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QUANTUM DIFFUSION OF ULTRA-COLD NEUTRONS IN A ROUGH WAVEGUIDE IN A GRAVITY FIELD

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QUANTUM DIFFUSION OF ULTRA-COLD NEUTRONS IN A ROUGH
WAVEGUIDE IN A GRAVITY FIELD

BY

MAURICIO ESCOBAR

A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF THE
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ABSTRACT

We report the results of our study of propagation of gravitationally quantized ultracold neutrons in rough waveguides in conjunction with GRANIT experiments (ILL, Grenoble). Our theoretical study is done within the frame of the general theory of transport in systems with random rough boundaries developed by Meyerovich *et al.* We present a theoretical description of GRANIT experiments in the biased diffusion approximation for waveguides with one- and two-dimensional ($1D$ and $2D$) roughness. All system parameters collapse into a single constant (Φ) which determines the depletion times for the gravitational quantum states and the exit neutron count. Φ is determined by a complicated integral of the correlation function (CF) of surface roughness. For waveguides with $1D$ roughness most of the calculations can be performed analytically for the main common types of CF. For waveguides with $2D$ roughness the final calculations are mostly numerical. We also developed useful scaling equations for Φ which can allow experimentalists to accommodate our results to different experimental setups. The reliable identification of the CF is always hindered by the presence of long fluctuation-driven correlation tails in finite-size samples. In order to deal with this issue, we perform numerical experiments relevant for the identification of the roughness CF. We generate surfaces with predetermined CF using rotation of uncorrelated surfaces or using Monte Carlo simulations based on the Ising model. These numerical experiments show how to circumvent the difficulties that arise in extracting the correlation properties of surface roughness using the data on the surface profile obtained in STM-like experiments. This experience helps us to analyze the new rough mirror and make theoretical predictions for ongoing GRANIT experiments. We also propose an alternative waveguide design which can improve the accuracy of experimental results.

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DEDICATION

To my mother...

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CHAPTER 1

Introduction

1.1 Preliminary Comments

The main purpose of this thesis is to present a rigorous theoretical description of the propagation of ultracold neutrons (UCN) through a rough waveguide based on the theory of quantum transport in systems with rough boundaries formulated by Meyerovich *et al.* [1–12]. We plan to formulate predictions for experimental results within this theoretical framework. An additional goal is to build computational models that allow testing the effect of wall roughness on particle transport in different scenarios. We use our experience with simulated rough mirrors in numerical experiments to confidently identify the roughness correlation function (CF) for the real rough ceiling mirror which is being built at the Institute Laue-Langevin (ILL), in Grenoble, France. This allows us to suggest improvements for the experimental setup.

The observation of discrete quantum gravitational states of UCN in Earth’s gravitational field has been one of the most interesting recent achievements in neutron physics. The most representative experimental results were obtained by Nesvizhevsky *et al.* after 2002 [13–24] by implementation of the GRANIT spectrometer [19–21] at ILL.

The lowest quantum gravitational states of UCN are observed by projecting a collimated beam of UCN with large horizontal but small vertical velocities between two parallel horizontal mirror surfaces (the “waveguide”). The surface of the upper mirror has microscale roughness and, therefore, scatters away the neutrons in the

higher gravitational states when they reach it. On the other hand, the bottom mirror is a perfect reflector which specularly reflects the neutrons. After several collisions with the rough walls neutrons incident at high angles are lost. As a result, only UCN in the lowest gravitational states, which cannot reach the upper mirror, continue bouncing and get to a detector.

The detection of quantum gravitational states of UCN encouraged the use of rough mirrors as quantum state selectors to resolve the ultra-low energies required in the experiments (~ 1 peV). Rough surfaces in GRANIT experiments are important because they ensure non-specular reflection. State selectors of this type can have a wide range of applications, not only for the UCN beams. The advantageous implementation of rough scatterer surfaces has inspired the design of numerous promising GRANIT-like experiments [1–12, 25–43]. Two examples are the resolution of centrifugal quantum states in UCN in the so-called “whispering gallery” of quantum states of UCN [25, 26] and the observation of quantum gravitational states for other ultracold particles and anti-particles within the framework of the GBAR project at CERN [27–31]. Other interesting experiments include the search for fundamental forces at extra-short ranges as predicted by grand unified theories [32–40, 44], tests of the weak equivalence principle [34, 35, 38–41, 44], extensions of quantum mechanics [42, 43] and surface studies [1–12]. GRANIT-like experiments may also be helpful to advance investigations of fundamental properties of neutrons, such as, for example, the search of the electric dipole moment of the neutron [45, 46], the search for the neutron charge [47, 48] and the precise measurement of the neutron life-time [49].

The resolution and quality of the observed quantum gravitational states of UCN rely heavily on the quality of roughness of the upper “ceiling” mirror. Earlier, Meyerovich *et al.* proposed a theory of particle diffusion along random rough walls

in which the experimental results are linked to the roughness parameters of the absorber mirror [1–12]. The agreement between this theory and the experimental results on UCN is surprisingly good, despite the existing uncertainties of the input parameters. Other theoretical approaches to GRANIT experiments do not fully account for the roughness of the waveguide [22–24].

Meyerovich *et al.* emphasized the role played by the roughness correlation function of surface inhomogeneities (CF) in the diffusion of UCN along rough walls. It turned out that the roughness-driven transition probabilities between two quantum states $(j, \mathbf{q})$ and $(j', \mathbf{q}')$ are directly proportional to the power spectrum (Fourier image) of the CF, where $\mathbf{q}$ is the particle momentum along the wall [1–12]. All the information about the imperfections of the surface enter the neutron count via a single constant, Φ , which is a complicated integral of the power spectrum [8], see Eqs. (30) and (43). This shows the paramount importance of an *accurate* identification of the surface correlator for the use of rough mirrors in precision measurements.

Treating a real surface to create imperfections with a pre-determined CF is extremely impractical, if not impossible [50]. Even if this were possible, the identification of the CF for a given surface is highly non-trivial [51–54]. As result, the common theoretical practice is to designate its shape *ad hoc* [1, 2], despite the impact of the functional form of the CF on the physical observables [1–8]. The best way to approach this issue is to computationally generate random rough surfaces where the surface correlations are known *exactly*. One can obtain the generated discrete surface profile by measuring it with the computational analog of a STM (Scanning Tunneling Microscope) needle. The correlator is extracted by direct computation, compared with the CF used to generate the surface and analyzed using various fitting functions. Another option is to feed the extracted correlator

directly into the equations for the observables without using the fitting functions. The importance of numerical experiments with the simulated surfaces is to show how to circumvent the possible pitfalls that hinder the reliable identification of a surface correlator for a real surface. We will show below that a proper identification of the surface correlator is fundamental for increasing the resolution of the observed quantum gravitational states of UCN in the GRANIT spectrometer. A better control in the way the roughness of the scatterer/absorber mirror is prepared will open ways to optimize the results for current experiments.

Recent measurements of roughness parameters for a new rough glass mirror, which will be used as a scatterer/absorber in upcoming UCN experiments [10–12], offer us the opportunity to test the effectiveness of the numerical experiments [9] and apply the experience gained identifying correlators with simulated surfaces to a real rough surface. The ongoing experiments implementing this new mirror should also serve to test the theory of biased quantum diffusion approximation developed in Refs. [1–12].

This thesis is arranged as follows:

In Section 1.2 we provide a description of the experimental setup used to observe quantum gravitational states in UCN [13–23]. We describe the GRANIT spectrometer and introduce the main parameters of the system. We also introduce the proper dimensionless variables and the roughness parameters describing the coarseness of the surfaces. In Section 1.3 we also discuss the details of design of the new mirror and the characteristics of its roughness. In Section 1.4 we present the main equations and the theoretical framework of the bias quantum diffusion approximation.

In Chapter 2 we derive our expressions for the exit neutron count based on the theoretical framework for one-dimensional ($1D$) and two-dimensional ($2D$) rough

waveguides. The main conclusion is that all the system parameters collapse into a single constant (Φ) which determines the depletion times for the gravitational states through a complicated integral of the power spectrum of the CF ($\tilde{\zeta}$). We perform these integrations numerically and, where possible, analytically. Finally, we show the effects of different types of roughness in the value of Φ and how this impacts the neutron count, $N(\Phi)$. Our conclusion is that an optimal value to observe the step-wise behavior of $N(\Phi)$ is $\Phi > 40$ for $1D$ rough waveguides [8]. A value of $\Phi \sim 5 \times 10^3$ in the case of the new $2D$ rough waveguide gives a neutron count with very well defined quantum steps [10–12], but might be too large for precise measurements.

In Chapter 3 we discuss the computational methods of generation of $1D$ and $2D$ rough surfaces with desired correlations between inhomogeneities. We perform numerical experiments with different kinds of roughness in which we evaluate how the observables are impacted by features of the extracted CF such as long-range correlations (tails), sample size effects, step size, and anisotropies exhibited by the generated surfaces. Special care should be taken in dealing with the long fluctuation-driven tails and the anisotropy of the CF. The treatment of these effects is highly non-trivial. We propose procedures for dealing with these issues and test their effectiveness. Towards the end of the chapter, we extend our numerical experiments to surfaces with atomic roughness which are generated via Monte Carlo simulations with Ising chains in one and two dimensions.

In Chapter 4 we focus our attention on the reliable identification of the CF for the new rough surface mirror. First, we extract the correlator from the datasets containing the surface measurements (see Section 1.3 for a primer). Later, we apply the criteria developed from the numerical experiments of Chapter 3 for the appropriate identification of the surface correlator. We compare the main issues in

the identification of the extracted CF with those encountered with the simulated rough surfaces. The main distinctions are the difference in size of the sampled areas and the step size of the instrument used in the measurements when compared to those for our simulated surfaces. Finally, we identify the functional form of the CF as two-dimensional isotropic exponential function [10–12].

In Chapter 5 we offer our theoretical predictions for the neutron count of future GRANIT experiments with the new mirror, based on our conclusions regarding the correlation function identified in Chapter 4.

Finally, in Chapter 6 we summarize the results and formulate our main conclusions and suggestions. In addition, we put forward our proposal for an alternative design of the rough ceiling mirror based on our numerical experiments with Ising chains developed in Chapter 2. This new design might significantly improve the quality of GRANIT experiments. We provide suggestions for its implementation and show the predicted observables.

1.2 The GRANIT Experiment

A quasiclassical estimation of the energy levels of a quantum particle bouncing on a horizontal surface in the presence of Earth’s gravitational field gives a spectrum of a few peV for the lowest energy states of neutrons [55–57], making the observation of gravitational quantum bound states extremely challenging. The main reason is the extreme weakness of the gravitational interaction when compared to electromagnetic or nuclear forces. Neutrons are elementary particles with no charge and a relatively long lifetime, which makes them the most favorable candidates for the experimental observation of quantum bound states in a gravitational field¹ [58].

¹Anti-hydrogen and positronium have emerged recently as interesting alternatives. See Refs. [27–30]

Figure 1: Scheme of the rough neutron waveguide in GRANIT experiment.

The first experimental evidence of the observation of the lowest quantum states of neutrons in Earth’s gravitational field was reported in 2002 by Nesvizhevsky *et al.* [13–23] after a series of experiments in a high-precision neutron gravitational spectrometer. The GRANIT spectrometer takes advantage of the long storage time of neutrons by sending a collimated beam of UCN through a long waveguide with reflecting walls. The details of operation of the GRANIT spectrometer can be found in Refs. [13–23] and references therein. The basic idea for the observation of the gravitationally induced quantum states of UCN is summarized in Figure 1.

A collimated flux of UCN with a horizontal velocity of $\sim (5 \div 15)$ m/s and a small vertical velocity of a few cm/s is allowed to propagate between two parallel horizontal mirrors made of sapphire (the “waveguide”). The bottom “floor” mirror is in practice perfectly flat [15, 59, 60]. This ensures high probability of specular reflection for the bouncing neutrons. On the other hand, the top “ceiling” mirror

is made intentionally rough for the purpose of serving as a selector for the vertical component of the velocity of the neutrons. The coarse surface of the ceiling causes turning of the velocity vector thus increasing the probability of absorption via quantum mechanical tunneling. In this way, only the neutrons with vertical velocity smaller than a critical value (~ 4 m/s) remain unabsorbed and can exit the waveguide and reach a detector.

The waveguide is installed in the uppermost part of the spectrometer, where it has been isolated from the effects of external vibrations, electromagnetic fields and other external factors. The mirrors in the waveguide can be set up in several configurations in which they can be interchanged and their position can be adjusted horizontally and vertically for different purposes [22–24]. In this thesis, we adopt the configuration shown in Figure 1, in which the edge of mirrors are perfectly aligned and each is ~ 10 cm long. This length is the minimum horizontal distance covered by the UCN during their estimated flight time (~ 20 ms). The vertical separation of the mirrors (the width of the waveguide, H) can be changed. The minimal width is ~ 15 μm , which is comparable to the semi-classical amplitude of bounces of UCN in the ground state. The quantization of the vertical motion of neutrons by Earth’s gravity field translates into the quantization of the amplitudes of bounces from the floor mirror. Consequently, the neutron count at the location of the detector should be a step-wise function of the width of the waveguide [1, 2] (see also Figure 4 on page 18).

The main mechanism of neutron loss within the waveguide is the absorption of neutrons with vertical velocity above the critical value by the mirror material [1, 2]. The scattering of neutrons by the rough ceiling turns the velocity vector thus increasing its vertical component for neutrons that reach the ceiling. The imperfections of the ceiling mix the gravitational quantum states and broadens

the energy levels. Therefore, it is necessary to provide a quantitative description of the roughness parameters governing the surface inhomogeneities.

The roughness of a surface is described in terms of its deviation with respect to a perfectly flat reference plane that is chosen in accordance to the long-range behavior of the surface [50]. If $z(x, y)$ is the height of the surface relative to the mean plane then the strength of the roughness is characterized by the average *amplitude of roughness* of the inhomogeneities, $\ell = \sqrt{\langle z^2 \rangle}$, where the averaging occurs over the size of the surface for a given height-to-height distribution². However, two surfaces with the same average height and distribution might still look considerably different from each other if the horizontal length scale over which the heights are varying is different. Such horizontal length scale is referred to as *correlation radius*, R . One way of interpreting R is as the mean lateral size of the imperfections of the surface.

Although an increase of the roughness amplitude ℓ should make the selection of the gravitational states more pronounced, it is not convenient to make it large since it causes uncertainties when measuring the positions of the mirrors. Instead, one should stay within the *weak roughness domain*, $\ell \ll R, H$.

Consider the motion of a quantum particle in the gravity field above a perfectly reflecting mirror. This corresponds to an open geometry where the ceiling is absent (see Figure 1). In this case, the Schödinger equation reads

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + mgz \right) \psi(z) = E\psi(z), \quad (1)$$

where $\psi(z)$, the wavefunction in the z -direction, must satisfy $\psi(0, \infty) = 0$. The solution of Eq. (1), together with the boundary conditions, is a popular problem in introductory quantum mechanics whose solution is a linear combination of the

²For simplicity, one assumes a suitable choice of a reference plane such that $\langle z \rangle = 0$ [50].

Airy functions, Ai and Bi [55–57]. In this geometry, one finds useful to measure all relevant lengths in units of

$$l_0 = \left(\frac{\hbar^2}{2m^2g} \right)^{1/3} \approx 5.87 \text{ } \mu\text{m}, \quad (2)$$

which is the *characteristic length scale* of our system. This value describes the amplitude of particle bounces in the lowest quantum state.

From Eq. (2), we can introduce other relevant scales. The energy scale is defined by $e_0 = mgl_0 \sim 0.602 \text{ peV}$ (the energy of the neutron in the ground state), while $v_0 = \sqrt{2gl_0} = \hbar/ml_0 \sim 1.1 \times 10^{-2} \text{ m/s}$ defines the velocity scale. The time scale is given by

$$\frac{1}{\tau_0} = \frac{\sqrt{2\pi} \hbar}{4m l_0^2} \sim 1149 \text{ s}^{-1}. \quad (3)$$

It is also convenient to adopt some notation which will become useful later:

- The width of the waveguide in units of l_0 is $h = H/l_0$.
- The correlation radius and the amplitude of roughness are expressed in the dimensionless variables $r = R/l_0$ and $\eta = \ell/l_0$. After inspection under the microscope, it was estimated that the rough mirror of Ref. [13] had the roughness parameters $R \simeq 7 \text{ } \mu\text{m}$ and $\ell \simeq 0.7 \text{ } \mu\text{m}$. This corresponds to $r \simeq 1.19$ and $\eta \simeq 0.119$. The floor mirror, on the other hand, had an amplitude of roughness in the order of $10 \text{ } \text{\AA}$ and a correlation radius of a few hundred nm [59, 60].
- The quantized energy levels of the UCN are represented by $\lambda_j = E_j/e_0$. In Ref. [13], the typical overall kinetic energy of the particles in the beam ranged between $u_c = 1.4 \times 10^5 < \varepsilon = E/e_0 < 8.7 \times 10^5$. Here, $u_c = U_c/e_0$

is absorption threshold of the mirror surfaces³, $U_c \approx 100$ neV. Notice that λ_0/u_c , $mgh/u_c \sim 10^{-5}$. This indicates that the details of the potential well close to the absorption threshold ($j \gg 1$) are negligible for the lowest gravitational quantum states (see Ref. [2]).

- It is useful to introduce the ratio $\chi = u_c/\varepsilon$. In Ref. [13], $0.16 \lesssim \chi < 1$. The dimensionless momenta are $\beta_j = v_j/v_0 = \sqrt{\varepsilon - \lambda_j} = \sqrt{\varepsilon}(1 - \lambda_j/2\varepsilon) = q_j l_0/\hbar$, for $\lambda_j \ll \varepsilon$.
- The UCN flight time corresponds to $t_L = L/v_x$, where L is the length of the mirrors. In Ref. [13], $t_L \approx 2 \times 10^{-2}$ s. In dimensionless units, $t_L/\tau_0 \approx 23$.

1.3 New Mirror and Roughness Measurements

Since 2002, the GRANIT spectrometer has been subject to various upgrades [11, 21, 63, 64]. Several uncertainties in the waveguide have been reduced or eliminated and many parameters have been measured more accurately. The main objective of the improvements is to refine the observation of the UCN spectrum. The major modification in the latest upgrade is the installation of a new large rough ceiling mirror for upcoming UCN experiments at ILL. Consequently, we have to distinguish between the data-set corresponding to the experiments performed with the old mirror from 2002 until recently and those for the new waveguide. In both cases, the setups maintain the geometry of Figure 1.

The design of the new, larger ceiling mirror should serve to improve the shape of the UCN spectrum. Since the main application of the ceiling mirror is to serve as a selector of quantum gravitational states, the roughness has to be large in order to maximize its scattering/absorption efficiency. As commented earlier, this

³This is the so-called Fermi pseudopotential of the surface mirror [61, 62].

Figure 2: The latest rough mirror surface with five control patches [11]. The mirror is 90 mm long in the direction of propagation of the UCN.

is done at the expense of loosing precision in the measurements of the position of the absorber.

The dimensions of the new mirror are shown in Figure 2. The neutrons propagate parallel to the 90 mm long edge. The surface roughness is measured using a Vertical Scanning Interferometry (VSI) technique [65] in the five control patches shown in the Figure. Each patch is $0.504 \times 0.504 \text{ mm}^2$ and consists of a matrix of $\sim 2500 \times 2500$ data points representing the amplitude of roughness of the inhomogeneities of the scatterer with respect to a mean reference plane. The scanning is done using a light source that splits into two coherent light beams. One of the beams is sent onto the mirror and is coupled with another light beam that has been reflected from a flat control sample (amplitude of roughness of $0.5 \text{ \AA}$). The emergent resulting beam is then analyzed in a CCD camera where the interference patterns provide the surface profile. The technique is not perfect. If the inhomogeneities are too sharp at a particular position, the beam doesn't reflect back into the detector. The CCD mechanism recognizes this as a "bad pixel" and enters the

data set under the label “Bad”. About $(1.5 \div 2)\%$ of the data points per patch were cataloged “Bad”. The “Bad” points appeared scattered across the patch, often forming clusters. The largest cluster found contained 8 adjacent “Bad” points. A more thorough discussion on how these faulty entries were dealt with will be offered in Chapter 4.

The VSI technique is more advantageous than other scanning techniques, such as Atomic Force Spectroscopy (AFM), for several reasons. First, the extension of the scanned surface has to be considerably larger than the correlation radius, at least a few hundred μm . Such area is too large for standard AFM, which is more appropriate for measurements in the angstrom range. Second, the lateral correlation radius should be comparable to $l_0 \gg 1 \text{ \AA}$ for optimal absorption efficiency. Each data point in the patch has the spatial separation of the instrument’s horizontal step size, $\sim 0.2 \mu\text{m} \ll l_0$. Here, the range of application of AFM would have been constraining.

Other parameters of the new waveguide are slightly different from the original GRANIT data. The average kinetic energy is $\varepsilon = 1.4 \times 10^5 = u_c$, or $\chi = 1$. This puts the average horizontal UCN velocity in $\sim 4 \text{ m/s}$. The time of flight for the new mirror is $9 \text{ cm}/4 \text{ m/s} = 22.5 \text{ ms} = 26\tau_0$. Finally, the most significant differences occur obviously in the roughness of the mirror itself. This will be the topic of discussion in Chapter 4.

1.4 Theoretical Background

Studies of the effects of random surface roughness on wave and particle scattering are important for the description of the diffusion flows of particles along rough walls in thin films, wires, layers, quantum wells and rough waveg-

guides [3–7, 52–54, 66–69]. Earlier, Meyerovich *et al.* developed a versatile theoretical framework of particle transport in systems with random rough boundaries which incorporates the boundary scattering directly into the bulk transport equation [1–5]. The main idea is to include the roughness of the walls into the roughness-driven transition probabilities between quantum states, $W(\mathbf{q}, \mathbf{q}')$ (see below). The diffusion along the rough channel is described by the Boltzmann-like transport equation

$$\dot{n}(\mathbf{q}) = 2\pi \int \frac{d^3\mathbf{q}'}{(2\pi\hbar)^3} W(\mathbf{q}, \mathbf{q}') (n(\mathbf{q}) - n(\mathbf{q}')) \delta(\epsilon_{\mathbf{q}} - \epsilon_{\mathbf{q}'}), \quad (4)$$

where $n(\mathbf{q})$ is the distribution function of the particles and $\epsilon(\mathbf{q})$ is the energy spectrum. Here, $\mathbf{q} = (p, q)$ is the momentum along xy in the waveguide with the geometry of Figure 1.

Eq. (4) is readily adjusted to the neutron problem. The motion perpendicular to the walls is quantized by gravity, whereas the motion parallel to the walls is quasi-classical with continuous spectrum. Consequently,

$$\dot{n}_j(\mathbf{q}) = 2\pi \sum_{j'} \int \frac{d^2\mathbf{q}'}{(2\pi\hbar)^2} W_{jj'}(\mathbf{q}, \mathbf{q}') (n_{j\mathbf{q}} - n_{j'\mathbf{q}'}') \delta(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'}'). \quad (5)$$

The contribution from transitions to the states within continuous spectrum above the absorption threshold U_c , for which there are no reverse processes, is negligible [1, 2]. Thus, upon the substitution $q_j^2/2m = E - \epsilon_j$, one can carry out the integration over the energies which yields [10–12]

$$\frac{\partial N_j}{\partial t} = \frac{m}{2\pi} \sum_{j'} \int d\theta W_{jj'}(|\mathbf{q}_j - \mathbf{q}_{j'}|) (N_{j'} - N_j), \quad (6)$$

where N_j is the neutron population per unit length of the beam and θ is the angle between $\mathbf{q}_j$ and $\mathbf{q}_{j'}$.

