Propagation of quantized ultracold neutrons in a narrow rough waveguide: application to GRANIT experiments

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Transport along rough walls

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Collaborators & publications

V. Nesvizhevsky, Institute Laue-Langevin, Grenoble

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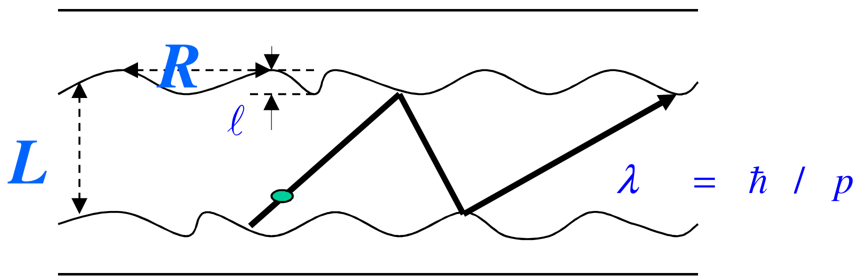
*R. Adhikari, Y. Cheng, AEM, and V.V. Nesvizhevsky, PRA **75**, 063613 (2007)*
*M. Escobar, and AEM, PRA **83**, 033618 (2011)*
M. Escobar, and AEM, to be published (2014)

Transport: Schematics



$\ell \ll R, L$

L – average spacing

R – (average) lateral size (correlation radius) of inhomogeneities

ℓ - (average) height of inhomogeneities

λ - (Fermi) wavelength of particles

The surface modulation can be either random or regular (*i.e.*, periodic)

Theoretical Approaches

- Direct perturbative calculation (*Fishman & Calecki, 1989)* – the best approach in ***simple*** cases

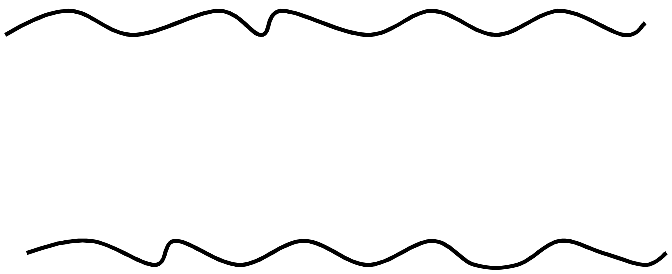
- S-matrix approach (*Voronovich, 1984, 1994)* – difficult to account for interference effects

- Adiabatic approach (*Kawabata, 1993)* – works well for "adiabatic" (slowly changing) inhomogeneities

- Quasiclassical approach (*Makarov et al, 1995)* – difficult to account for interference effects

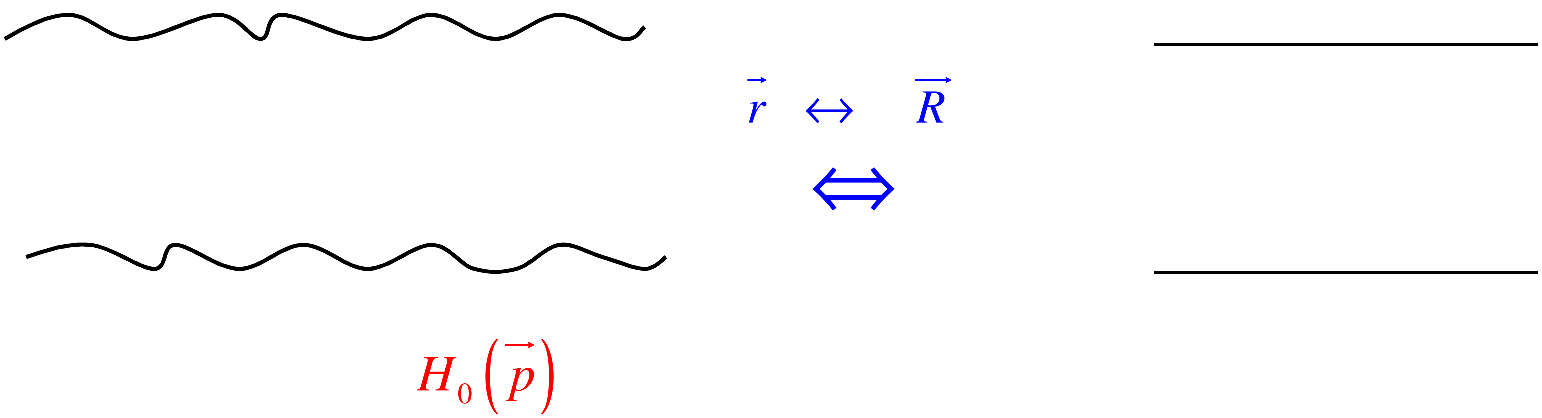
- Mapping transformation *(Tesanovic et al, 1986; Meyerovich et al, 1994 -2002)* – the most rigorous and physically transparent approach

Mapping transformation method



$H_0\left(\vec{p}\right)$

Mapping transformation method



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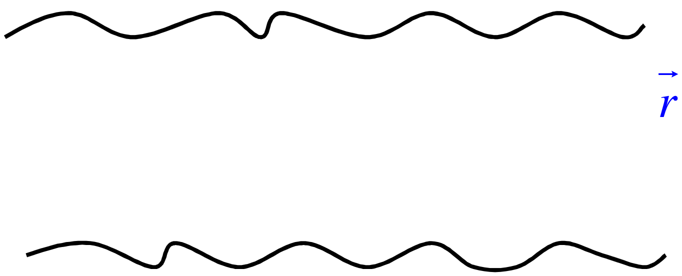
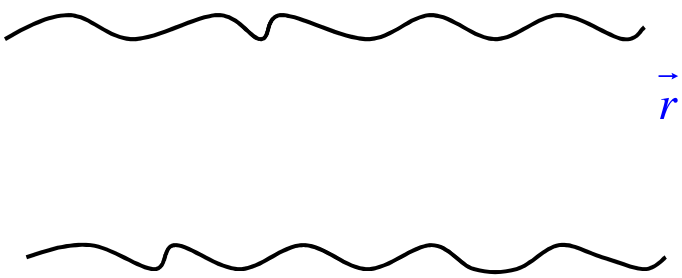


$$\vec{r}\,,\ \vec{p} \ \leftrightarrow\ \vec{R}\,,\ \vec{P}$$

$$\Leftrightarrow$$

$$H_0\left(\vec{p}\right) \quad \leftrightarrow \quad H_0\left(\vec{P}\right) + V\left(\vec{P}, \vec{R}\right)$$

Mapping transformation method



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If the film surface is random, the "perturbation"

$V\left(\vec{P},\vec{R}\right)$ *is random.*

If the film surface is periodic, the "perturbation"

$V\left(\vec{P},\vec{R}\right)$ *is periodic.*

The function $V\left(\vec{P},\vec{R}\right)$ *can be explicitly expressed*

via the ***exact*** *profile of the film surface.*

Example

"Old" boundaries $$x = \pm L/2 \mp \xi_{1,2}(y,z)$$

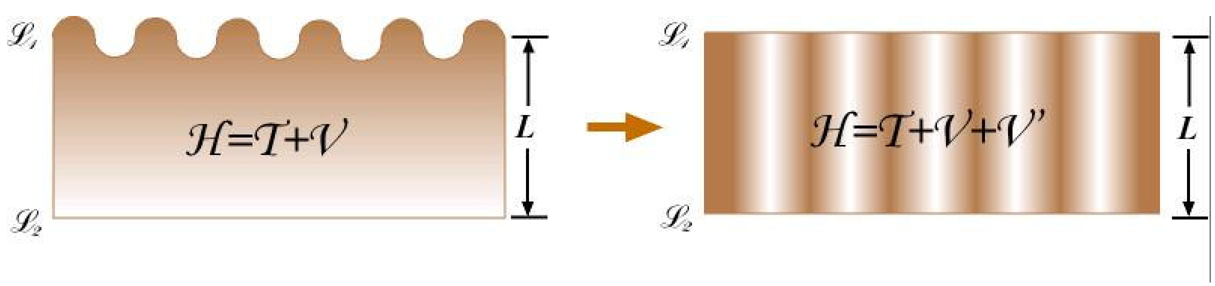
Transformation $$X = \frac{x + \xi_1/2 - \xi_2/2}{1 - \xi_1/L - \xi_2/L}, Y = y, Z = z$$

"New" boundaries $$X = \pm L/2$$

"New" momenta $$\hat{P}_x = \frac{\hbar}{i}\frac{\partial}{\partial X} = \cdots$$

"Old" Hamiltonian $$\hat{H} = p^2/2m$$

"New" Hamiltonian $$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{\xi_1 + \xi_2}{mL}\hat{P}_x^2 + \frac{1}{2m\ell}\left[X\frac{\xi'_{1y} + \xi'_{2y}}{L} - \frac{\xi'_{1y} - \xi'_{2y}}{2}\right]\hat{P}_x\hat{P}_y + \ldots$$



"Bulk perturbation" *V'* closely follows the wall modulation!

