Energetic Spectrum of a Particle in Three-Dimensional Infinite Potential Square Well in Point of View of Number Theory and Bayesian Statistics

Pavel JAHODA, Jan KRACIK, David ULCAK

Department of Applied Mathematics, Faculty of Electrical Engineering and Computer Science, VSB–Technical University of Ostrava, 17. listopadu 15/2172, 708 33 Ostrava, Czech Republic

pavel.jahoda@vsb.cz, jan.kracik@vsb.cz, david.ulcak.st@vsb.cz

DOI: 10.15598/aeee.v15i2.2248

Abstract. *Using results of number theory we develop an approximate statistical model of energy levels of particles in a three-dimensional infinite potential well depending on whether there is exactly one particle or more than one particles in the well. The model is used to perform a statistical inference about the number of particles in the well. The estimation procedure is developed within the Bayesian framework.*

Keywords

Asymptotic density, Bayesian inference, number theory, potential well.

1. Introduction

An idealized statistical model of a potential well is considered in this article. Its link with some of known results of number theory and quantum physics is described.

Theoretical model of a finite potential square well has found its application in theory of quantum well lasers [8]. Quantum well structures can be grown by Molecular Beam Epitaxy (MBE) [2] and then used in active regions of lasers [1]. Models of finite potential square wells can be approximated by a model of an infinite potential square well.

We use number theory to describe and distinguish energetic spectrum of a single particle enclosed within a cubic potential well from energetic spectrum of total energy of a system of several particles. Measured values of total energy are used to estimate whether there is only one or more particles in the potential well.

We are concerned with a well-known model of a three-dimensional infinite potential square well. Infinite depth of the well could be interpreted as the infinite stiffness of walls of this cube. Thus, a particle does not loose anything of its energy by collisions with walls. Potential energy V of a particle is equal to 0 inside the well and $V = \infty$ outside. In other words, it is impossible for a particle to leave the well.

Solving stationary Schrodinger equation we obtain the energetic spectrum of a particle enclosed within a cubic potential well with an edge of length l. It is given by the formula

$$E = (a^2 + b^2 + c^2)\frac{\hbar^2\pi^2}{2ml^2}, \tag{1}$$

where m is a mass of the particle, $\hbar$ is the reduced Planck constant, and $a, b, c \in \mathbb{N}$, referred to as quantum numbers, describe a state of the particle. For details see, e.g. [11].

It follows from the formula Eq. (1) that

$$\frac{E}{\frac{\hbar^2\pi^2}{2ml^2}} = a^2 + b^2 + c^2, \tag{2}$$

belongs to the set of natural numbers. It means that the rescaled energy on the left–hand side of Eq. (2) of a single particle belongs to the set $S_E = \{a^2 + b^2 + c^2 : a, b, c \in \mathbb{N}\}$. We call this set an energetic spectrum. From now on we assume that the total energy is expressed in this rescaled form.

We would like to estimate the probability that a randomly chosen natural number from the interval $\langle 1, n\rangle$,

$n \in \mathbb{N}$, belongs to the set S_E. For "large" n we approximate this probability by the number

$$d(S_E) = \lim_{n\to\infty} \frac{S_E(n)}{n}, \tag{3}$$

where $S_E(n)$ is a number of elements of the set S_E which are less than or equal to n. The number $d(S_E)$ is called the asymptotic density of the set S_E.

2. Asymptotic Density of the Spectrum

Asymptotic density of the set $A \subseteq \mathbb{N}$, well-known concept from number theory, is defined as follows.

Definition 1. *Let $A \subseteq \mathbb{N}$. A number of elements of the set $A \subseteq \mathbb{N}$, which are less than or equal to n, is denoted by $A(n)$. The number $\bar{d}(A)$, where*

$$\bar{d}(A) = \limsup_{n\to\infty} \frac{A(n)}{n}, \tag{4}$$

is called upper asymptotic density of the set A and the number $\underline{d}(A)$, where

$$\underline{d}(A) = \liminf_{n\to\infty} \frac{A(n)}{n}, \tag{5}$$

is called lower asymptotic density of the set A.

If $\bar{d}(A) = \underline{d}(A)$, then value $d(A) = \bar{d}(A) = \underline{d}(A) = \lim_{n\to\infty} \frac{A(n)}{n}$ is called asymptotic density of set A.

We immediately obtain from the definition the following basic properties of asymptotic density, which are further used.

