993-I

Band-offset ratio dependence on the effective-mass Hamiltonian based on a modified profile of the GaAs-$Al_xGa_{1-x}As$ quantum well

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This paper suggests a simple permutation scheme to construct the Hermitian Hamiltonian utilized in the effective-mass equation, introduces a smoothed profile to more accurately model heterojunctions, and illustrates the dependence of the band-offset ratio of a GaAs-$Al_xGa_{1-x}As$ quantum well on the particular Hermitian Hamiltonian used in the calculation. The permutation scheme produces the BenDaniel and Duke Hamiltonian, the Bastard Hamiltonian, the Zhu and Kroemer Hamiltonian, and a Hamiltonian termed the redistributed Hamiltonian in this paper. The heterojunction is modeled by an error function rather than a step function to more accurately model the material transition region at the interface between the two materials. The 11 heavy-hole (HH) transition energy obtained by BenDaniel and Duke Hamiltonian with a particular band-offset ratio is reproduced by utilizing non-BenDaniel and Duke Hamiltonians with appropriate band-offset ratios. This process is repeated for BenDaniel and Duke Hamiltonian band-offset ratios varying from 0.5 to 0.8, and then proceeds to 11 light-hole (LH), 22 HH, and 22 LH transitions. It is found that the Hamiltonian dependence of the band-offset ratio is significant.

I. INTRODUCTION

The conduction-band-offset ratio, which is the ratio of the conduction-band offset to the total band gap of the heterojunction, has been investigated in GaAs-$Al_xGa_{1-x}As$ quantum wells because of its fundamental importance and application. The ratio has been measured by spectroscopic[1–6] and electrical[7–9] methods, and the reported value ranges from 0.88 to 0.57. From Duggan's[10] and Kroemer's[11] review articles about the ex-

well, the position-dependent potential is frequently modeled by a discontinuous profile, namely, a step function.[1,2,4,6] However, in this paper, the step change of the profile is replaced by an error function because, in the real world, neither the potential nor the effective mass can change abruptly across the heterojunction.

In the work published by Chomette *et al.* in 1986,[21] it was shown that the band-offset ratio depends on the analytic model and the interface conditions employed to compute the transition energy. This observation initiates

Li-Kuhn kinetic energy operator – explicitly

$$\hat{H}^{LK} = -\frac{\hbar^2}{4}\left[\frac{d}{dx}\frac{1}{\sqrt{M(x)}}\frac{d}{dx}\frac{1}{\sqrt{M(x)}} + \frac{1}{\sqrt{M(x)}}\frac{d}{dx}\frac{1}{\sqrt{M(x)}}\frac{d}{dx}\right] + V(x)$$

$$\left\{\frac{d}{dx}\frac{1}{\sqrt{M(x)}}\frac{d}{dx}, \frac{1}{\sqrt{M(x)}}\right\} = \frac{2}{M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{4}\frac{M''}{M} + \frac{1}{2}\left(\frac{M'}{M}\right)^2\right]$$

Li-Kuhn kinetic energy operator – explicitly

$$\hat{H}^{LK} = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{4}\frac{M''}{M} + \frac{1}{2}\left(\frac{M'}{M}\right)^2\right] + V(x)$$

$$\frac{d^2\psi}{dx^2} - \frac{M'}{M}\frac{d\psi}{dx} - \frac{1}{4}\frac{M''}{M} + \frac{1}{2}\left(\frac{M'}{M}\right)^2 + \left(\frac{2ME}{\hbar^2} - \frac{M^2\omega^2x^2}{\hbar^2}\right)\psi = 0$$

Li-Kuhn kinetic energy operator – Schrödinger equation

$$\frac{d^2\psi}{dx^2} - \frac{2x}{a^2 - x^2}\frac{d\psi}{dx} + \frac{c_0 - \frac{1}{2}}{a^2 - x^2}\psi + \frac{(c_0 - c_2)x^2}{(a^2 - x^2)^2}\psi = 0$$

Wavefunction

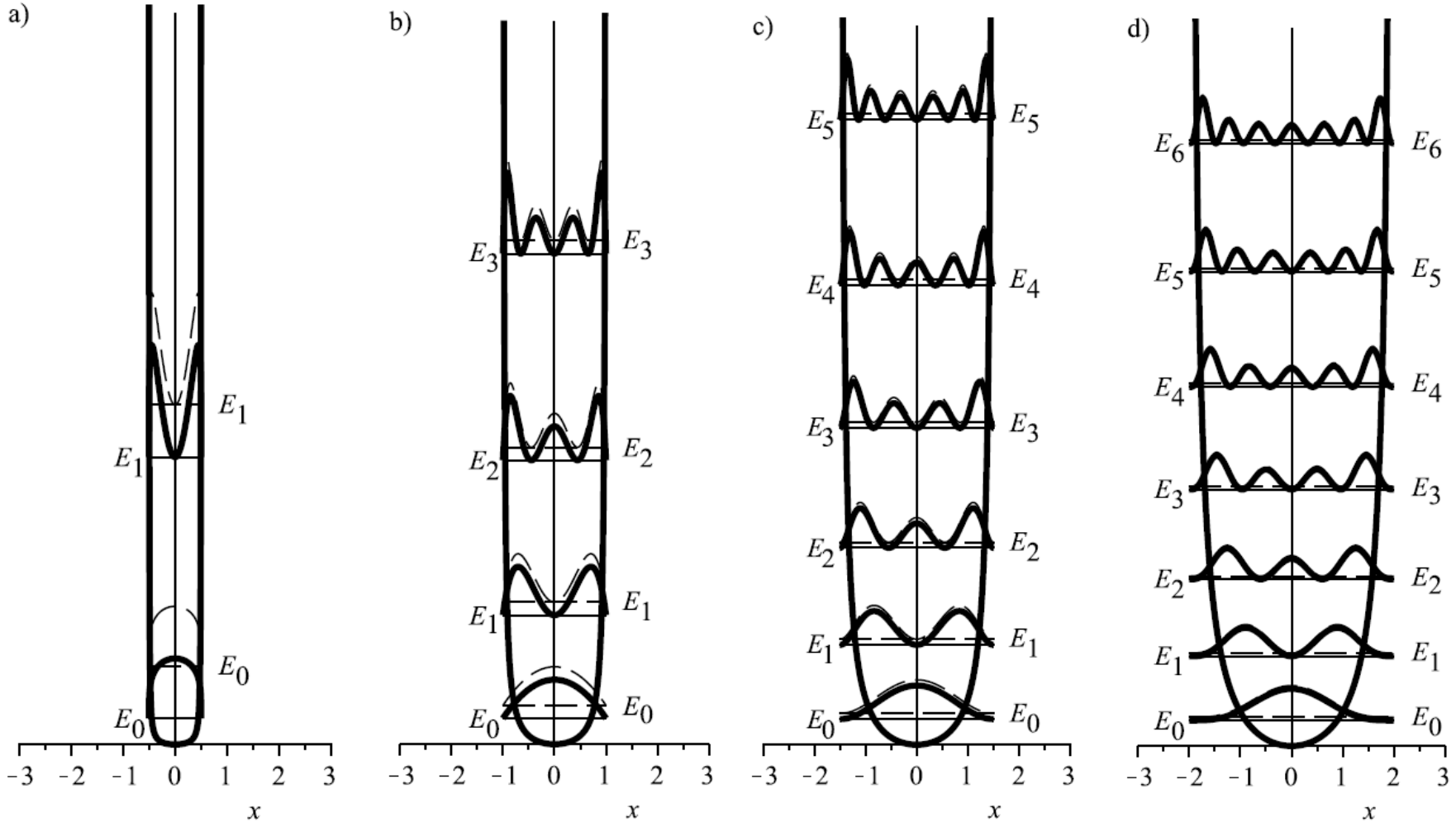
$$\psi_n^{LK}(x) = \psi_n^{BD}(x) = c_n^{BD}\left(1-\frac{x^2}{a^2}\right)^{\frac{\lambda_0^2 a^2}{2}} C_n^{\left(\lambda_0^2 a^2+\frac{1}{2}\right)}\left(\frac{x}{a}\right)$$

$$c_n^{BD} = 2^{\lambda_0^2 a^2}\Gamma\left(\lambda_0^2 a^2+\tfrac{1}{2}\right)\sqrt{\frac{\left(n+\lambda_0^2 a^2+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+2\lambda_0^2 a^2+1\right)}}$$