Transport problems

The transport calculations follow the standard scheme:

1. Perform the mapping transformation

$$\widehat{H}_0(\vec{p},\vec{r}) \to \widehat{H}_0(\vec{P},\vec{R}) + \widehat{V}(\vec{P},\vec{R},\{\xi_{1,2}(R)\})$$

2. Calculate the matrix elements of the "perturbation" and the averaged scattering probabilities

$$W(\vec{p},\vec{p}\,') = \left\langle \left| V_{\vec{p},\vec{p}\,'} \right|^2 \right\rangle_\xi$$

3. Apply these scattering probabilities to the collision operator in the transport equation

$$\frac{dn}{dt} = \int W(\vec{p},\vec{p}\,')\left[n(\vec{p}) - n(\vec{p}\,')\right]\delta\left(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}\,'}\right) d^3p'/(2\pi\hbar)^3$$

Randomly modulated surfaces:
Scattering & transition probabilities

$$W_{jj'} = \zeta\left(\vec{q} - \vec{q}\,'\right) U_c^2 \left|\Psi_j\left(H\right)\right|^2 \left|\Psi_{j'}\left(H\right)\right|^2$$

inside finite well

Randomly modulated surfaces: Scattering & transition probabilities

$$W_{jj'} = \zeta\left(\vec{q}-\vec{q}\,'\right)U_c^2\left|\Psi_j\left(H\right)\right|^2\left|\Psi_{j'}\left(H\right)\right|^2$$

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$$W_{jj'} = \tfrac{1}{4m^2}\zeta\left(\vec{q}-\vec{q}\,'\right)\left|\Psi_j{}'\left(H\right)\right|^2\left|\Psi_{j'}{}'\left(H\right)\right|^2$$

inside infinite well

Randomly modulated surfaces: Scattering & transition probabilities

$$W_{jj'} = \zeta\left(\vec{q}-\vec{q}\,'\right)U_c^2\left|\Psi_j(H)\right|^2\left|\Psi_{j'}(H)\right|^2$$ *inside finite well*

$$W_{jj'} = \frac{1}{4m^2}\zeta\left(\vec{q}-\vec{q}\,'\right)\left|\Psi_j'(H)\right|^2\left|\Psi_{j'}'(H)\right|^2$$ *inside infinite well*

$$W_{jj'} = \frac{2\pi^4 j^2 j'^2}{m^2 L^6}\zeta\left(\vec{q}-\vec{q}\,'\right)$$ *inside infinite square well*

The correlation function of surface roughness plays the same role for scattering by surface inhomogeneities as the impurity cross-section for scattering by bulk impurities!

Quantized systems

Restricted motion between the walls is quantized: $p_x \to \pi\hbar j / L$

The energy spectrum splits into minibands:

$$\varepsilon\left(\vec{p}\right) \to \varepsilon\left(\pi\hbar j / L, p_y, p_z\right) = \varepsilon_j\left(\vec{q}\right)$$

$$p^2 / 2m \to \frac{1}{2m}\left(\frac{\pi\hbar j}{L}\right)^2 + \frac{q^2}{2m}$$

… and the equienergy (Fermi) surface is sliced into a set of (Fermi) curves by the planes $p_x \to \pi\hbar j / L$

Quantizing Slicer ©

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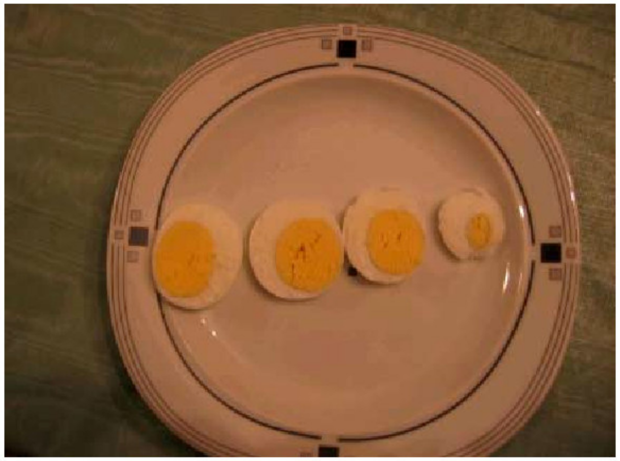
… and the Fermi surface is sliced into a set of Fermi curves by the planes $p_x \to \pi\hbar j / L$



Change in film thickness L can result in abrupt change in the number of "slices" – *i.e.*, in a topological phase transition

Correlation function of surface roughness

The correlation function of surface roughness plays the same role for scattering by surface inhomogeneities as the impurity cross-section for scattering by bulk impurities.

The usual advice is to extract this correlation function from precise data on the surface profile obtained using STM, AFM, or light scattering measurements

Correlation function of surface roughness

The possibility of having an accurate description of experiment hinges on knowing the correlation function of surface roughness. Is it possible identify the correlation function from precise measurements of the surface profile?

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We generated various 1D *and* 2D *rough surfaces with known correlation functions, measured the profile, and tried to identify the extracted correlation functions by fitting it to different fitting functions.*

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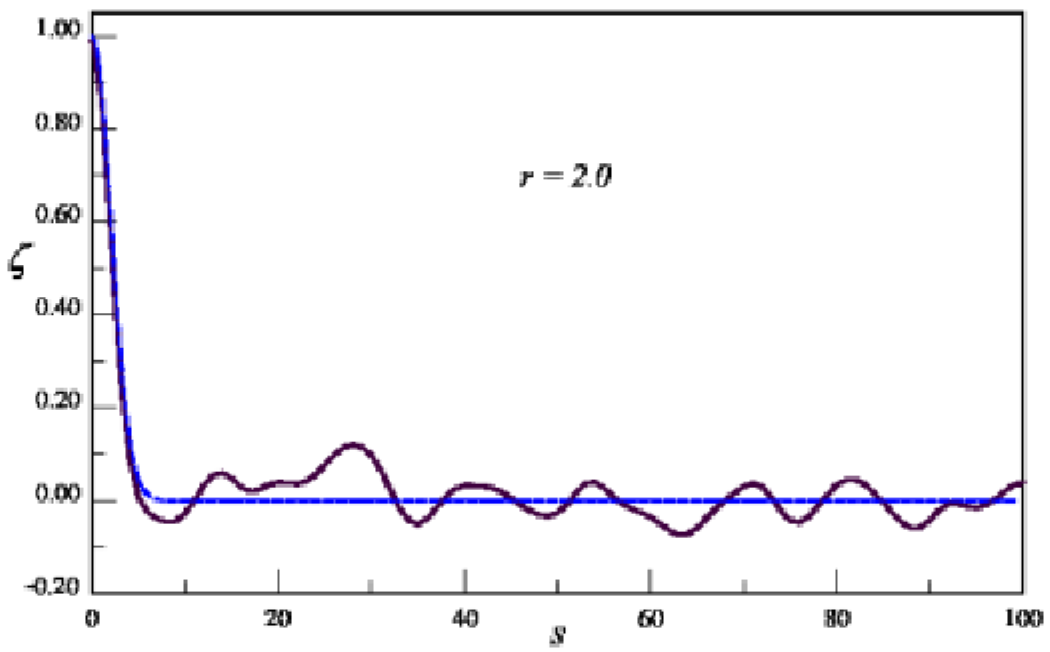
We generated various 1D *and* 2D *rough surfaces with known correlation functions, measured the profile, and tried to identify the extracted correlation functions by fitting it to different fitting functions.*

In most cases the presence of fat fluctuation-driven tails in extracted correlation functions prevented unambiguous identification of surface correlators!