Lemma 1. *Let $A \subseteq \mathbb{N}$. Then $\bar{d}(A)$ and $\underline{d}(A)$ exist and the following statements hold:*

1. $d(\mathbb{N}) = 1$.
2. $0 \le \underline{d}(A) \le \bar{d}(A) \le 1$.
3. *Let $K \subseteq \mathbb{N}$ be a finite set. If $d(A)$ exists, then it holds that $d(A \cup K) = d(A - K) = d(A)$.*
4. *Let $A, D, \Omega \subseteq \mathbb{N}$, $A \cap D = \emptyset$ and $A \cup D = \Omega$. If there exist $d(\Omega)$ and $d(D)$, then it holds that $d(A) = d(\Omega) - d(D)$.*
5. *Let $A, D \subseteq \mathbb{N}$ and $A = \mathbb{N} - D$. If $d(D)$ exists, then $d(A) = 1 - d(D)$.*
6. *Let $A \subseteq B \subseteq \mathbb{N}$ and $d(B)$ exists. It holds that $0 \le \underline{d}(A) \le \bar{d}(A) \le d(B) \le 1$.*

Proof. The statements follow from basic properties of limes superior and limes inferior of sequences and from the following facts:

- For every natural number n it holds $0 \le A(n) \le n$.
- If $K \subseteq \mathbb{N}$ is a finite set, then there exists $k \in \mathbb{N}$ such that for every sufficiently large $n \in \mathbb{N}$ it holds $A(n) \le (A \cup K)(n) \le A(n) + k$ and $A(n) \ge (A - K)(n) \ge A(n) - k$.
- If $A \cap D = \emptyset$ and $A \cup D = \Omega$, then for every natural number n it holds $\Omega(n) = (A \cup D)(n) = A(n) + D(n)$.
- If $A \subseteq B$ and $d(B)$ exists, then $\forall n \in \mathbb{N} : \frac{A(n)}{n} \le \frac{B(n)}{n}$ and thus:

$$\bar{d}(A) = \limsup_{n\to\infty} \frac{A(n)}{n} \le \limsup_{n\to\infty} \frac{B(n)}{n} = d(B). \tag{6}$$

□

We introduce two important theorems which we use later to determine the asymptotic density of spectrum.

Theorem 1 (Legendre)**.** *Let $n \in \mathbb{N}$. Then n can be represented as $n = a^2 + b^2 + c^2$, $a, b, c \in \mathbb{Z}$ if and only if $n \neq 4^{j-1}(8k + 7)$, $j, k \in \mathbb{N}$.*

The proof can be found e.g. in [6].

Theorem 2 (Bachet's conjecture)**.** *Every $n \in \mathbb{N}$ can be represented as $n = a^2 + b^2 + c^2 + d^2$, $a, b, c, d \in \mathbb{Z}$.*

The proof can be found e.g. in [7].

We determine asymptotic density of energetic spectrum of a single particle at first.

Theorem 3. *If $S_E = \{a^2 + b^2 + c^2 : a, b, c \in \mathbb{N}\}$, then $d(S_E) = \frac{5}{6}$.*

Proof. Let us denote $B_3 = \{a^2 + b^2 + c^2 \in \mathbb{N} : a, b, c \in \mathbb{Z}\}$ a $B_2 = \{a^2 + b^2 \in \mathbb{N} : a, b \in \mathbb{Z}\}$. Then

$$B_3 - B_2 \subseteq S_E \subseteq B_3. \tag{7}$$

First, we determine $d(B_2)$. It is known (see [11] and [5]) that $B_2(n) = \frac{c.n}{\sqrt{\log n}} + o(1)$. Hence $d(B_2) = \lim_{n\to\infty} \frac{B_2(n)}{n} = 0$.

We determine $d(B_3)$ now. Theorem 1 says that a natural number n can be expressed as a um of three squares of integers if and only if the number n does not belong to the set $A = \{4^j(8k-1) \mid j \in \mathbb{N} \cup \{0\}, k \in \mathbb{N}\}$. We can see that

$$B_3 = \mathbb{N} - A. \tag{8}$$

We prove that $d(A) = \frac{1}{6}$.

It can be easily verified that sets $A_j = \{4^j(8k-1) \,|k \in \mathbb{N}\}$, $j \in \mathbb{N} \cup \{0\}$ are pairwise disjoint and

$$A_j(n) = \left[\frac{1}{4^j}\frac{n}{8} + \frac{1}{8}\right]. \tag{9}$$

Since $A = \cup_{j=0}^{\infty} A_j$ and sets A_j are pairwise disjoint, it must hold

$$A(n) = \sum_{j=0}^{j_n} \left[\frac{1}{4^j}\frac{n}{8} + \frac{1}{8}\right], \tag{10}$$

where j_n is the least integer such that there exists $k \in \mathbb{N}$ satisfying $4^{j_n}(8k-1) \leq n$. Hence

$$\begin{aligned} 4^{j_n}(8\cdot 1 - 1) \quad &\leq \quad n \quad < \quad 4^{j_n+1}(8\cdot 1 - 1) \\ j_n \leq \frac{\ln n - \ln 7}{\ln 4} &< j_n + 1, \end{aligned} \tag{11}$$

and we find out that $j_n = \left[\frac{\ln n - \ln 7}{\ln 4}\right]$.