The simplest approach to the determination of the transition probabilities $W_{jj'}$ in Eq. (6) consists of using the small corrugation of the wall as a perturbation parameter within the weak roughness domain [3–5]. Let $\xi(x, y)$ be a random variable describing the surface roughness of the ceiling mirror with respect to the plane $z = H$. This corresponds to a barrier of height U_c at position $z = H + \xi(x, y)$. Since $mgH \ll U_c$, the magnitude of the perturbation is described by $V(x, y, z) \approx -\xi(x, y)U_c\delta(z - H)$, where the roughness-driven transition probabilities are

$$W_{jj'}(\mathbf{q}, \mathbf{q}') = \langle |V_{j\mathbf{q}, j'\mathbf{q}'}|^2 \rangle. \quad (7)$$

The matrix element should be determined by using the wavefunction

$$\Psi_j(x, y, z) = \phi(\mathbf{x})\psi_j(z), \quad (8)$$

where $\mathbf{x} = (x, y)$. The functions ψ_j correspond to the unperturbed quantized eigenstates of neutrons in the presence of a gravity field in the *closed* geometry with flat walls, as found in Ref. [1]. The functions $\phi(\mathbf{x})$ are properly normalized plane waves. If the absorption barrier U_c is finite, the calculation of $W_{jj'}$ in (7) yields [1, 2]:

$$W_{jj'}(\mathbf{q}, \mathbf{q}') = \tilde{\zeta}(|\mathbf{q} - \mathbf{q}'|)U_c^2|\psi_j(H)|^2|\psi_{j'}(H)|^2, \quad (9)$$

otherwise, if $U_c \rightarrow \infty$, then [3–6]

$$W_{jj'}(\mathbf{q}, \mathbf{q}') = \frac{1}{4m^2}\tilde{\zeta}(|\mathbf{q} - \mathbf{q}'|)|\psi'_j(H)|^2|\psi'_{j'}(H)|^2, \quad (10)$$

where the function $\tilde{\zeta}$ is the *power spectrum* (Fourier image) of the *correlation function of inhomogeneities* (CF) [50], defined as

$$\zeta(\mathbf{x}) = \langle \xi(\mathbf{x}')\xi(\mathbf{x}' + \mathbf{x}) \rangle = \lim_{A \rightarrow \infty} A^{-1} \int d^2\mathbf{x}' \xi(\mathbf{x}')\xi(\mathbf{x}' + \mathbf{x}), \quad (11)$$

Name	$\varphi(\mathbf{x}/r)$
Gaussian, G	$\exp(-\mathbf{x}^2/2r^2)$
Power Law, PL	$2\mu/(1 + \mathbf{x}^2/r^2)^{1+\mu}$
Exponential, E	$(\mathbf{x} /r)^\lambda K_\lambda(\mathbf{x} /r)/2^\lambda \Gamma(1 + \lambda)$

Table 1: Most common mathematical forms of the correlation functions.

where A is the averaging area.

The mathematical form of the CF cannot be found theoretically, except for very few exactly solvable realistic models of surface interaction. In theoretical calculations, the shape of the CF is assumed to be known. However, there are many equally justifiable forms of the CF [23, 70]. The most common choices are the Gaussian (G), exponential (E) or power law (PL) correlators, see Table 1. All these mathematical models follow the general form

$$\zeta(\mathbf{x}) = \eta^2 \varphi(\mathbf{x}/r), \quad (12)$$

where the dimensionless roughness parameters η and r can be used as free parameters in the identification of surface correlations. The use of additional fitting parameters might improve the description of the surface roughness but it will not offer any new physics. In general, the function φ in Eq. (12) is smooth and satisfies $\varphi(0) = 1$ and $\varphi(\infty) = 0$. However, in practice, the CF does not monotonically decay to zero. Instead, it might exhibit a long oscillating tail (see Figure 3 on page 17). This noise-like oscillating tail has an important impact on the identification of surface correlations and on the calculation of observables (see Eq. (9)). We will return to this in more detail in Chapter 3.

The short-range behavior of the surface correlations is determined by a peak area of size $\sim r$. The reliable identification of the CF depends on the quality of the data in and around the peak area, see Chapter 3 and Refs. [50, 51].

Figure 3: (Solid line) CF for a one-dimensional surface with Gaussian correlations among inhomogeneities. (Dotted line) Gaussian fitting function corresponding to $\exp(-x^2/8)$, i.e., $r = 2$.

The diffusion of neutrons between discrete gravitational states has a strong directional bias upward [1, 2]. The bias is explained by the rapid growth of the product of the wavefunctions at the boundary with increasing j and j' (see Eqs. (9) and (10)). This product grows roughly as $j^2 j'^2$. The increase in the rate of the jumps $j \rightarrow j' > j$ is compensated only by the decay of $\tilde{\zeta}(|\mathbf{q}_j - \mathbf{q}_{j'}|)$ at large $|\mathbf{q}_j - \mathbf{q}_{j'}|$, which is determined by $|\mathbf{q}_j - \mathbf{q}_{j'}| \lesssim 1/R$. As a result, the transition rates $W_{j'>j}$ display a narrow peak around some $j_1 \gg j$.

The consequences of the strong upward bias are twofold. First, almost all the time necessary for a neutron initially in a low gravitational state j to diffuse upwards towards the absorption barrier is spent in the first transition upward. Further transitions to higher states occur much faster. Second, the strong upward bias allows us to neglect particles returning back to the lowest states. This results

Figure 4: (Crosses) Experimental neutron count as measured by Nesvizhevsky *et al.* in Ref. [13]. (Solid curve) Neutron count as a function of the width of the waveguide as predicted by the quantum transport theory for biased diffusion. The parameters of the original mirror are $\eta = 0.119$, $r = 1.19$, $\chi = 0.16$. The initial occupancy of states in front of the waveguide is chosen $N_j(0) = N_0 = 1$.

in a decoupling of Eqs. (6):

$$\frac{\partial N_j}{\partial t} = -\frac{N_j}{\tau_j}, \quad (13)$$

where $\tau_j = \tau_j(h)$ are the relaxation times of neutrons in the j^{th} gravitational state.

The set of linear differential equations (13) can be readily solved in terms of the relaxation times to yield the exit UCN count [1, 2, 10–12]:

$$N_e = \sum_j N_j(0) \exp(-t_L/\tau_j), \quad (14)$$

where the initial distribution of neutrons entering the waveguide, $N_j(0)$, is usually assumed uniform, $N_j(0) = N_0$.

Figure 4 on page 18 compares the experimental data from Ref. [13] (crosses) with the calculations, Eq. (14) (solid curve), see Ref. [2]. The roughness parameters are those of the original ceiling mirror (i.e., $\eta = 0.119$, $r = 1.19$). There is a good agreement between the theoretical and the experimental curves despite of low accuracy for the estimates of the roughness parameters of $\sim (10\div 20)\%$. This is rather surprising, given the high sensitivity of the theoretical curve to the amplitude of roughness and correlation radius. There are other uncertainties associated with the width of the slit [13] and the lack of knowledge of the initial neutron distribution, $N_j(0)$ [2].

In the next chapter we will improve and refine the theoretical approach.

List of References

- [1] A. Meyerovich and V. V. Nesvizhevsky, “Gravitational quantum states of neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 73, 063616, June 2006.
- [2] R. Adhikari, Y. Cheng, and A. E. Meyerovich, “Quantum size effect and biased diffusion of gravitationally bound neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 75, 063613, June 2007.
- [3] A. E. Meyerovich and A. Stepaniants, “Quantized systems with randomly corrugated walls and interfaces,” *Phys. Rev. B*, vol. 60, no. 12, p. 9129, 1999.
- [4] A. E. Meyerovich and A. Stepaniants, “Transport equation and diffusion in ultrathin channels and films,” *Phys. Rev. B*, vol. 58, p. 13 242, Nov. 1998.
- [5] A. E. Meyerovich and A. Stepaniants, “Transport phenomena at rough boundaries,” *Phys. Rev. Lett.*, vol. 73, no. 2, p. 316, July 1994.
- [6] Y. Cheng and A. E. Meyerovich, “Mode coupling in quantized high-quality films,” *Phys. Rev. B*, vol. 73, 085404, Feb. 2006.
- [7] A. E. Meyerovich and I. V. Ponomarev, “Surface roughness and size effects in quantized films,” *Phys. Rev. B*, vol. 65, 155413, 2002.

- [8] M. Escobar and A. Meyerovich, “Beams of gravitationally bound ultracold neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 83, 033618, Mar. 2011.
- [9] M. Escobar and A. Meyerovich, “Applications and identification of surface correlations,” arXiv:1404.1291, 2014.
- [10] M. Escobar and A. Meyerovich, “Quantized ultracold neutrons in rough waveguides: GRANIT experiments and beyond,” *Advances in High Energy Physics*, vol. 2014, Article ID: 185414, July 2014.
- [11] M. Escobar, F. Lamy, A. E. Meyerovich, and V. V. Nesvizhevsky, “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- [12] M. Escobar and A. E. Meyerovich, “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.
- [13] V. V. Nesvizhevsky, H. G. Börner, A. K. Petukhov, H. Abele, S. Baessler, F. J. Rueb, T. Stöferle, A. Westphal, A. M. Gagarski, G. A. Petrov, and A. V. Strelkov, “Quantum states of neutrons in Earth’s gravitational field,” *Nature*, vol. 415, pp. 297–299, Nov. 2002.
- [14] V. V. Nesvizhevsky, “Investigation of quantum neutron states in the terrestrial gravitational field above a mirror,” *Physics-Uspekhi*, vol. 47 (5), p. 515, 2004.
- [15] V. V. Nesvizhevsky, H. G. Börner, A. M. Gagarski, A. K. Petoukhov, G. A. Petrov, H. Abele, S. Baessler, G. Divkovic, F. J. Rueb, T. Stöferle, A. Westphal, A. V. Strelkov, K. V. Protasov, and A. Y. Voronin, “Measurement of quantum states of neutrons in the Earth’s gravitational field,” *Phys. Rev. D*, vol. 67, 102002, 2003.
- [16] V. V. Nesvizhevsky, A. K. Petukhov, H. G. Börner, T. A. Baranova, A. M. Gagarski, G. A. Petrov, K. V. Protasov, A. Y. Voronin, S. Baessler, H. Abele, A. Westphal, and L. Lucovac, “Study of the neutron quantum states in the gravity field,” *Eur. Phys. J. C*, vol. 40, pp. 479–491, 2005.
- [17] V. V. Nesvizhevsky, H. Börner, A. M. Gagarski, G. A. Petrov, A. K. Petukhov, H. Abele, S. Baessler, T. Stöferle, and S. M. Soloviev, “Search for quantum states of neutron in a gravitational field: gravitational levels,” *Nuclear Instruments and Methods in Physics Research A*, vol. 440, pp. 754–759, 2000.
- [18] V. V. Nesvizhevsky and K. V. Protasov, *Trends in Quantum Gravity Research*. Nova Science Publishers, Inc., 2006.

- [19] I. Antoniadis, S. Baessler, O. Bertolami, D. Dubbers, A. Meyerovich, V. V. Nesvizhevsky, K. Protasov, and S. Reynaud, *C. R. Physique* 12, vol. 8, pp. 703–706, Oct. 2011.
- [20] S. Baessler, M. Beau, M. Kreuz, V. N. Kurlov, V. V. Nesvizhevsky, G. Pignol, K. V. Protasov, F. Vezzu, and A. Y. Voronin, “The GRANIT spectrometer,” *C. R. Physique*, vol. 12, pp. 707–728, 2011.
- [21] S. Baessler, A. M. Gagarski, E. V. Lychagin, A. Mietke, A. Y. Muzychka, V. V. Nesvizhevsky, G. Pignol, A. V. Strelkov, B. P. Toperverg, and K. Zhernenkov, “New methodical developments for GRANIT,” *C. R. Physique*, vol. 12, pp. 729–754, 2011.
- [22] A. Westphal, “Quantum Mechanics and Gravitation,” Ph.D. dissertation, University of Heidelberg, 2001. [Online]. Available: arxiv.org/pdf/gr-qc/0208062.
- [23] C. Krantz, “Quantum States of Neutrons in the Gravitational Field,” Ph.D. dissertation, University of Heidelberg, 2006. [Online]. Available: <http://www.physi.uni-heidelberg.de/Publications/>
- [24] A. Y. Voronin, H. Abele, S. Baessler, K. V. Protasov, and A. Westphal, “Quantum motion of a neutron in a wave-guide in the gravitational field,” *Phys. Rev. D*, vol. 73, 044029, Feb. 2006.
- [25] V. V. Nesvizhevsky, K. Petukhov, K. V. Protasov, and A. Y. Voronin, “Centrifugal quantum states of neutrons,” *Phys. Rev. A*, vol. 78, 033616, 2008.
- [26] V. V. Nesvizhevsky and A. Y. Voronin, “Centrifugal quantum states of neutrons,” *C. R. Physique*, vol. 12, pp. 791–795, 2011.
- [27] A. Y. Voronin, P. Froelich, and V. V. Nesvizhevsky, “Gravitational quantum states of antihydrogen,” *Phys. Rev. A*, vol. 83, 032903, Mar. 2011.
- [28] A. Y. Voronin, V. V. Nesvizhevsky, and S. Reynaud, “Whispering-gallery of antihydrogen near a curved surface,” *Phys. Rev. A*, vol. 85, 014902, 2012.
- [29] G. Dufour, P. Debu, A. Lambrecht, V. V. Nesvizhevsky, S. Reynaud, and A. Y. Voronin, “Shaping the distribution of vertical velocities of antihydrogen in GBAR,” arXiv:1312.5534v1 [quant-ph], 2012.
- [30] P. Crivelli, V. V. Nesvizhevsky, and A. Y. Voronin, “Can we observe the gravitational quantum states of Positronium?” arXiv:1408.7051v1 [physics.atom-ph], 2014.
- [31] A. Y. Voronin, V. V. Nesvizhevsky, and S. Reynaud, “Whispering-gallery states of antihydrogen near a curved surface,” *Nature Physics*, vol. 6, 114–117, 2010.

- [32] I. Antoniadis, S. Baessler, M. Büchner, V. V. Fedorov, S. Hoedl, A. Lambrecht, V. V. Nesvizhevsky, G. Pignol, K. V. Protasov, S. Reynaud, and Y. Sobolev, “Short-range fundamental forces,” *C. R. Physique*, vol. 12, pp. 775–778, 2011.
- [33] S. Baessler, V. V. Nesvizhevsky, G. Pignol, K. V. Protasov, and A. Y. Voronin, “Constraints on spin-dependent short-range interactions using gravitational quantum levels of ultracold neutrons,” arXiv:0902.3139, 2009.
- [34] M. Kreuz, V. V. Nesvizhevsky, P. Schmidt-Wellenburg, T. Soldner, M. Thomas, H. G. Börner, F. Naraghi, G. Pignol, K. V. Protasov, D. Rebreyend, F. Vezzu, R. Flaminio, C. Michel, N. Morgado, L. Pinard, S. Baessler, A. M. Gagarski, L. A. Grigorieva, T. M. Kuzmina, A. E. Meyerovich, L. P. Mezhov-Deglin, G. A. Petrov, A. V. Strelkov, and A. Y. Voronin, “A method to measure the resonance transitions between the gravitationally bound quantum states of neutrons in the GRANIT spectrometer,” *Nucl. Instrum. Meth. A*, vol. 611, pp. 326–330, 2009.
- [35] T. Jenke, P. Geltenbort, H. Lemmel, and H. Abele, “Realization of a gravity-resonance-spectroscopy technique,” *Nature Physics*, vol. 7, pp. 468–472, 2011.
- [36] G. L. Greene and V. Gudkov, “Neutron interferometric method to provide improved constraints on non-newtonian gravity at the nanometer scale,” *Phys. Rev. C*, vol. 75, 015501, 2007.
- [37] V. V. Nesvizhevsky, G. Pignol, and K. V. Protasov, “Neutron scattering and extra-short-range interactions,” *Phys. Rev. D*, vol. 77, 034020, 2008.
- [38] T. Jenke, G. Cronenberg, J. Burgdörfer, L. A. Chizova, P. Geltenbort, A. N. Ivanov, T. Lauer, T. Lins, S. Rotter, H. Saul, U. Schmidt, and H. Abele, “Gravity Resonance Spectroscopy Constrains Dark Energy and Dark Matter Scenarios,” *Phys. Rev. Lett.*, vol. 112, p. 151105, 2014.
- [39] S. Schleich and E. Rasel, “Neutrons knock at the cosmic door,” *Physics*, vol. 7, no. 39, Apr. 2014.
- [40] O. Bertolami and F. M. Nunes, “Ultracold neutrons, quantum effects of gravity and the weak equivalence principle,” arXiv:hep-ph/0204284, 2002.
- [41] T. Bourdel, M. Doser, A. D. Ernest, A. Y. Voronin, and V. V. Voronin, “Quantum phenomena in gravitational field,” *C. R. Physique*, vol. 12, pp. 779–790, 2011.
- [42] O. Bertolami, J. G. Rosa, C. M. L. de Aragao, P. Castorina, and D. Zappala, “Noncommutative gravitational quantum well,” *Phys. Rev. D*, vol. 72, 025010, July 2005.
- [43] O. Bertolami, “Nonlinear corrections to quantum mechanics from quantum gravity,” *Phys. Lett. A*, vol. 154, pp. 225–229, Apr. 1991.

- [44] P. Brax and G. Pignol, “Strongly coupled chameleons and the neutronic quantum bouncer,” *Physics Review Letters*, vol. 107, p. 111301.
- [45] J. H. Smith, E. M. Purcell, and N. F. Ramsey, “Experimental limit to the electric dipole moment of the neutron,” *Phys. Rev.*, vol. 108, no. 1, Oct. 1957.
- [46] C. A. Baker, D. D. Doyle, K. Green, M. G. D. van der Grinten, P. G. Harris, P. Iadjiev, S. N. Ivanov, D. J. R. May, J. M. Pendlebury, J. D. Rischardson, D. Shiers, and K. F. Smith, “Improved experimental limit on the electric dipole moment of the neutron,” *Phys. Rev. Lett*, vol. 97, 131801, Sept. 2006.
- [47] H. F. Dylla and J. C. King, “Neutrality of Molecules by a New Method,” *Phys. Rev.*, vol. A7, pp. 1224–1229, 1973.
- [48] K. Durstberger-Rennhofer, T. Jenke, and H. Abele, “Probing neutron’s electric neutrality with ramsey spectroscopy of gravitational quantum states of ultra-cold neutrons,” *Phys. Rev. D*, vol. 84, 036004, 2011.
- [49] A. T. Yue, M. S. Dewey, D. M. Gilliam, G. L. Greene, A. B. Laptev, J. S. Nico, W. M. Snow, and F. E. Wietfeldt, “Improved Determination of the Neutron Lifetime,” *Phys. Rev. Lett.*, vol. 111, 22501, Nov. 2013.
- [50] J. A. Ogilvy, *Theory of wave scattering from random surfaces*. IOP Publishing, 1991.
- [51] J. A. Ogilvy and J. R. Foster, “Rough surfaces: gaussian or exponential statistics?” *J. Phys. D: Appl. Phys.*, vol. 22, pp. 1243–1251, 1989.
- [52] R. C. Munoz, G. Vidal, G. Kremer, L. Moraga, and C. Arenas, “Surface-induced resistivity of gold films on mica: comparison between the classical and the quantum theory,” *J. Phys.: Condens. Matter*, vol. 11, pp. L299–L307, 1999.
- [53] R. C. Munoz, G. Vidal, G. Kremer, L. Moraga, and C. Arenas, “Surface roughness and surface-induced resistivity of gold films on mica: influence of roughness modelling,” *J. Phys.: Condens. Matter*, vol. 12, pp. 2903–2912, 2000.
- [54] R. C. Munoz, A. Concha, F. Mora, and R. Espejo, “Surface roughness and size effects of thin gold films on mica,” *Phys. Rev. B*, vol. 61, no. 7, p. 4514, Feb. 2000.
- [55] J. Gea-Banacloche, “A quantum bouncing ball,” *Am. J. Phys.*, vol. 67, p. 776, 1999.
- [56] M. N. Berberan-Santos, E. N. Bodunov, and L. Pogliani, “Classical and quantum study of the motion of a particle in a gravitational field,” *Journal of Mathematical Chemistry*, vol. 37, no. 2, 2005.

- [57] S. Flugge, *Practical Quantum Mechanics I*. Springer-Verlag, 1999.
- [58] V. I. Luschikov and A. I. Frank, *JETP Lett.*, vol. 28, p. 59, 1978.
- [59] V. V. Nesvizhevsky, “Polished sapphire for ultracold-neutron guides,” *Nuclear Instruments and Methods in Physics Research A*, vol. 557, pp. 576–579, 2006.
- [60] V. V. Nesvizhevsky, G. Pignol, K. V. Protasov, G. Quemener, D. Forest, P. Ganau, J. M. Mackowski, C. Michel, J. L. Montorio, N. Morgado, L. Pinard, and A. Remillieux, “Comparison of specularly reflecting mirrors for GRANIT,” *Nuclear Instruments and Methods in Physics Research A*, vol. 578, pp. 435–438, 2007.
- [61] R. Golub, D. Richardson, and S. K. Lamoreaux, *Ultracold neutrons*. IOP Publishing, 1991.
- [62] R. Golub and J. M. Pendlebury, “Ultra-cold neutrons,” *Rep. Prog. Phys.*, vol. 42, p. 3, 1979.
- [63] V. V. Nesvizhevsky, A. K. Petukhov, H. G. Börner, T. Soldner, P. Schmidt-Wellenburg, M. Kreuz, G. Pignol, K. V. Protasov, D. Rebreyend, F. Vezzu, D. Forest, P. Ganau, J. M. Mackowski, C. Michel, J. L. Montorio, N. Morgado, L. Pinard, A. Remillieux, A. M. Gagarski, G. A. Petrov, A. M. Kusmina, A. V. Strelkov, H. Abele, S. Baessler, and A. Y. Voronin, “GRANIT project: a trap for gravitational quantum states of ultracold neutrons,” arXiv:0708.2541v1, 2007.
- [64] D. Roulier, F. Vezzu, S. Baessler, B. Clément, D. Morton, V. Nesvizhevsky, G. Pignol, and D. Rebreyend, “Status of the GRANIT facility,” arXiv:1410.1376v1[physics.ins-det], 2014.
- [65] I. Kurganskaya, A. Luttge, and A. R. Barron, “The application of VSI to the Study of Crystal Surface Processes ,” *Connexions*, 2009. [Online]. Available: <http://cnx.org/content/m22326/1.4/>
- [66] G. Fishman and D. Calecki, “Influence of surface roughness on the conductivity of metallic and semiconducting quasi-two-dimensional structures,” *Phys. Rev. B*, vol. 43, no. 14, 1991.
- [67] G. Fishman and D. Calecki, “Surface-induced resistivity of ultrathin methallic films: a limit law,” *Phys. Rev. Lett.*, vol. 62, no. 11, 1989.
- [68] S. M. Goodnick, D. K. Ferry, C. W. Wilmsen, Z. Liliental, D. Fathy, and O. L. Krivanek, “Surface roughness at the Si(100)-SiO₂ interface,” *Phys. Rev. B*, vol. 32, no. 12, Dec. 1985.
- [69] F. G. Bass and I. M. Fuks, *Wave scattering from statistically rough surfaces*. Pergamon, New York, 1979.