Correlation function of surface roughness

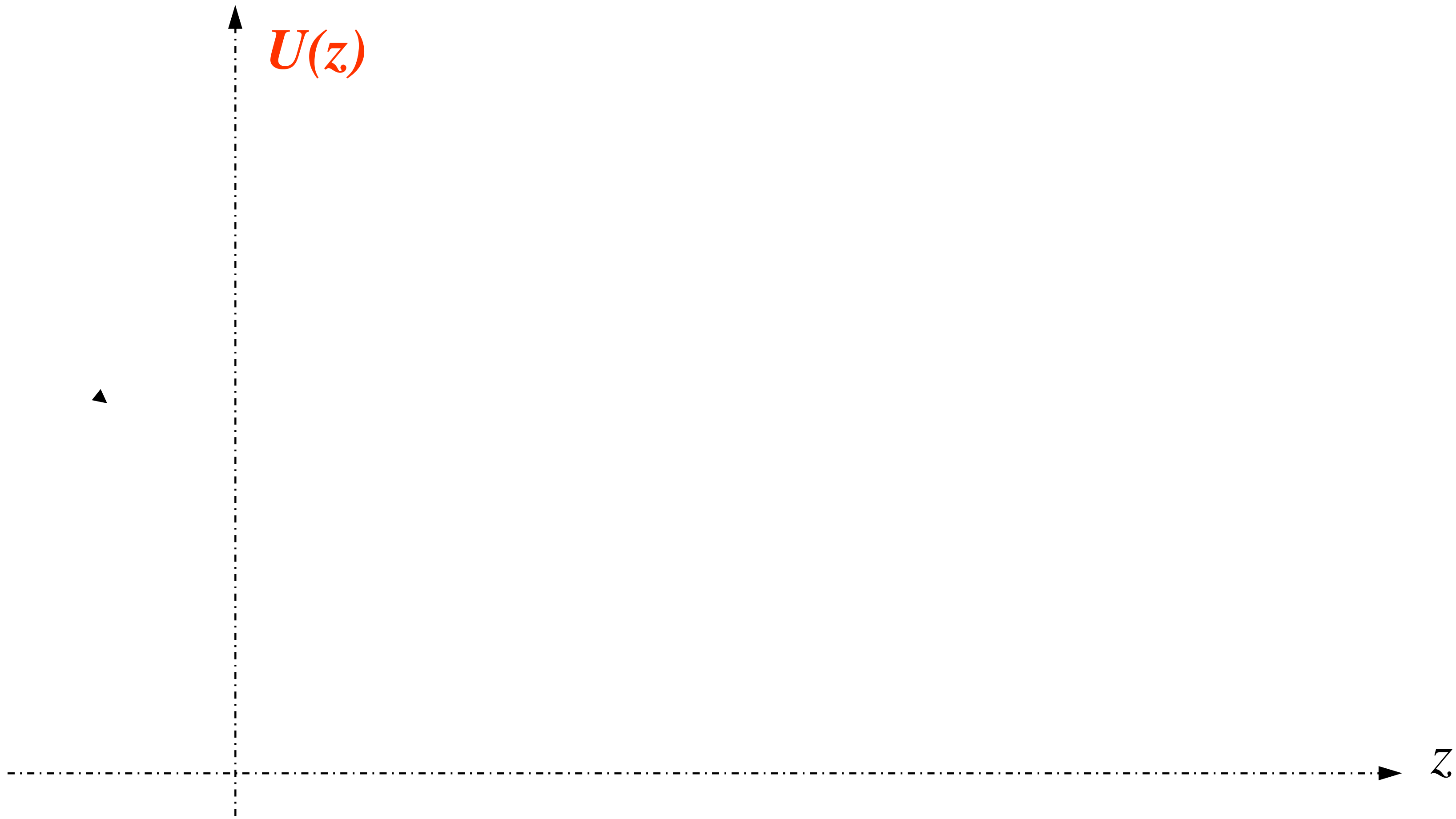
Example of a numerically extracted correlation function for a surface generated with Gaussian roughness



The fitting error σ *comes mostly not from the peak area where the shape of the fitting function is important, but mostly from the tail and is nearly the same for all fitting functions all of which are near zero in the tail area!*

Gravitational quantum states

*Neutron beam between two **horizontal** plates*



Gravitational quantum states

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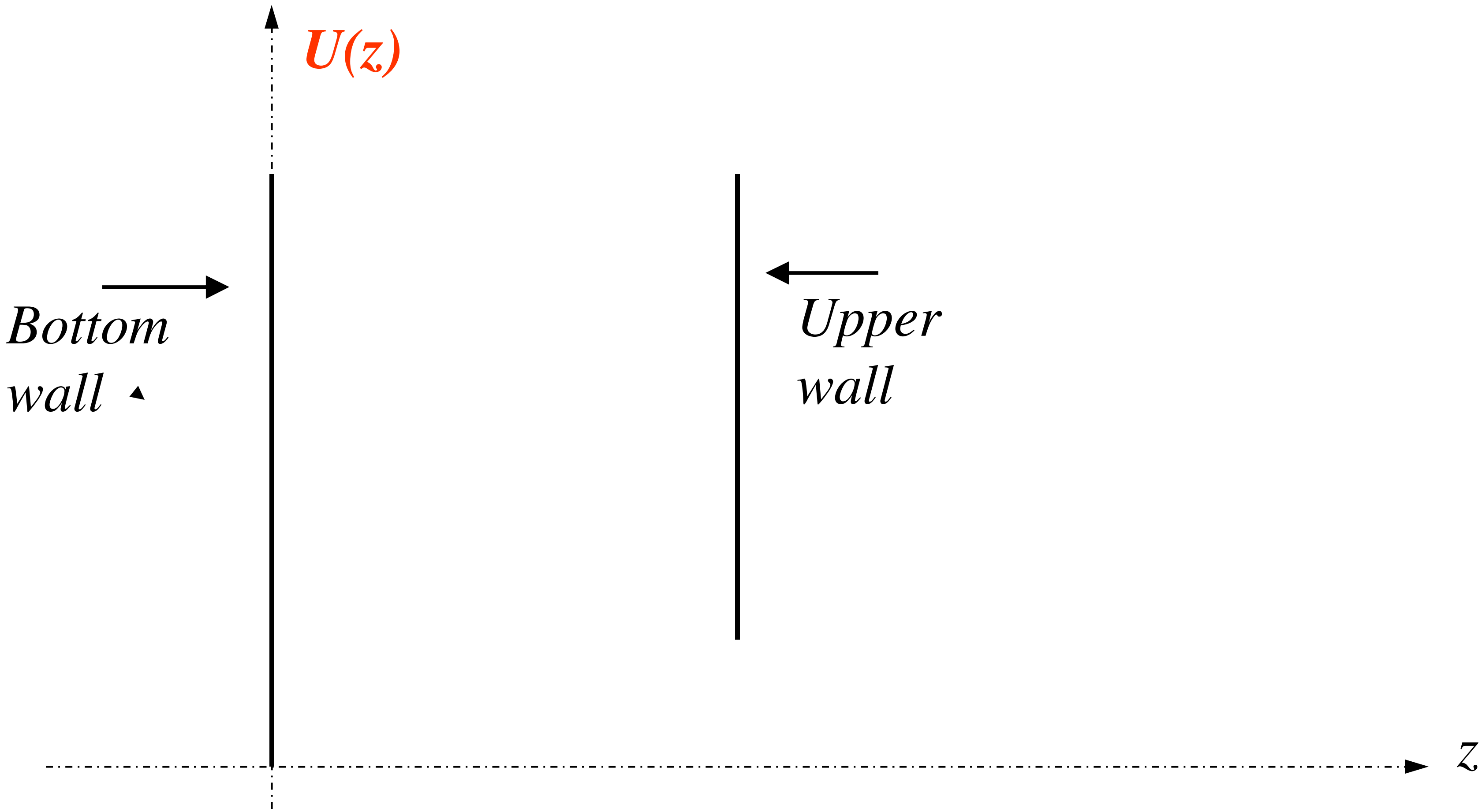