Thus

$$\frac{A(n)}{n} = \frac{1}{n}\sum_{j=0}^{\left[\frac{\ln n - \ln 7}{\ln 4}\right]} \left(\frac{1}{4^j}\frac{n}{8} + \frac{1}{8} - \varepsilon_j\right), \tag{12}$$

where $0 \leq \varepsilon_j < 1$.

With $n \to \infty$ we obtain $d(A) = \frac{1}{6}$. From Eq. (8) it follows that $d(B_3) = 1 - \frac{1}{6} = \frac{5}{6}$. And using Eq. (7) we get

$$\begin{aligned} d(B_3) - d(B_2) \quad \leq \quad \underline{d}(S_E) \quad \leq \quad \overline{d}(S_E) \quad \leq \quad d(B_3) \\ \tfrac{5}{6} - 0 \quad \leq \quad \underline{d}(S_E) \quad \leq \quad \overline{d}(S_E) \quad \leq \quad \tfrac{5}{6} \\ d(S_E) = \frac{5}{6}. \end{aligned} \tag{13}$$

□

The following theorem will be useful in the next section.

Theorem 4. *Let* $E_k = \{n_1^2 + n_2^2 + \cdots + n_k^2 : n_1, n_2, \ldots, n_k \in \mathbb{N}\}$. *Then for every* $k \in \mathbb{N}$, $k \geq 4$ *it holds that* $d(E_k) = 1$.

Proof. We will prove this theorem by induction with respect to k. First, we will show that $d(E_4) = 1$.

Let us denote $B_4 = \{n_1^2 + n_2^2 + n_3^2 + n_4^2 : n_1, n_2, n_3, n_4 \in \mathbb{Z}\}$. Lagrange four square theorem (Bachet's conjecture) says that $B_4 = \mathbb{N}$. Furthermore, it is known (see [3] and sequence A000534 in the OEIS) that

$$E_4 = B_4 - A, \tag{14}$$

where $A = A_1 \cup A_2 \cup A_3 \cup A_4$, $A_1 = \{1, 3, 5, 9, 11, 17, 29, 41\}$, $A_2 = \{2 \cdot 4^m : m \in \mathbb{N} \cup \{0\}\}$, $A_3 = \{6 \cdot 4^m : m \in \mathbb{N} \cup \{0\}\}$, $A_4 = \{14 \cdot 4^m : m \in \mathbb{N} \cup \{0\}\}$.

It is obvious that for a sufficiently large n it holds $A_1(n) = 8$, $A_2(n) = \left[\frac{\ln n - \ln 2}{\ln 4}\right]$, $A_3(n) = \left[\frac{\ln n - \ln 6}{\ln 4}\right]$ and $A_4(n) = \left[\frac{\ln n - \ln 14}{\ln 4}\right]$. Thus $d(A_1) = d(A_2) = d(A_3) = d(A_4) = d(A) = 0$ and, using Eq. (14), it follows that $d(E_4) = d(B_4) = d(\mathbb{N}) = 1$.

Now, let us assume that $d(E_k) = 1$ and let us denote $B = \{n_1^2 + n_2^2 + \cdots + n_k^2 + 1^2 : n_1, n_2, \ldots, n_k \in \mathbb{N}\}$. It holds that

$$B \subseteq E_{k+1} \subseteq \mathbb{N}. \tag{15}$$

For a sufficiently large n it holds $B(n) = E_k(n-1)$. Hence $d(B) = d(E_k) = 1$ and from Eq. (15) it follows that $d(E_{k+1}) = 1$.

□

3. Statistical Inference

The three-dimensional infinite potential square well is just a simplified model approximating physical potential wells which exist in real world. Even so, let us assume that such potential wells are available and we want to decide whether there is exactly one particle or there are more particles in a particular well. For that purpose we perform a virtual experiment based on repeated measurements of total energy of the system. We assume certain "ideal" properties of the particles: They are all of the same kind and they do not interact with each other.

We already know that energy E of a single particle belongs to the set S_E (Eq. (2)) with the asymptotic density $\frac{5}{6}$ (Thm. 3). If there are $k \geq 2$ particles in the well, the total energy of the system is equal to a sum of $3k$ squares of natural numbers. It means that in this case (Thm. 4) the total energy of the particles can be equal to an arbitrary value from $\mathbb{N}$ excluding a set of zero asymptotic density.