Energy spectrum

$$E_n^{LK} = \hbar\omega \left(n + \tfrac{1}{2} + \frac{n(n+1) + \frac{1}{2}}{2\lambda_0^2 a^2} \right), \quad n = 0, 1, 2, \ldots$$

$$E_0^{LK} = E_0 \left(1 + \frac{1}{2\lambda_0^2 a^2} \right)$$


a)
b)
c)
d)
E_0
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E_5
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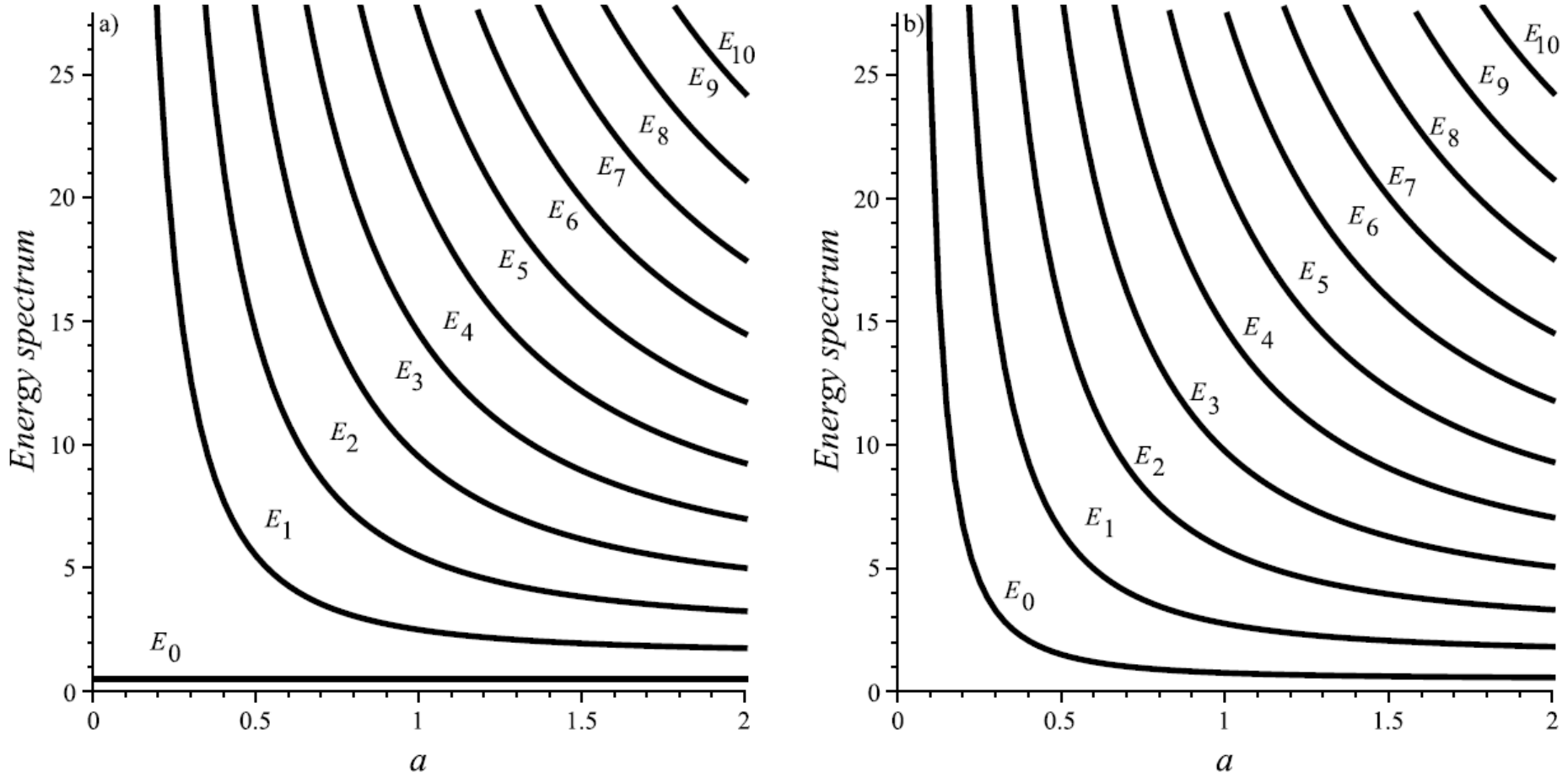
a)
b)
Energy spectrum
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E_3
E_4
E_5
E_6
E_7
E_8
E_9
E_{10}

Gora-Williams kinetic energy operator

PHYSICAL REVIEW VOLUME 177, NUMBER 3 15 JANUARY 1969

Theory of Electronic States and Transport in Graded Mixed Semiconductors*

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Semiconductors which are slowly graded in composition can be shown to have position-dependent band gaps and position-dependent effective masses, describable in terms of an effective Hamiltonian in an effective-mass equation. The effective Hamiltonian previously obtained is, in the present work, rendered Hermitian. Electronic minority-carrier transport for graded systems is described in terms of an effective field which includes the electrostatic field plus a term in the gradient of the band edge and another in the gradient of the effective mass. The local radiative-recombination lifetime and local density of states for inhomogeneous semiconductors are discussed. The equation for the excess minority-carrier concentration in an inhomogeneous semiconductor is deduced and is found to differ from that in an homogeneous system, by the effective field replacing the electric field, by the position dependences of lifetime and mobility, and by terms in the mobility gradient. Some phenomena specific to graded mixed semiconductors are considered on the basis of the theoretical analysis.

I. INTRODUCTION

SEVERAL unique phenomena and device applications have been described for semiconductors which are slowly graded in composition, based on the assumption that such graded systems exhibit graded band gaps.[1–3] Of interest here is the phenomenon of anti-Stokes radiative emission. Van Ruyven and Williams[4] have proposed field-enhanced minority carrier transport and recombination in graded band-gap systems as an anti-Stokes mechanism. The present paper examines

in average unit cell is entirely in the unit-cell potential with no change in lattice constant.

Assuming that $L(x)$ varies slowly over the spatial extent of the Wannier functions of the homogeneous systems, and that interband coupling of $S(\mathbf{r})$ can be neglected, we obtained an effective masslike equation[5] which is valid for states near each band edge

$$[1/2m_n^*+\beta_n L(x)](-\nabla^2)F_n(\mathbf{r})+\alpha_n L(x)F_n(\mathbf{r}) = E_n F_n(\mathbf{r}), \quad (1)$$

Gora-Williams kinetic energy operator – explicitly

$$\hat{H}_0^{GW} = -\frac{\hbar^2}{4}\left\{M^{-1}(x), \frac{d^2}{dx^2}\right\}$$

Gora-Williams kinetic energy operator – solution

$$\left\{ M^{-1}(x), \frac{d^2}{dx^2} \right\} = \frac{2}{M} \left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{2}\frac{M''}{M} + \left(\frac{M'}{M} \right)^2 \right]$$

$$\hat{H}^{GW} = -\frac{\hbar^2}{2M} \left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{2}\frac{M''}{M} + \left(\frac{M'}{M} \right)^2 \right] + \frac{M\omega^2 x^2}{2}$$

Gora-Williams kinetic energy operator – PDEM ***M(x)***

$$M(x) = \frac{a^2 m}{a^2 - x^2}$$

$$\lim_{a \to \infty} \frac{a^2 m}{a^2 - x^2} = m$$

$$V(-a) = V(a) = \infty.$$

Gora-Williams kinetic energy operator – solution

$$\left[\frac{d^2}{dx^2} - \frac{2x}{a^2 - x^2}\frac{d}{dx} - \frac{1}{a^2 - x^2}\right]\psi + \left(\frac{2ma^2E}{\hbar^2(a^2 - x^2)} - \frac{m^2\omega^2a^4x^2}{\hbar^2(a^2 - x^2)^2}\right)\psi = 0$$

Schrödinger equation with the Gora-Williams kinetic energy operator – solution

$$\psi'' - \frac{2\xi}{1-\xi^2}\psi' + \frac{c_0 - 1 + (1 - c_0 - c_2)\,\xi^2}{(1-\xi^2)^2}\psi = 0$$

$$\xi = \frac{x}{a}, \quad \frac{d}{dx} = \frac{1}{a}\frac{d}{d\xi}, \quad \frac{d^2}{dx^2} = \frac{1}{a^2}\frac{d^2}{d\xi^2}$$

$$c_0 = \frac{2ma^2E}{\hbar^2}, \quad c_2 = \frac{m^2\omega^2a^4}{\hbar^2}$$

Nikiforov-Uvarov method

$$\psi = \varphi(\xi)\, y, \quad \varphi(\xi) = e^{\int \frac{\pi(\xi)}{\sigma(\xi)} d\xi}.$$