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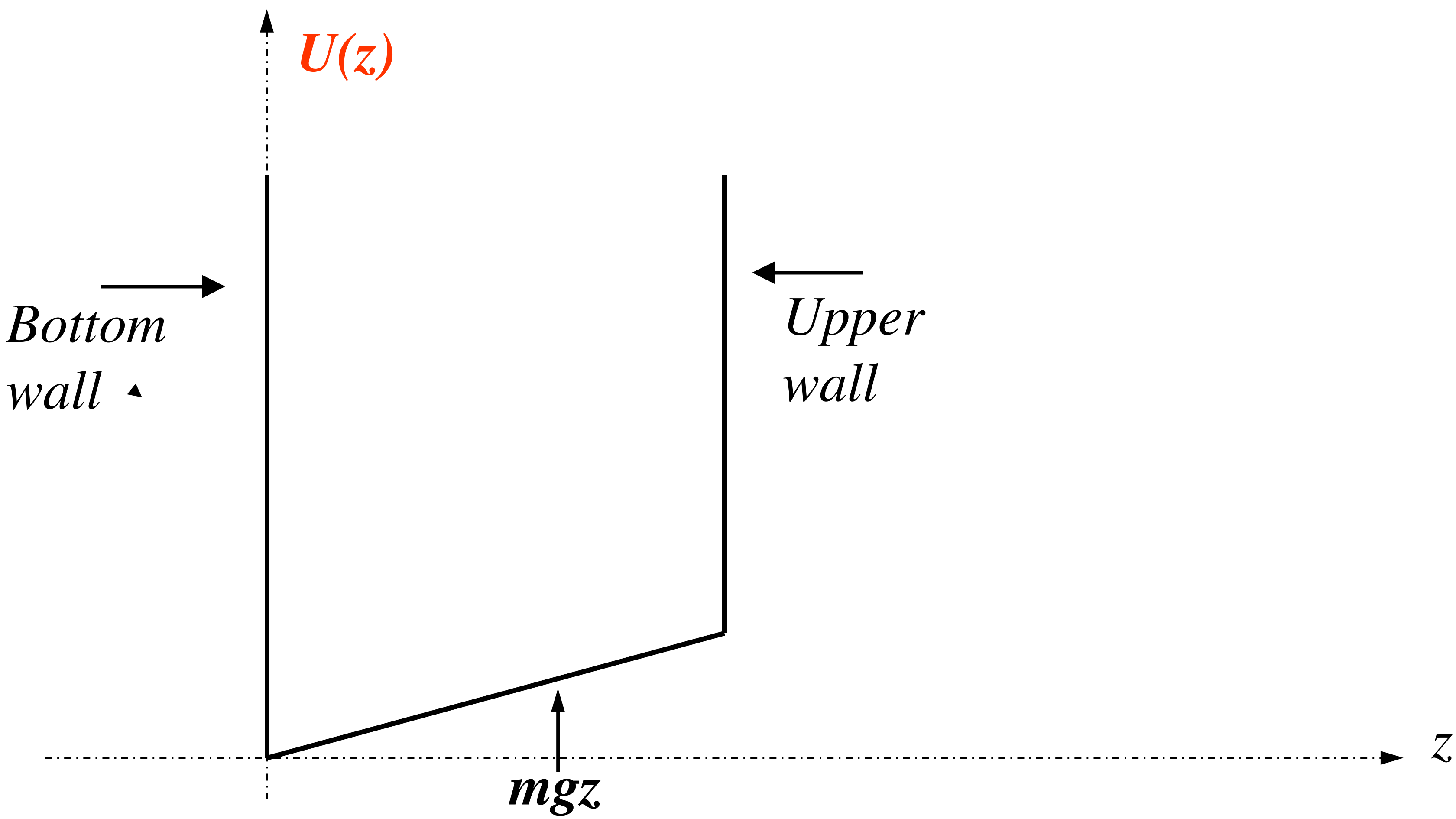

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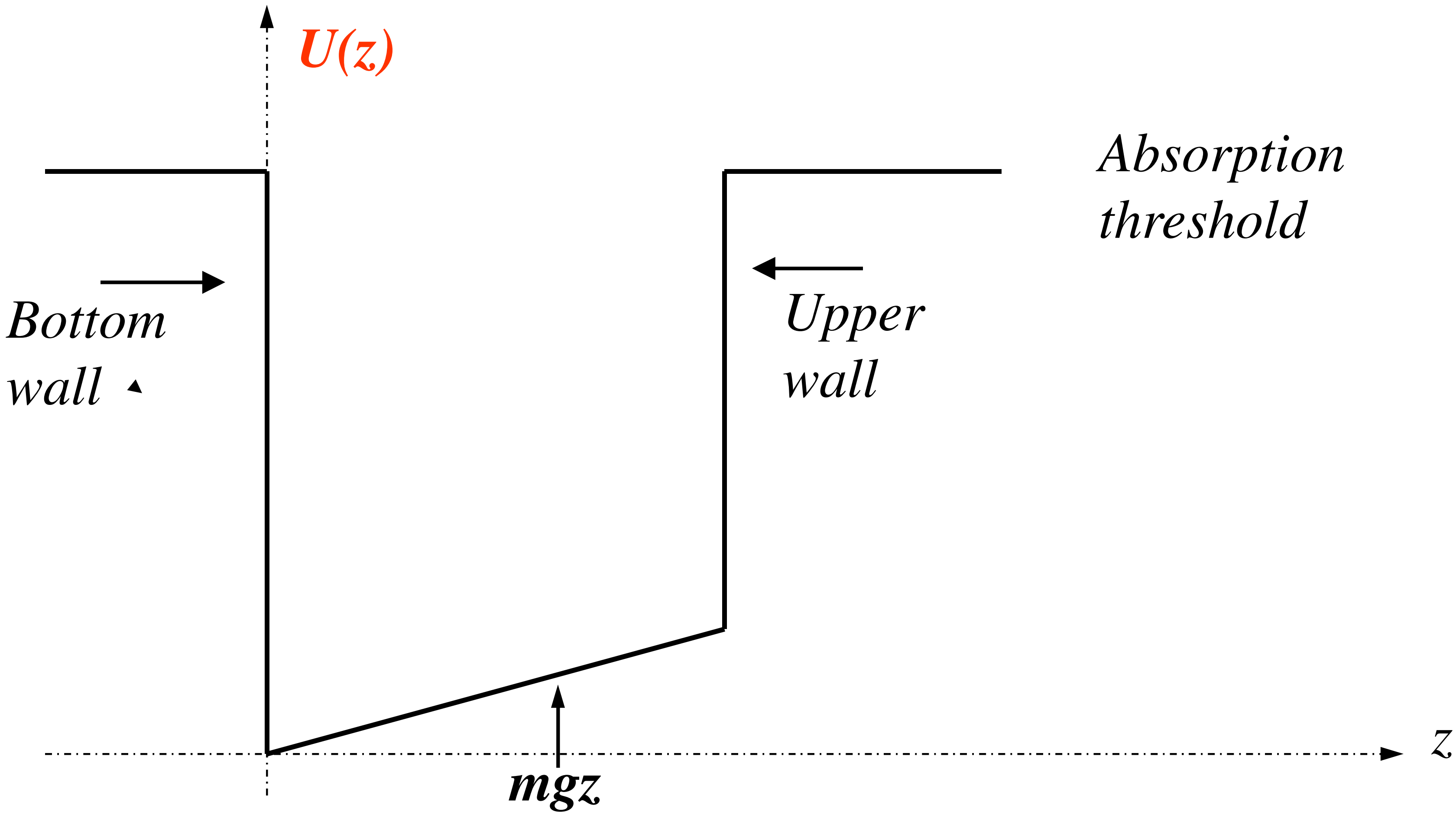