Now, suppose, that we are able to change the energy in a potential well and measure it repeatedly. Moreover, we suppose that the measurements are independent. Under appropriate conditions the asymptotic density of S_E can be used to establish a statistical model of observed energies depending on the number of particles in the well. Particularly, if there is exactly one particle in the well, then the energy is surely in S_E. If there are more than one particle, then we approximate the probability that the energy is in S_E with the asymptotic density $d(S_E)$. The model can be accepted under quite general conditions: Let us denote with $p(\epsilon)$ the probability that a system with multiple particles has energy equal to ϵ. The probability that

the energy is in S_E is then $\sum_{\epsilon\in S_E} p(\epsilon)$. The approximate equality

$$\sum_{\epsilon\in S_E} p(\epsilon) \approx d(S_E), \tag{16}$$

is satisfied, e.g., if the energy E is approximately uniformly distributed on a set $\{1,\dots,N\}$, where $N\in\mathbb{N}$ is large enough so that $\frac{S_E(N)}{N} \approx d(S_E)$. Another condition under which Eq. (16) is satisfied is that $p(\epsilon)$ is concentrated on a discrete interval $\{M,\dots,N\}$ where $M,N\in\mathbb{N}$ are large enough so that

$$\frac{S_E(N)-S_E(M)}{N-M} \approx d(S_E), \tag{17}$$

and points in S_E are approximately uniformly distributed on $\{M,\dots,N\}$. For example, if $M=1, N=10^4$ and $p(\epsilon)$ is the probability mass function of the binomial distributions with parameters $(10^4, 0.5)$, we get $\sum_{\epsilon\in S_E} p(\epsilon) - d(S_E) \doteq -0.002$.

Remark 1. *We can verify whether measured energy E belongs to S_E algorithmically, see [9].*

In what follows we derive a statistical procedure through which the number of particles can be inferred. Bayesian paradigm [10] is used for this purpose as it allows to employ prior knowledge. In problems of this type the prior information can be naturally acquired from similar experiments.

3.1. Notational Remarks

In this section random variables are denoted by uppercase Roman or Greek letters and their values by corresponding lowercase letters. However, often the random variables and their values need not be formally distinguished. In such cases lowercase letters are used whereas the exact meaning is clear from the context. All probability density functions – conditional as well as non-conditional – are solely denoted by the symbol f. Random variables to which they are related are distinguished by the arguments. For example, $f(x,y)$ denotes the joint density of the random vector (X,Y) at the point (x,y), $f(x)$ is the marginal density of X at x , and $f(x|y)$ is the conditional density of X at x given $Y=y$. By $f(x|y=\xi)$ we denote the conditional density of X at x given $Y=\xi$. Random vector $(X_1,X_2,\dots,X_t)$ and its value $(x_1,x_2,\dots,x_t)$ are denoted by $X_{1:t}$ and $x_{1:t}$, respectively.

Throughout this section the distributions of random variables are assumed to have densities with respect to either Lebesgue measure on $\mathbb{R}$ or counting measure on $\mathbb{N}_0 = \mathbb{N}\cup\{0\}$. Distributions of random vectors are represented by densities with respect to a suitable product measure.

3.2. Bayesian Approach

Within the Bayesian paradigm the beliefs about the values of unknown quantities are represented with probability measures. In other words, the unknown quantities are taken as random quantities. Let θ be an unknown (vector) parameter. Its probability density function $f(\theta)$, referred to as prior probability density, is determined by the statistician so that it reflects the available prior information about θ, i.e., the knowledge which is available before data are observed or processed. The statistical model which describes dependence of a random quantity x on the unknown parameter θ is now understood as a conditional density $f(x|\theta)$. After observing the value of x the conditional density $f(\theta|x)$ represents the overall knowledge about the parameter θ. It can be taken as a prior knowledge combined with the information acquired from data. The conditional density $f(\theta|x)$ is referred to as posterior density and relates to the model and prior density via Bayes rule

$$f(\theta|x) = \frac{f(x|\theta)f(\theta)}{f(x)}, \tag{18}$$

where

$$f(x) = \int f(x|\theta)f(\theta)\mathrm{d}\theta. \tag{19}$$

The integral Eq. (19) is understood as a Lebesgue integral over the range of θ with respect to the appropriate measure.

Because the denominator in Eq. (18) is completely determined by the product in the nominator the relation Eq. (18) can be shorten to

$$f(\theta|x) \propto f(x|\theta)f(\theta), \tag{20}$$

where $\propto$ means proportionality up to a constant independent of θ. Bayesian calculations are typically made easier with this convention.

3.3. Statistical Model

In what follows it is assumed that individual realizations of a potential well are produced under identical conditions, whereas the numbers of particles in individual wells are independent. Each well is repeatedly inspected by measuring the total energy of particles in the system. Before each measurement the energy of the system is randomly changed so that the energies measured for a particular well can be taken as independent random quantities. Moreover, the energies are assumed to be uniformly distributed over $\{1,2,\dots,N\}$ for some large $N\in\mathbb{N}$. For simplicity it is also assumed the same number, say $n\in\mathbb{N}$, of measurements is done for each well.