- [70] S. K. Sinha, E. B. Sirota, S. Garoff, and H. B. Stanley, “X-ray and neutron scattering from rough surfaces,” *Phys. Rev. B*, vol. 38, no. 4, p. 2297, 1998.

CHAPTER 2

Waveguides with 1D and 2D Roughness

2.1 Waveguides with 1D Roughness

The values of $\tau_j = \tau_j(h)$ in Eq. (13) determine the depletion times of each quantum state j and the overall neutron count, Eq. (14). These depletion times in the biased diffused approximation, in which only the upward transition rates $j \rightarrow j' > j$ are significant, are given by [1, 2]:

$$\frac{1}{\tau_j} = \frac{1}{\tau_j^{(0)}} + \sum_{j'} \frac{1}{\tau_{jj'}}, \quad (15)$$

where $\tau_j^{(0)}$ are the characteristic times for direct transitions over the absorption threshold u_c and $\tau_{jj'}$ are the transition times between the discrete gravitational states j and j' . Since the absorption threshold u_c is very high ($\sim 10^5$) the direct transitions over the threshold are negligible in comparison to the second term in Eq. (15). Consequently, Eqs. (6), (13) and (15), yield [1–5]:

$$\frac{1}{\tau_j} = m \sum_{j' > j} \int \frac{d\theta}{2\pi} W_{jj'}(|\mathbf{q}_j - \mathbf{q}_{j'}|), \quad (16)$$

where θ is the angle between the momenta $\mathbf{q}_j$ and $\mathbf{q}_{j'}$.

When we substitute Eq. (9) into Eq. (16), we find that the relaxation times τ_j differ from each other only by the values of $\psi_j^2(H)$ [1, 2],

$$\frac{1}{\tau_j} = \frac{b_j}{b_1} \frac{1}{\tau_1}, \quad (17)$$

Figure 5: The ratios $\tau_j(h)/\tau_1(h)$, Eq. (17), for the lowest quantum levels $j = 2, 3, 4, 5$ as a function of the slit width h . The curves are labeled by the values of j . These functions are the same for 1D and 2D roughness and do not depend on the roughness parameters.

where τ_1 is the depletion time for the lowest gravitational state (see Eq. (16)),

$$\frac{1}{\tau_1} = m \sum_{j' > 1} \int \frac{d\theta}{2\pi} W_{1j'}(|\mathbf{q}_1 - \mathbf{q}_{j'}|). \quad (18)$$

We define b_j in Eq. (17) as

$$b_j = \frac{l_0}{2} \cdot 10^5 \psi_j^2(H), \quad (19)$$

where the coefficient 10^5 is introduced only for the computational convenience.

The ratios $\tau_j(h)/\tau_1(h)$, Eq. (17), are plotted in Figure 5 on page 27 for $j = 2, 3, 4, 5$ as a function of the width of the waveguide, h . These ratios measure the relative widths of the eigenstates in the biased diffusion approximation. It is important to note that these ratios are the same for $1D$ and $2D$ roughness and do *not* depend on the roughness parameters at all. Figure 5 also illustrates the fact that the depletion times τ_j can be relatively close to each other. The stepwise dependence of the exit neutron count N_e on h can be observed only if the values of $t_L/\tau_j = (t_L/\tau_1)(b_j/b_1)$ are not too close to each other, which requires relatively long times of flight, i.e., a relatively long waveguide.

Eqs. (17) and (18) show that for the lowest quantum gravitational levels all the relevant parameters of roughness and the waveguide entering the exit neutron count collapse into a single dimensionless constant Φ [3–7],

$$\frac{N_e(h)}{N_0} = \sum_j \exp\left(-\frac{t_L}{\tau_j(h)}\right) = \sum_j \exp(-\Phi b_j(h)), \quad (20)$$

where

$$\Phi = \frac{t_L}{\tau_1(h)b_1(h)}, \quad (21)$$

and $t_L = L/v_j \approx L/\sqrt{\epsilon}v_0$ for the lowest levels.

What makes Φ the most important parameter of the problem (even more important than $1/\tau_1$) is that it does *not* depend on the waveguide width, h , unlike the relaxation time $\tau_1 = \tau_1(h)$ which is inversely proportional to $b_1(h)$ in Eq. (17). The calculation of Φ in Eq. (21) obviously depends on the dimensionality of the roughness and the shape of the surface CF. The value of the dimensionless constant Φ also depends on the properties of the waveguide. Regardless, the moment we determine Φ we know the dependence of the neutron count on the waveguide

width irrespective of the origin of this particular value of Φ , see Figure 6 on page 31. Therefore, the calculation of Φ becomes the prime target of the theory.

We calculate Φ starting from the waveguides with $1D$ roughness for which most of the calculations can be carried out analytically. $1D$ roughness is a random grating perpendicular to the direction of the beam and the $2D$ momentum both before and after the scattering has only one component along the beam, $\mathbf{q} = (p, 0)$. Later, we will mention why $1D$ roughness is important though the existing rough mirrors exhibit $2D$ roughness [4, 5, 7] (Chapter 6). It is more convenient to start not from Eq. (18) but from Eq. (16). The transition probabilities and the distribution function have the form [1, 5]

$$W_{jj'}(\mathbf{q}, \mathbf{q}') = \delta(q - q')W_{jj'}(p, p'), \quad (22)$$

$$n_j(\mathbf{q}) = \frac{(2\pi)^2}{L_p L_q} \delta(q) \delta(p - p_j) N_j, \quad (23)$$

where $p_j = \sqrt{2m(E - \epsilon_j)}$. Consequently, Eq. (16) reduces to [1, 2]

$$\frac{1}{\tau_j} = \frac{1}{\tau_0} \sum_{j' > j} \frac{w_{jj'}(p_j - p_{j'})}{v_{j'}}, \quad (24)$$

where, in our dimensionless variables, the scattering probabilities have the form

$$w_{jj'} = 4 \times 10^{-10} \frac{\eta^2 r}{\beta_j} u_c^2 \psi_1(y_{jj'}) b_j b_{j'}, \quad (25)$$

where $y_{jj'} = y_j - y_{j'} = r(\beta_j - \beta_{j'})$ and ψ_1 stands for the dimensionless part of the $1D$ Fourier image of the CF (12), i.e.:

$$\tilde{\zeta}_1(p_j - p_{j'}) = \sqrt{2\pi} l_0^3 \eta^2 r \psi_1(y_{jj'}). \quad (26)$$

The lower index “1” in Eqs. (25), (26) and below indicates $1D$ roughness.

Because of the upward bias in the UCN diffusion, only the terms with large j' , $1 \ll j' \ll u_c$, make a noticeable contribution to the sum (24). This leads to two important conclusions. First, the important final states $j' \gg 1$ are far away from the bottom of the well where the presence of the gravitational field can be neglected and the energy states can be described by a deep square well approximation [1, 3, 5],

$$\lambda_{j'} = \pi^2 j'^2 / h^2, \quad b_{j'} = 10^5 \lambda_{j'} / h u_c. \quad (27)$$

Second, the rapid increase of the transition rate for $j' \gg 1$ allows us to replace the sum in Eq. (24) by an integration,

$$\frac{\tau_0}{\tau_1} = 2 \times 10^{-5} u_c^2 \left(\frac{\eta}{r} \right)^2 b_1(h) F_1(r, h), \quad (28)$$

where

$$\begin{aligned} F_1(r, h) &= 2 \times 10^{-5} r^3 \varepsilon^{-1/2} \sum_{j' > 1} b_{j'} \psi_1(y_{1j'}) \\ &\simeq \frac{2r^3 \varepsilon}{\pi u_c} \int_0^1 dz \, z^2 \psi_1(y), \quad y(z) = r \sqrt{\varepsilon} \left(1 - \sqrt{1 - z^2} \right). \end{aligned} \quad (29)$$

Eqs. (28) and (29) allow us to write our main parameter Φ_1 in Eq. (21) in a very simple form (see Appendix A for details):

$$\Phi_1(\eta, r) = A_1 \eta^2 r \int_0^1 dz \, z^2 \psi_1(y), \quad (30)$$

where

$$A_1 = \frac{4}{\pi} \times 10^{-5} \frac{t_L}{\tau_0} \frac{\varepsilon}{u_c}. \quad (31)$$

As stated earlier, the width of the waveguide h does not appear in Eq. (30). Φ_1 depends *only* on the parameters of roughness (η and r), the profile of the CF

Figure 6: Experimental neutron count as measured by Nesvizhevsky *et al.* in Ref. [8] (Crosses). The solid curves show the theoretical exit neutron count (20) as a function of the width of the waveguide for various values of Φ_1 . The curves are marked by the values of Φ_1 used in calculations. The curve corresponding to $\Phi_1^G \approx 23.5$ is equivalent to the theoretical fit [1] to experimental data using the one-dimensional Gaussian CF. The parameters of the original mirror are $\eta = 0.119$, $r = 1.19$, $\chi = 0.16$. The initial occupancy of states in front of the waveguide assumed to be $N_j(0) = N_0 = 1$.

(ψ_1) and on the properties of the experimental setup (the neutron flight time (t_L), the penetration barrier (u_c) and the total kinetic energy (ε)) which are collected in the constant A_1 .

The only remaining task is the calculation of the integral (30) for CF of various functional forms, see Table 2. For example, if the correlation function is Gaussian, its Fourier image is also Gaussian,

$$\varphi_1^G(x/r) = \exp(-x^2/2r^2), \quad \psi_1^G(y) = \exp(-y^2/2). \quad (32)$$

Name	$\varphi_1(x/r)$	$\psi_1(y)$	$\Phi_1/A_1\eta^2$
Gaussian, G	$\exp(-x^2/2r^2)$	$\exp(-y^2/2)$	$\frac{1}{3\sqrt{r}} \left(\frac{8}{\varepsilon}\right)^{3/4} \Gamma\left(\frac{7}{4}\right)$
Power law, PL	$\frac{2\mu}{(1+x^2/r^2)^{1+\mu}}$	$\frac{y^\mu K_\mu(y)}{2^{\mu-1}\Gamma(\mu)}$	$\sqrt{\frac{\pi}{r}} \varepsilon^{-3/4} 2^{1-\mu} \mu$
Exponential, E	$\left(\frac{x}{r}\right)^\lambda \frac{K_\lambda(x/r)}{2^\lambda \Gamma(1+\lambda)}$	$\frac{1}{(1+y^2)^{1+\lambda}}$	$\frac{1}{3\sqrt{r}} \left(\frac{4}{\varepsilon}\right)^{3/4} \frac{\Gamma(\lambda+1/4)}{\Gamma(\lambda+1)}$

Table 2: The most important 1D CF, their power spectrum, and the analytical expressions for Φ_1 after integrating Eq. (30).

The integration in Eq. (30) yields:

$$\frac{\Phi_1^G}{A_1\eta^2} = \frac{1}{3\sqrt{r}} \left(\frac{8}{\varepsilon}\right)^{3/4} \Gamma\left(\frac{7}{4}\right). \quad (33)$$

This equation has been used in Ref. [3] when fitting the experimental data from Ref. [8]. Assuming that the measured roughness parameters of the original mirror are accurate and that we are dealing with 1D Gaussian roughness, we obtain $\Phi_1^G \approx 23.5$. The curve corresponding to $\Phi_1^G \approx 23.5$ is indistinguishable from the theoretical fit to the experimental data [3, 8] shown in Figures 4 and 6 as crosses.

It is important to note that η and r in Figure 6 are not fitting parameters, but were the observed values of the amplitude and lateral size of roughness in experiment ($\eta = 1.19$, $r = 0.119$). The only fitting parameter is the value of N_0 (the vertical scale of Figure 6) under the assumption $N_0 = N_j(0)$. For the experimental setup of Ref. [8], $A_1 = 3.53 \times 10^7$ and Φ_1 acquires a normal order of magnitude between 1 and 100. It is clear from Figures 4 and 6 that one requires $\Phi \gtrsim 40$ in order to see well-developed quantum gravitational steps in the dependence of the exit neutron count on the waveguide width, h .

Table 2 summarizes the most common forms of 1D surface correlations (Gaussian, power law and exponential) and their power spectra. In the case of the power

law CF, the Fourier image behaves like an exponential function,

$$\varphi_1^{PL}(x/r) = \frac{2\mu}{(1 + x^2/r^2)^{1+\mu}}, \quad \psi_1^{PL}(y) = \frac{y^\mu K_\mu(y)}{2^{\mu-1}\Gamma(\mu)}, \quad (34)$$

and the constant Φ_1 has the form

$$\frac{\Phi_1^{PL}}{A_1\eta^2} = \sqrt{\frac{\pi}{r}} \varepsilon^{-3/4} 2^{1-\mu} \mu. \quad (35)$$

where K_n is the modified Bessel function of the second kind.

In the opposite case, when the power spectrum of roughness ψ_1 is given by a power law function, the CF φ_1 behaves exponentially, i.e.,

$$\psi_1^E(y) = \frac{1}{(1 + y^2)^{1+\lambda}}, \quad \varphi_1^E(x/r) = \frac{(x/r)^\lambda K_\lambda(x/r)}{2^\lambda \Gamma(1 + \lambda)}, \quad (36)$$

$$\frac{\Phi_1^E}{A_1\eta^2} = \frac{1}{3\sqrt{r}} \left(\frac{4}{\varepsilon}\right)^{3/4} \frac{\Gamma(\lambda + 1/4)}{\Gamma(\lambda + 1)}. \quad (37)$$

The functions ψ_1^{PL} and φ_1^E in Eqs. (34) and (36) become purely exponential when $\mu = \lambda = 1/2$, since

$$\exp(-x) = \sqrt{\frac{2x}{\pi}} K_{1/2}(x). \quad (38)$$

The parameter Φ_1 and the relaxation times τ_j exhibit a universal dependence on the amplitude η , the correlation radius of the surface roughness r , and the overall kinetic energy of particles in the beam ε :

$$\Phi_1, \frac{1}{\tau_j} \propto \frac{\eta^2}{r^{1/2} \varepsilon^{3/4}}. \quad (39)$$

This scaling is precise when $u_c \rightarrow \infty$. For finite u_c , $u_c \approx 10^5$, the power of r is slightly different, $r^{-0.493}$.

Figure 7: The inverse depletion times $1/\tau_j$ for the lowest gravitational states $j = 1, 2, 3, 4, 5$ for a waveguide with $1D$ exponential roughness with $\eta = r = 1$. The curves are marked by the values of j . The vertical scale is in kHz.

The expressions for Φ_1 in Eqs. (33), (35) and (37) allow us to find the depletion times τ_j for each gravitational state, Eq. (17). In Figure 7, we plot the inverse of the depletion times $1/\tau_j(h)$ in kHz for $j = 1, 2, 3, 4, 5$, in the case of a waveguide with pure exponential $1D$ roughness $\eta = r = 1$. Eq. (39) allows recalculating the relaxation times for different roughness parameters. The parameters of the waveguide (neutron velocity, neutron flight time, etc.) correspond to the original GRANIT cell.

The relaxation times $\tau_j(h)$ describe the depletion and broadening of the quantum gravitational states, $\epsilon_j(h)$. In Figure 8 on page 35, we plot $\epsilon_j(h)$ for $j = 1, 3, 5$ as a function of the waveguide width h (solid lines) together with the line broadening $\epsilon_j(h) \pm 1/2\tau_j(h)$ (dashed lines) in kHz. The roughness is exponential in $1D$ with $\eta = r = 1$. Eq. (39) extends the results to different values of η and r . The

Figure 8: The energies of the gravitational quantum states $\epsilon_j(h)$ for $j = 1, 3, 5$ as a function of the waveguide width (h) (solid lines). The dashed lines show the line broadening $\epsilon_j \pm 1/2\tau_j$ in kHz. The roughness is exponential in one dimension with $\eta = r = 1$.

broadening of the state j increases dramatically and rapidly reaches the separation between the states after the width of the waveguide becomes smaller than some critical value, $h_{c,j}$. Below $h_{c,j}$ the gravitational state ϵ_j loses its discrete quantum nature. This occurs simultaneously with the depletion of the neutron population of this state.

Name	$\varphi_2(\mathbf{x}/r)$	$\psi_2(Q, Q')$
Gaussian, G	$\exp(-\mathbf{x}^2/2r^2)$	$4\pi e^{-QQ'} I_0(QQ') e^{-(Q-Q')^2/2}$
Power Law, PL	$(1 + \mathbf{x}^2/r^2)^{-3/2}$	Numerical integration required.
Exponential, E	$\exp(- \mathbf{x} /r)$	$\frac{8E(\Omega)}{[1+(Q-Q')^2]\sqrt{1+(Q+Q')^2}}$

Table 3: Most commonly used correlators in two dimensions and their dimensionless zeroth angular harmonic.

2.2 Waveguides with 2D Roughness

We can extend the above results to waveguides with 2D roughness. In contrast to the systems with 1D roughness, most of the calculations in the 2D cases can be done only numerically. Starting from Eq. (18), and substituting Eqs. (9) and (27), we find

$$\frac{\tau_0}{\tau_1} = 2 \times 10^{-5} u_c^2 \left(\frac{\eta}{r}\right)^2 b_1(h) F_2(r, h), \quad (40)$$

where

$$\begin{aligned} F_2(r, h) &= \sqrt{\frac{2}{\pi}} \times 10^{-5} r^4 \sum_{j' > 1} b_{j'} \psi_2(y_1, y_{j'}) \\ &\simeq r^4 \sqrt{\frac{2u_c}{\pi\chi^3}} \int_0^1 dz \, z^2 \psi_2(y_1, y), \quad y_1 = r\sqrt{\varepsilon}, \quad y(z) = y_1 \sqrt{1 - z^2} \end{aligned} \quad (41)$$

where ψ_2 is the dimensionless zeroth harmonic of the CF, $\tilde{\zeta}^{(0)}(|\mathbf{q}_j - \mathbf{q}_{j'}|)$, over the angle between the vectors $\mathbf{q}_j$ and $\mathbf{q}_{j'}$ [9], see Eq. (18):

$$\tilde{\zeta}_2^{(0)}(|\mathbf{q}_j - \mathbf{q}_{j'}|) = \ell^2 R^2 \psi_2(Q_j, Q_{j'}), \quad (42)$$

where $q_j R = Q_j$. The subscript “2” in Eqs. (40), (41) and (42) refers to 2D roughness. The argument to transform the sum (41) into an integral is the same used to derive Eqs. (29) and (30).

After combining Eqs. (40) and (41), we get an equation similar to Eq. (30) (see Appendix A for more details):

$$\Phi_2(\eta, r) = A_2 \eta^2 r^2 \int_0^1 dz z^2 \psi_2(y_1, y), \quad (43)$$

where

$$A_2 = \left(\frac{2}{\pi}\right)^{3/2} \times 10^{-5} \frac{t_L}{\tau_0} u_c \varepsilon^{3/2}. \quad (44)$$

The calculation of the zeroth angular harmonic of the $2D$ CF in momentum space can be done analytically for the Gaussian CF [9],

$$\psi_2^G(Q, Q') = 4\pi e^{-QQ'} I_0(QQ') e^{-(Q-Q')^2/2}, \quad (45)$$

and exponential CF [9],

$$\psi_2^E(Q, Q') = \frac{8E(\Omega)}{[1 + (Q - Q')^2] \sqrt{1 + (Q + Q')^2}}. \quad (46)$$

In Eq. (45), I_0 is the modified Bessel function of the first kind and in Eq. (46), $E(\Omega)$ is the complete elliptic integral with

$$\frac{\Omega}{2} = \sqrt{\frac{QQ'}{1 + (Q + Q')^2}}. \quad (47)$$

The analytical expressions are summarized in Table 3. Further calculations have to be done numerically.

As in the case of $1D$ roughness, both Φ and $1/\tau_j$ remain proportional to η^2 . However, the dependence on the correlation radius is more elusive because we lack analytical expressions for Φ_2 . In the case of $2D$ exponential roughness (see Table

Figure 9: The same as in Figure 7 for 2D exponential roughness in the new GRANIT cell.

3), our numerical data show that the scaling for $r \gtrsim 0.3$ remains similar to Eq. (39), i.e.,

$$\Phi_2, 1/\tau_j \propto \eta^2 r^\gamma \epsilon^\delta. \quad (48)$$

At $u_c \rightarrow \infty$, we find $\gamma = -1/2$, the same as in the case of 1D roughness. However, at finite u_c the deviation of the index γ from the 1D case is more pronounced: $\gamma = -0.465$ instead of -0.493 at $u_c \sim 10^5$. The scaling index for the energy in the 2D case is different from Eq. (39) because of the different dependencies on velocities in the integrand of Eq. (43). Instead of $\delta = -3/4$ we find $\delta \approx -1.165$.

Figure 9 presents the inverse depletion times $1/\tau_j(h)$ in kHz for $j = 1, 2, 3, 4, 5$ in a waveguide with the 2D exponential roughness and $\eta = r = 1$. The values of the neutron velocity and time of flight entering Eq. (44) correspond to the new

Figure 10: The same as in Figure 8. The dashed lines show the line broadening $\epsilon_j \pm 1/2\tau_j$ in kHz for $1D$ exponential roughness. The dotted lines show the line broadening for $2D$ exponential roughness in the new GRANIT cell. In both cases the roughness parameters are $\eta = r = 1$. The critical values $h_{c,j}$ above which the depletion and broadening of $\epsilon_j(h)$ explode in $2D$ are above those in $1D$ rough waveguides. The broadening rate is also higher in $2D$ rough waveguides.

GRANIT cell, see Section 1.3. The scaling relation in Eq. (48) allows us to get $1/\tau_j$ for other values of the roughness parameters.

The depletion and the broadening of the energy states $\epsilon_j(h)$ in the $2D$ case are shown in Figure 10 (dotted lines) and compared with the line broadening in $1D$ (dashed lines). The critical values of $h_{c,j}$ below which the broadening explodes is slightly larger in $2D$ than those for $1D$ roughness. The slope of the energy broadenings is also slightly higher in $2D$ rough waveguides. This is explained by the role of the sideways scattering which is absent in the $1D$ case.

The values of the line broadening/depletion times in Figures 7, 8, 9 and 10 should allow us to provide the full description of the problem and predict the neutron count, Eq. (20). The only remaining issue is the value of the correlation parameters and the shape of the CF for real mirrors. We will deal with these issues in the following sections.