$\pi(\xi)$ is a first degree polynomial

Nikiforov-Uvarov method – polynomial solution

$$y'' + \frac{\tau}{\sigma} y' + \frac{\bar{\sigma}}{\sigma^2} y = 0$$

$$\tau = 2\pi + \tilde{\tau} \text{ and } \bar{\sigma} = \tilde{\sigma} + \pi^2 + \pi\left(\tilde{\tau} - \sigma'\right) + \pi'\sigma$$

$$\tilde{\tau} = -2\xi, \qquad \sigma = 1 - \xi^2,$$

$$\tilde{\sigma} = c_0 - 1 + \left(1 - c_0 - c_2\right)\xi^2$$

$$\bar{\sigma} = \lambda\sigma, \quad \lambda = const.$$

Nikiforov-Uvarov method – polynomial solution-2

$$\sigma(\xi)y'' + \tau(\xi)y' + \lambda y = 0.$$

$$\pi^2(\xi) + \left[\tilde{\tau}(\xi) - \sigma'(\xi)\right]\pi(\xi) + \tilde{\sigma}(\xi) - \mu\sigma(\xi) = 0$$

$$\mu = \lambda - \pi'(\xi)$$

Wavefunction

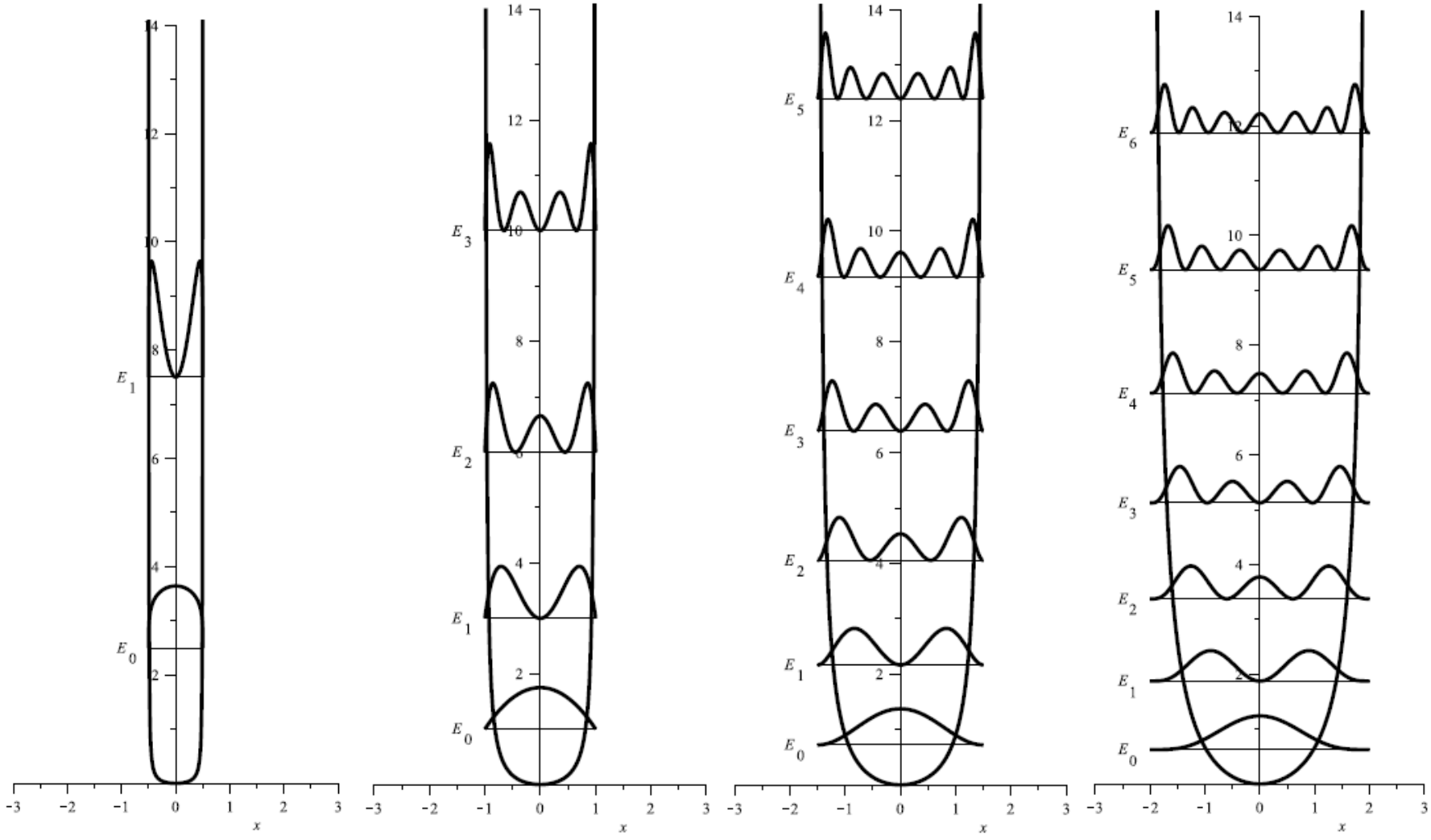
$$\psi_n^{GW}(x) = c_n^{GW}\left(1-\frac{x^2}{a^2}\right)^{\frac{m\omega a^2}{2\hbar}} C_n^{\left(\frac{m\omega a^2}{\hbar}+\frac{1}{2}\right)}\left(\frac{x}{a}\right)$$

$$c_n^{GW} = 2^{\frac{m\omega a^2}{\hbar}}\Gamma\left(\frac{m\omega a^2}{\hbar}+\frac{1}{2}\right)\sqrt{\frac{\left(n+\frac{m\omega a^2}{\hbar}+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+\frac{2m\omega a^2}{\hbar}+1\right)}}$$

$$\int_{-a}^{a}\left[\psi_m^{GW}(x)\right]^*\psi_n^{GW}(x)dx = \delta_{mn}$$

Energy spectrum

$$E_n^{GW} = \hbar\omega\left(n+\frac{1}{2}\right)+\frac{\hbar^2}{2ma^2}\left(n^2+n+1\right)$$


E0
E1
E0
E1
E2
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E2
E3
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E0
E1
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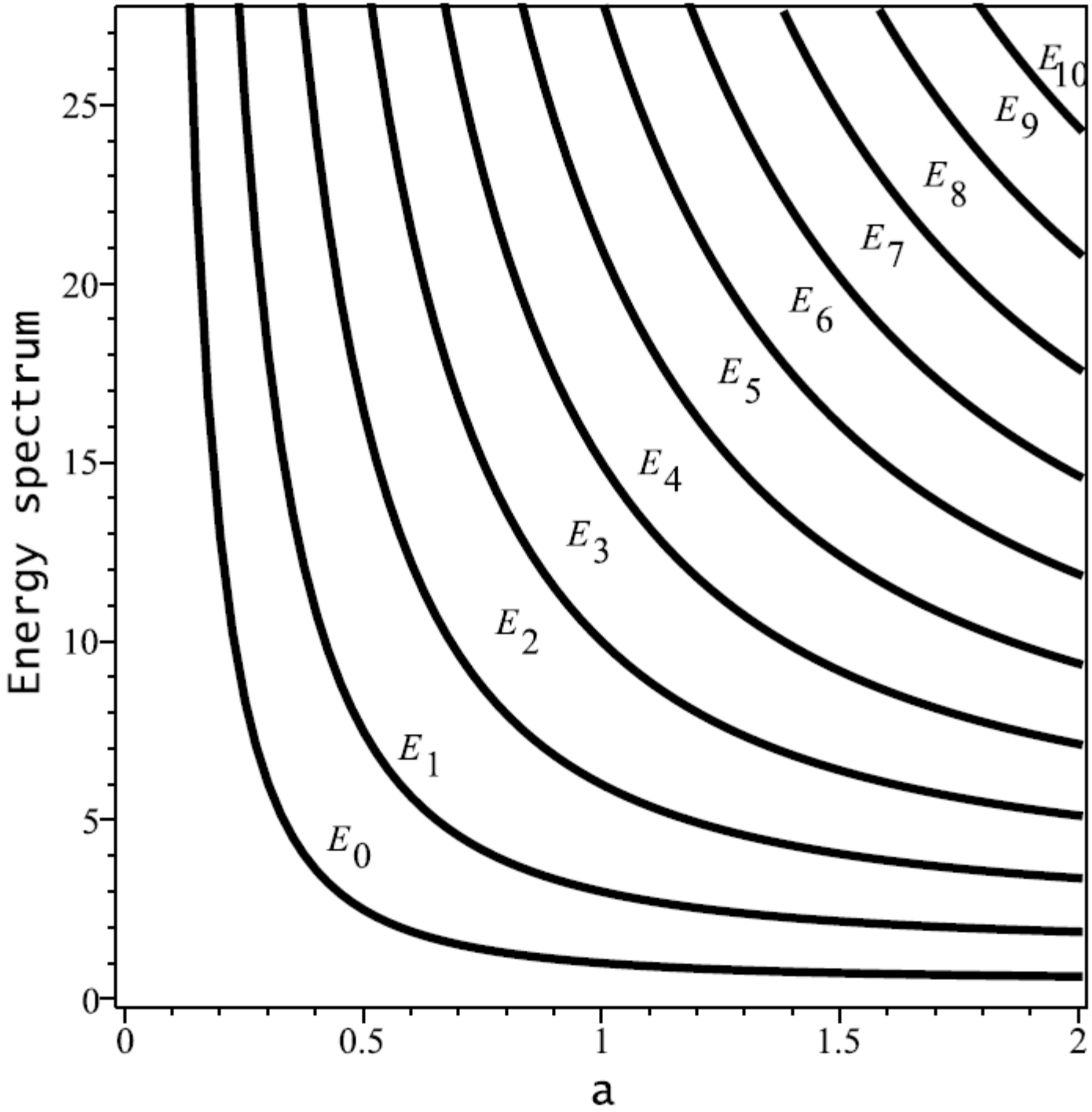
E4
E5
E6
x