Let k_i be a number of particles in the i-th potential well and $E_{i,j}$ be a result of j-th energy measurement in

the i-th well. We define the following random variables:

$$s_i = \begin{cases} 0 \text{ if } k_i > 1, \\ 1 \text{ if } k_i = 1, \end{cases} \tag{21}$$

$$m_i = \begin{cases} 0 \text{ if } \exists j \in \{1,2,\ldots,n\}: \ E_{i,j} \notin S_E, \\ 1 \text{ if } \forall j \in \{1,2,\ldots,n\}: \ E_{i,j} \in S_E. \end{cases}$$

In words, $s_i = 1$ if there is a single particle in the i-th well and $m_i = 1$ iff all of the energy measurements of the i-th system can be expressed as a sum of three squares of natural numbers. The variables s_i are not observed and constitute a part of unknown parameter vector, while m_i are observed and their values represent data.

The statistical model through which the data m_i are related to the unobserved states s_i is now given by

$$f(m_i|s_i=0) = \begin{cases} 1-\left(\frac{5}{6}\right)^n \text{ if } m_i = 0, \\ \left(\frac{5}{6}\right)^n \text{ if } m_i = 1, \end{cases} \tag{22}$$

$$f(m_i|s_i=1) = \begin{cases} 0 \text{ if } m_i = 0, \\ 1 \text{ if } m_i = 1. \end{cases}$$

From the assumptions formulated at the beginning of this subsection it follows that the parameters s_i can be modelled as conditionally independent Bernoulli random variables given the probability that a well contains exactly one particle. This probability, denoted θ, does not change across individual potential wells and it is assumed to be unknown. Thus, θ is another part of the parameter vector. The joint density of $s_{1:t}$, for any $t \in \mathbb{N}$, given θ is then

$$f(s_{1:t}|\theta) = \prod_{i=1}^{t} f(s_i|\theta), \tag{23}$$

where

$$f(s_i|\theta) = \begin{cases} 1-\theta \text{ if } s_i = 0, \\ \theta \text{ if } s_i = 1. \end{cases} \tag{24}$$

To specify the prior density of the parameter $(s_{1:t}, \theta)$ completely it remains to select a marginal prior distribution of θ. For simplicity, the prior density is selected as a beta density being a conjugate prior for the Bernoulli model, i.e.,

$$f(\theta) = \begin{cases} \dfrac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{B(\alpha,\beta)} & \text{for } \theta \in [0,1], \\ 0 & \text{for } \theta \notin [0,1]. \end{cases} \tag{25}$$

$B(\cdot,\cdot)$ in Eq. (25) denotes the beta function. If no relevant prior information is available before the first measurement, the parameters can be set to $(\alpha,\beta) = (\frac{1}{2},\frac{1}{2})$, which corresponds to a non-informative Jeffreys prior for the Bernoulli model. For details see, e.g., [10].

The energy levels E_{ij} and thus also data m_i depend only on the corresponding parameters s_i, i.e., given s_i data m_i are conditionally independent of all other quantities. Particularly, for all $t \in \mathbb{N}$ we get

$$f(m_{1:t}|s_{1:t},\theta) = \prod_{i=1}^{t} f(m_i|s_i). \tag{26}$$

The joint density of $m_{1:t}, s_{1:t}, \theta$ thus can be factorized as follows:

$$f(m_{1:t}, s_{1:t}, \theta) = \left(\prod_{i=1}^{t} f(m_i|s_i) f(s_i|\theta)\right) f(\theta). \tag{27}$$

The conditional independence structure can be represented through a directed acyclic graph (DAG) $D = (V,H)$ at Fig. 1 with V and H being a set of vertices and a set of edges, respectively. Its vertices are the random quantities $\theta, s_1, \ldots, s_t, m_1, \ldots m_t$. The joint probability density function Eq. (27) is factorized with respect to D in the following sense:

$$f(\theta, s_1, \ldots, s_t, m_1, \ldots m_t) = \prod_{x \in V} f(x|Pa(x)), \tag{28}$$

where $Pa(x)$ denotes a random vector represented by the parents of node x.

From Eq. (27) any conditional or marginal density of interest can be derived. Namely, for the posterior density of θ we get

$$\begin{aligned} f(\theta|m_{1:t}) &\propto f(m_{1:t}|\theta) f(\theta) = \\ &= \sum_{s_{1:t} \in \{0,1\}^t} \left(\prod_{i=1}^{t} f(m_i|s_i) f(s_i|\theta)\right) f(\theta) \\ &= \left(\prod_{i=1}^{t} \sum_{s_i \in \{0,1\}} f(m_i|s_i) f(s_i|\theta)\right) f(\theta). \end{aligned} \tag{29}$$

Denoting $v_t = \sum_{i=1}^{t} m_i$, the posterior density can be written

$$\begin{aligned} &f(\theta|m_{1:t}) \\ &\quad \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}\left(\left(1-\left(\tfrac{5}{6}\right)^n\right)(1-\theta)\right)^{t-v_t} \\ &\qquad \left(\left(\tfrac{5}{6}\right)^n (1-\theta)+\theta\right)^{v_t} \\ &\quad \propto \theta^{\alpha-1}\left(\left(\tfrac{5}{6}\right)^n (1-\theta)+\theta\right)^{v_t} (1-\theta)^{\beta+t-v_t-1}, \end{aligned} \tag{30}$$

for $\theta \in [0,1]$ and $f(\theta|m_{1:t}) = 0$ for $\theta \notin [0,1]$.