List of References

- [1] R. Adhikari, Y. Cheng, and A. E. Meyerovich, “Quantum size effect and biased diffusion of gravitationally bound neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 75, 063613, June 2007.
- [2] A. Meyerovich and V. V. Nesvizhevsky, “Gravitational quantum states of neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 73, 063616, June 2006.
- [3] M. Escobar and A. Meyerovich, “Beams of gravitationally bound ultracold neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 83, 033618, Mar. 2011.
- [4] M. Escobar and A. E. Meyerovich, “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.
- [5] M. Escobar and A. Meyerovich, “Quantized ultracold neutrons in rough waveguides: GRANIT experiments and beyond,” *Advances in High Energy Physics*, vol. 2014, Article ID: 185414, July 2014.
- [6] M. Escobar and A. Meyerovich, “Applications and identification of surface correlations,” arXiv:1404.1291, 2014.
- [7] M. Escobar, F. Lamy, A. E. Meyerovich, and V. V. Nesvizhevsky, “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- [8] V. V. Nesvizhevsky, H. G. Börner, A. K. Petukhov, H. Abele, S. Baessler, F. J. Rueb, T. Stöferle, A. Westphal, A. M. Gagarski, G. A. Petrov, and A. V. Strelkov, “Quantum states of neutrons in Earth’s gravitational field,” *Nature*, vol. 415, pp. 297–299, Nov. 2002.
- [9] A. E. Meyerovich and I. V. Ponomarev, “Surface roughness and size effects in quantized films,” *Phys. Rev. B*, vol. 65, 155413, 2002.

CHAPTER 3

Numerical Experiments With Random Rough Surfaces

3.1 General Comments

Most of the contents of this chapter can be found in Ref. [1].

The effects of the waveguide roughness on the exit neutron count (20) are summarized in Eqs. (30) and (43). The value of $\Phi_{1,2}$ is sensitive to both the roughness parameters, η and r , and the *shape* of the power spectrum of surface correlations, $\psi_{1,2}$. The practical applications of the transport theory require the CF of surface inhomogeneities as an input. The problem is that the form of the CF for real surfaces can neither be predicted theoretically nor be known beforehand. Consequently, it is common practice in theoretical calculations to choose the CF to be Gaussian, exponential, or power law functions (see Tables 2 or 3) without further justification despite the existence of evidence that the choice of CF with similar correlation parameters but *different* functional forms can lead to very different physical results, see Refs. [2–6]. This degrades the application of theoretical results to real surfaces.

This problem is much more general and important than just the UCN problem in GRANIT-like experiments.

The most effective way to deal with this issue is to study rough surfaces where the surface roughness CF is *known* exactly. However, it is virtually impossible to prepare a real surface in which the inhomogeneities display a roughness CF of desired mathematical form¹. Even if this were possible, special care is required to

¹In Ref. [7] the author briefly discusses the application of thermalized acid to produce roughness of “white” random nature on a surface.

identify accurately the surface correlator (see below).

The best alternative is to *computationally* generate surfaces with predetermined CF. Then, one can “measure” their profiles imitating the probing needle of a STM (Scanning Tunneling Microscope) or an AFM (Atomic Force Microscope), extract the correlators, and compare them to the “true” CF used to generate the surface [1, 8–10].

The profile measurements provide a big data-set of discrete correlation parameters. One could extract the CF, ζ_{ex} , via Eq. (11) and fit it to Gaussian, exponential and power law functions in Tables 2 and 3 using the amplitude of roughness and the correlation radius as fitting parameters, $\zeta_f(\mathbf{x}) = \eta_f^2 \varphi_f(|\mathbf{x}|/r_f)$. The potential shortcoming of this approach is that the values of the fitting correlation parameters, η_f and r_f , depend on the ad hoc choice of the fitting function, φ_f . Moreover, this can become a real problem when the correlation radius r is either comparable to the step size in scanning microscopy [11] or when the size of the inhomogeneities is large. Even if the value of the correlation radius is not so extreme, how can one evaluate the reliability of ζ_f when compared to ζ_{ex} ? As we will see, the statistical quality of the fit is *not* the answer. The standard deviation (σ) between $\zeta_{ex}(\mathbf{x})$ and $\zeta_f(\mathbf{x})$ does *not* translate into the quality of the predictions for the physical observables. We will discuss this in detail in Sections 3.3 through 3.5.

The alternative is to use the raw correlation data directly in transport computations, for example, for $\Phi_{1,2}$ for our neutron problem. However, as we will see below, the use of the raw experimental data can often be even more dangerous than using the wrong fitting function.

The knowledge of the exact CF for numerically generated rough surfaces will allow us to judge the quality of the identification process not by the statistical

properties of the fits, but by how well the physical observables are reproduced. The issues in identifying the form of the surface correlations for real and computationally generated surfaces are more or less the same [12, 13] and our results should provide a roadmap for dealing with experimental data (see Chapter 4). This will also allow us to design a random surface with desirable correlation properties which can be reproduced experimentally (see Chapter 6).

The purpose of our numerical experiments is to see how sensitive the results for observables such as $\Phi_{1,2}$ are to a choice of fitting function and, by extension, how we should use the correlation data sets extracted from the real experimental data. In this Chapter, we test this idea in systems with both large scale roughness (Section 3.3) and atomic roughness (Section 3.6) and apply our procedures to other roughness-sensitive systems besides our neutron problem.

3.2 Generation of Random Profiles with Predetermined Roughness Correlations

For simplicity, let us start from a 1D discretized random rough profile, $\mathbf{g} = (g_1, g_2, \dots, g_N)$, where $g_i = g_i(x_i)$ is the height of the inhomogeneities with respect to some reference plane. The random profile $\mathbf{g}$ is generated using a Gaussian distribution, $P(\mathbf{g}) = (2\pi)^{-N/2} \exp(-\mathbf{g}^2/2)$, which is used in many random number generators. The rough profile $\mathbf{g}$ is clearly uncorrelated since the CF (11) corresponds to white noise, $\langle g_i g_k \rangle \propto \delta_{ik}$. We wish to use the profile $\mathbf{g}$ to produce a surface $\mathbf{h}$ with predetermined binary correlations,

$$\zeta_{ik} = \zeta(|i - k|) = \langle h_i h_k \rangle = \int d^N \mathbf{h} h_i h_k P(\mathbf{h}), \quad (49)$$

where

$$P(\mathbf{h}) = C_N \exp \left(-\frac{1}{2} \mathbf{h}^\dagger \hat{\mathbf{G}} \mathbf{h} \right), \quad (50)$$

$\hat{\mathbf{G}}$ is an $N \times N$ matrix, and $1 = \int d^N \mathbf{h} P(\mathbf{h})$. If we rotate the vector $\mathbf{h}$ in such a way that the quadratic form $\mathbf{h}^\dagger \hat{\mathbf{G}} \mathbf{h}$ in Eq. (50) is diagonalized, we obtain

$$\begin{aligned} -\frac{1}{2} \mathbf{h}^\dagger \hat{\mathbf{G}} \mathbf{h} &= -\frac{1}{2} (\hat{\mathbf{A}} \mathbf{g})^\dagger \hat{\mathbf{G}} (\hat{\mathbf{A}} \mathbf{g}) \\ &= -\frac{1}{2} \mathbf{g}^\dagger (\hat{\mathbf{A}}^\dagger \hat{\mathbf{G}} \hat{\mathbf{A}}) \mathbf{g} \\ &= -\frac{1}{2} \mathbf{g}^2, \end{aligned} \quad (51)$$

where $\hat{\mathbf{A}}$ satisfies

$$\hat{\mathbf{A}}^\dagger \hat{\mathbf{G}} \hat{\mathbf{A}} = \delta_{ik}. \quad (52)$$

Substituting this into Eq. (49):

$$\begin{aligned} \zeta_{ik} &= \int d^N \mathbf{h} h_i h_k P(\mathbf{h}) \\ &\propto \int d^N \mathbf{g} \left(\sum_l A_{il} g_l \right) \left(\sum_m A_{km} g_m \right) P(\mathbf{g}) \\ &= \sum_{lm} A_{il} A_{km} \int d^N \mathbf{g} g_i g_k P(\mathbf{g}) = (\mathbf{A}^\dagger \mathbf{A})_{ik}, \end{aligned} \quad (53)$$

(the g_i are uncorrelated). Hence,

$$\hat{\mathbf{A}} = \hat{\mathbf{G}}^{-1} = \sqrt{\hat{\boldsymbol{\zeta}}}, \quad (54)$$

where $\hat{\boldsymbol{\zeta}}$ is the *correlation matrix* [11] that contains the desired functional form of the correlations,

$$\zeta_{ik} = \eta^2 \varphi_{ik}. \quad (55)$$

Figure 11: An example of a 1D rough surface profile generated using Eq. (54) for Gaussian CF with $N = 2000$, $\eta = 1$ and $r = 2$.

In Eq. (55), the symmetric matrix element φ_{ik} behaves as the functions defined in Table 1 with x substituted by $|i - k| = s_{ik}$, the separation between imperfections on the 1D rough surface.

Generating the 1D rough surface numerically is relatively straightforward: compute the rotation matrix $\hat{\mathbf{A}}$ in Eq. (54) and apply it to the uncorrelated vector $\mathbf{g}$. The only limitation is in the computational resources required to perform this operation for large matrices $\hat{\boldsymbol{\zeta}}$ whose size is determined by the step size $b = x_{i+1} - x_i$. In our numerical experiments, we choose $b = l_0$, and available computational resources allows us to work with a matrix $\hat{\mathbf{A}}$ of maximum size $N_{max} \sim 5000$. In Figure 11 we show an example of a 1D rough surface generated by this procedure.

The above process can be extended to $2D$ surfaces in two different ways. In principle, one can designate the uncorrelated (**g**) and rotated (**h**) profiles as two-dimensional arrays of inhomogeneities and consider the rotation operator $\hat{\mathbf{A}}$ as a 4-component tensor. We prefer instead to make a flat file out of the $2D$ surface profile. This is done by introducing a projection rule in which the double index (i, j) associated with the two dimensions of the rough profile is relabeled into one (α) . Let the rough surface profile $\hat{\mathbf{g}}$ be represented by a $N \times N$ matrix, where g_{ij} is the height of the grid point (x_i, y_j) with respect of a mean plane. Then, the projection process can occur as illustrated below²

$$\hat{\mathbf{g}} = \begin{pmatrix} g(1, N) \leftarrow g(N) & g(2, N) \leftarrow g(2N) & \cdots & g(N, N) \leftarrow g(N^2) \\ \vdots & \vdots & \ddots & \vdots \\ g(1, 2) \leftarrow g(2) & g(2, 2) \leftarrow g(N+2) & \cdots & g(N, 2) \leftarrow g(N^2 - N + 2) \\ g(1, 1) \leftarrow g(1) & g(2, 1) \leftarrow g(N+1) & \cdots & g(N, 1) \leftarrow g(N^2 - N + 1) \end{pmatrix}. \quad (56)$$

Therefore, the $2D$ profile now can be treated as a $1D$ “flat” vector $\mathbf{g} = (g_1, \dots, g_\alpha, \dots, g_{N^2})$, where

$$\alpha(i, j) = (i - 1)N + j, \quad (57)$$

$1 \leq \alpha \leq N^2$, is the mapping rule from the $2D$ to the $1D$ flat index, and

$$i(\alpha) - 1 = \lfloor \frac{\alpha}{N} \rfloor, \quad j(\alpha) = \alpha - \lfloor \frac{\alpha}{N} \rfloor N \quad (58)$$

is the inverse map. The only remaining task is to rotate $\mathbf{g}$ into $\mathbf{h}$ by means of Eq. (54) and project the flat file back onto the original surface grid using Eq. (58).

²This particular rule for counting is completely arbitrary. All we require is a rule that reduces the double index into a single one.

The price to pay is a more cumbersome expression for the separation between inhomogeneities,

$$s_{\alpha\beta}^2 = \left(\left[\frac{\alpha}{N} \right] - \left[\frac{\beta}{N} \right] \right)^2 + \left((\alpha - \beta) - N \left(\left[\frac{\alpha}{N} \right] - \left[\frac{\beta}{N} \right] \right) \right)^2. \quad (59)$$

In flat file indices, the correlation matrix (55) is now given by

$$\zeta_{\alpha\beta} = \eta^2 \varphi_{\alpha\beta}. \quad (60)$$

Figure 12 on page 48 shows an example of a $2D$ surface generated with roughness parameters $\eta = 1$, $r = 2$ and $2D$ Gaussian CF of surface roughness.

Notice that the obvious size explosion due to the increase in dimensionality restricts dramatically the linear size of the generated $2D$ rough surfaces, see Figure 12. Whereas the matrix $\hat{\mathbf{A}}$ has size $N \times N$ for $1D$ rough surfaces, in $2D$ systems the size blows up to $N^2 \times N^2$. In addition, the matrix $\hat{\mathbf{A}}$ in $2D$ loses completely its nearly diagonal structure, even if the CF is very steep, due to the “flattening” process in Eq. (56).

We should emphasize that we can computationally imprint correlations of *any* desired functional form, including $\varphi_{1,2}$ in Tables 2 and 3, by means of the rotation operation in Eq. (54). The process is only limited by the computational power required to handle the size of $\hat{\mathbf{A}}$ which rapidly grows with the size of the surface.

The difficulties encountered in the generation of the rough surfaces and the extraction of the CF are beyond trivial, although they are typical. In the following sections we will discuss the main features of the extracted CF, ζ_{ex} , and how these features impact the observables. We will also mention how to deal with the issues hindering the accurate identification of surface correlations both in one and two dimensions.

Figure 12: An example of a $2D$ roughness profile with Gaussian CF among inhomogeneities with $\eta = 1$ and $r = 2$. The size of the surface is $60l_0 \approx 352 \mu\text{m}$.

3.3 Extraction of Correlations from 1D Random Rough Profiles

The calculation of the correlation properties of our generated discrete rough profiles $\mathbf{h}$ is done by direct calculation, Eq. (11). Regardless of the dimensionality of the surface, the main issue is our inability to let the size $A \rightarrow \infty$ in Eq. (11) since any generated (or real) surface is always finite. To increase accuracy, one should allow A , meaning N_{max} , to grow as large as possible.

In order to make the most with this computational limit, we introduce periodic boundary conditions for the 1D rough strings, $h_{i+N} = h_i$, so that the extracted 1D CF is

$$\zeta_{ex}(s \leq N/2) = \langle h_i h_k \rangle = \frac{1}{N} \sum_k h_k h_{k+s}. \quad (61)$$

Notice that under this condition, one cannot extend the evaluation of Eq. (61) beyond $s_{max} = N/2$: $\zeta_{ex}(s \geq N/2)$ is simply a mirror image of $\zeta_{ex}(s \leq N/2)$.

Figure 13 on page 50 illustrates a typical CF calculated using Eq. (61) from the 1D rough profile shown in Figure 11, where the “true” roughness correlations are known *exactly*, namely, 1D Gaussian CF with $\eta = 1$ and $r = 2$, $\exp(-s^2/8)$. In general, the typical CF consists of a peak area of size $\sim r$ describing the short-range correlations and a long oscillating tail associated with long-range correlations. The fluctuations in the tail are an inevitable consequence of the finite surface size [11]. Such fluctuations appear in physical experiments with restricted scanning areas as well.

Figures 14 and 15 on pages 51 and 52 show the extracted CF (61) for three different 1D rough surfaces ($\mathbf{h}$) generated starting from the *same* uncorrelated rough profile ($\mathbf{g}$) using Eq. (54). The “true” correlations are supposed to be Gaussian (solid, curve 1), exponential (dashed, curve 2) and power law (dotted, curve 3),

Figure 13: CF extracted using Eq. (61) for the 1D surface rough profile shown in Figure 11. The original profile was generated having 1D Gaussian correlations with roughness parameters $\eta = 1$, $r = 2$. The surface size is $N/2 = 1000$ points long.

respectively. The roughness parameters are $\eta = 1$, $r = 2$ for all three. Notice that whereas the CF are distinguishable from each other inside the peak area (Figure 14), the shape of the correlations is more or less the same in the tail area (Figure 15).

The presence of the alternating long correlation tail for finite surfaces, whether real or simulated, has two important consequences. First, the value of the standard deviation σ between ζ_{ex} and the fitting function ζ_f ,

$$\sigma^2 = \langle (\zeta_{ex} - \zeta_f)^2 \rangle, \quad (62)$$

cannot serve as a statistical measure of the quality of the fit. The fitting functions

Figure 14: CF for numerically generated 1D surface profiles emulating Gaussian (solid, curve 1), exponential (dashed, curve 2), and power law (dotted, curve 3). The original uncorrelated rough profile ($\mathbf{g}$) was the same. The CF differ mostly within the peak area (at distances $\lesssim r$)

ζ_f in Table 4 on page 58 go to zero at large x and, as a result, the value of σ mostly reflects the large tail area instead of the shape of the peak area where both the extracted CF and the fitting functions ζ_f differ from each other. This conclusion is evident from Figure 15. Second, the oscillations in the tails make a non-negligible contribution to the power spectrum of the CF, ψ . Because of the similarity of the tails produced by different correlators (Figure 15), using the same raw data as an input for the calculation of the observables may become counterproductive if the tail is not treated with care, especially in 2D systems where one has to deal with even larger and more volatile fluctuations (see Section 3.5.2).

Figure 15: Same as in Figure 14. At distances much bigger than r (tail area), the shapes of the correlations are indistinguishable from each other.

Increasing the size of the sample with the hope of improving σ often doesn't make the identification of the CF easier, since a larger N also means a longer tail (Figure 16, page 53). Changing the step size b is not helpful either. If one increases the number of points under the peak by decreasing b by some factor (which is equivalent to increasing the correlation radius r by the same factor), the number of points in the tails decreases accordingly and the accuracy in the long-range correlations, and therefore on σ , deteriorates. Unless one can compensate the decrease in b by at the same time increasing N , making b smaller is useless in view of our computational limitations.

The implications of decreasing the sample step b are even deeper. In addition

Figure 16: The quality factor σ as a function of the size of the generated surface N for exact Gaussian (crosses), exponential (squares) and power law (triangles) CF. The solid curve is $\sqrt{2/N}$.

to the loss of accuracy in the tails, it has the obvious downside of limiting the surface size even further, to $Nb/2$ in 1D rough systems. As a consequence, the surface is covered by fewer large size inhomogeneities (domains) that may emulate the presence of an additional correlation radius. The inter-domain correlations give rise to spurious secondary peaks at separations that correspond to integer numbers of the average distances between the domains. These peaks reflect correlations between the domains and not physical interactions [1].

The conclusion is therefore inescapable: The value of σ is misleading in judging the statistical quality of the choice of the fitting function. We will emphasize this in Sections 3.5 and 3.6 where we will offer more examples.

3.4 Extraction of Correlations from 2D Random Rough Profiles

The generation of 2D rough surfaces requires more computational resources. Since our largest generated rough surfaces were about 70×70 , the largest generated 2D CF were about 40×40 . Computations beyond this limit required special efforts.

In 2D rough systems, imposing periodic boundary conditions on the surface profiles to extract the CF is no longer practical. Instead, one can perform the averaging in Eq. (11) by maximizing the utilization of available points while simultaneously trying to avoid double-counting of correlations (see Appendix B for details).

An example of 2D CF extracted from the 2D rough profile shown in Figure 12 on page 48 is given in Figure 17 on page 55, in which the roughness correlations are emulating the isotropic Gaussian CF with $\eta = 1$, $r = 2$, $\exp[-(s^2 + t^2)/8]$. Once again, the function ζ_{ex} exhibits a peak area and oscillating tails.

The anisotropy of the extracted CF in Figure 17 is well pronounced. (Similar anisotropy in the extracted correlator is also observed in STM experiments, see Refs. [2–5]). This issue becomes evident after averaging over the angles. The result is the “flat” CF, $\zeta_{fl}(\rho)$, shown in Figure 18 (solid curve) on page 56, where $\rho = \sqrt{s^2 + t^2}$. Since the exact correlator is known, one can compare it with the function $\exp(-\rho^2/8)$ (dashed curve). Surprisingly, the standard deviation between these two curves is very small, $\sigma \approx 0.057$, despite of these two curves being visually very different in the tail region. This confirms our conclusion in Section 3.3 regarding the effect of the tail of the CF on the value of σ . In 2D rough systems this issue is exacerbated by both the effect of the anisotropy (Figure 17) and the smaller linear size of the generated surface.

The high volatility in the tail of ζ_{fl} in Figure 18 is due to differences in orientations in the xy plane for nearby points along the ρ axis: Adjacent points

Figure 17: An example of a 2D CF for the two-dimensional rough profile shown in Figure 12. The roughness emulates 2D isotropic Gaussian correlations with $\eta = 1$, $r = 2$, $\exp[-(s^2 + t^2)/8]$. The anisotropy of the profile is well pronounced.

Figure 18: Same as Figure 17 after averaging over the angles (solid line). A comparison with the exact CF, $\exp(-\rho^2/8)$ (dashed line), yields a surprisingly low value of standard deviation, $\sigma \sim 0.057$. Notice the high-frequency, volatile behavior of the tail of $\zeta_{fl}(\rho)$ due to the anisotropy of Figure 17.

along the ρ axis can be very far away from each other on the xy plane. For example, for $\rho = 4$ the correlations between the grid points $(x, y) = (4, 0)$ and $(0, 4)$ are averaged; for $\rho = 5$ a total of four grid points $(x, y) = (5, 0), (0, 5), (3, 4)$ and $(4, 3)$ contribute to the average. This volatility becomes more pronounced as ρ increases.

In the following Section we will show more examples of the results of our numerical experiments described above and the ways of dealing with the oscillating tails, both in $1D$ and $2D$ rough systems. We will highlight the inherent pitfalls and risks that one might encounter in identifying the surface correlators. This should

prepare us for accurately identifying the surface correlations governing GRANIT’s new rough mirror, as well as other physical rough surfaces in general (Chapter 4).

3.5 Results of Numerical Experiments

Our goal here is to show that the use of a fitting function of a wrong shape can invalidate both the computations and the experiments. First, the parameters of the fitting CF (ζ_f), obtained from the best fit to the extracted CF (ζ_{ex}), strongly depend on the *assumption* about the functional shape of the “real” correlator. For example, in Refs. [2–5] the authors obtain vastly different values of the correlation radius after analysis of the same STM measurements of ζ_{ex} using the fit to Gaussian and exponential CF (see also Table 5). Since the shape of the “true” correlator in experiment is not known a priori, it is almost impossible to know what function should be fitted to ζ_{ex} and what is the reliability of the extracted fitting parameters.

Below, we show the results for $1D$ and $2D$ rough systems. In $1D$, we concentrate on applications to our neutron diffusion problem [14]. In $2D$, we apply our results to transport phenomena for ballistic degenerate fermions in quantized films [15–19], where the observables are also sensitive to surface correlations.

3.5.1 Results for $1D$ Rough Surfaces

It was mentioned earlier that Eq. (62) is highly weighted towards the tail of the correlator, especially when the correlation radius is comparable to the probing step. If the fitting CF rapidly approaches zero at large separations, σ in Eq. (62) is essentially independent of the choice of ζ_f whereas the physical results for the observables could be.