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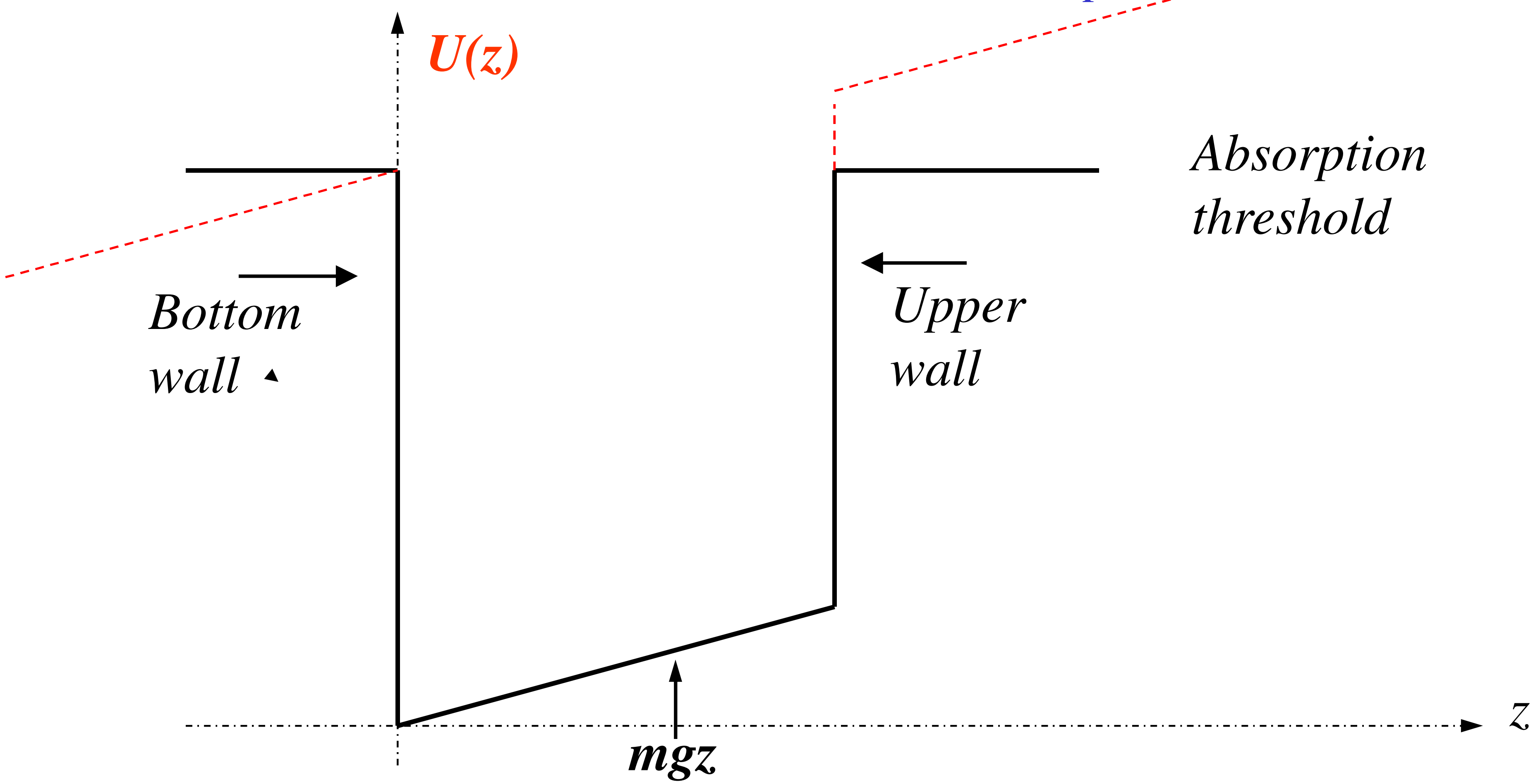
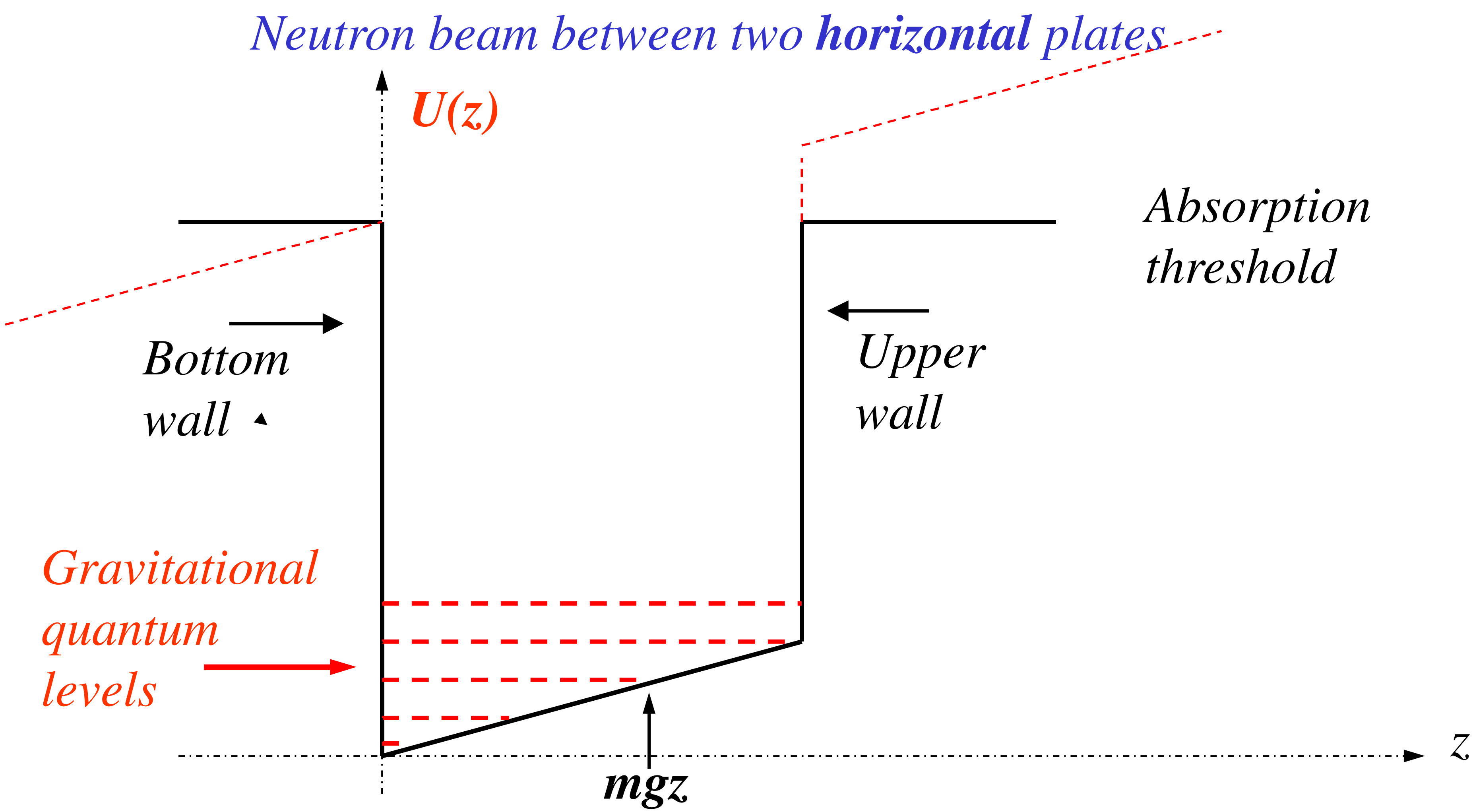


Gravitational quantum states



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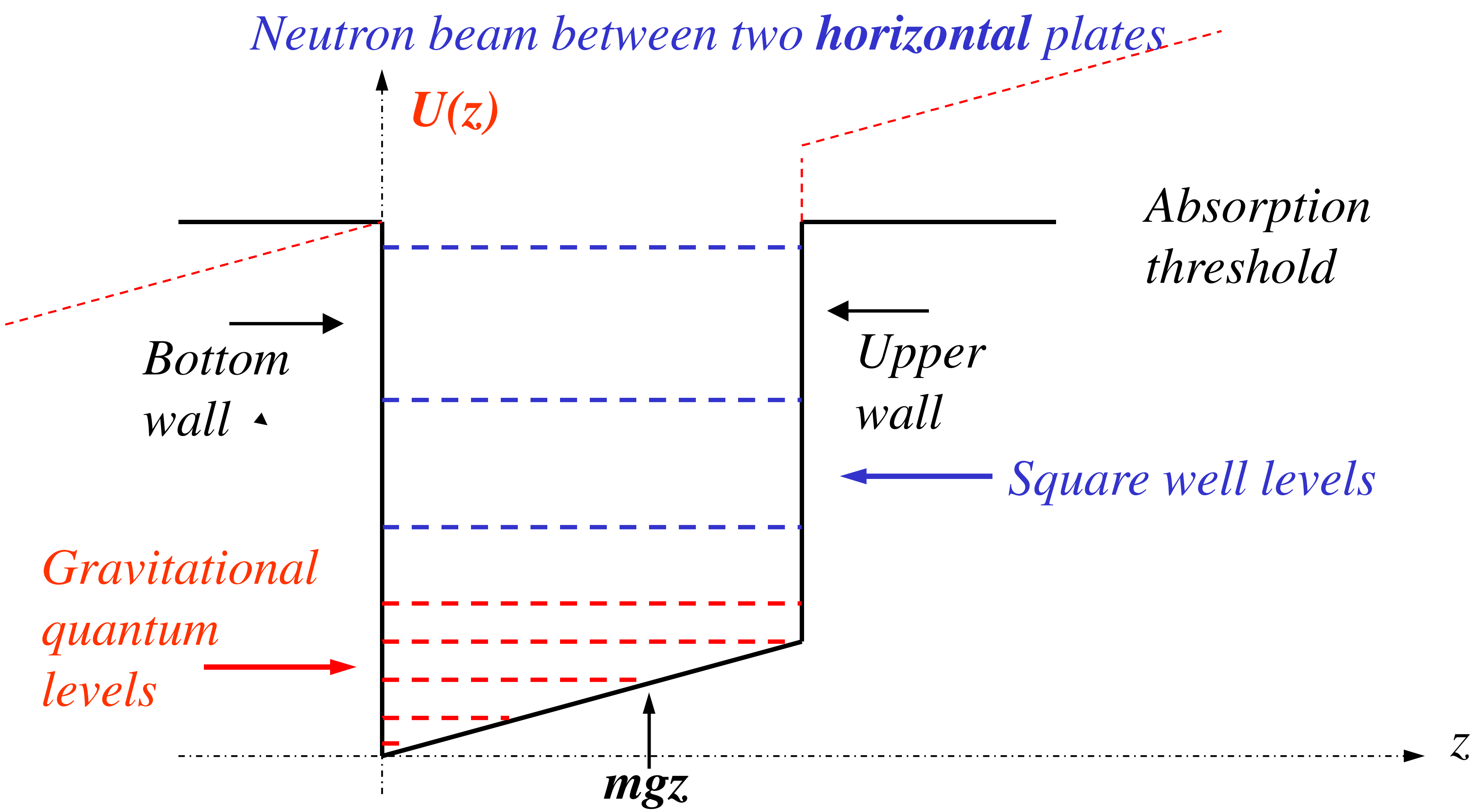