The main concern is in a probability distribution of a number of particles in, say, the $(t+1)$-th system given the measurements of the energies in the system and all preceding measurements which serve as a source of prior information about the $(t+1)$-th system. The conditional density $f(s_{t+1}|m_{1:t}, m_{t+1})$ can be again de-

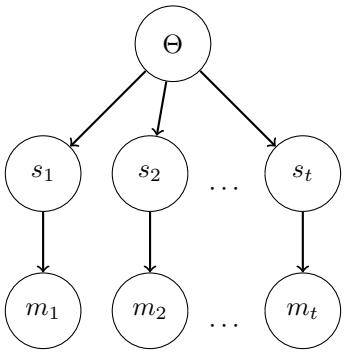


Fig. 1: DAG representing conditional independence structure.

rived from Eq. (27) for $(t+1)$ instead of t.

$$\begin{aligned} f(s_{t+1}|m_{1:t}, m_{t+1}) &\propto f(s_{t+1}, m_{1:t}, m_{t+1}) \\ &= \int_0^1 \sum_{s_{1:t}\in\{0,1\}^t} f(s_{1:t}, m_{1:t}, \theta) \\ &\quad f(m_{t+1}|s_{t+1}) f(s_{t+1}|\theta)\mathrm{d}\theta \\ &\propto f(m_{t+1}|s_{t+1}) \int_0^1 f(s_{t+1}|\theta) f(\theta|m_{1:t})\mathrm{d}\theta. \end{aligned} \tag{31}$$

Particularly, we get

$$f(s_{t+1}|m_{1:t}, m_{t+1}=0) = \begin{cases} 1 & \text{if } s_{t+1}=0, \\ 0 & \text{if } s_{t+1}=1, \end{cases} \tag{32}$$

and

$$\begin{aligned} &f(s_{t+1}|m_{1:t}, m_{t+1}=1) \\ &= \begin{cases} \dfrac{\left(\frac{5}{6}\right)^n \int_0^1 (1-\theta) f(\theta|m_{1:t})\mathrm{d}\theta}{Z_t} & \text{if } s_{t+1}=0, \\ \dfrac{\int_0^1 \theta f(\theta|m_{1:t})\mathrm{d}\theta}{Z_t} & \text{if } s_{t+1}=1, \end{cases} \end{aligned} \tag{33}$$

where

$$\begin{aligned} Z_t = \left(\tfrac{5}{6}\right)^n \int_0^1 (1-\theta) f(\theta|m_{1:t})\mathrm{d}\theta + \\ \int_0^1 \theta f(\theta|m_{1:t})\mathrm{d}\theta. \end{aligned} \tag{34}$$

3.4. Simulations

In this paragraph we give several illustrative examples of posterior densities derived above. In all of the examples the prior density is selected as the Jeffreys prior. We start with posterior densities $f(\theta|m_{1:t})$ estimated from simulated data for various numbers of measurements in each well, namely $n = 2, 10, 20$, and various numbers of produced wells t. The true value of the parameter θ used for simulation is $\theta = 0.3$. The posterior densities are plotted in Fig. 4. From the graphs it is seen how increasing number of observations, i.e., number of measurements in each well and/or number of wells, provides more information about the unknown parameter θ. With increasing number of observations the posterior densities gradually concentrate about the true value $\theta = 0.3$.

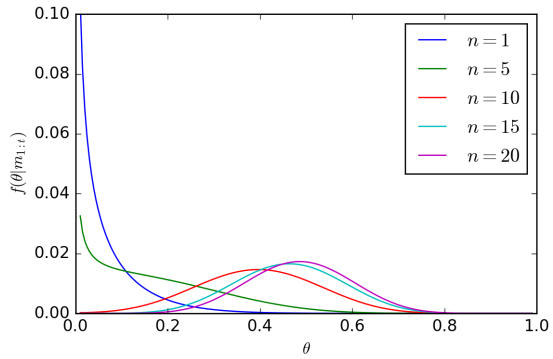


Fig. 2: Posterior density $f(\theta|m_{1:t})$ for $t = 20, v_t = 10$, and $n = 1, 5, 10, 15, 20$.