Energy spectrum
a
0
5
10
15
20
25
0
0.5
1
1.5
2
E_0
E_1
E_2
E_3
E_4
E_5
E_6
E_7
E_8
E_9
E_{10}

Zhu-Kroemer kinetic energy operator

PHYSICAL REVIEW B VOLUME 27, NUMBER 6 15 MARCH 1983

Interface connection rules for effective-mass wave functions at an abrupt heterojunction between two different semiconductors

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The problem of the connection rules for effective-mass wave functions across an abrupt heterojunction is investigated by expressing the results of a one-dimensional tight-binding approximation in terms of effective-mass wave functions. The widely used conventional connection rules of continuous-wave function and first derivative are only an approximation, invalid in all but the simplest limiting case. The connection-rule problem is reformulated by first extrapolating the effective-mass wave functions on the two sides of the heterojunction across the interface, as if the semiconductor were homogeneous. In each of the two lattice planes adjacent to the interface, the extrapolated wave function must then be proportional to the true wave function, with two proportionality coefficients that depend on certain matrix elements. By suitably renormalizing the wave function, the connection rules for type-I heterojunctions become, to the first order, the same as if a δ-function scatterer were superimposed on the band-edge discontinuity. The effects of the new connection rules on the ground state of a symmetric square well are discussed as an example.

I. INTRODUCTION

A. The problem

In the theory of semiconductor heterostructure, especially of the quantum wells that have become technologically possible in recent years, one frequently encounters the problem of connecting effective-mass wave functions across an interface

nection rules for WKB wave functions across a classical turning point, we refer to it as a connection-rule problem.

The majority of those working in the field of semiconductor heterostructures and quantum wells, and especially those using the effective-mass approximation for the interpretation (or prediction) of *experimental* properties, have taken for granted that the conventional connection rules from ordinary

Zhu-Kroemer kinetic energy operator – explicitly

$$\hat{H}_0^{ZK} = -\frac{\hbar^2}{2}\frac{1}{\sqrt{M(x)}}\frac{d^2}{dx^2}\frac{1}{\sqrt{M(x)}}$$

Zhu-Kroemer kinetic energy operator – solution

$$\frac{1}{\sqrt{M(x)}}\frac{d^2}{dx^2}\frac{1}{\sqrt{M(x)}} = \left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{2}\frac{M''}{M} + \frac{3}{4}\left(\frac{M'}{M}\right)^2\right]$$

$$\hat{H}^{ZK} = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{2}\frac{M''}{M} + \frac{3}{4}\left(\frac{M'}{M}\right)^2\right] + \frac{M\omega^2 x^2}{2}$$

Zhu-Kroemer kinetic energy operator – PDEM ***M(x)***

$$M(x) = \frac{a^2 m}{a^2 - x^2}$$

$$\lim_{a \to \infty} \frac{a^2 m}{a^2 - x^2} = m$$

$$V(-a) = V(a) = \infty.$$

Zhu-Kroemer kinetic energy operator – solution

$$\left[\frac{d^2}{dx^2}-\frac{2x}{a^2-x^2}\frac{d}{dx}-\frac{1}{a^2-x^2}-\frac{x^2}{\left(a^2-x^2\right)^2}\right]\psi+\left(\frac{2ma^2E}{\hbar^2\left(a^2-x^2\right)}-\frac{m^2\omega^2a^4x^2}{\hbar^2\left(a^2-x^2\right)^2}\right)\psi=0$$

Schrödinger equation with the Zhu-Kroemer kinetic energy operator – solution

$$\psi'' - \frac{2\xi}{1-\xi^2}\psi' + \frac{(c_0 - 1) - (c_0 + c_2)\,\xi^2}{(1-\xi^2)^2}\psi = 0$$

$$\xi = \frac{x}{a}, \quad \frac{d}{dx} = \frac{1}{a}\frac{d}{d\xi}, \quad \frac{d^2}{dx^2} = \frac{1}{a^2}\frac{d^2}{d\xi^2}$$

$$c_0 = \frac{2ma^2E}{\hbar^2}, \quad c_2 = \frac{m^2\omega^2a^4}{\hbar^2}$$

Nikiforov-Uvarov method

$$\psi = \varphi(\xi)\, y, \quad \varphi(\xi) = e^{\int \frac{\pi(\xi)}{\sigma(\xi)} d\xi}.$$

$\pi(\xi)$ is a first degree polynomial

Nikiforov-Uvarov method – polynomial solution

$$y'' + \frac{\tau}{\sigma} y' + \frac{\bar{\sigma}}{\sigma^2} y = 0$$

$$\tau = 2\pi + \tilde{\tau} \text{ and } \bar{\sigma} = \tilde{\sigma} + \pi^2 + \pi\left(\tilde{\tau} - \sigma'\right) + \pi'\sigma$$

$$\tilde{\tau} = -2\xi, \qquad \sigma = 1 - \xi^2,$$

$$\tilde{\sigma} = \left(c_0 - 1\right) - \left(c_0 + c_2\right)\xi^2,$$

$$\bar{\sigma} = \lambda\sigma, \quad \lambda = const.$$

Nikiforov-Uvarov method – polynomial solution-2

$$\sigma(\xi)y'' + \tau(\xi)y' + \lambda y = 0.$$

$$\pi^2(\xi) + \left[\tilde{\tau}(\xi) - \sigma'(\xi)\right]\pi(\xi) + \tilde{\sigma}(\xi) - \mu\sigma(\xi) = 0$$

$$\mu = \lambda - \pi'(\xi)$$

Wavefunction

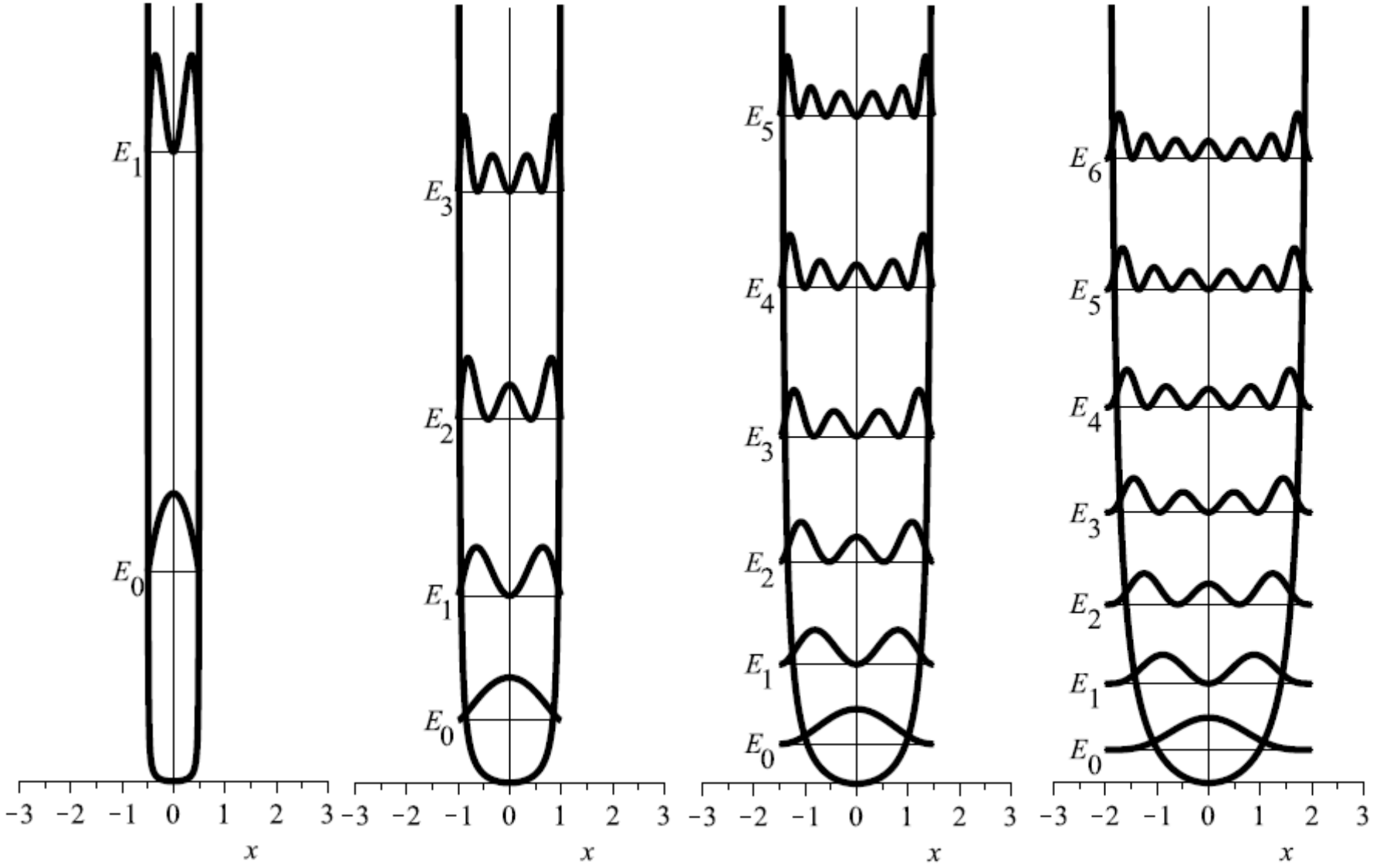
$$\psi_n^{ZK}(x) = c_n^{ZK}\left(1-\frac{x^2}{a^2}\right)^{\frac{1}{2}\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+1}} C_n^{\left(\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+1}+\frac{1}{2}\right)}\left(\frac{x}{a}\right)$$