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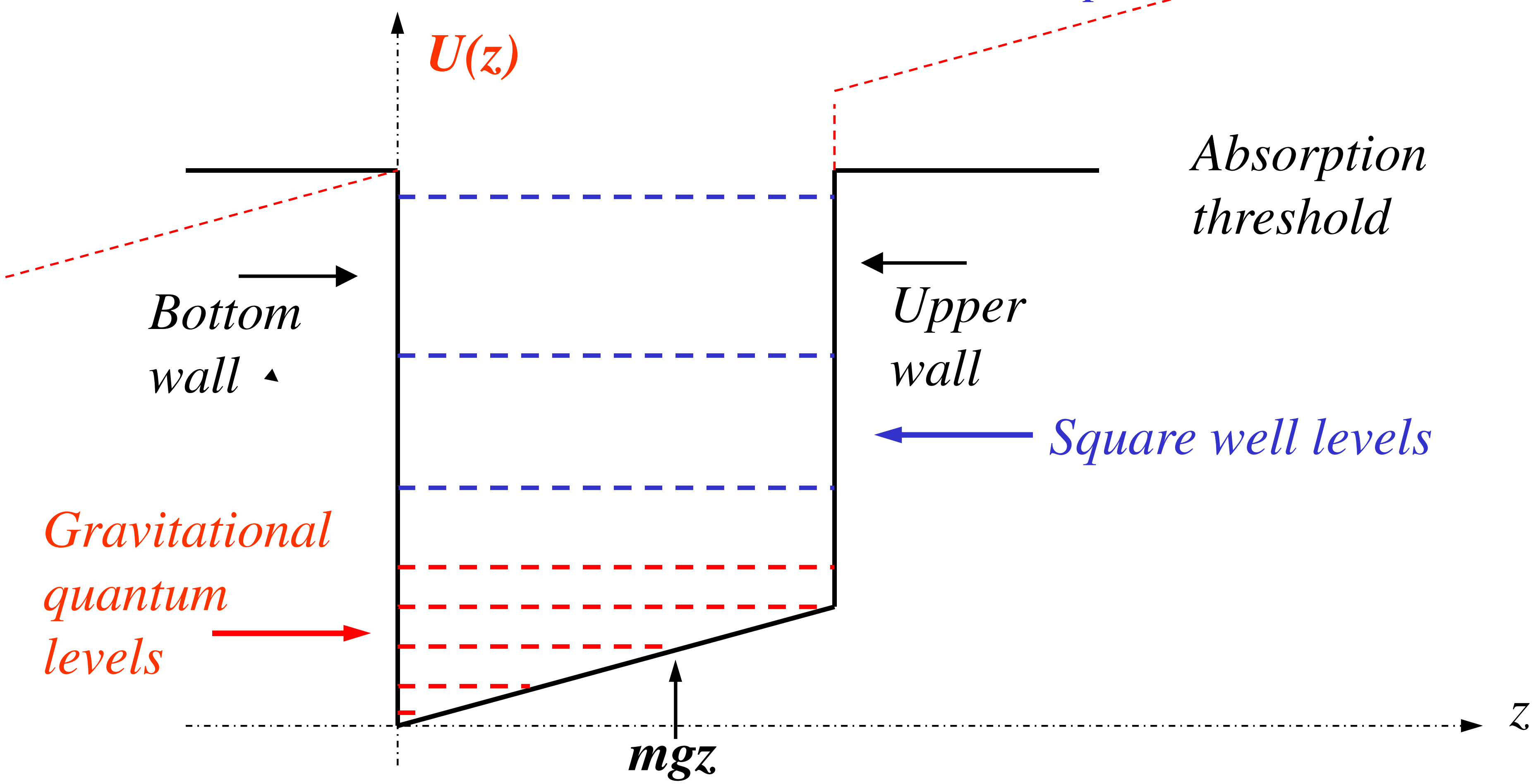
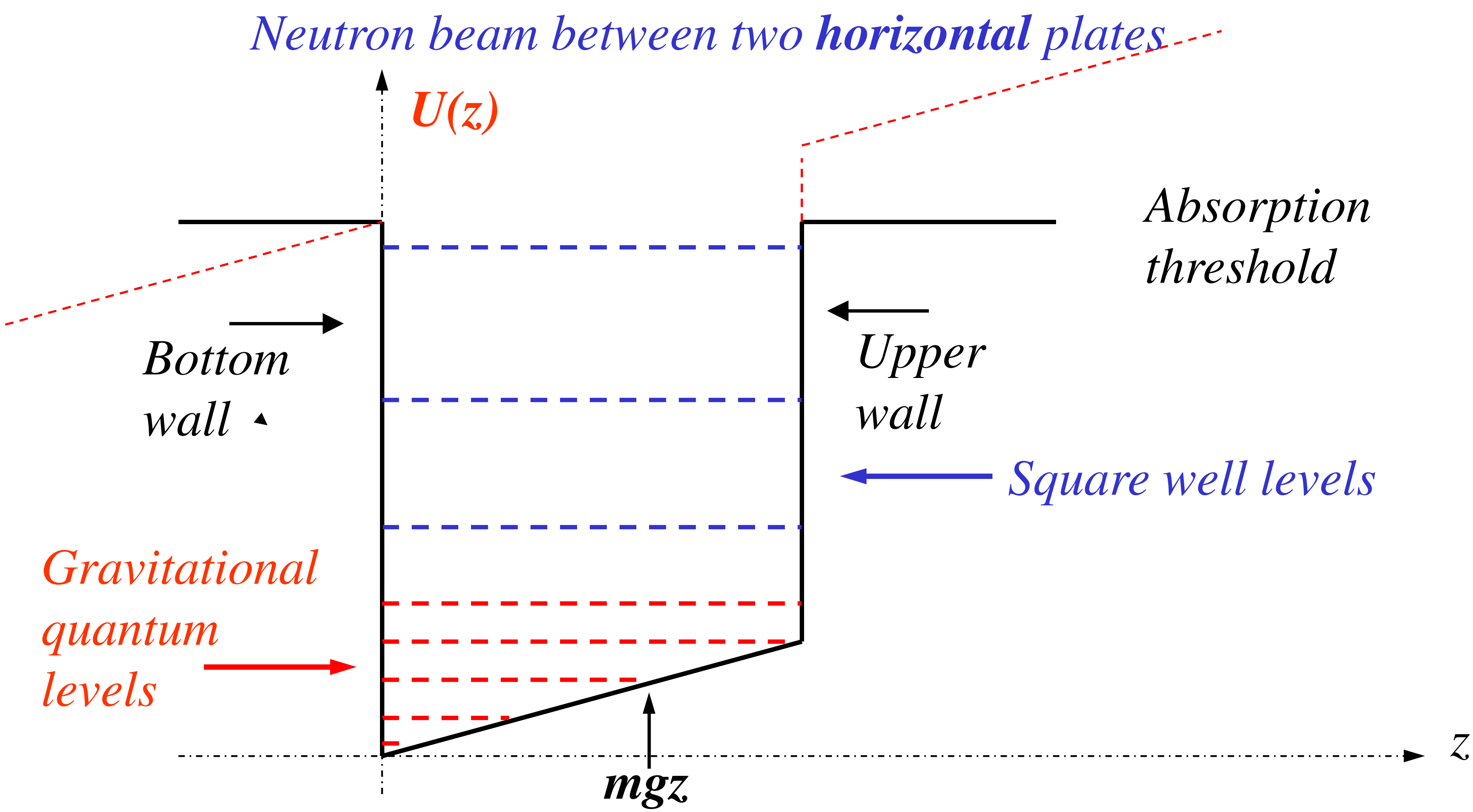


Problem: Thousands of discrete states which can hardly be resolved!

Gravitational quantum states



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Gravitational quantum states