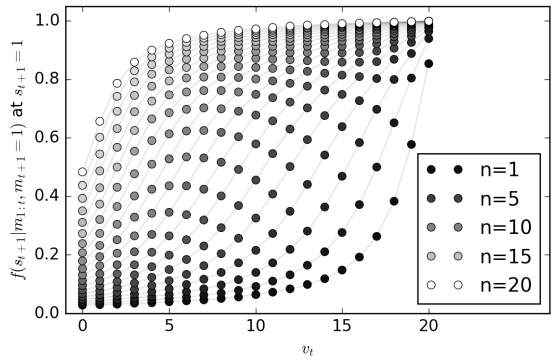
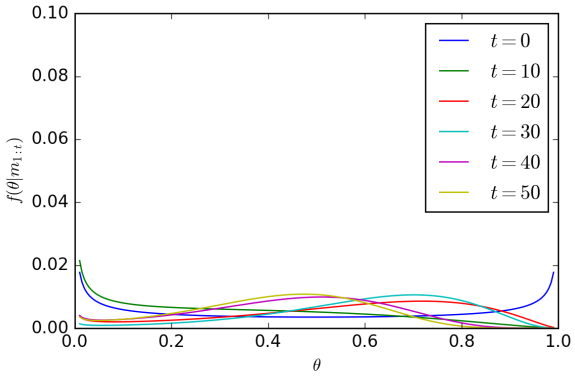


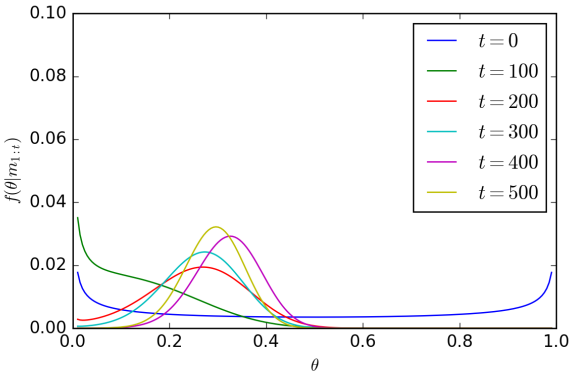
Fig. 3: Density $f(s_{t+1}|m_{1:t}, m_{t+1}=1)$ at $s_{t+1}=1$ for $t = 20, v_t = 0, \ldots, 20$, and $n = 1, \ldots, 20$.

Figure 2 illustrates five examples of posterior densities $f(\theta|m_{1:t})$ for different numbers of measurements n in each well. Namely, we assume $t = 20, v_t = 10$, and $n = 1, 5, 10, 15, 20$. In this case the data are not sampled. Instead, it is assumed that for 10 of the 20 wells all measured energies were in the set S_E. Although t and v_t are the same in all situations, the acquired information about θ naturally varies with increasing number of measurements n.

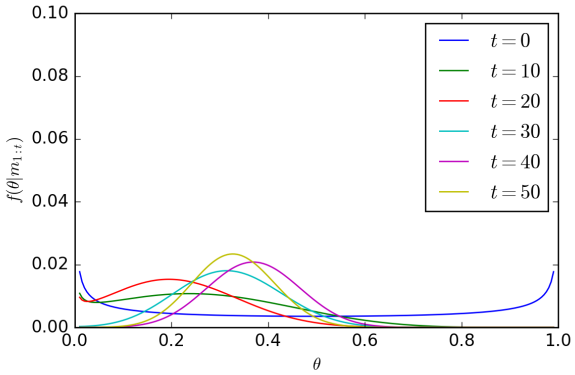
Finally, in Fig. 3 it is shown how the density $f(s_{t+1}|m_{1:t}, m_{t+1})$ with $m_{t+1} = 1$ depends on previous observations (represented by v_t) for different n. For $t = 20, v_t = 0, \ldots, 20$, and $n = 1, \ldots 20$ the values of $f(s_{t+1}|m_{1:t}, m_{t+1}=1)$ at $s_{t+1} = 1$ are plotted.