$$c_n^{ZK} = 2^{\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+1}}\Gamma\left(\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+1}+\frac{1}{2}\right)\sqrt{\frac{\left(n+\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+1}+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+2\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+1}+1\right)}}$$

$$\int_{-a}^{a}\left[\psi_m^{ZK}(x)\right]^*\psi_n^{ZK}(x)dx = \delta_{mn}$$

Energy spectrum

$$E_n^{ZK} = \hbar\sqrt{\omega^2 + \frac{\hbar^2}{m^2a^4}}\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2ma^2}\left(n^2 + n + 1\right)$$


E_1
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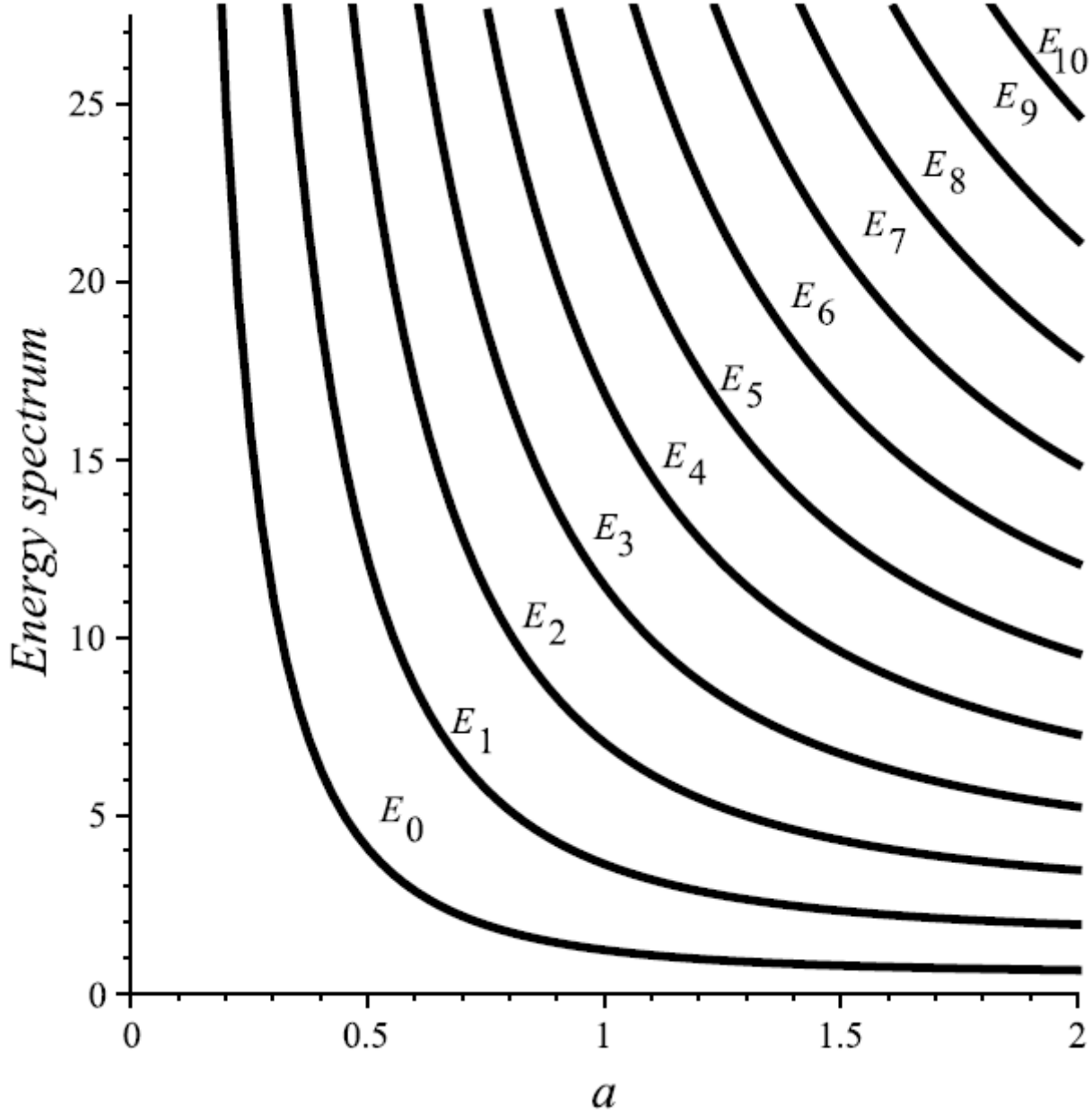
Energy spectrum
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E_{10}

Morrow-Brownstein kinetic energy operator

PHYSICAL REVIEW B VOLUME 30, NUMBER 2 15 JULY 1984

Model effective-mass Hamiltonians for abrupt heterojunctions and the associated wave-function-matching conditions

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We consider a class of Hermitian effective-mass Hamiltonians whose kinetic energy term is $(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma}+m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha})/4$ with $\alpha+\beta+\gamma=-1$. We apply these Hamiltonians to an abrupt heterojunction between two crystals and seek the matching conditions across the junction on the effective-mass wave function (ψ) and its spatial derivative ($\dot{\psi}$). For $\alpha\neq\gamma$ we find that the wave function must vanish at the junction thus implying that the junction acts as an impenetrable barrier. Consequently, the only viable cases are for $\alpha=\gamma$ where we show that $m^{\alpha}\psi$ and $m^{\alpha+\beta}\dot{\psi}$ must be continuous across the junction.

I. INTRODUCTION

Effective-mass theory (EMT) has been used to calculate physical quantities in crystals when the desired accuracy did not justify the use of a more complete theory.[1] Although originally[2] developed to treat impurities in an otherwise perfect crystal, EMT has been extended to crystals whose chemical composition changes from region to region—the so-called graded crystals.[3–6] The new feature appearing in these latter applications is that the effective theory. Actually, in slowly graded crystals the distinction between the different operators in Eq. (1) is not important, since the derivations of EMT there are valid only when the chemical composition changes appreciably over a distance that is large in comparison to a lattice constant; all operators of the type in Eq. (1) are equivalent in that limit.[8]

In treatments of abrupt heterojunctions the situation is more confused. Instead of trying to derive the correct form of the kinetic energy operator (if indeed one exists)

Morrow-Brownstein kinetic energy operator – explicitly

$$\hat{H}_0^{MB} = \frac{1}{2} M^{\alpha}(x)\hat{p}_x M^{\beta}(x)\hat{p}_x M^{\alpha}(x), \quad 2\alpha+\beta=-1$$

Morrow-Brownstein kinetic energy operator – solution

$$\hat{H}^{MB} = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} + \alpha\frac{M''}{M} - \alpha(\alpha+2)\left(\frac{M'}{M}\right)^2\right] + \frac{M\omega^2 x^2}{2}$$