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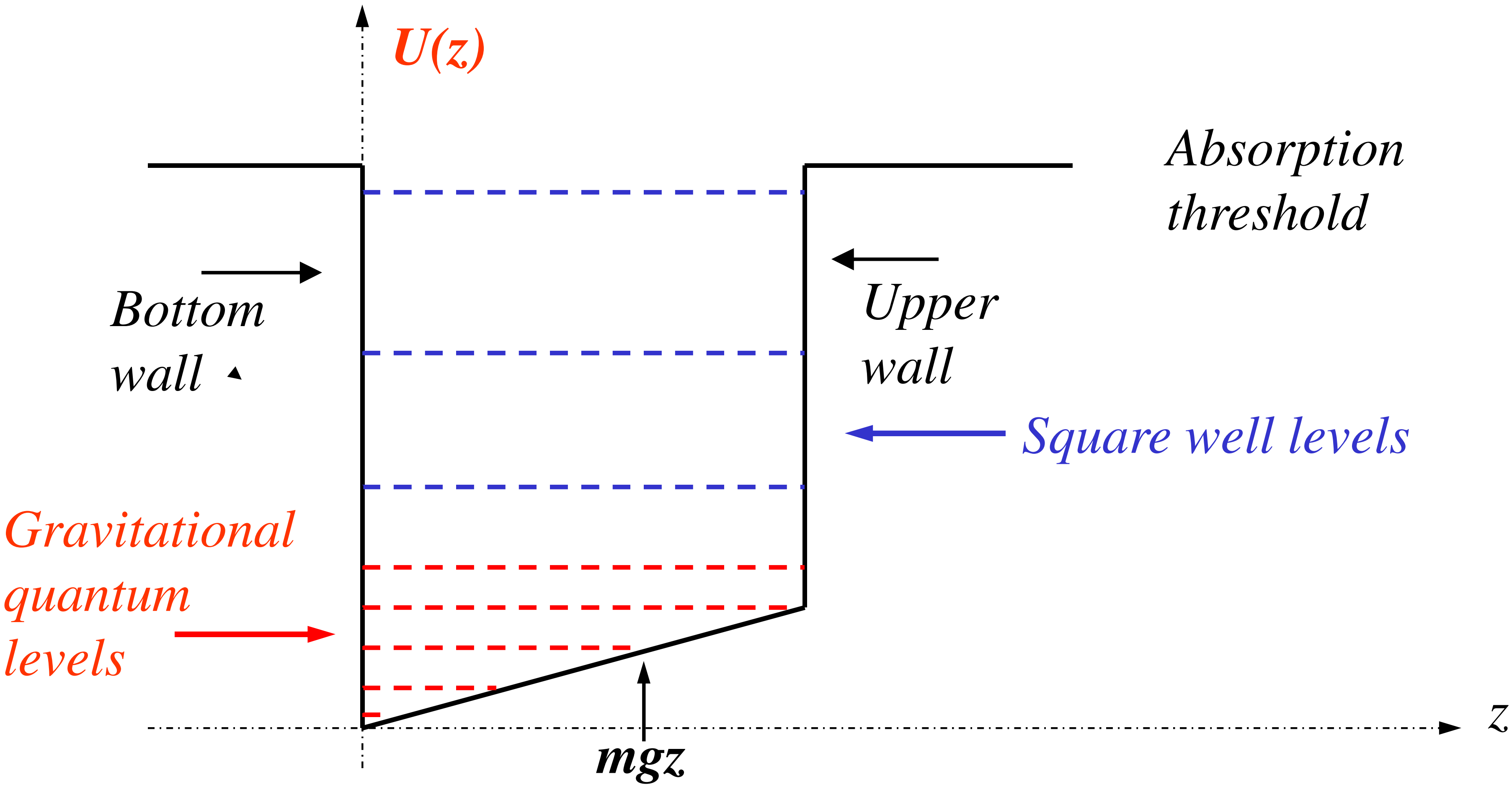
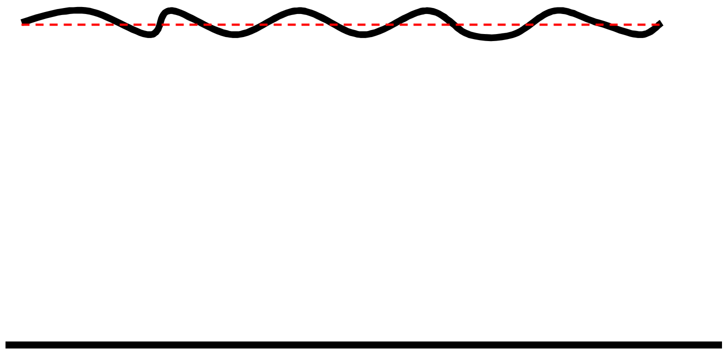


Problem: Thousands of discrete states which can hardly be resolved!

Problem: The gravitational energy *mgH* is 10^{-5} of the threshold!

Resolving the gravitational states: classical language

Let us make the ***upper*** *plate (mirror) rough:*



Resolving the gravitational states: classical language

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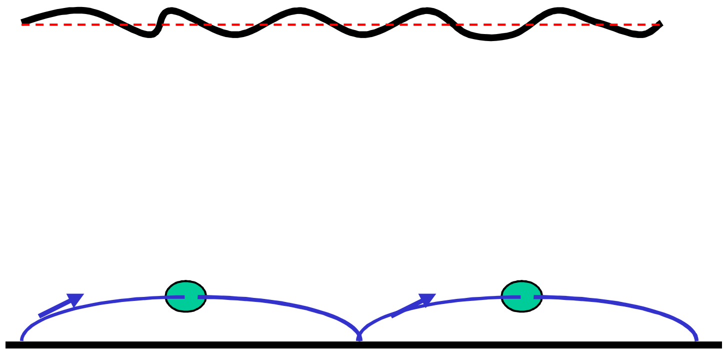

The particles with low vertical velocity are unaffected and continue to bounce along the bottom mirror

Resolving the gravitational states: classical language

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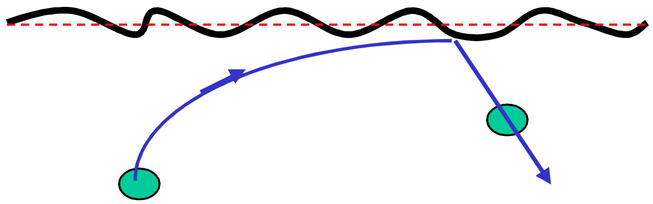
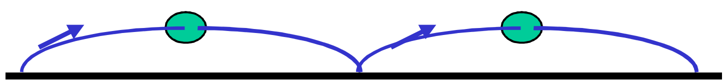


The particles with higher vertical velocity reach the upper, rough mirror and can acquire an even larger vertical velocity after scattering



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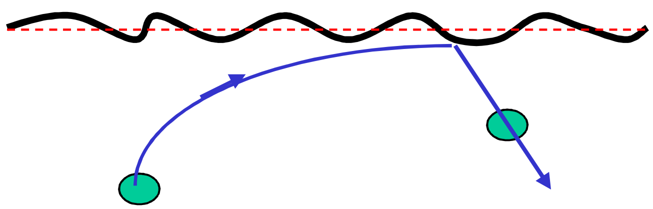

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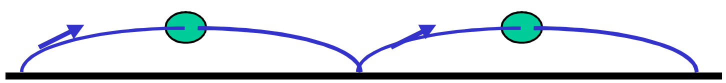

The particles with low vertical velocity are unaffected and continue to bounce along the bottom mirror

Since the horizontal beam velocity *V* is relatively high, consecutive collisions with the rough wall will provide the neutron with the vertical velocity above the absorption threshold.

Resolving the gravitational states: classical language

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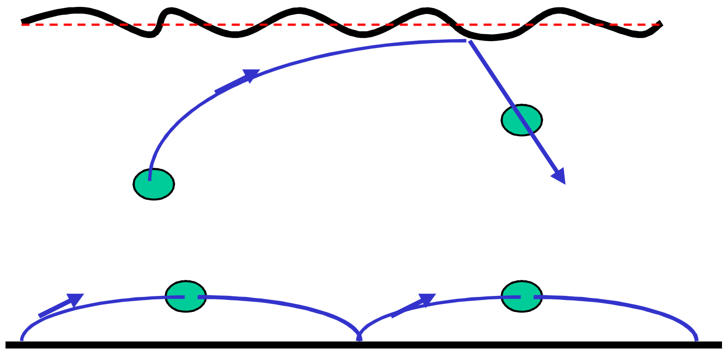


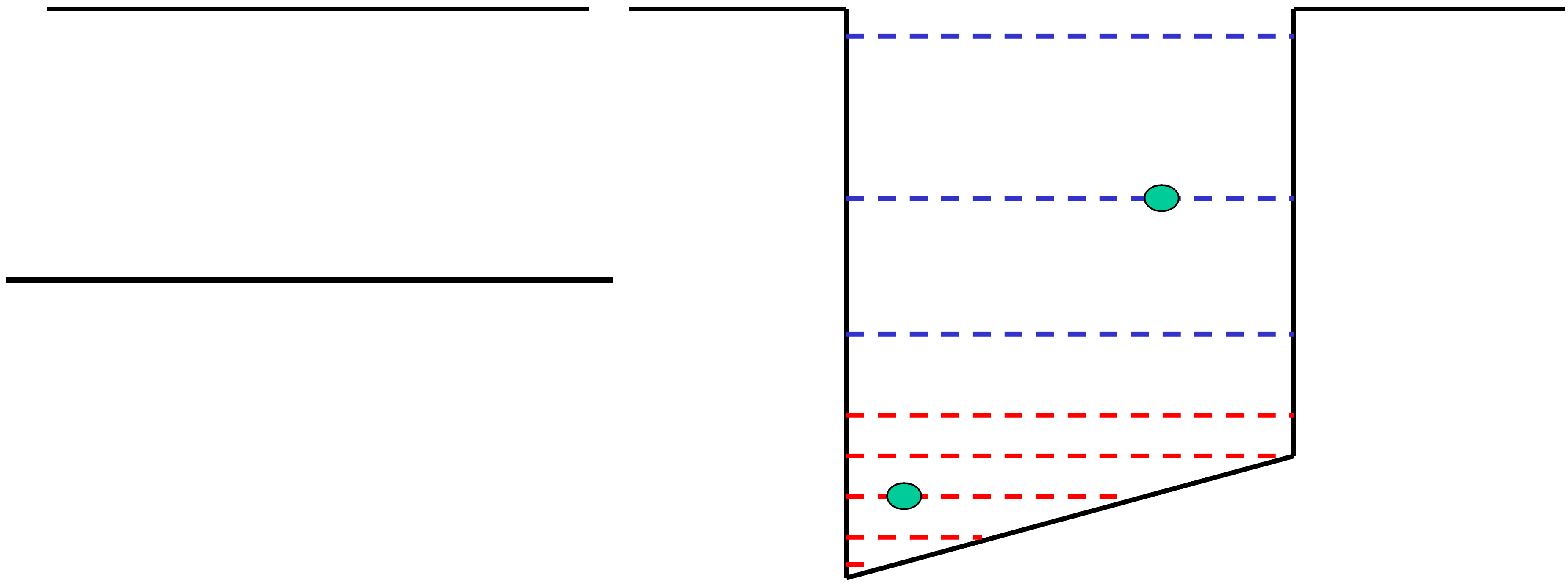
The particles with higher vertical velocity reach the upper, rough mirror and can acquire an even larger vertical velocity after scattering