There is an alternative: In addition to analyzing the extracted correlators using fitting functions, we can perform the direct Fourier analysis of the correlation

Name	$\varphi_f(x)$
Gaussian, G	$\exp(-x^2/2r_f^2)$
Power Law, PL	$(1 + x^2/r_f^2)^{-3/2}$
Exponential, E	$\exp(-x/r_f)$

Table 4: 1D fitting functions $\zeta_f(x) = \eta_f^2 \varphi_f(x/r_f)$ used to determine the correlation parameters from the extracted correlation function, Eq. (61).

data sets as it is sometimes done for experimental data. This should give us the full power spectrum of the CF which can be used for direct calculation of the observables. This approach allows us to avoid the pitfalls of using the “wrong” shape of ζ_f . However, this is also problematic because this procedure utilizes all the erroneous information contained in the tail fluctuations. One can introduce a cutoff in the spectral analysis to avoid this, but then the physical results become dependent on the guess for the cutoff.

We illustrate all this starting from the 1D case in application to our neutron problem. Table 5 on page 59 contains examples of three numerical runs based on the methods from Section 3.2. In each run we generate a 1D rough surface with Gaussian correlation of inhomogeneities with $\eta = 0.119$ and $r = 1.19$ (the roughness parameters measured experimentally in Ref. [14]). The main physical observable is Φ_1 , Eq. (30), which determines the neutron count at the exit of the waveguide, Eq. (20), and which should be ≈ 23.5 for this roughness (see Figure 6). After each numerical run, we fit the observed CF with a Gaussian (G), exponential (E) and power law (PL) correlators (Table 4), and extract the best fitting values $\eta_f^{G,E,PL}$ and $r_f^{G,E,PL}$ for the amplitude of roughness and correlation radius. Then, we recalculate Φ_1 , Eqs. (33), (35) and (37), using these fitting parameters. Table 5 contains values of Φ_1 for these three types of fitting correlators ($\Phi_1^{G,E,PL}$), the standard deviations for the fittings ($\sigma^{G,E,PL}$), and the fitting parameter ($r_f^{G,E,PL}$) which provided the best fits. We do not present the fitting parameters $\eta_f^{G,E,PL}$,

#	$r_f^G, \sigma^G \times 10^4$	$r_f^E, \sigma^E \times 10^4$	$r_f^{PL}, \sigma^{PL} \times 10^4$	$\Phi_1^G, \Phi_1^E, \Phi_1^{PL}, \Phi_1^r$
1	1.19, 5.24	1.59, 5.81	1.44, 5.81	23.86, 18.19, 18.81, 21.96
2	1.15, 4.49	1.53, 4.56	1.36, 4.64	23.33, 17.84, 18.65, 21.14
3	1.25, 4.37	1.69, 4.40	1.54, 4.47	23.56, 17.26, 17.85, 20.96

Table 5: Three numerical runs based on the methods shown in Section 3.2 in application to our neutron problem. Rough 1D surfaces emulate 1D Gaussian correlations of inhomogeneities with $\eta = 0.119$ and $r = 1.19$, as assumed in experiment [14]. The expected value of the main physical parameter Φ_1 , Eq. (30), is $\Phi_1 \approx 23.5$. The extracted correlators were fitted to Gaussian (G), exponential (E) and power law (PL) fitting functions from in Table 4. The table contains the best fitting values of $r_f^{G,E,PL}$ together with $\sigma^{G,E,PL}$ and the recalculated values of $\Phi_1^{G,E,PL}$. The column with Φ_1^r gives the values of Φ when the raw spectral decomposition of the data was put directly into the equations without fitting.

which all were in the range $0.118 \div 0.123$. In Table 5 we also show the values of Φ_1^r and σ^r obtained from the direct Fourier analysis of the raw data with a large number of harmonics ($N/2$). As a consequence, σ^r is vanishingly small, $\sim 2 \times 10^{-17}$ for all three runs. This procedure is equivalent to performing the integration of the power spectrum of the observed correlator in Eq. (30) including its fluctuation-driven tails.

The results of Table 5 are very informative. The quality of the fits for all three types of fitting functions was more or less the same, $\sigma^{G,E,PL} \sim 5 \times 10^{-4}$, but the results for the physical observable, $\Phi_1^{G,E,PL}$, differed significantly. The “true” correlation among the generated inhomogeneities is 1D Gaussian and, not surprisingly, the values of Φ_1^G are the closest to the “true” value of 23.5. This confirms our conclusion that the statistical quality of the fit (σ) of the measured surface correlations to some ad hoc correlator does not tell much about the quality of the predictions of the physical observables.

Feeding the Fourier image of the extracted CF directly into the equations without any fitting does not improve the quality of the conclusions either. The reason is simple: with this approach one uses too much information about the long

distance correlations, which are determined by the fluctuations and not by any physical forces. Still, feeding the equations with the raw CF works slightly better than making the wrong guess of shape of the CF. The values of Φ_1^r determined from the raw data without fitting were actually closer to those calculated from the Gaussian fits, differing from them by $\sim 9\%$. In contrast, the results for fitting with the power law and exponential fitting functions were relatively close to each other ($\Phi_1^{E,PL} \sim 18$) but they differ from those for the Gaussian fit by about 23%. The reason is that the Gaussian function has a much shorter tail.

3.5.2 Results for 2D Rough Surfaces

The results for 2D rough systems are impacted by increase in dimensionality and the smaller linear size of our samples [1]. We will postpone the discussion of the applications to UCN until Chapter 4. Instead, we apply our results to the conductivity of quantized ultra-thin films (UTF) in quantum size effect (QSE) conditions (see Refs. [15–19] and references therein). The QSE is a manifestation of the quantization of the motion in the direction perpendicular to the film, in a way very similar to the gravity-induced quantization of motion perpendicular to the bottom mirror in the diffusion of UCN in rough waveguides. This QSE leads to a split in the energy spectrum into a set of mini-bands $\epsilon(\mathbf{p}) \rightarrow \epsilon_j(\pi j/L, \mathbf{q})$ and manifests itself as large fluctuations of the conductivity (Σ_c) as a function of the UTF thickness, L [15].

In Refs. [15–19], Meyerovich *et al.* found that the scattering by random surface inhomogeneities is sensitive to the type of surface roughness correlations governing the rough boundaries through the intra/inter-band transition probabilities,

$$W_{jj'}(\mathbf{q}, \mathbf{q}') = \frac{\hbar}{m^2 L^2} \left[\zeta_{11} + \zeta_{22} + 2(-1)^{j+j'} \zeta_{12} \right] \left(\frac{\pi j}{L} \right)^2 \left(\frac{\pi j'}{L} \right)^2, \quad (63)$$

where the correlation functions ζ_{11} , ζ_{22} describe intrawall correlations of roughness and ζ_{12} describes interwall correlations [16].

The solution of Eq. (4) with $W_{jj'}$ given by Eq. (63) in the long-wave limit $qR \ll 1$ yields [15–19],

$$\Sigma_c = \frac{2e^2}{\hbar} \frac{(L/\pi)^4}{2S(S+1)(2S+1)\tilde{\zeta}(0)} \sum_j \left(\frac{Lq_j}{\hbar j} \right)^2, \quad (64)$$

where $\tilde{\zeta}(0) = \tilde{\zeta}_0 \simeq \tilde{\zeta}(qR \ll 1)$ is the zeroth harmonic of the Fourier spectrum of $\zeta(\mathbf{x})$ and $S = \lfloor p_F L / \pi \hbar \rfloor$ is the total number of occupied mini-bands. The value of $\tilde{\zeta}_0$ is important not only for the conductivity of UTF but also for a much more general class of problems associated with scattering long-wave particles (or waves) on rough surfaces. The scattering in the long-wave limit ($q \rightarrow 0$) is always described by a single constant which in this case is $\tilde{\zeta}_0$.

Note that with our definition of $\tilde{\zeta}$ one must have $\tilde{\zeta}(q \rightarrow 0) = 2\pi\ell^2 R^2$ in the long-wave limit. Here again one can either choose to fit the extracted CF to the fitting functions or determine $\tilde{\zeta}_0$ by direct numerical integration, just as we did with Φ_1 in the previous Section.

The results below (see Tables 6(a) and (b) in page 62) describe 3 rough surfaces with the “true” CF being the isotropic 2D Gaussian ($G2$), $\exp[-(s^2 + t^2)/8]$, with $\eta = 1$, $r = 2$ (see Figures 12 and 17). In this case, $\tilde{\zeta}_0$ should be equal to $8\pi \approx 25.13$. The last row in each table shows the data extracted from the averaging of ten independent runs with the same Gaussian generating function. In experiment, this is equivalent to averaging the data extracted from 10 different regions of the same surface [2–5]. The linear size of the samples is 60×60 points. The Table shows the values of the extracted fitting parameter r_f , the values of σ and, most importantly, the calculated values of the physical observable $\tilde{\zeta}_0$. The values of η_f are not shown but they fell within the range $0.90 \div 1.20$.

#	$r^{G1}, \sigma^{G1} \times 10^2$	$r^{G2}, \sigma^{G2} \times 10^2$	$\tilde{\zeta}_0^{G1}, \tilde{\zeta}_0^{G2}$
1	1.04, 1.97, 5.7	1.04, 1.95, 9.5	25.3, 25.89
2	1.10, 1.80, 6.5	1.10, 1.78, 8.5	24.4, 24.37
3	0.90, 1.84, 4.1	0.91, 1.82, 6.0	17.4, 17.09
Av.	1.00, 1.98, 1.9	1.00, 1.97, 2.4	25.0, 25.0

(a)

#	$r^E, \sigma^E \times 10^2$	$r^{PL}, \sigma^{PL} \times 10^2$	$\tilde{\zeta}_0^E, \tilde{\zeta}_0^{PL}$
1	1.14, 2.04, 6.2	1.08, 2.45, 5.9	33.81, 44.03
2	1.20, 1.76, 7.4	1.14, 2.15, 7.2	27.91, 37.75
3	0.98, 2.05, 4.3	0.94, 2.40, 4.1	25.17, 31.04
Av.	1.10, 2.11, 2.9	1.05, 2.49, 2.4	33.8, 42.9

(b)

Table 6: Three numerical runs using the methods of Section 3.2 for generated 2D rough Gaussian surfaces with $\eta = 1$ and $r = 2$. The expected value of the main physical observable is $\tilde{\zeta}_0 = 8\pi \approx 25.13$. Tables 6 (a) and (b) contain the extracted fitting parameter $r^{G,E,PL}$, the standard deviation $\sigma^{G,E,PL}$, and the recalculated values of $\tilde{\zeta}_0$. The Gaussian fit was done independently for the 1D flat CF, $\zeta(\rho)$ (index 1; see Table 6(a) and Figure 18) and the 2D CF using the fitting function $\eta_f^2 \exp[-(x^2 + y^2)/2r_f^2]$ (index 2; see Table 6(b)). The range of the fitting parameter η_f (not shown) in all fits was $0.90 \div 1.20$. The fourth row gives the results for the CF resulting from averaging over 10 independent runs.

As mentioned in Section 3.4, the tails of our 2D CF exhibit anisotropy even though the underlying “true” correlator is isotropic (Figure 17). One can treat the anisotropy of $\zeta_{ex}(s, t)$ in two ways: We can either deal with the anisotropic 2D CF and fit it directly with 2D equivalent of the fitting functions from Table 4 or we can flatten the observed 2D correlator into a 1D function, $\zeta(\rho)$, and average away the anisotropy.

We use both options when fitting the Gaussian correlator. In the first column of Table 6, we present the results obtained from the flat 1D CF when fitted with the 1D Gaussian fitting correlator of Table 4 (the index “1” refers to 1D). The second column gives the results of fitting by a 2D isotropic Gaussian correlator (the index “2” refers to 2D), $\eta_f^2 \exp[-(x^2 + y^2)/2r_f^2]$. For exponential and power

Figure 19: Average of 10 extracted 2D CF after flattening into 1D file (solid line; see last row of Tables 6(a) and (b)). The dashed line is the “true” 1D flat CF, $\exp(-\rho^2/8)$ with roughness parameters $\eta = 1$ and $r = 2$. Compare with Figure 18. The averaging process seems to help to reduce the amplitude and volatility of the oscillating tails. However, important physical information of the CF might be lost.

law fitting functions in columns 3 and 4 we use only the flat file $\zeta(\rho)$.

When we fed the results of the spectral analysis of the extracted raw CF directly into the equations, we obtained poor and unstable results due to the anisotropy of the extracted correlator. As shown in Figure 18, this flat 1D version of the 2D CF exhibits high volatility in the tails. The volatility doesn’t affect much the values of σ or the quality of the fits, but makes it impossible to be used for the direct Fourier analysis of the raw experimental data. By manipulating the number of harmonics one can obtain either a good spectral decomposition of the tail or of the main peak, but not of both. This procedure might have worked if we

would have been able to increase the sample size. However, an increase in sample size would have also implied an increase of volatility for the reasons explained in Section 3.4.

The best way to deal with these issues is working with the CF averaged over 10 runs (last row in Table 6), as sometimes done in experiments [3]. This procedure seemed to produce stable results and a significant reduction of the volatility (see Figure 19, page 63). However, the quality of the results was still not very good. The value of $\tilde{\zeta}_0$ after the 1D Fourier analysis of the flat averaged 1D CF in Figure 19 is 18.79 and the value obtained from the 2D Fourier analysis of the averaged 2D CF is 17.6. Note that these two numbers are much worse than those obtained using exponential and power law fitting functions (Table 6).

Averaging the extracted CF over several runs (or averaging over several parts of the rough surface as in experiments) is not an entirely safe procedure. If, for example, the true CF contains an oscillating tail, the averaging might destroy important physical information contained in it. This same uncertainty does not allow us to choose a cutoff of the fluctuations. However, this procedure might work well if one knows beforehand that the “true” correlator is a monotonically decreasing function of the distance.

Note that, as in the case of neutrons, the behavior of σ in Table 6 is similar to that of Table 5 in that the values of σ remain more or less the same across the Table. The values of σ in Table 6 are larger than those in Table 5 because of the reduction of the lateral size of our samples. As always, fitting CF with the correct Gaussian shape yields $\tilde{\zeta}_0$ the closest to its true value. In contrast to the 1D problem, the accuracy of the results for 2D rough surfaces obtained using the wrong fitting functions is nevertheless preferable to feeding the Fourier image of the raw data directly into the equations.

The methods discussed above work well for systems with macroscopic roughness, where the CF of our rough surfaces can be described by smooth functions. These methods are justified when the natural scale of the system is much larger than the atomic size a . For our neutron problem, $a \ll l_0 = 5.87\mu\text{m}$. However, this approximation is not as good in the case of electrons in UTF, since the amplitude of the rough inhomogeneities can be the order of a . In the following Section we propose a method to deal with this type of rough systems.

3.6 Surfaces with Quantized Amplitude of Inhomogeneities: Ising Roughness

We start our approach to quantized surface roughness by considering a modification of the method described in Section 3.2. It is easy to see that the rotation matrix $\hat{\mathbf{A}}$ in Eq. (54) is determined solely by the desirable correlation ζ_{ik} . The generated surface profile h_i (in 1D or 2D) does not reduce to a set of integer numbers in terms of a when one starts from a uncorrelated string of integers, g_i . The best we can do is to generate the correlated string h_i and then round the values to the nearest integer number. This new rough string, $\bar{h}_i$, will obviously possess a somewhat different CF.

The results of this procedure are illustrated in Figure 20, page 66. Here we generated a 1D surface with “true” 1D exponential surface correlator with $\eta = 2$ and $r = 1$ (line 3, dashed) and then rounded the data points in the generated string to the nearest integer (line 1, solid). For illustrative purposes, we show the extracted CF (line 2, dot-dashed). As one can see, this procedure can work at best qualitatively.

It might be impossible to computationally emulate a random rough surface with an integer profile with an arbitrary predetermined CF, except, of course,

Figure 20: Line 1, solid: CF extracted from the generated string after rounding the profile data points $\bar{h}_i$ to the nearest integer number, $N^{-1}\langle\bar{h}_i\bar{h}_k\rangle$. Line 2, dot-dashed: CF extracted from the generated string, h_i , $N^{-1}\langle h_i h_k \rangle$. Line 3, dashed: “true” CF of the rough strings h_i and $\bar{h}_i$ with $\eta = 2$ and $r = 1$, $4 \exp(-x/2)$, see Table 2.

for “classical” surfaces with very large amplitude of roughness. However, several specific “quantized” correlators can still be generated based on Monte Carlo simulations for spin lattice models with various Hamiltonians. Numerical experiments with these systems might help in extracting the proper CF from experimental data of the surface profile based on realistic assumptions on the interaction of the surface defects. This can also help to guess which CF to use in theoretical calculations. Needless to say, many of the lattice models produce CF which are exponential at large distances but have complicated, often analytically unresolved structure in the peak area [20–22].

Unfortunately, the universe of CF which are accessible in this way is limited

by the number of known exactly solvable lattice models, mostly in $1D$, some of which may have little resemblance to real surfaces. It is even unclear whether there are any restrictions on allowed forms of the CF. In $2D$ systems even the simplest models, such as the Ising model, lead to correlators for which we do not have explicit analytical expressions making them virtually useless for our purposes.

The simplest case is, of course, the ferromagnetic Ising lattice, $\tilde{h}_i = \pm 1$, for which the CF is determined by the attractive coupling constant J in the Hamiltonian (or, equivalently, by the Boltzmann factors $\exp(\pm 2J/k_B T)$). In the $1D$ case, the CF is exponential,

$$\zeta^E(x) = \eta^2 \exp(-x/r), \quad r = \frac{1}{2} \exp(2J/k_B T). \quad (65)$$

For the $2D$ Ising model, though the CF is known in principle, it is described by a set of complicated equations involving elliptical integrals [20–22].

We performed Monte Carlo simulations of $1D$ and $2D$ rough surfaces on the basis of the Ising model. In $1D$ computations, we generated strings of 1000 entries each and performed 10^6 Metropolis “cooling” cycles³. By selecting appropriately the Boltzmann factor in Eq. (65), we could generate spin profiles with exponential CF with known correlation radius. In illustrations below we emulate correlations with roughness parameters equal to those measured earlier in GRANIT experiments [14], $\eta = 0.119$ and $r = 1.19$. Since the “true” CF is now exponential, the theoretical value of the observable Φ_1 for these roughness parameters should be $\Phi_{1th}^E = 19.5$ according to Eq. (37). For these same parameters, $\Phi_{1th}^G = 23.7$ and $\Phi_{1th}^{PL} = 20.4$ (Eqs. (33) and (35)). We extracted the correlator by the same methods used in the previous sections, Eq. (61), and recalculated the observable (Φ_1) using

³It is important to note that for numerical experiments with the Ising model the computational limit is the number of Metropolis cycles, $N_{max}^{cycle} = 10^6$, and *not* the lateral length of our rough profiles.

#	$r_f^E, \sigma^E \times 10^4$	$r_f^G, \sigma^G \times 10^4$	$r_f^{PL}, \sigma^{PL} \times 10^4$	$\Phi_1^E, \Phi_1^G, \Phi_1^{PL}, \Phi_1^r$
1	1.27, 6.69	0.85, 6.93	1.26, 6.72	18.6, 27.4, 19.6, 25.8
2	1.23, 6.83	0.88, 6.94	1.25, 6.84	19.1, 26.8, 19.7, 26.2
3	1.04, 6.51	0.73, 6.74	1.07, 6.54	20.7, 30.2, 21.4, 27.3
4	1.18, 6.65	0.87, 6.71	1.23, 6.62	19.7, 27.1, 20.0, 26.1
5	0.94, 6.44	0.74, 6.42	1.03, 6.38	22.2, 29.8, 21.9, 27.7

Table 7: Five Monte Carlo runs for the 1D Ising model. The “true” CF is exponential with $\eta = 0.119$ and $r = 1.19$, which yields $\Phi_{1th}^E = 19.5$ (Eq. 37). The extracted CF from the generated rough surfaces were fitted with the exponential (E), Gaussian (G), and power law (PL) functions. The table contains the best fitting values of $r^{E,G,PL}$ and the corresponding values of $\sigma^{E,G,PL}$ and $\Phi_1^{E,G,PL}$. The best fitting values of η (not shown) differed from that of the “true” correlator by less than 1% for all fitting functions. The values of Φ_1^r were obtained by direct spectral decomposition of the raw correlation data. Each rough string was $N = 1000$ points long and we performed 10^6 Metropolis cycles.

the two alternatives implemented earlier: Fitting to various fitting functions (see Table 4) and direct spectral decomposition of the raw data.

The result of 5 runs are summarized in Table 7. We used the amplitude of roughness (η_f) and the correlation radius (r_f) as fitting parameters as before. Whereas the values of $r_f^{E,G,PL}$ were obviously different, the values of $\eta_f^{E,G,PL}$ differed from the theoretical value ($\eta = 0.119$) by less than 1% for all fitting functions, thus we omitted them from the Table. As expected, the fit corresponding to the exponential correlator provides the best values of Φ_1 . The values of $\sigma^{E,G,PL}$ for all fitting functions are practically indistinguishable from each other, similarly to our previous numerical experiments (Tables 5 and 6). Of the other two fits, it is not clear why the power law fit provides much better values of Φ_1 than the Gaussian one.

The last column in Table 7 also shows the values of Φ_1^r obtained by direct spectral analysis using $N/2$ harmonics of the raw correlation data without any fitting. These results display the worst agreement with $\Phi_{1th}^E = 19.5$ (about 36% difference) whereas the value of σ^r was 13 orders of magnitude better than σ for any of our fitting functions. The explanation is the same as before: the full set of

Figure 21: An example of extracted CF for a 1D surface, $h(x)$, generated using the Ising model (solid line 1), Eq. (65), with correlation parameters $\eta = 0.119$ and $r = 1.19$ and its fitting CF (dashed line 2). The standard deviation between the fit and the extracted CF was $\sim 6.83 \times 10^{-4}$. The fitting roughness parameters, recalculated observables and values of standard deviations for other 5 runs can be found in Table 7.

raw data is dominated by the long range fluctuating correlation tails (see Figure 21).

The last table, Table 8 on page 72, presents the results for three rough surfaces generated using the 2D Ising model plus a row for the CF averaged over ten runs, as we did in Section 3.5.2. The best fitting parameters are shown in Table 8(a) while the recalculated observables are shown in Table 8(b). We performed 10^6 Metropolis cycles at $T = 1.2T_c$ (correlation radius $r \approx 1.04$). One of the generated 2D Ising rough profiles is shown in Figure 22, page 70. The surface size is relatively large, 100×100 . The correlators were extracted implementing the same techniques used in previous Sections (see Figure 23, page 71).

Figure 22: An example of a $2D$ rough surface with quantized amplitude of roughness, $\tilde{h}_i \pm 1$, generated using the Ising model at $T = 1.2T_c$.

In the second column of Table 8(b), the observable is now Φ_2 which was calculated using Eq. (43). The extracted correlation data was fitted for both the $1D$ flat CF (index “1”) using the fitting correlators from Table 4, and the $2D$ CF (index “2”) using the isotropic exponential fitting correlator $\eta_f^2 \exp[-\sqrt{x^2 + y^2}/r_f]$. Unlike $1D$ spin rough systems, here we do not know the exact “true” value of Φ_2 . We expect that at $T = 1.2T_c$ the domains are relatively small and the relaxation times are manageable. We expect that the exponential correlator in Table 8 provides the best estimate for Φ_{2th} .