Morrow-Brownstein kinetic energy operator – PDEM ***M(x)***

$$M(x) = \frac{a^2 m}{a^2 - x^2}$$

$$\lim_{a \to \infty} \frac{a^2 m}{a^2 - x^2} = m$$

$$V(-a) = V(a) = \infty.$$

Morrow-Brownstein kinetic energy operator – solution

$$\left[\frac{d^2}{dx^2}-\frac{2x}{a^2-x^2}\frac{d}{dx}+\frac{2\alpha}{a^2-x^2}-\frac{4\alpha^2x^2}{(a^2-x^2)^2}\right]\psi+\left(\frac{c_0}{a^2-x^2}-\frac{c_2x^2}{(a^2-x^2)^2}\right)\psi=0$$

Schrödinger equation with the Morrow-Brownstein kinetic energy operator – solution

$$\psi'' + \frac{\tilde{\tau}}{\sigma}\psi' + \frac{\tilde{\sigma}}{\sigma^2}\psi = 0$$

$$\tilde{\tau} = -2\xi, \qquad \sigma = 1 - \xi^2,$$

$$\tilde{\sigma} = (2\alpha + c_0) - (4\alpha^2 + 2\alpha + c_0 + c_2)\,\xi^2$$

$$\xi = \frac{x}{a}, \quad \frac{d}{dx} = \frac{1}{a}\frac{d}{d\xi}, \quad \frac{d^2}{dx^2} = \frac{1}{a^2}\frac{d^2}{d\xi^2}$$

$$c_0 = \frac{2ma^2E}{\hbar^2}, \quad c_2 = \frac{m^2\omega^2a^4}{\hbar^2}$$

Nikiforov-Uvarov method

$$\psi = \varphi(\xi)\, y, \quad \varphi(\xi) = e^{\int \frac{\pi(\xi)}{\sigma(\xi)} d\xi}.$$

$\pi(\xi)$ is a first degree polynomial

Nikiforov-Uvarov method – polynomial solution

$$y'' + \frac{\tau}{\sigma} y' + \frac{\bar{\sigma}}{\sigma^2} y = 0$$

$$\tau = 2\pi + \tilde{\tau} \text{ and } \bar{\sigma} = \tilde{\sigma} + \pi^2 + \pi\left(\tilde{\tau} - \sigma'\right) + \pi'\sigma$$

$$\bar{\sigma} = \lambda\sigma, \quad \lambda = const.$$

Nikiforov-Uvarov method – polynomial solution-2

$$\sigma(\xi)y'' + \tau(\xi)y' + \lambda y = 0.$$

$$\pi^2(\xi) + \left[\tilde{\tau}(\xi) - \sigma'(\xi)\right]\pi(\xi) + \tilde{\sigma}(\xi) - \mu\sigma(\xi) = 0$$

$$\mu = \lambda - \pi'(\xi)$$

Wavefunction

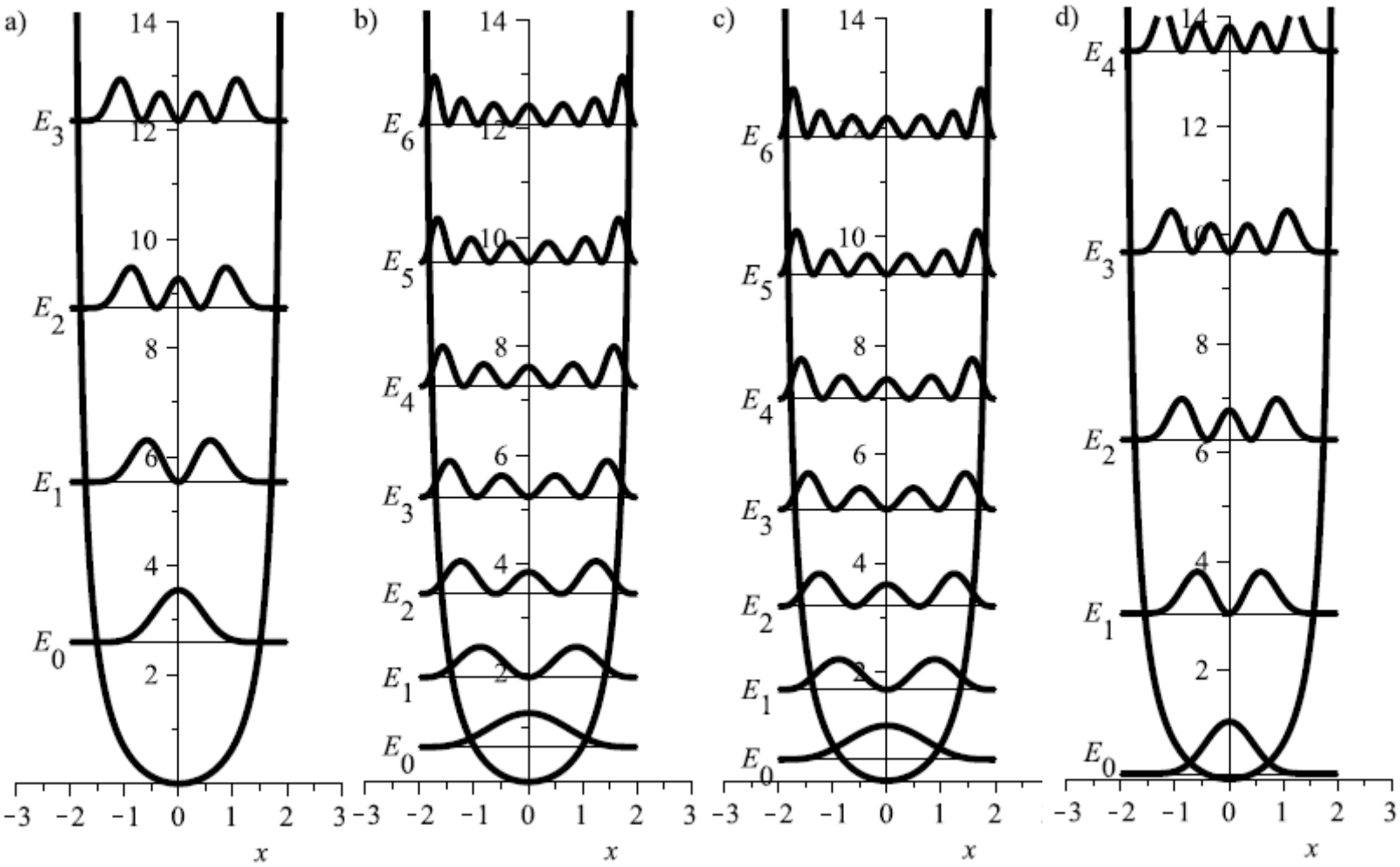
$$\psi_n^{MB}(x) = c_n^{MB}\left(1-\frac{x^2}{a^2}\right)^{\frac{1}{2}\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha^2}} C_n^{\left(\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha^2}+\frac{1}{2}\right)}\left(\frac{x}{a}\right)$$

$$c_n^{MB} = 2^{\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha^2}}\Gamma\left(\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha^2}+\frac{1}{2}\right)\sqrt{\frac{\left(n+\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha^2}+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+2\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha^2}+1\right)}}$$

$$\int_{-a}^{a}\left[\psi_m^{MB}(x)\right]^*\psi_n^{MB}(x)dx = \delta_{mn}$$

Energy spectrum

$$E_n^{MB} = \hbar\sqrt{\omega^2 + \frac{4\alpha^2\hbar^2}{m^2a^4}}\left(n+\frac{1}{2}\right) + \frac{\hbar^2}{2ma^2}\left(n^2+n-2\alpha\right)$$