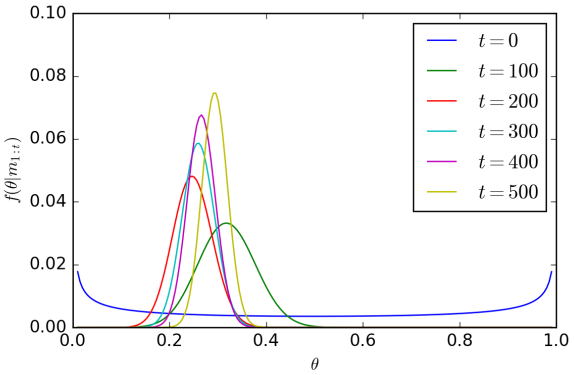
(a) $n = 2$



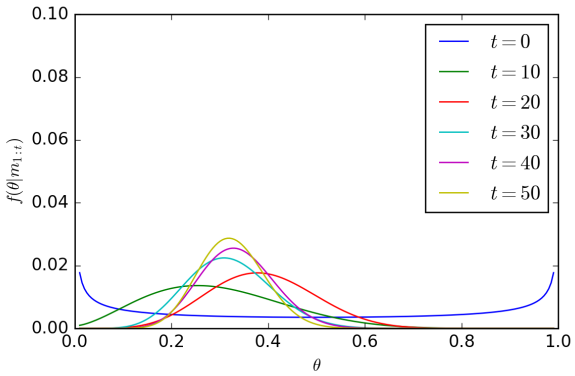
(b) $n = 2$



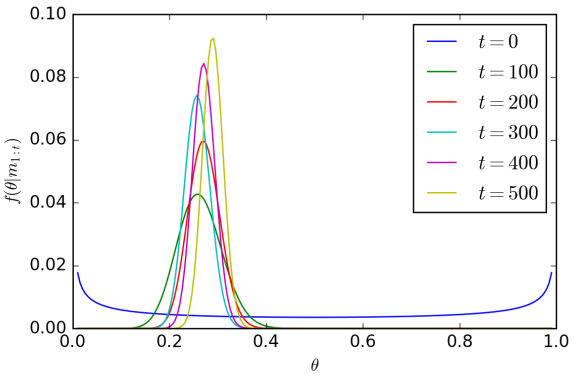
(c) $n = 10$



(d) $n = 10$



(e) $n = 20$



(f) $n = 20$

Fig. 4: Posterior densities $f(\theta|m_{1:t})$ estimated from simulated measurements for $n = 2, 10, 20$ depending on a number of potential wells t. True $\theta = 0.3$.

4. Conclusions

The considered model of a potential well is definitely an idealized one. In this case known results of number theory can be used to derive a simple statistical model of the energy levels. In the future it would be interesting to compare the model with models constructed under more realistic assumptions including, e.g., finiteness of the well or specific assumptions about particle energies. Nevertheless, with more realistic models the posterior and predictive densities will be intractable and Monte Carlo algorithms or other approximation techniques will be required.

Acknowledgement

The work is supported by Grant of SGS No. SP2017/56, VSB–Technical University of Ostrava, Czech Republic.

References

[1] FAIST, J., F. CAPASSO, D. L. SIVCO, C. SIRTORI, A. L. HUTCHINSON and A. Y. CHO. Quantum Cascade Laser. *Science*. 1994, vol. 264, iss. 5158, pp. 553–556. ISSN 0036-8075. DOI: 10.1126/science.264.5158.553.

[2] CHO, A. Y. Advances in molecular beam epitaxy. *Journal of Crystal Growth*. 1991, vol. 111, iss. 1–4, pp. 1–13. ISSN 0022-0248. DOI: 10.1016/0022-0248(91)90938-2.

[3] GROSSWALD, E. *Representations of Integers as Sums of Squares*. New York: Springer-Verlag, 1985. ISBN 978-1461385684.

[4] LANDAU, E. Uber die Einteilung der positiven ganzen Zahlen in vier Klassen nach der Mindeszahl der zu ihrer additiven Zusammensetzung erforderlichen Quadrate. *Archiv der Mathematik und Physik*. 1908, vol. 13, pp. 305–312.

[5] RIEGER, G. J. Zum Satz von Landau uber die Summe aus zwei Quadraten. *Journal fur die reine und angewandte Mathematik*. 1970, vol. 244, pp. 198–200.

[6] HEASLET, M. A. and J. V. USPENSKY. *Elementary number theory*. New York: McGraw-Hill, 1939.

[7] HARDY, G. H. and E. M. WRIGHT. *An Introduction to the Theory of Numbers*. New York: Oxford University Press, 1979. ISBN 978-0198531715.

[8] ZORY, P. S. *Quantum Well Lasers*. San Diego: Academic Press, 1993. ISBN 978-0127818900.

[9] RABIN, M. O. and J. O. SHALLIT. Randomized Algorithms in Number Theory. *Communications on Pure and Applied Mathematics*. 1986, vol. 39, iss. S1, pp. S239–S256. ISSN 1097-0312. DOI: 10.1002/cpa.3160390713.

[10] ROBERT, C. P. *The Bayesian choice: from decision-theoretic foundations to computational implementation*. New York: Springer, 2007. ISBN 978-0387715988.

[11] LANDAU, L. D. and E. M. LIFSHITZ. *Quantum Mechanics (Non-Relativistic Theory): Course of Theoretical Physics Volume 3*. Oxford: Pergamon Press, 1977. ISBN 978-0080209401.

About Authors

Pavel JAHODA was born in Ostrava, Czech Republic. He received his Ph.D. from University of Ostrava in 2006. His research interests include analytic and statistical number theory.

Jan KRACIK was born in Opava, Czech Republic. He received his Ph.D. from Czech Technical University in Prague in 2009. His research interests include applied statistics and Bayesian decision making.

David ULCAK was born in Brno, Czech Republic. He received his Bachelor degree from VSB–Technical University of Ostrava in 2016. His research interests include numerical number theory and numerical analysis.