The values of σ for all the fits in Table 8(a) are again close to each other, while the values of r_f and Φ_2 are noticeably different. The results for the exponential

Figure 23: (a) An example of the extracted 2D CF of a rough surface using the Ising model at $T = 1.2T_c$, Figure 22. (b) The same CF after averaging over the angles.

fit should be the closest to the true value of Φ_2 . The first column shows the exponential fitting from the flat file, $\zeta_{fl}(\rho)$. The second column gives the results of fitting $\zeta_{ex}(s, t)$ directly by the 2D isotropic exponential function and for Gaussian and power law correlators (columns 3 and 4) we used again the flat file, $\zeta_{fl}(\rho)$.

The last column of Table 8(b) shows our results for atomic roughness in UTF systems, where the observable is $\tilde{\zeta}_0$, Eq. (64). We found somewhat surprising that the results for our choice of the power law correlator, which is the Fourier image of the exponential correlator (Eqs. (34) and (36)), are close to those using the

#	$r^{E1}, \sigma^{E1} \times 10^2$	$r^{E2}, \sigma^{E2} \times 10^2$	$r^G, \sigma^G \times 10^2$	$r^{PL}, \sigma^{PL} \times 10^2$
1	1.56, 2.03	1.60, 2.75	1.06, 2.41	1.55, 2.12
2	1.43, 1.56	1.43, 2.27	1.06, 1.89	1.48, 1.63
3	1.53, 1.66	1.53, 2.49	1.11, 2.04	1.57, 1.75
Av.	1.54, 0.69	1.57, 0.89	1.10, 1.42	1.57, 0.91

(a)

#	$(\Phi_2^{E1}, \Phi_2^{E2}, \Phi_2^G, \Phi_2^{PL}) \times 10^3$	$\tilde{\zeta}_0^{E1}, \tilde{\zeta}_0^{E2}, \tilde{\zeta}_0^G, \tilde{\zeta}_0^{PL}$
1	3.37, 3.32, 2.53, 2.58	15.33, 16.18, 7.01, 15.16
2	2.53, 2.53, 2.53, 2.64	12.80, 12.94, 7.11, 13.78
3	3.40, 3.40, 2.48, 2.57	14.61, 14.75, 7.80, 15.43
Av.	3.39, 3.36, 2.49, 2.57	14.99, 15.43, 7.67, 15.46

(b)

Table 8: (a) Best fitting values of $r^{E,G,PL}$ and the corresponding values of $\sigma^{E,G,PL}$ for three rough surfaces generated using the 2D Ising model (first three rows) and for the CF averaged over ten surfaces (last row). (b) The results for the observables $\Phi_2^{E1,E2,G,PL}$ and $\tilde{\zeta}_0^{E1,E2,G,PL}$ using the fitting parameters from (a). The Monte Carlo simulations have been done at $T = 1.2T_c$ with 10^6 Metropolis cycles. The surface size is 101×101 . The results for the fits $E1$ and $E2$ should be the closest to the true physical parameters Φ_2 and $\tilde{\zeta}_0$.

exponential fit. What is even more surprising, the values of $\tilde{\zeta}_0$ for the power law fit using the 1D CF (PL) are systematically closer to the exponential fit using the 2D CF ($E2$) than to the exponential fit using the 1D CF ($E1$). The Gaussian fit yields a very different value of $\tilde{\zeta}_0$. Note that the values of σ are comparable to each other in all the cases. The direct spectral analysis of the raw correlator data again yields the worst physical results and changes from run to run; these results were not worth listing. The spectral analysis of the CF averaged over ten runs yielded results that were not as bad as the Gaussian fit, 17.42 for the 1D case and 18.70 for the 2D case. The difference between results obtained using different fitting functions once again illustrates the uncertainty in comparing computational and experimental data to the theoretical results. One should have at least some information about the shape of the “true” CF.

3.7 Closing Comments

In summary, we looked at reconciling numerical and physical measurements of random rough surfaces with theoretical results using the roughness CF. We demonstrated that data extracted from scanning microscopy of the surface profile can be insufficient for unambiguous determination of the shape of the CF. The same is true for computational experiments in which a random surface is generated without an effort to reproduce a known CF.

There are two main obstacles, apart from the accuracy of the measurements, that affect the correct identification of surface correlations. The first one is the presence of the fluctuating tails in the extracted CF in $1D$ and $2D$ rough systems which is an unavoidable result of the finite size of the samples. The second one is the relationship between the step size b , the correlation radius r and the overall number of data points N . In order to properly recover the surface correlator one should have a step size as small as possible (at most $b \lesssim r/10$ [6, 11, 23]). If one decreases b while keeping the overall number of data points N constant, the data-set measured in units of r shrinks and is covered by smaller number of bigger domains. Decreasing b while keeping the sample size constant is therefore counterproductive and gives rise to spurious, purely geometrical correlations between clusters of inhomogeneities that have no physical significance and can mimic the presence of additional, larger correlation radii. One can decrease the step size while increasing the number of data points which is difficult to do with limited computational capabilities. This same effect makes reproducing surfaces with very large correlation radii virtually impossible with the methods of Section 3.2.

We analyzed two methods of numerical generation of surfaces with predetermined roughness CF. This was done with two practical physical applications in mind: the quantum diffusion $1D$ beams of UCN in a rough waveguide and the

resistivity of UTF in QSE conditions. We judged the quality of the analysis of the extracted CF by the accuracy of the predictions for the observables for these applications.

There are several challenges for identifying the roughness correlator both from experimental and numerical data on the surface profile. Most importantly, the standard deviation σ between the measured correlation and some fitting function cannot be considered a good predictor for the physical results because the value of σ extracted from fitting is strongly weighted towards the tail of the CF. If the CF decreases rapidly at large distances, the values of σ are more or less the same for all reasonable fitting functions and measure the fluctuations without providing information about the appropriateness of the chosen fitting CF. Meanwhile, the physical observables are very sensitive to the shape of the correlator. As a result, the error in physical results can exceed σ by far.

One option for suppressing the fluctuation-driven tails is to average the numerically or experimentally measured CF over several samples, as in experiments [2–5]. However, this operation is inherently dangerous when, for example, the CF itself has long tails of alternating sign. The operation might be helpful if there is prior knowledge that there are no long range correlations in the sample.

We also tried the alternative approach to data analysis without using fitting functions by performing the spectral analysis of the raw correlation data and feeding the results directly into the equations for the calculation of the observables. In $1D$ samples, this approach worked somewhat, but not much, better than using a fitting function of the wrong shape, but still noticeably worse than using the “right” fitting function. This approach did not work in our generated $2D$ samples because of the fluctuation-driven anisotropy which was exacerbated by the smaller sizes of the samples compared with those in $1D$.

If there are no restrictions on the amplitudes of inhomogeneities, as in the case of macroscopic roughness, one can easily generate a surface with any given CF. Generating random surfaces with discretized, atomic inhomogeneities, i.e., inhomogeneities with amplitudes of integer sizes, presents unique challenges. Here the only reliable method is to use a solvable spin lattice model (Ising model). However, this approach works only in 1D rough systems since the universe of exactly solvable models is limited and, therefore, one can generate the surfaces with discrete amplitude of inhomogeneities with just few types of predetermined surface correlators which may or may not reflect real rough surfaces.

For the neutron problem, for which the roughness of the waveguide is introduced on purpose, our numerical experiments with the Ising model might prove to be helpful. One can generate a random rough profile using the Monte Carlo simulations on the basis of the 1D Ising model with predetermined correlation radius and amplitude of roughness and to transfer this profile onto the mirror surface. We will make use of this idea in Chapter 6.

In the following Chapter, we will use our experience with simulated rough surfaces to identify accurately the rough CF of GRANIT’s new mirror.

List of References

- [1] M. Escobar and A. Meyerovich, “Applications and identification of surface correlations,” arXiv:1404.1291, 2014.
- [2] R. C. Munoz, G. Vidal, G. Kremer, L. Moraga, and C. Arenas, “Surface-induced resistivity of gold films on mica: comparison between the classical and the quantum theory,” *J. Phys.: Condens. Matter*, vol. 11, pp. L299–L307, 1999.
- [3] R. C. Munoz, G. Vidal, G. Kremer, L. Moraga, and C. Arenas, “Surface roughness and surface-induced resistivity of gold films on mica: influence of roughness modelling,” *J. Phys.: Condens. Matter*, vol. 12, pp. 2903–2912, 2000.

- [4] R. C. Munoz, A. Concha, F. Mora, and R. Espejo, “Surface roughness and size effects of thin gold films on mica,” *Phys. Rev. B*, vol. 61, no. 7, p. 4514, Feb. 2000.
- [5] R. C. Munoz, G. Vidal, M. Muslow, J. G. Lisoni, C. Arenas, A. Concha, F. Mora, R. Espejo, G. Kremer, L. Moraga, R. Esparza, and P. Haberle, “Surface roughness and surface-induced resistivity of gold films on mica: Application of quantitative scanning tunneling microscopy,” *Phys. Rev. B*, vol. 62, no. 7, p. 4686, 2000.
- [6] J. A. Ogilvy and J. R. Foster, “Rough surfaces: gaussian or exponential statistics?” *J. Phys. D: Appl. Phys.*, vol. 22, pp. 1243–1251, 1989.
- [7] A. Westphal, “Quantum Mechanics and Gravitation,” Ph.D. dissertation, University of Heidelberg, 2001. [Online]. Available: arxiv.org/pdf/gr-qc/0208062.
- [8] M. Escobar and A. E. Meyerovich, “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.
- [9] M. Escobar, F. Lamy, A. E. Meyerovich, and V. V. Nesvizhevsky, “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- [10] M. Escobar and A. Meyerovich, “Quantized ultracold neutrons in rough waveguides: GRANIT experiments and beyond,” *Advances in High Energy Physics*, vol. 2014, Article ID: 185414, July 2014.
- [11] J. A. Ogilvy, *Theory of wave scattering from random surfaces*. IOP Publishing, 1991.
- [12] G. Palasantzas, “Roughness spectrum and surface width of self-affine fractal surfaces via the K-correlation model,” *Phys. Rev. B*, vol. 48, no. 19, p. 14472, 1993.
- [13] S. M. Goodnick, D. K. Ferry, C. W. Wilmsen, Z. Liliental, D. Fathy, and O. L. Krivanek, “Surface roughness at the Si(100)-SiO₂ interface,” *Phys. Rev. B*, vol. 32, no. 12, Dec. 1985.
- [14] V. V. Nesvizhevsky, H. G. Börner, A. K. Petukhov, H. Abele, S. Baessler, F. J. Rueb, T. Stöferle, A. Westphal, A. M. Gagarski, G. A. Petrov, and A. V. Strelkov, “Quantum states of neutrons in Earth’s gravitational field,” *Nature*, vol. 415, pp. 297–299, Nov. 2002.
- [15] A. E. Meyerovich and I. V. Ponomarev, “Surface roughness and size effects in quantized films,” *Phys. Rev. B*, vol. 65, 155413, 2002.

- [16] A. E. Meyerovich and A. Stepaniants, “Transport equaiton and diffusion in ultrathin channels and films,” *Phys. Rev. B*, vol. 58, p. 13 242, Nov. 1998.
- [17] A. E. Meyerovich and A. Stepaniants, “Transport phenomena at rough boundaries,” *Phys. Rev. Lett.*, vol. 73, no. 2, p. 316, July 1994.
- [18] A. E. Meyerovich and A. Stepaniants, “Interference of bulk and boundary scattering in films with a quantum size effect,” *J. Phys.: Condens. Matter*, vol. 12, pp. 5575–5597.
- [19] Y. Cheng and A. E. Meyerovich, “Mode coupling in quantized high-quality films,” *Phys. Rev. B*, vol. 73, 085404, Feb. 2006.
- [20] H. Cheng and T. T. Wu, “Theory of toeplitz determinants and the spin correlations of the two-dimensional Ising model III,” *Phys. Rev.*, vol. 164, no. 2, pp. 719–735, 1967.
- [21] J. D. Johnson, S. Krinsky, and B. M. McCoy, “Vertical-arrow correlation length in the eight-vertex model and the low-lying excitations of the X-Y-Z-Hamiltonian,” *Phys. Rev. A*, vol. 8, no. 5, pp. 2526–2547, 1973.
- [22] T. T. Wu, B. M. McCoy, C. A. Tracy, and E. Barouch, “Spin-spin correlation functions for the two-dimensional Ising model: Exact theory in the scaling region,” *Phys. Rev. B*, vol. 13, no. 1, p. 316, 1976.
- [23] J. A. Ogilvy, “Computer simulation of acoustic wave scattering from rough surfaces,” *J. Phys. D: Appl. Phys.*, vol. 21, pp. 260–277, 1988.

CHAPTER 4

Correlation Properties of the Real GRANIT Mirror

4.1 Extraction of the Roughness CF

Most of the contents of this chapter can be found in Ref. [1].

As mentioned earlier in Section 1.3, we analyzed the experimental data on the roughness of a new large glass mirror produced for ongoing GRANIT experiments at ILL [1–4].

The design and construction of the new mirror are determined by the following considerations. This mirror should serve for shaping of the initial UCN spectrum and will be installed at the most upstream part of the transport mirror. In first test experiments, it will be used also for measurements of parameters of gravitational quantum states of UCN. Since the main application of the mirror is to serve as a gravitational state selector, the mirror has large roughness amplitudes thus maximizing its efficiency at the expense of absolute measurements with this rough scatterer/absorber. The total length along the beam of UCN is restricted by the length of the flat bottom mirror; therefore, the length of the rough mirror is restricted by some reasonable small value (9 cm). The width of the rough mirror is similar to the width of the bottom mirror (30 cm). The schematics of the mirror is given in Figure 24 on page 79.

The roughness profile of this new mirror was measured in the five patches shown in Figure 24 using the vertical scanning interferometry (VSI) technique, see Section 1.3 and Ref. [5]. Light is split into two coherent light beams. One beam is sent onto the measured mirror and is coupled after reflection with another light

Figure 24: The latest rough mirror surface with five control patches [1]. The mirror is 90 mm long in the direction of propagation of the UCN. The surface roughness is assumed to be uniform across the mirror.

beam reflected from a perfectly flat sample. The resulting beam is analyzed in a CCD camera and the interference pattern gives the profile of the rough mirror. Scanning over a certain area of the rough mirror allows one to measure the distribution of roughness. If the roughness is too sharp in a particular point, the beam deviates from its vertical trajectory and it does not get back into the detector resulting in a “Bad” point in the data set. The fabrication of the rough mirror favors producing moderate roughness without large angles between the local surface and the global reference plane (too large amplitudes have been eliminated by the surface production technique). There are about $(1.5 \div 2)\%$ of “Bad” points among the whole data-set, which sometimes formed clusters. The largest cluster contained 8 “Bad” points.

The raw data set contains surface profiles $h_i(x, y)$ measured in five patches ($i = 1, 2, 3, 4, 5$), Figure 24. The mirror is 90 mm long in the direction of the UCN beam and 300 mm wide. The size of each patch is $0.504 \times 0.504 \text{ mm}^2$. The data

set for each patch contains $2557 \times 2557 \sim 6.5 \times 10^6$ points. The distance between individual data points (step size) is $b = 0.2 \text{ } \mu\text{m} \ll l_0, \ell$.

4.1.1 Data Set Preparation

The data analysis consists of several steps. First, thin stripes of “Bad” points located at the edges of the measured profiles were eliminated. The “Bad” data points within the remaining 2537×2537 square were replaced by the averages of surrounding points. Second, the proper reference planes for individual patches are restored by fitting each of the five data sets h_i to the planes $p_i(x, y) = a_i + b_i x + c_i y$ to eliminate the tilting and ensure that $\langle h_i \rangle = 0$. The set of coefficients a_i, b_i, c_i provides the best fit to the profile data for the i^{th} patch and the values of $p_i(x, y)$ are subtracted from $h_i(x, y)$, $\bar{h}_i(x, y) = h_i(x, y) - p_i(x, y)$. By itself, eliminating the tilting in this way is not controversial. The only potential problem here could arise if the mirror as a whole is slightly curved and the reference planes for the individual patches are different from each other.

4.1.2 Computation of the CF

The analysis of the data sets and the results are similar to our numerical experiments in Chapter 3 and Ref. [6]. We improve the accuracy by maximizing utilization of the data points. We define the extracted CF as

$$\zeta_{ex}(s > 0, t > 0) = \frac{1}{(N-s)(N-t)} \sum_{i=1+t}^N \sum_{j=1}^{N-s} \bar{h}_{i,j} \bar{h}_{i-t,j+s}, \quad (66)$$

where $\bar{h}_{ij}$ is the height of the point at coordinates (x_i, y_j) and $N = 2537$ is the lateral size of the sample. Just as in numerical experiments, the finite size of the patches degrades the accuracy of the computations for large s and t in Eq. (66). This degradation becomes rapid at $s, t > N/2$ resulting in the large fluctuations in the tail.

Figure 25: Light surface: Extracted 2D CF, $\zeta_{ex}(s, t)$ in Eq. (66), for patch #2 (see Figure 24). Dark surface: Best fit for $\zeta_{ex}(s, t)$ by isotropic exponential fitting function, $\zeta_f(\rho) = \eta^2 \exp(-\rho/r_f^E)$, $\rho = \sqrt{s^2 + t^2}$, where $\eta = \sqrt{\zeta_{ex}(0, 0)} = 1.14$ and $r_f^E = 0.72$. The best fitting values of the correlation radius r^E for all extracted CF are summarized in Tables 9 and 10. The horizontal axes are in units of l_0 while the ζ axis is in units of l_0^2 .

The extraction of the correlation information from the profile data sets is routine with the only limitation being the large volume of profile data. Our computational capabilities allowed us to compute the 2D ζ_{ex} in Eq. (66) up to $s_{max} = t_{max} = 200$ points $\approx 7l_0^1$. Due to the rapid increase of operations with increasing s and t we calculated $\zeta_{ex}(100 < s, t < 200)$ with step size equal to $2b$. An example of 2D CF for one of the patches is shown in Figure 25 (light surface). The extracted correlators for the other patches look similar. All extracted correlators exhibit sharp peaks which might indicate an exponential decay of the CF.

We checked the isotropy of the five extracted CF by fitting them to anisotropic

¹This value defines our computational limit.

#	η	$r_s^E, r_t^E \sigma^E \times 10^2$	$r_s^{PL}, r_t^{PL}, u, \sigma^{PL} \times 10^2$
1	1.03	0.62, 0.63, 1.42	0.45, 0.45, 0.9997, 1.56
2	1.14	0.70, 0.73, 2.69	0.44, 0.46, 0.864, 2.04
3	0.97	0.64, 0.74, 2.71	0.28, 0.31, 0.658, 1.37
4	0.99	0.64, 0.66, 2.35	0.32, 0.34, 0.73, 1.26
5	0.96	0.57, 0.60, 0.83	0.46, 0.48, 1.10, 1.20
Av.	1.02	0.64, 0.67, 1.84	0.38, 0.40, 0.842, 1.33

Table 9: The parametrization of the extracted CF, $\zeta_{ex}(s, t)$, by anisotropic exponential and power law fitting functions (see Eqs. (67) and (68)). Rows 1-5 give the data for the individual patches (see Figure 24) and the last row gives the CF averaged over all patches. The values of the amplitude of roughness in the second column correspond to $\eta = \sqrt{\zeta_{ex}(0, 0)}$ (see Eq. (66)) and it is not a fitting parameter.

#	$r_f^E, \sigma^E \times 10^2$	$r_f^G, \sigma^G \times 10^2$	$r_f^{PL}, \sigma^{PL} \times 10^2$	$(\Phi_2^E, \Phi_2^G, \Phi_2^{PL}) \times 10^{-3}$
1	0.62, 1.42	0.49, 3.93	0.66, 2.04	5.44, 3.94, 4.18
2	0.72, 2.44	0.56, 5.75	0.76, 3.15	6.23, 4.52, 4.78
3	0.68, 2.61	0.50, 4.94	0.70, 3.23	4.63, 3.46, 3.60
4	0.65, 2.25	0.49, 4.56	0.68, 2.80	4.92, 3.64, 3.81
5	0.58, 0.68	0.47, 3.00	0.62, 1.48	4.87, 3.50, 3.75
Av.	0.65, 1.75	0.50, 4.39	0.69, 2.44	5.22, 3.83, 4.01

Table 10: Results of the fit of the extracted CF for five patches (see Figure 24) and for the averaged CF (last row) by the exponential (E), Gaussian (G), and power law (PL) fitting functions as defined in Table 2. For each fitting function the table shows the correlation radii $r^{E,G,PL}$ and the quality of the fits, $\sigma^{E,G,PL}$ (Eq. (62)). The last column shows the calculated parameter $\Phi_2^{E,G,PL}$ (Eq. (43)) responsible for the exit neutron count, Eq. (20).

exponential and power law fitting functions:

$$\zeta_f^E(s, t) = \eta^2 \exp \left(-\sqrt{(s/r_s^E)^2 + (t/r_t^E)^2} \right), \quad (67)$$

$$\zeta_f^{PL}(s, t) = \frac{\eta^2}{[1 + (s/r_s^{PL})^2 + (t/r_t^{PL})^2]^u}, \quad (68)$$

where $\eta^2 = \zeta_{ex}(0, 0) = N^{-2} \sum_i \bar{h}_i^2$, and is not a fitting parameter. The best fitting values for $r_{s,t}$ are summarized in Table 9.

The first five rows in Table 9 provide the data for the individual patches, while the last row describes the CF averaged over all patches. One can make two

Figure 26: The illustration of the fluctuation-driven tails of the CF, $\zeta(s, 0)$, for patch #2 of the actual mirror (solid curve) and for the numerically generated surface with roughness emulating the exponential CF with $\eta = 1.14$ and $r = 0.72$ (see the second row of Table 10)

conclusions. First, as in our numerical experiments the statistical quality of the fit by each fitting function, which is measured by σ^2 in Eq. (62), is roughly the same for both ζ_f^E and ζ_f^{PL} and it is dominated by the oscillations in the tails. Second, the anisotropy of the CF, as measured by the difference in the correlation radii $r_{s,t}$ in the s and t directions, is of the order of $(3 \div 4)\%$. This is smaller than the difference in the correlation radii between the patches, which is rather pronounced. For this reason, in further analysis we neglect the anisotropy and concentrate on analyzing the extracted CF averaged over the angles, $\zeta_{fl}(\rho)$, $\rho = \sqrt{s^2 + t^2}$ (see Figure 27).

Figure 27: Solid line, 1: Extracted correlator after averaging over the angles and over all patches, last row in Table 10. Dashed line, 2: The fitting 1D exponential correlator of the form $\zeta_f^E(\rho) = \zeta_{ex}(0,0) \exp(-\rho/r_f^E)$. Dotted line, 3: The fitting 1D power law correlator of the form $\zeta_f^{PL}(\rho) = \zeta_{ex}(0,0)[1 + (\rho/r^{PL})^2]^{-3/2}$. The fitting E correlator describes the peak area of the extracted CF much better than the PL fitting correlator. The extracted fitting parameters and values of σ are shown in Table 10.