a)
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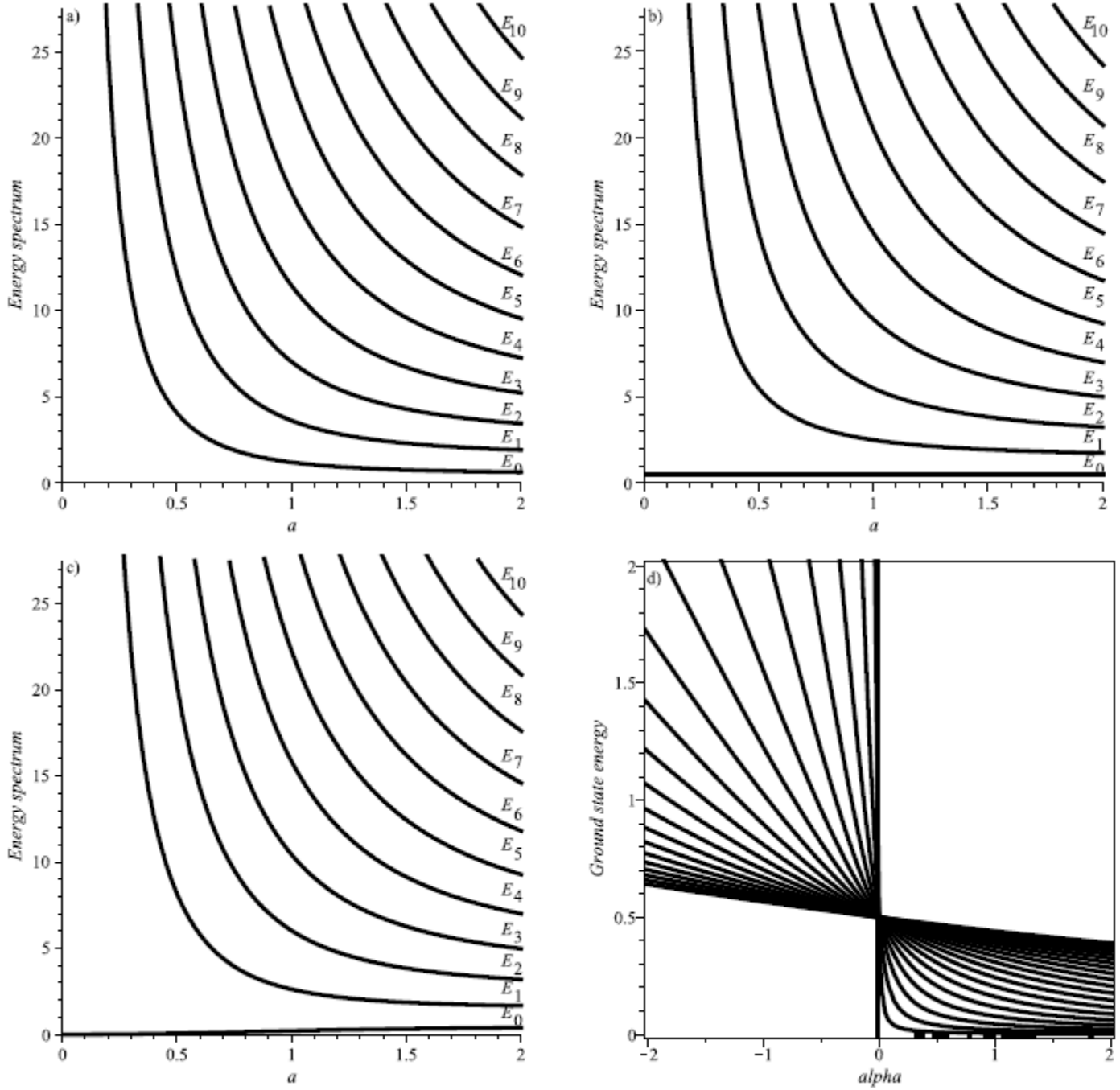
a)
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Energy spectrum
Ground state energy
a
alpha
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E_3
E_4
E_5
E_6
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E_8
E_9
E_{10}

von Roos kinetic energy operator

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Position-dependent effective masses in semiconductor theory

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The motion of free carriers (electrons and holes) in semiconductors of nonuniform chemical composition is sometimes described by means of a Hamiltonian possessing a position-dependent effective mass. In previous work we have shown that position-dependent masses lead to inconsistencies on account of Bargmann's theorem, which postulates that a coherent superposition of states of different masses (wave packets) is forbidden. We have also shown how to circumvent this selection rule. We derive an extension of Bargmann's theorem to the effect that Hamiltonians with position-dependent masses are not Galilean invariant. Furthermore, it is also shown that the customary derivation of position-dependent effective-mass Hamiltonians is by no means unique. There exist, in general, many nonequivalent Hamiltonians within the same approximation, all derivable from the basic many-body Hamiltonian, as long as the concept of a position-dependent mass is maintained. Because of the lack of uniqueness and the lack of Galilean invariance of variable-effective-mass theories it seems appropriate to abandon the concept of a position-dependent mass. In previous work we have shown how to do this successfully.

I. INTRODUCTION

The importance of a theoretical understanding of transport phenomena in semiconductors of a variable, position-dependent chemical composition for modern device technology does not need to be emphasized. The Wannier-Slater theorem[1] valid for homogeneous semiconductors of a uniform chemical given by $E_c(0)+U(\vec{r})$. For details, particularly in more complicated situations (several minima, degeneracy of energy eigenvalues, band mixing, etc.), the reader is referred to Ref. 2. An extension of the Wannier-Slater theorem to nonuniform semiconductors, material possessing a position-dependent varying chemical composition, has been attempted by a number of authors.[3–6] Since we are primarily

von Roos kinetic energy operator – explicitly

$$\hat{H}_0^{vR} = \frac{1}{4}\left[M^{\alpha}(x)\hat{p}_x M^{\beta}(x)\hat{p}_x M^{\gamma}(x) + M^{\gamma}(x)\hat{p}_x M^{\beta}(x)\hat{p}_x M^{\alpha}(x)\right]$$

$$\alpha + \beta + \gamma = -1$$

von Roos kinetic energy operator – solution

$$\hat{H}^{vR} = -\frac{\hbar^2}{4}\left[M^{\alpha}(x)\frac{d}{dx}M^{\beta}(x)\frac{d}{dx}M^{\gamma}(x) + M^{\gamma}(x)\frac{d}{dx}M^{\beta}(x)\frac{d}{dx}M^{\alpha}(x)\right] + \frac{M(x)\omega^2 x^2}{2}$$

$$\hat{H}^{vR} = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} + \frac{\alpha+\gamma}{2}\frac{M''}{M} - (\alpha+\alpha\gamma+\gamma)\left(\frac{M'}{M}\right)^2\right] + \frac{M\omega^2 x^2}{2}$$

von Roos kinetic energy operator – PDEM ***M(x)***

$$M(x) = \frac{a^2 m}{a^2 - x^2}$$

$$\lim_{a \to \infty} \frac{a^2 m}{a^2 - x^2} = m$$

$$V(-a) = V(a) = \infty.$$

von Roos kinetic energy operator – solution

$$\left[\frac{d^2}{dx^2} - \frac{2x}{a^2-x^2}\frac{d}{dx} + \frac{\alpha+\gamma}{a^2-x^2} - \frac{4\alpha\gamma x^2}{(a^2-x^2)^2}\right]\psi + \left(\frac{2ME^{vR}}{\hbar^2} - \frac{M^2\omega^2x^2}{\hbar^2}\right)\psi^{vR} = 0$$

Schrödinger equation with the von Roos kinetic energy operator – solution

$$\psi'' + \frac{\tilde{\tau}}{\sigma}\psi' + \frac{\tilde{\sigma}}{\sigma^2}\psi = 0$$

$$\tilde{\tau} = -2\xi, \qquad \sigma = 1 - \xi^2,$$

$$\tilde{\sigma} = (\alpha + \gamma + c_0) - (4\alpha\gamma + \alpha + \gamma + c_0 + c_2)\,\xi^2$$

$$\xi = \frac{x}{a}, \quad \frac{d}{dx} = \frac{1}{a}\frac{d}{d\xi}, \quad \frac{d^2}{dx^2} = \frac{1}{a^2}\frac{d^2}{d\xi^2}$$

$$c_0 = \frac{2ma^2E}{\hbar^2}, \quad c_2 = \frac{m^2\omega^2a^4}{\hbar^2}$$

Nikiforov-Uvarov method

$$\psi = \varphi(\xi)\, y, \quad \varphi(\xi) = e^{\int \frac{\pi(\xi)}{\sigma(\xi)} d\xi}.$$