In Figure 25 in page 81 we plotted the best fit for the CF from patch #2 to isotropic exponential fitting function (dark surface). The value of the fitting correlation radius is indistinguishable from that of the corresponding flat 1D CF (Table 10, second row). Figure 26 gives a comparison between the CF for patch #2 and for a computationally generated rough surface (see Chapter 3) emulating the exponential correlation with roughness parameters identical to those extracted from patch #2, namely, $\eta = 1.14$ and $r = 0.72$ (see Table 10). The similarity in fluctuating tails is striking. Similar long oscillations tails are observed for all other

patches.

Though the exponential and power law fits yield similar values of σ because of the dominant contribution of the tail, in the peak area the exponential fit worked visually much better. This is evidenced in Figure 27 on page 84 where we present the flat CF obtained from the $2D$ correlator averaged over the five patches in the last row of Table 10 (solid line 1), together with the exponential (dashed line 2) and power law (dotted line 3) fitting correlators. For this reason we choose to use the results of the exponential fits for calculating the observable Φ_2 , Eq. (43), in the last column of Table 10.

In Table 10, we present the results of fitting $\zeta_{fl}(\rho)$ for the five patches and for the averaged CF (last row) using the exponential (E), Gaussian (G), and power law functions (PL) from Table 2 together with the values of the fitting correlation radii, the standard deviation and the observable Φ_2 . The values of η remain the same as those of the second column in Table 9.

4.2 Experimental Consequences

The main conclusion from the previous sections is that the difficulties that we experience trying to identify the CF for the actual mirror are exactly the same as in our numerical experiments in Chapter 3. Our extensive numerical data show that the best way of identification seems to be the averaging over several samples in combination with the graphical and numerical analysis of the peak area without much reliance on the overall standard deviation, σ .

Our reluctant conclusion from the analysis of the experimental data on the roughness of the actual mirror is that its roughness CF is close to the isotropic exponential function, $\zeta_{\text{actual}}(\rho) = \eta^2 \exp(-\rho/r)$, with roughness amplitude $\eta = 1.02$

and correlation radius $r = 0.65$ (Table 10). This yields the value $\Phi_2 \simeq 5.22 \times 10^3$. The uncertainty in the parameters is about 10% given the presence of “Bad” points in the data sets, residual anisotropy and, most of all, difference in values between the patches.

Knowing the value of Φ_2 we can predict the exit neutron count in experiments with this mirror. Luckily, the uncertainty in Φ_2 in this range of values does not affect much the dependence of the exit neutron count on the waveguide width. We will present our main predictions for the neutron count in function of the waveguide width in the next chapter.

List of References

- [1] M. Escobar, F. Lamy, A. E. Meyerovich, and V. V. Nesvizhevsky, “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- [2] M. Escobar and A. Meyerovich, “Quantized ultracold neutrons in rough waveguides: GRANIT experiments and beyond,” *Advances in High Energy Physics*, vol. 2014, Article ID: 185414, July 2014.
- [3] M. Escobar and A. E. Meyerovich, “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.
- [4] G. Pignol, S. Baessler, V. V. Nesvizhevsky, K. Protasov, D. Rebreyend, and A. Voronin, “Gravitational Resonance Spectroscopy with Oscillating Magnetic Field Gradient in the GRANIT Flow through Arrangement,” *Advances in High Energy Physics*, vol. 2014, Article ID: 628125, Aug. 2014.
- [5] I. Kurganskaya, A. Luttge, and A. R. Barron, “The application of VSI to the Study of Crystal Surface Processes,” *Connexions*, 2009. [Online]. Available: <http://cnx.org/content/m22326/1.4/>
- [6] M. Escobar and A. Meyerovich, “Applications and identification of surface correlations,” arXiv:1404.1291, 2014.

CHAPTER 5

Predictions For Ongoing GRANIT Experiments

Most of the contents of this chapter can be found in Ref. [1].

Figure 28 on page 88 shows the predicted exit neutron count for our extracted roughness parameters $\eta = \ell/l_0 = 1.02$, $r = R/l_0 = 0.65$, and $\Phi_2 \simeq 5.22 \times 10^3$ (last row in Table 10) as a function of the spacing between the rough and flat mirrors, h (Figure 1) [1–3]. The steps in the figure are the long-sought demonstration of the consecutive depletion of the quantum gravitational steps (see Chapter 2).

The accuracy of this prediction is limited by a relatively large value of the roughness amplitude, which breaks our main theoretical assumption $\eta \ll r, h$ [1, 3–6]. The same factor limits the accuracy of measuring the spacing between mirrors, as mentioned earlier, making the measurements at small h virtually impossible.

From the point of view of the experiment, a large η is not very good either. It results in a noticeable broadening of the levels and in the smearing of the gravitational quantum states [3]. In addition, both theory and experiment require better information on the distribution of neutrons entering the slit over the quantum states, N_0 (see Eq. (20)).

The uncertainty of about 10% in our predicted value of Φ_2 (see Section 4.2) does not affect the dependence of the exit neutron count on the slit width as opposed to smaller values of Φ found in Refs. [4–6] (see Figure 6). This is illustrated in Figure 29 on page 88. The eight curves in this figure show (from left to right) the exit neutron count N_e/N_0 with respect to the slit width, h , for $\Phi_2 \times 10^{-3} = 1; 2; 3; 4; 5; 6; 7; 8$ (see Eq. (20)). All curves in Figure 29 show well pronounced

Figure 28: Predicted exit neutron count $N_e(h)/N_0$, Eq. (20), as a function of the waveguide width, h (see Figure 1). Calculations for the new GRANIT mirror with isotropic exponential roughness yield $\Phi_2 \simeq 5.22 \times 10^3$.

Figure 29: Exit neutron count $N_e(h)/N_0$ as a function of the waveguide width, h for several values of Φ_2 . N_0 represents the number of neutron entering the slit in each quantum state, Eq. (20). Eight curves from left to right correspond to $\Phi_2 \times 10^{-3} = 1; 2; 3; 4; 5; 6; 7; 8$. The neutron count decreases with increasing Φ_2 .

predicted quantum steps which allows using the setup for precise measurements of fundamental forces [7–15].

It is worth mentioning that the neutron count is less sensitive to the value of Φ when Φ is in the $(2 \div 8) \times 10^3$ range than when it is in the $5 \div 40$ range (compare Figures 6 and 29).

List of References

- [1] M. Escobar, F. Lamy, A. E. Meyerovich, and V. V. Nesvizhevsky, “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- [2] M. Escobar and A. Meyerovich, “Quantized ultracold neutrons in rough waveguides: GRANIT experiments and beyond,” *Advances in High Energy Physics*, vol. 2014, Article ID: 185414, July 2014.
- [3] M. Escobar and A. E. Meyerovich, “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.
- [4] A. Meyerovich and V. V. Nesvizhevsky, “Gravitational quantum states of neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 73, 063616, June 2006.
- [5] R. Adhikari, Y. Cheng, and A. E. Meyerovich, “Quantum size effect and biased diffusion of gravitationally bound neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 75, 063613, June 2007.
- [6] M. Escobar and A. Meyerovich, “Beams of gravitationally bound ultracold neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 83, 033618, Mar. 2011.
- [7] I. Antoniadis, S. Baessler, M. Büchner, V. V. Fedorov, S. Hoedl, A. Lambrecht, V. V. Nesvizhevsky, G. Pignol, K. V. Protasov, S. Reynaud, and Y. Sobolev, “Short-range fundamental forces,” *C. R. Physique*, vol. 12, pp. 775–778, 2011.
- [8] S. Baessler, V. V. Nesvizhevsky, G. Pignol, K. V. Protasov, and A. Y. Voronin, “Constraints on spin-dependent short-range interactions using gravitational quantum levels of ultracold neutrons,” arXiv:0902.3139, 2009.
- [9] M. Kreuz, V. V. Nesvizhevsky, P. Schmidt-Wellenburg, T. Soldner, M. Thomas, H. G. Börner, F. Naraghi, G. Pignol, K. V. Protasov, D. Rebreyend, F. Vezzu, R. Flaminio, C. Michel, N. Morgado, L. Pinard, S. Baessler,

- A. M. Gagarski, L. A. Grigorieva, T. M. Kuzmina, A. E. Meyerovich, L. P. Mezhev-Deglin, G. A. Petrov, A. V. Strelkov, and A. Y. Voronin, “A method to measure the resonance transitions between the gravitationally bound quantum states of neutrons in the GRANIT spectrometer,” *Nucl. Instrum. Meth. A*, vol. 611, pp. 326–330, 2009.
- [10] G. L. Greene and V. Gudkov, “Neutron interferometric method to provide improved constraints on non-newtonian gravity at the nanometer scale,” *Phys. Rev. C*, vol. 75, 015501, 2007.
 - [11] V. V. Nesvizhevsky, G. Pignol, and K. V. Protasov, “Neutron scattering and extra-short-range interactions,” *Phys. Rev. D*, vol. 77, 034020, 2008.
 - [12] T. Jenke, P. Geltenbort, H. Lemmel, and H. Abele, “Realization of a gravity-resonance-spectroscopy technique,” *Nature Physics*, vol. 7, pp. 468–472, 2011.
 - [13] T. Jenke, G. Cronenberg, J. Burgdörfer, L. A. Chizova, P. Geltenbort, A. N. Ivanov, T. Lauer, T. Lins, S. Rotter, H. Saul, U. Schmidt, and H. Abele, “Gravity Resonance Spectroscopy Constrains Dark Energy and Dark Matter Scenarios,” *Phys. Rev. Lett.*, vol. 112, p. 151105, 2014.
 - [14] S. Schleich and E. Rasel, “Neutrons knock at the cosmic door,” *Physics*, vol. 7, no. 39, Apr. 2014.
 - [15] O. Bertolami and F. M. Nunes, “Ultracold neutrons, quantum effects of gravity and the weak equivalence principle,” arXiv:hep-ph/0204284, 2002.

CHAPTER 6

Summary and Conclusions

6.1 Main Conclusions

In summary, we have applied the general theory of transport of particles along rough surfaces [1–6] to the gravitationally quantized diffusion of UCN in a rough waveguide. We demonstrated that all the information about the properties of the waveguide (length, roughness, absorption threshold, etc.) collapse into a single dimensionless constant $\Phi_{1,2}$ which determines the exit neutron count (see Eqs. (20) and (21)). The parameter Φ is determined by a complicated integral involving the roughness CF whose shape should be known a priori (see Eqs. (30) and (43)). In waveguides with $1D$ roughness the integration could be carried analytically for most common types of correlators (see Table 2). In waveguides with $2D$ roughness the calculations were mostly numerical (see Table 3)

In general, the larger the value of Φ , the more pronounced are the quantum steps on the dependence of the neutron count on the waveguide width. These quantum steps become very clear at $\Phi \gtrsim 40$ for a waveguide with $1D$ roughness as described in Ref. [7] (compare Figures 6 and 28). Experimentally, the value of Φ can be increased by increasing η while still staying within the weak roughness domain, $r > \eta$. However, one should keep in mind that an increase in the amplitude of roughness η also degrades the accuracy of the measurement of the waveguide width [8].

We found that in the biased diffusion approximation the constant Φ is closely related to the depletion times (line broadenings) for the gravitational states, τ_j

(Eq. (16)), which have simple scaling properties (Eqs. (39) and (48)). The ratios τ_j/τ_1 are universal functions of the waveguide width (Figures 7 and 9), independent of the waveguide parameters.

We also derived useful scaling relationships which will allow experimentalists to extend our theoretical predictions in different experimental setups (Eqs. (39) and (48)).

We performed numerical experiments aimed at the identification of the CF extracted from computationally generated rough surfaces with predetermined correlators (Chapter 3). Our method allowed us to generate surfaces with macroscopic roughness ($\eta, l_0 \gg a$, where a is the atomic size) and atomic roughness ($\eta \sim a \ll l_0$), both in $1D$ and $2D$. In the case of macroscopic roughness we generated surfaces with desired CF by rotating an uncorrelated profile vector (see Eq. (54)), while in the case of atomic roughness we used a Monte Carlo simulation for a spin lattice model (see Eq. (65)).

The objective of the numerical experiments was to identify the difficulties in the accurate extraction of the roughness CF from profile data for computationally generated rough surfaces. We did this by fitting the extracted $1D$ and $2D$ CF to reasonable fitting correlators (Tables 2 and 3) and by inputting the spectral decomposition of the extracted raw CF directly into the equations for the observables.

We found two main obstacles for the unambiguous extraction of the roughness correlator:

The first of them is the presence of fluctuation-driven tails in extracted CF which is unavoidable for finite samples. All the fitting functions which we used (see Tables 2, 3 and Eqs. (67) and (68)) exhibited more or less the same statistical quality of the fit (σ) but lead to considerably different predictions for the observables. The statistical quality of the fits is heavily weighted towards the fluctuating

tail region of the CF rather than the peak area. In consequence, the quality of the fit should *not* be judged by the value of σ in Eq. (62). Suppressing the fluctuations in the tails by averaging of the CF extracted from several independent samples might be beneficial if there are no long-range oscillating correlations in the sample; otherwise it might be dangerous.

The second obstacle is the relationship between the step size b , which should be as small as possible, and the correlation radius. Decreasing b without proportionally increasing the size of the samples gives rise to geometrical interdomain correlations that are not related to physical interactions. These interdomain correlations can masquerade as the presence of an additional, larger correlation radius.

Avoiding the use of fitting functions by feeding the equations with the raw correlation data seems to be marginally acceptable for $1D$ rough surfaces and did not work at all for $2D$ surfaces. Our main conclusion here is that the direct use of the raw correlator is worse than the careful analysis of the fitting functions.

In conclusion, the identification of the roughness CF should not be undertaken lightly. The results of the numerical experiments lead us to believe that the proper identification of the CF requires using the statistical quality of the fittings (σ) in combination with averaging the extracted CF over different samples plus a graphical and numerical analysis of the averaged correlator in the peak area.

Based on this experience, we identified the CF for the new GRANIT mirror as isotropic exponential with roughness parameters $\eta = 1.04$ and $r = 0.65$ (see Section 4.2). This roughness correlator yields the value $\Phi_2 \simeq 5.22 \times 10^3$ which allows us to predict the exit neutron count as a function of the neutron width for the new GRANIT experiments utilizing this rough mirror (Figure 28). Despite uncertainties in the measurements and the quality of the data, the predicted neutron count exhibits well-developed quantum steps corresponding to the consecutive depletion

of lower gravitational states.

6.2 Recommendations For Future Work: The Ising Mirror

The presence of well-formed steps on the neutron count curve (Figure 28) is explained mostly by a relatively large amplitude of roughness (η), about 10 times bigger than for the older cell. This large value of the amplitude of roughness presents challenges for both theory and experiment. On the theoretical side, the main assumption of the theory, $\eta \ll r, h$ (weak roughness) is violated. For experiment, the large amplitude of roughness degrades the accuracy of measurements. It also means that the energy levels become broad and not very well defined even if inter-level transitions are disregarded.

Most of these uncertainties disappear if a future rough mirror is fabricated utilizing a drastically different design based on the 1D Ising model described in Section 3.6. In essence, we are proposing to make the rough mirror looking like an interferometric grating with trenches of constant depth but with randomly varying widths and separations [9, 10]. Such an Ising grating can be easily generated computationally with the methods used in Section 3.6. Since the characteristic length is macroscopic, $l_0 \sim 5.87\mu\text{m}$, the generated pattern can then be transferred to the mirror surface.

An element of such a mirror is shown in Figure 30. The thick dark line shows the surface of the mirror. Since this is an upper mirror for a GRANIT-like experiment, the mirror material is above the thick line (gray region) and the neutron beam is propagating below it (white region). The dark rectangles of width l_0 are the “Ising spins”. Both axes are measured in units of l_0 .

Since the real mirror is continuous, in contrast to the discrete Ising model,

Figure 30: A fragment of the proposed rough upper “Ising mirror” based on the Monte Carlo simulations of Section 3.6 for the 1D Ising model with $J/k_B T \approx 0.7$. The thick black line is the surface profile and the dark bars are the “Ising spins”. The mirror material is the filled gray area. The amplitude of roughness is $\eta = 0.2$, the correlation radius is $r = 2$ and the value of the observable is $\Phi_1 \approx 43.5$. All axes are in units of l_0 . The vertical scale is about 100 times smaller than the horizontal one. The value of η can be changed by simply rescaling the vertical axis.

the roughness CF coincides with the Ising exponent (Eq. (65)) only in the integer points and is slightly different elsewhere:

$$\zeta(x) = \eta^2 \left[\exp\left(-\frac{\lfloor x \rfloor}{r}\right) + (x - \lfloor x \rfloor) \left(\exp\left(-\frac{\lceil x \rceil}{r}\right) - \exp\left(-\frac{\lfloor x \rfloor}{r}\right) \right) \right] \quad (69)$$

The neutron count predictor Φ_1 for the CF in Eq. (69) can be calculated only numerically. It differs from the one for a purely exponential function by not more than 5%. Since the value of Φ_1^E in Eq. (37) is more sensitive to η than to r ,

Figure 31: Predicted exit neutron count $N_e(h)/N_0$ for the Ising mirror described in Figure 30 generated using Monte Carlo simulations for the 1D Ising model described in Section 3.6. In this figure, the roughness amplitudes are $\eta = 0.3$ (solid line) and $\eta = 0.4$ (dashed line), and the correlation radius is $r = 2$. The steps can be made more pronounced by further increasing η while still remaining in the weak roughness limit, $\eta \ll r$.

one should increase η as much as possible while remaining in the weak roughness limit, $\eta < r$. Another limit is imposed by the width of the waveguide which in experiments comes down to $h \sim 2$. Therefore, the optimal waveguide should have roughness correlation radius $r \simeq 2$ and amplitude $\eta < 2$. We would not recommend making η much larger than $0.2 \div 0.4$, since the ratio η/h limits the accuracy of measuring the waveguide width, as mentioned earlier. The values of Φ_1 with $r = 2$ and $\eta = 0.2 \div 0.4$ are in the range $42.5 \div 170$ with the parameters of the original waveguide and in the $30.3 \div 121.5$ range with the parameters of the

new waveguide. These values of Φ_1 are sufficient for exhibiting the quantum steps in the exit neutron count (see Figure 31) and for producing neutrons with well-defined energies in the peV range. Because the amplitude of roughness is quite small, these values are much smaller than the ones in Figure 29 and the quantum steps are less pronounced.

Note that most of the sources of error mentioned earlier disappear for this design since the width of the slit can be accurately measured and the energy levels are much better defined. The loss of neutrons due to sideways scattering is minimized as well. This design is easily scalable in both vertical and horizontal directions and creates a well-controlled environment.

List of References

- [1] A. Meyerovich and V. V. Nesvizhevsky, “Gravitational quantum states of neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 73, 063616, June 2006.
- [2] R. Adhikari, Y. Cheng, and A. E. Meyerovich, “Quantum size effect and biased diffusion of gravitationally bound neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 75, 063613, June 2007.
- [3] A. E. Meyerovich and A. Stepaniants, “Quantized systems with randomly corrugated walls and interfaces,” *Phys. Rev. B*, vol. 60, no. 12, p. 9129, 1999.
- [4] A. E. Meyerovich and A. Stepaniants, “Transport equaiton and diffusion in ultrathin channels and films,” *Phys. Rev. B*, vol. 58, p. 13 242, Nov. 1998.
- [5] Y. Cheng and A. E. Meyerovich, “Mode coupling in quantized high-quality films,” *Phys. Rev. B*, vol. 73, 085404, Feb. 2006.
- [6] A. E. Meyerovich and I. V. Ponomarev, “Surface roughness and size effects in quantized films,” *Phys. Rev. B*, vol. 65, 155413, 2002.
- [7] V. V. Nesvizhevsky, H. G. Börner, A. K. Petukhov, H. Abele, S. Baessler, F. J. Rueb, T. Stöferle, A. Westphal, A. M. Gagarski, G. A. Petrov, and A. V. Strelkov, “Quantum states of neutrons in Earth’s gravitational field,” *Nature*, vol. 415, pp. 297–299, Nov. 2002.

- [8] M. Escobar and A. Meyerovich, “Beams of gravitationally bound ultracold neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 83, 033618, Mar. 2011.
- [9] M. Escobar, F. Lamy, A. E. Meyerovich, and V. V. Nesvizhevsky, “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- [10] M. Escobar and A. E. Meyerovich, “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.

APPENDIX A

Proofs of Eqs. (30) and (43)

A.1 Proof of Eq. (30)

With the help of Eq. (27), Eq. (29) can be rewritten as:

$$\begin{aligned}
 F_1(r, h) &= 2 \times 10^{-5} r^3 \varepsilon^{-1/2} \sum_{j' > 1} b_{j'} \psi_1(y_{1j'}) \\
 &= \frac{2\pi^2 r^3 \sqrt{\chi}}{h^3 u_c^{3/4}} \sum_{j' > 1}^{\mathcal{N}} j'^2 \psi_1(y_{1j'}), \quad \mathcal{N} = \frac{h}{\pi} \varepsilon^{1/2} \\
 &\simeq \frac{2r^3 \varepsilon}{\pi u_c} \frac{1}{\mathcal{N}^3} \int_1^{\mathcal{N}} j'^2 \psi_1(y_{1j'}) dj',
 \end{aligned} \tag{A.1}$$

where $y_{jj'} = y_j - y_{j'} = r(\beta_j - \beta_{j'})$. The substitution $z_{j'} = j'/\mathcal{N}$ in Eq. (A.1) at $\mathcal{N} \rightarrow \infty$ (or $u_c \rightarrow \infty$) yields:

$$F_1(r, h) \simeq \frac{2r^3 \varepsilon}{\pi u_c} \int_0^1 dz \, z^2 \psi_1(y), \tag{A.2}$$

where $y_{1j'} \rightarrow y(z) = r\sqrt{\varepsilon}(1 - \sqrt{1 - z^2})$. Eq. (A.2) is the last line of Eq. (29). Substituting this expression into Eq. (21), we obtain Eqs. (30) and (31).

A.2 Proof of Eq. (43)

The integration over the angle in Eq. (6) yields the zeroth harmonic of the transition probabilities $W_{jj'}(|\mathbf{q}_{j'} - \mathbf{q}_j|)$ which can be written as¹:

$$W_{jj'}^{(0)} = \int_0^{2\pi} W_{jj'}(|\mathbf{q}_{j'} - \mathbf{q}_j|) d\theta = \pi \tilde{\zeta}_2^{(0)}(Q_j, Q_{j'}) U_c^2 \psi_j^2(H) \psi_{j'}^2(H), \tag{A.3}$$

¹Compare Eq. (A.3) with Eq. (9).

where $|\mathbf{q}_{j'} - \mathbf{q}_j| = \sqrt{|\mathbf{q}_{j'}|^2 + |\mathbf{q}_j|^2 - 2|\mathbf{q}_{j'}||\mathbf{q}_j|\cos\theta}$ (see Ref. [1]), and

$$\tilde{\zeta}_2^{(0)}(Q_{j'}, Q_j) = \ell^2 R^2 \psi_2(Q_{j'}, Q_j), \quad (\text{A.4})$$

with $Q_j = q_j R$.