$\pi(\xi)$ is a first degree polynomial

Nikiforov-Uvarov method – polynomial solution

$$y'' + \frac{\tau}{\sigma} y' + \frac{\bar{\sigma}}{\sigma^2} y = 0$$

$$\tau = 2\pi + \tilde{\tau} \text{ and } \bar{\sigma} = \tilde{\sigma} + \pi^2 + \pi\left(\tilde{\tau} - \sigma'\right) + \pi'\sigma$$

$$\bar{\sigma} = \lambda\sigma, \quad \lambda = const.$$

Nikiforov-Uvarov method – polynomial solution-2

$$\sigma(\xi)y'' + \tau(\xi)y' + \lambda y = 0.$$

$$\pi^2(\xi) + \left[\tilde{\tau}(\xi) - \sigma'(\xi)\right]\pi(\xi) + \tilde{\sigma}(\xi) - \mu\sigma(\xi) = 0$$

$$\mu = \lambda - \pi'(\xi)$$

Wavefunction

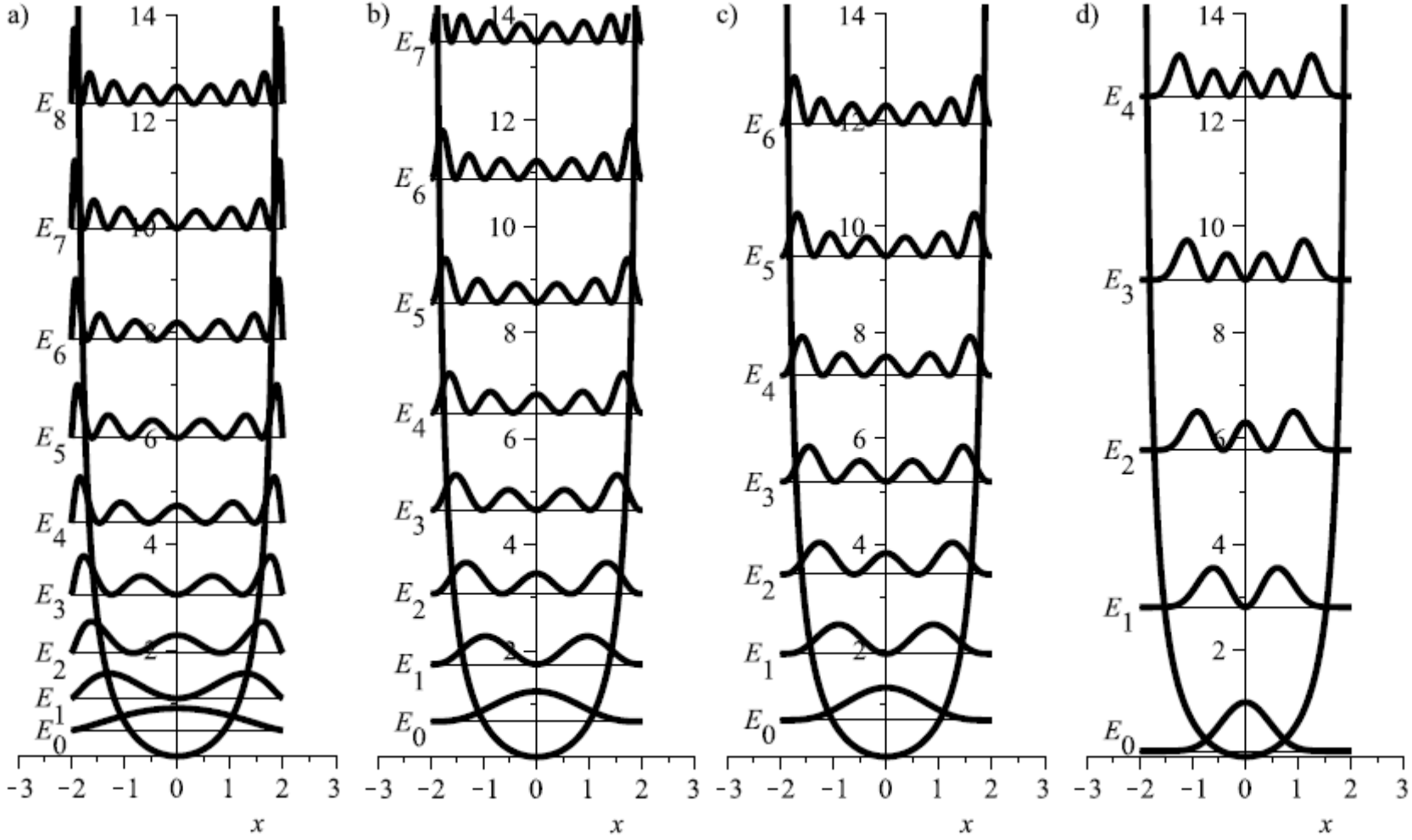
$$\psi_n^{vR}(x) = c_n^{vR}\left(1-\frac{x^2}{a^2}\right)^{\frac{1}{2}\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha\gamma}} C_n^{\left(\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha\gamma}+\frac{1}{2}\right)}\left(\frac{x}{a}\right)$$

$$c_n^{vR} = 2^{\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha\gamma}}\Gamma\left(\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha\gamma}+\frac{1}{2}\right)\sqrt{\frac{\left(n+\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha\gamma}+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+2\sqrt{\frac{m^2\omega^2a^4}{\hbar^2}+4\alpha\gamma}+1\right)}}$$

$$\int_{-a}^{a}\left[\psi_m^{vR}(x)\right]^*\psi_n^{vR}(x)dx = \delta_{mn}$$

Energy spectrum

$$E_n^{vR} = \hbar\sqrt{\omega^2 + 4\alpha\gamma\frac{\hbar^2}{m^2a^4}}\left(n+\frac{1}{2}\right) + \frac{\hbar^2}{2ma^2}\left(n^2+n+\beta+1\right)$$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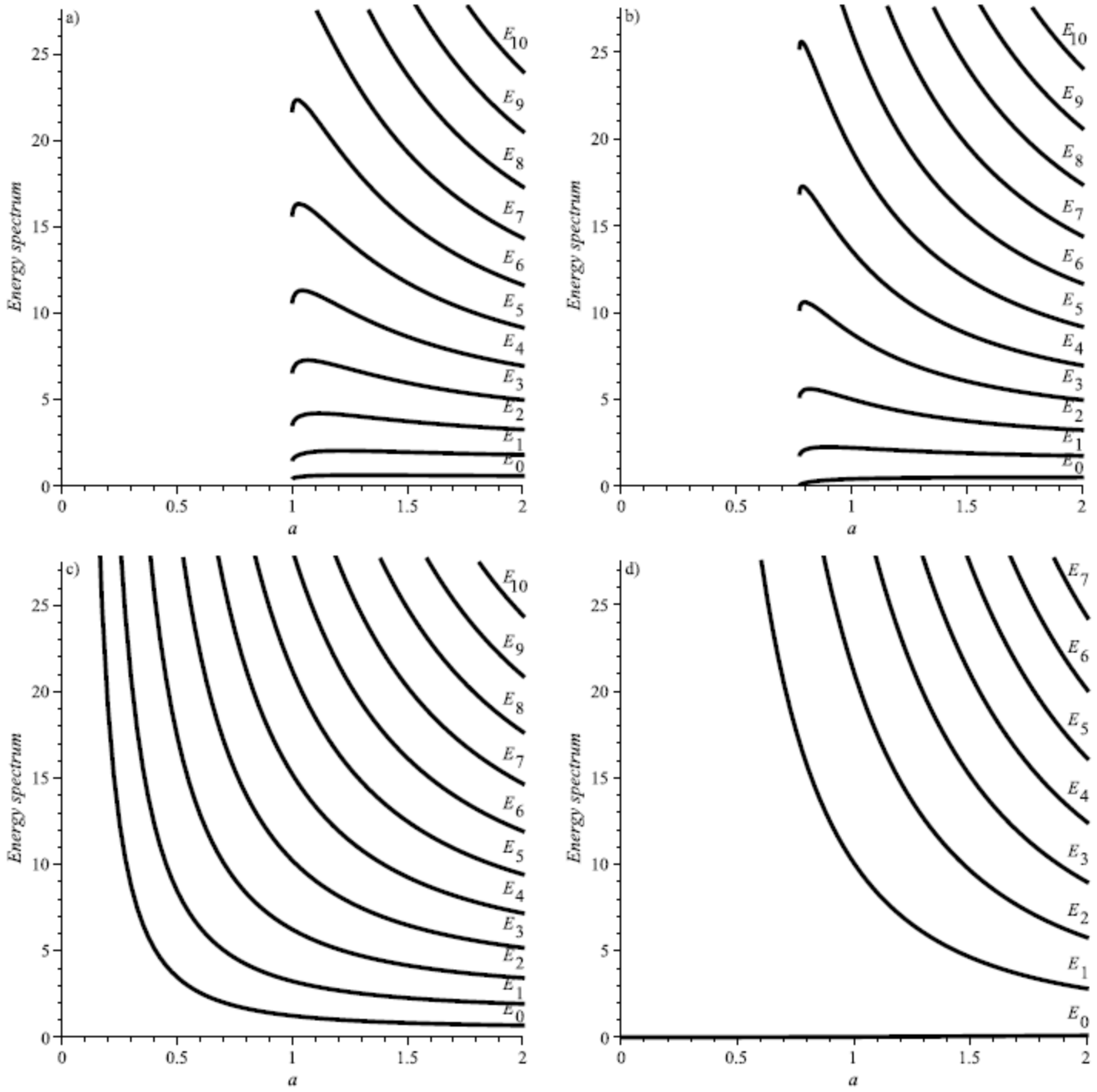
a)
b)
c)
d)
Energy spectrum
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E_2
E_3
E_4
E_5
E_6
E_7
E_8
E_9
E_{10}
0
0.5
1
1.5
2
5
10
15
20
25

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Thank you for your attention!