The expression for the dimensionless transition probability is obtained by substituting Eq. (A.4) into Eq. (A.3)²:

$$w_{jj'} = \frac{4}{\sqrt{2\pi}} \times 10^{-10} u_c^2 b_j b_{j'} \eta^2 r^2 \psi_2(y_{j'}, y_j). \quad (\text{A.5})$$

We transform Eq. (41) for $F_2(r, h)$ by replacing summation by integration in the same way as in Eq. (A.2):

$$\begin{aligned} F_2(r, h) &= \sqrt{\frac{2}{\pi}} \times 10^{-5} r^4 \sum_{j' > 1} b_{j'} \psi_2(y_1, y_{j'}) \\ &\simeq r^4 \sqrt{\frac{2u_c}{\pi^3 \chi^3}} \frac{1}{\mathcal{N}^3} \int_1^{\mathcal{N}} j'^2 \psi_2(y_1, y_{j'}) dj'. \end{aligned} \quad (\text{A.6})$$

The last line of Eq. (41) is obtained using $z_{j'} = j'/\mathcal{N}$ in Eq. (A.6) and letting $\mathcal{N} \rightarrow \infty$ as before. Substituting this expression into Eq. (21), we obtain Eqs. (43) and (44), where $y_1 \rightarrow r\sqrt{\varepsilon}$ and $y_{j'} \rightarrow y(z) = r\sqrt{\varepsilon}\sqrt{1 - z^2}$.

List of References

- [1] A. E. Meyerovich and I. V. Ponomarev, “Surface roughness and size effects in quantized films,” *Phys. Rev. B*, vol. 65, 155413, 2002.

²Compare with Eq. (25).

APPENDIX B

Calculation of ζ_{ex} for 2D Random Rough Profiles

The CF in our generated 2D rough profiles is extracted by optimizing the use of available points, N_{max} . Instead of considering the periodic boundary conditions as we did in 1D, we extract the correlations in different directions by following the pattern described in Figure B.1 and averaging the extracted CF over different quadrants. We use all points in these quadrants as starting points for pair correlations. The directions from starting to end points in pair correlations are shown by arrows. These directions are different for different quadrants. The starting and end points can belong to different quadrants. In all cases, one has to be careful to avoid the double-counting of the correlations, see Table B.1. The extracted CF is defined in Eq. (B.1) as follows:

$$\zeta_{ex}(s, t) = \begin{cases} C_1 \left(\sum_{k=1}^M \sum_{l=1}^M h_{kl} h_{k+s, l+t} + \sum_{k=1}^M \sum_{l=M}^N h_{kl} h_{k+s, l-t} \right), & s > 0, t > 0 \\ C_2(t) \left(\sum_{k=1}^M \sum_{l=1}^M h_{kl} h_{k, l+t} + \sum_{k=1}^M \sum_{l=M}^N h_{kl} h_{k, l-t} - \sum_{k=1}^M \sum_{l=M-t}^M h_{kl} h_{k, l+t} \right), & t > 0 \\ C_3 \left(\sum_{k=1}^M \sum_{l=1}^M h_{kl} h_{k+s, l} + \sum_{k=1}^M \sum_{l=M}^N h_{kl} h_{k+s, l} - \sum_{k=1}^M h_{kM} h_{k+s, M} \right), & s > 0 \\ C_4 \left(\sum_{k=1}^M \sum_{l=1}^M h_{kl}^2 + \sum_{k=1}^M \sum_{l=M}^N h_{kl}^2 - \sum_{k=1}^M h_{kM}^2 \right), & s = t = 0, \end{cases} \quad (B.1)$$

where N labels the lateral size of the surface (not the total number of generated points, which is $N^2 \leq N_{max}$) and $M = \frac{1}{2}(N + 1)$. In Eq. (B.1), C_i is the number of averaged points which is given by:

$$C_1 = \frac{1}{2M^2}, \quad C_2(t) = \frac{1}{2M^2 - M(t + 1)}, \quad C_3 = C_4 = \frac{1}{2M^2 - M}. \quad (B.2)$$

Figure B.1: The square above describes the extraction of the CF from our numerically generated 2D rough profiles. The size of the surface profile is $N^2 = N_{max} \sim 5000$. We optimize the use of the data points by calculating correlations in different directions following the patterns described in this figure and averaging the CF between the quadrants as described in Table B.1. One has to be careful to avoid double-counting of repeated correlations; see Eqs. (B.1) and (B.2).

Averaging squares	Comment
1 ($s > 0, t > 0$) & 2 ($s > 0, t < 0$)	No double-countings
1 ($t > 0$) & 2 ($t < 0$)	Exclude the overlapping bar
1 & 4 ($s > 0, t = 0$)	Exclude the overlapping border
1 & 2 ($s = t = 0$)	Exclude the overlapping border

Table B.1: This table describes the averaging of the extracted correlations among the quadrants defined by Figure B.1. In each case, one has to suppress the double-counted correlations.

BIBLIOGRAPHY

- Adhikari, R., Cheng, Y., and Meyerovich, A. E., “Quantum size effect and biased diffusion of gravitationally bound neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 75, 063613, June 2007.
- Antoniadis, I., Baessler, S., Büchner, M., Fedorov, V. V., Hoedl, S., Lambrecht, A., Nesvizhevsky, V. V., Pignol, G., Protasov, K. V., Reynaud, S., and Sobolev, Y., “Short-range fundamental forces,” *C. R. Physique*, vol. 12, pp. 775–778, 2011.
- Antoniadis, I., Baessler, S., Bertolami, O., Dubbers, D., Meyerovich, A., Nesvizhevsky, V. V., Protasov, K., and Reynaud, S., *C. R. Physique* 12, vol. 8, pp. 703–706, Oct. 2011.
- Baessler, S., Beau, M., Kreuz, M., Kurlov, V. N., Nesvizhevsky, V. V., Pignol, G., Protasov, K. V., Vezzu, F., and Voronin, A. Y., “The GRANIT spectrometer,” *C. R. Physique*, vol. 12, pp. 707–728, 2011.
- Baessler, S., Gagarski, A. M., Lychagin, E. V., Mietke, A., Muzychka, A. Y., Nesvizhevsky, V. V., Pignol, G., Strelkov, A. V., Toperverg, B. P., and Zhernenkov, K., “New methodical developments for GRANIT,” *C. R. Physique*, vol. 12, pp. 729–754, 2011.
- Baessler, S., Nesvizhevsky, V. V., Pignol, G., Protasov, K. V., and Voronin, A. Y., “Constraints on spin-dependent short-range interactions using gravitational quantum levels of ultracold neutrons,” arXiv:0902.3139, 2009.
- Baker, C. A., Doyle, D. D., Green, K., van der Grinten, M. G. D., Harris, P. G., Iadjev, P., Ivanov, S. N., May, D. J. R., Pendlebury, J. M., Rischardson, J. D., Shiers, D., and Smith, K. F., “Improved experimental limit on the electric dipole moment of the neutron,” *Phys. Rev. Lett*, vol. 97, 131801, Sept. 2006.
- Bass, F. G. and Fuks, I. M., *Wave scattering from statistically rough surfaces*. Pergamon, New York, 1979.
- Berberan-Santos, M. N., Bodunov, E. N., and Pogliani, L., “Classical and quantum study of the motion of a particle in a gravitational field,” *Journal of Mathematical Chemistry*, vol. 37, no. 2, 2005.
- Bertolami, O., “Nonlinear corrections to quantum mechanics from quantum gravity,” *Phys. Lett. A*, vol. 154, pp. 225–229, Apr. 1991.

- Bertolami, O. and Nunes, F. M., “Ultracold neutrons, quantum effects of gravity and the weak equivalence principle,” arXiv:hep-ph/0204284, 2002.
- Bertolami, O., Rosa, J. G., de Aragao, C. M. L., Castorina, P., and Zappala, D., “Noncommutative gravitational quantum well,” *Phys. Rev. D*, vol. 72, 025010, July 2005.
- Bourdel, T., Doser, M., Ernest, A. D., Voronin, A. Y., and Voronin, V. V., “Quantum phenomena in gravitational field,” *C. R. Physique*, vol. 12, pp. 779–790, 2011.
- Brax, P. and Pignol, G., “Strongly coupled chameleons and the neutronic quantum bouncer,” *Physics Review Letters*, vol. 107, p. 111301.
- Cheng, H. and Wu, T. T., “Theory of toeplitz determinants and the spin correlations of the two-dimensional Ising model III,” *Phys. Rev.*, vol. 164, no. 2, pp. 719–735, 1967.
- Cheng, Y. and Meyerovich, A. E., “Mode coupling in quantized high-quality films,” *Phys. Rev. B*, vol. 73, 085404, Feb. 2006.
- Crivelli, P., Nesvizhevsky, V. V., and Voronin, A. Y., “Can we observe the gravitational quantum states of Positronium?” arXiv:1408.7051v1 [physics.atom-ph], 2014.
- Dufour, G., Debu, P., Lambrecht, A., Nesvizhevsky, V. V., Reynaud, S., and Voronin, A. Y., “Shaping the distribution of vertical velocities of antihydrogen in GBAR,” arXiv:1312.5534v1 [quant-ph], 2002.
- Durstberger-Rennhofer, K., Jenke, T., and Abele, H., “Probing neutron’s electric neutrality with ramsey spectroscopy of gravitational quantum states of ultracold neutrons,” *Phys. Rev. D*, vol. 84, 036004, 2011.
- Dylla, H. F. and King, J. C., “Neutrality of Molecules by a New Method,” *Phys. Rev.*, vol. A7, pp. 1224–1229, 1973.
- Escobar, M., Lamy, F., Meyerovich, A. E., and Nesvizhevsky, V. V., “Rough mirror as a quantum state selector: analysis and design,” *Advances in High Energy Physics*, vol. 2014, Article ID: 764182, Aug. 2014.
- Escobar, M. and Meyerovich, A., “Applications and identification of surface correlations,” arXiv:1404.1291, 2014.
- Escobar, M. and Meyerovich, A., “Beams of gravitationally bound ultracold neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 83, 033618, Mar. 2011.
- Escobar, M. and Meyerovich, A., “Quantized ultracold neutrons in rough waveguides: GRANIT experiments and beyond,” *Advances in High Energy Physics*, vol. 2014, Article ID: 185414, July 2014.

- Escobar, M. and Meyerovich, A. E., “Quantum transport equation for systems with rough surfaces and its application to ultracold neutrons in a quantizing gravity field,” *Journal of Experimental and Theoretical Physics*, vol. 119, no. 6, pp. 1123–1133, 2014.
- Fishman, G. and Calecki, D., “Surface-induced resistivity of ultrathin methallic films: a limit law,” *Phys. Rev. Lett.*, vol. 62, no. 11, 1989.
- Fishman, G. and Calecki, D., “Influence of surface roughness on the conductivity of metallic and semiconducting quasi-two-dimensional structures,” *Phys. Rev. B*, vol. 43, no. 14, 1991.
- Flugge, S., *Practical Quantum Mechanics I*. Springer-Verlag, 1999.
- Gea-Banacloche, J., “A quantum bouncing ball,” *Am. J. Phys.*, vol. 67, p. 776, 1999.
- Golub, R. and Pendlebury, J. M., “Ultra-cold neutrons,” *Rep. Prog. Phys.*, vol. 42, p. 3, 1979.
- Golub, R., Richardson, D., and Lamoreaux, S. K., *Ultracold neutrons*. IOP Publishing, 1991.
- Goodnick, S. M., Ferry, D. K., Wilmsen, C. W., Liliental, Z., Fathy, D., and Krivanek, O. L., “Surface roughness at the Si(100)-SiO₂ interface,” *Phys. Rev. B*, vol. 32, no. 12, Dec. 1985.
- Greene, G. L. and Gudkov, V., “Neutron interferometric method to provide improved constraints on non-newtonian gravity at the nanometer scale,” *Phys. Rev. C*, vol. 75, 015501, 2007.
- Jenke, T., Cronenberg, G., Burgdörfer, J., Chizova, L. A., Geltenbort, P., Ivanov, A. N., Lauer, T., Lins, T., Rotter, S., Saul, H., Schmidt, U., and Abele, H., “Gravity Resonance Spectroscopy Constrains Dark Energy and Dark Matter Scenarios,” *Phys. Rev. Lett.*, vol. 112, p. 151105, 2014.
- Jenke, T., Geltenbort, P., Lemmel, H., and Abele, H., “Realization of a gravity-resonance-spectroscopy technique,” *Nature Physics*, vol. 7, pp. 468–472, 2011.
- Johnson, J. D., Krinsky, S., and McCoy, B. M., “Vertical-arrow correlation length in the eight-vertex model and the low-lying excitations of the X-Y-Z-Hamiltonian,” *Phys. Rev. A*, vol. 8, no. 5, pp. 2526–2547, 1973.
- Krantz, C., “Quantum States of Neutrons in the Gravitational Field,” Ph.D. dissertation, University of Heidelberg, 2006. [Online]. Available: <http://www.physi.uni-heidelberg.de/Publications/>

- Kreuz, M., Nesvizhevsky, V. V., Schmidt-Wellenburg, P., Soldner, T., Thomas, M., Börner, H. G., Naraghi, F., Pignol, G., Protasov, K. V., Rebreyend, D., Vezzu, F., Flaminio, R., Michel, C., Morgado, N., Pinard, L., Baessler, S., Gagarski, A. M., Grigorieva, L. A., Kuzmina, T. M., Meyerovich, A. E., Mezhov-Deglin, L. P., Petrov, G. A., Strelkov, A. V., and Voronin, A. Y., “A method to measure the resonance transitions between the gravitationally bound quantum states of neutrons in the GRANIT spectrometer,” *Nucl. Instrum. Meth. A*, vol. 611, pp. 326–330, 2009.
- Kurganskaya, I., Luttge, A., and Barron, A. R., “The application of VSI to the Study of Crystal Surface Proceses ,” *Connexions*, 2009. [Online]. Available: <http://cnx.org/content/m22326/1.4/>
- Luschikov, V. I. and Frank, A. I., *JETP Lett.*, vol. 28, p. 59, 1978.
- Meyerovich, A. and Nesvizhevsky, V. V., “Gravitational quantum states of neutrons in a rough waveguide,” *Phys. Rev. A*, vol. 73, 063616, June 2006.
- Meyerovich, A. E. and Ponomarev, I. V., “Surface roughness and size effects in quantized films,” *Phys. Rev. B*, vol. 65, 155413, 2002.
- Meyerovich, A. E. and Stepaniants, A., “Interference of bulk and boundary scattering in films with a quantum size effect,” *J. Phys.: Condens. Matter*, vol. 12, pp. 5575–5597.
- Meyerovich, A. E. and Stepaniants, A., “Transport phenomena at rough boundaries,” *Phys. Rev. Lett.*, vol. 73, no. 2, p. 316, July 1994.
- Meyerovich, A. E. and Stepaniants, A., “Transport equaiton and diffusion in ultrathin channels and films,” *Phys. Rev. B*, vol. 58, p. 13 242, Nov. 1998.
- Meyerovich, A. E. and Stepaniants, A., “Quantized systems with randomly corrugated walls and interfaces,” *Phys. Rev. B*, vol. 60, no. 12, p. 9129, 1999.
- Munoz, R. C., Concha, A., Mora, F., and Espejo, R., “Surface roughness and size effects of thin gold films on mica,” *Phys. Rev. B*, vol. 61, no. 7, p. 4514, Feb. 2000.
- Munoz, R. C., Vidal, G., Kremer, G., Moraga, L., and Arenas, C., “Surface-induced resistivity of gold films on mica: comparison between the classical and the quantum theory,” *J. Phys.: Condens. Matter*, vol. 11, pp. L299–L307, 1999.
- Munoz, R. C., Vidal, G., Kremer, G., Moraga, L., and Arenas, C., “Surface roughness and surface-induced resistivity of gold films on mica: influence of roughness modelling,” *J. Phys.: Condens. Matter*, vol. 12, pp. 2903–2912, 2000.

- Munoz, R. C., Vidal, G., Muslow, M., Lisoni, J. G., Arenas, C., Concha, A., Mora, F., Espejo, R., Kremer, G., Moraga, L., Esparza, R., and Haberle, P., “Surface roughness and surface-induced resistivity of gold films on mica: Application of quantitative scanning tunneling microscopy,” *Phys. Rev. B*, vol. 62, no. 7, p. 4686, 2000.
- Nesvizhevsky, V. V., “Investigation of quantum neutron states in the terrestrial gravitational field above a mirror,” *Physics-Uspekhi*, vol. 47 (5), p. 515, 2004.
- Nesvizhevsky, V. V., “Polished sapphire for ultracold-neutron guides,” *Nuclear Instruments and Methods in Physics Research A*, vol. 557, pp. 576–579, 2006.
- Nesvizhevsky, V. V., Börner, H., Gagarski, A. M., Petrov, G. A., Petukhov, A. K., Abele, H., Baessler, S., Stöferle, T., and Soloviev, S. M., “Search for quantum states of neutron in a gravitational field: gravitational levels,” *Nuclear Instruments and Methods in Physics Research A*, vol. 440, pp. 754–759, 2000.
- Nesvizhevsky, V. V., Börner, H. G., Gagarski, A. M., Petoukhov, A. K., Petrov, G. A., Abele, H., Baessler, S., Divkovic, G., Rueb, F. J., Stöferle, T., Westphal, A., Strelkov, A. V., Protasov, K. V., and Voronin, A. Y., “Measurement of quantum states of neutrons in the Earth’s gravitational field,” *Phys. Rev. D*, vol. 67, 102002, 2003.
- Nesvizhevsky, V. V., Börner, H. G., Petukhov, A. K., Abele, H., Baessler, S., Rueb, F. J., Stöferle, T., Westphal, A., Gagarski, A. M., Petrov, G. A., and Strelkov, A. V., “Quantum states of neutrons in Earth’s gravitational field,” *Nature*, vol. 415, pp. 297–299, Nov. 2002.
- Nesvizhevsky, V. V., Petukhov, A. K., Börner, H. G., Baranova, T. A., Gagarski, A. M., Petrov, G. A., Protasov, K. V., Voronin, A. Y., Baessler, S., Abele, H., Westphal, A., and Lucovac, L., “Study of the neutron quantum states in the gravity field,” *Eur. Phys. J. C*, vol. 40, pp. 479–491, 2005.
- Nesvizhevsky, V. V., Petukhov, A. K., Börner, H. G., Soldner, T., Schmidt-Wellenburg, P., Kreuz, M., Pignol, G., Protasov, K. V., Rebreyend, D., Vezzu, F., Forest, D., Ganau, P., Mackowski, J. M., Michel, C., Montorio, J. L., Morgado, N., Pinard, L., Remillieux, A., Gagarski, A. M., Petrov, G. A., Kusmina, A. M., Strelkov, A. V., Abele, H., Baessler, S., and Voronin, A. Y., “GRANIT project: a trap for gravitational quantum states of ultracold neutrons,” arXiv:0708.2541v1, 2007.
- Nesvizhevsky, V. V., Petukhov, K., Protasov, K. V., and Voronin, A. Y., “Centrifugal quantum states of neutrons,” *Phys. Rev. A*, vol. 78, 033616, 2008.
- Nesvizhevsky, V. V., Pignol, G., and Protasov, K. V., “Neutron scattering and extra-short-range interactions,” *Phys. Rev. D*, vol. 77, 034020, 2008.

- Nesvizhevsky, V. V., Pignol, G., Protasov, K. V., Quemener, G., Forest, D., Ganau, P., Mackowski, J. M., Michel, C., Montorio, J. L., Morgado, N., Pinard, L., and Remillieux, A., “Comparison of specularly reflecting mirrors for GRANIT,” *Nuclear Instruments and Methods in Physics Research A*, vol. 578, pp. 435–438, 2007.
- Nesvizhevsky, V. V. and Protasov, K. V., *Trends in Quantum Gravity Research*. Nova Science Publishers, Inc., 2006.
- Nesvizhevsky, V. V. and Voronin, A. Y., “Centrifugal quantum states of neutrons,” *C. R. Physique*, vol. 12, pp. 791–795, 2011.
- Ogilvy, J. A., “Computer simulation of acoustic wave scattering from rough surfaces,” *J. Phys. D: Appl. Phys.*, vol. 21, pp. 260–277, 1988.
- Ogilvy, J. A., *Theory of wave scattering from random surfaces*. IOP Publishing, 1991.
- Ogilvy, J. A. and Foster, J. R., “Rough surfaces: gaussian or exponential statistics?” *J. Phys. D: Appl. Phys.*, vol. 22, pp. 1243–1251, 1989.
- Palasantzas, G., “Roughness spectrum and surface width of self-affine fractal surfaces via the K-correlation model,” *Phys. Rev. B*, vol. 48, no. 19, p. 14472, 1993.
- Pignol, G., Baessler, S., Nesvizhevsky, V. V., Protasov, K., Rebreyend, D., and Voronin, A., “Gravitational Resonance Spectroscopy with Oscillating Magnetic Field Gradient in the GRANIT Flow through Arrangement,” *Advances in High Energy Physics*, vol. 2014, Article ID: 628125, Aug. 2014.
- Roulier, D., Vezzu, F., Baessler, S., Clément, B., Morton, D., Nesvizhevsky, V., Pignol, G., and Rebreyend, D., “Status of the GRANIT facility,” arXiv:1410.1376v1[physics.ins-det], 2014.
- Schleich, S. and Rasel, E., “Neutrons knock at the cosmic door,” *Physics*, vol. 7, no. 39, apr 2014.
- Sinha, S. K., Sirota, E. B., Garoff, S., and Stanley, H. B., “X-ray and neutron scattering from rough surfaces,” *Phys. Rev. B*, vol. 38, no. 4, p. 2297, 1998.
- Smith, J. H., Purcell, E. M., and Ramsey, N. F., “Experimental limit to the electric dipole moment of the neutron,” *Phys. Rev.*, vol. 108, no. 1, Oct. 1957.
- Voronin, A. Y., Abele, H., Baessler, S., Protasov, K. V., and Westphal, A., “Quantum motion of a neutron in a wave-guide in the gravitational field,” *Phys. Rev. D*, vol. 73, 044029, Feb. 2006.

- Voronin, A. Y., Froelich, P., and Nesvizhevsky, V. V., “Gravitational quantum states of antihydrogen,” *Phys. Rev. A*, vol. 83, 032903, Mar. 2011.
- Voronin, A. Y., Nesvizhevsky, V. V., and Reynaud, S., “Whispering-gallery of antihydrogen near a curved surface,” *Phys. Rev. A*, vol. 85, 014902.
- Voronin, A. Y., Nesvizhevsky, V. V., and Reynaud, S., “Whispering-gallery states of antihydrogen near a curved surface,” *Nature Physics*, vol. 6, 114-117 2010.
- Westphal, A., “Quantum Mechanics and Gravitation,” Ph.D. dissertation, University of Heidelberg, 2001. [Online]. Available: arxiv.org/pdf/gr-qc/0208062.
- Wu, T. T., McCoy, B. M., Tracy, C. A., and Barouch, E., “Spin-spin correlation functions for the two-dimensional Ising model: Exact theory in the scaling region,” *Phys. Rev. B*, vol. 13, no. 1, p. 316, 1976.
- Yue, A. T., Dewey, M. S., Gilliam, D. M., Greene, G. L., Laptev, A. B., Nico, J. S., Snow, W. M., and Wietfeldt, F. E., “Improved Determination of the Neutron Lifetime,” *Phys. Rev. Lett.*, vol. 111, 22501, Nov. 2013.