The particles with low vertical velocity are unaffected and continue to bounce along the bottom mirror

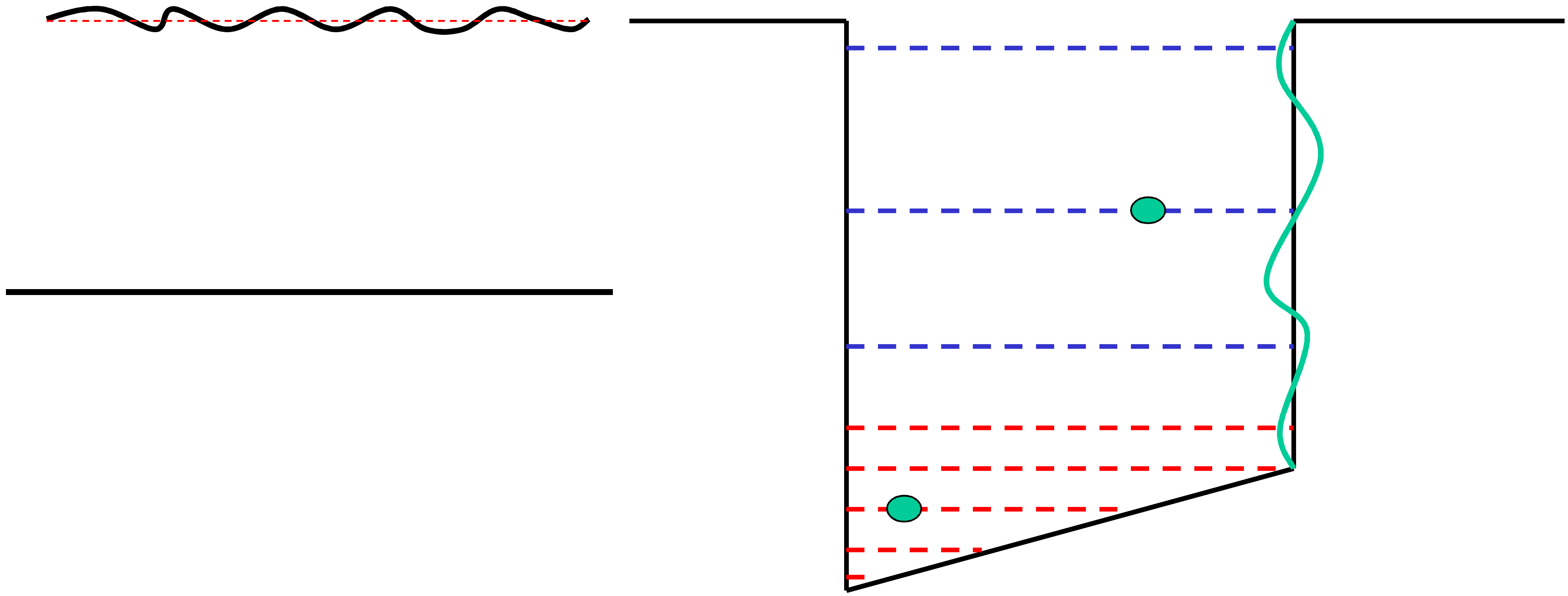
Since the horizontal beam velocity *V* is relatively high, numerous consecutive collisions with the rough wall will provide the neutron with the vertical velocity above the absorption threshold.

In the end, only the neutrons with the very small vertical velocity, which do not reach the rough upper wall, will survive.

Resolving the gravitational states: quantum language



Resolving the gravitational states: quantum language



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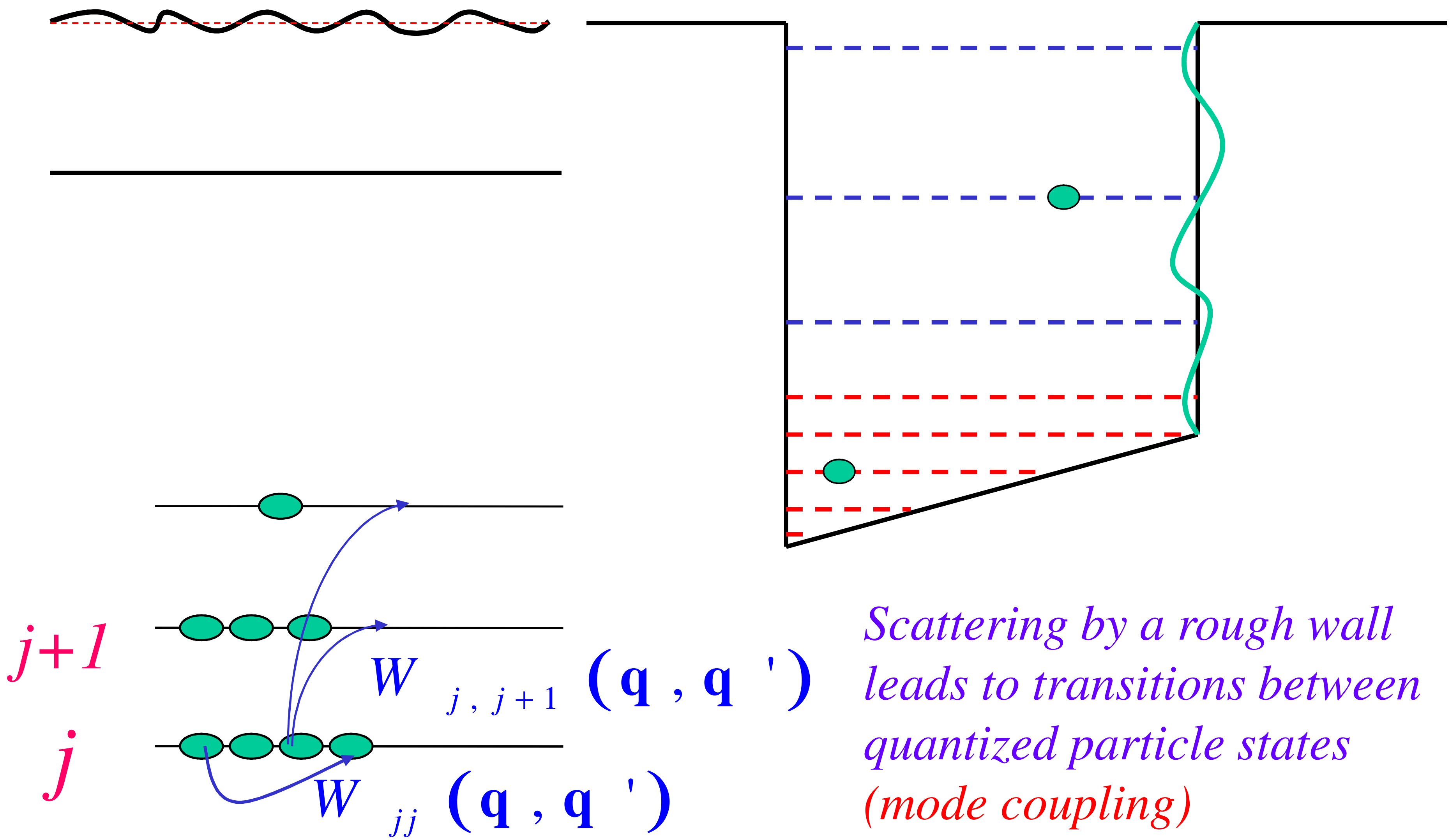
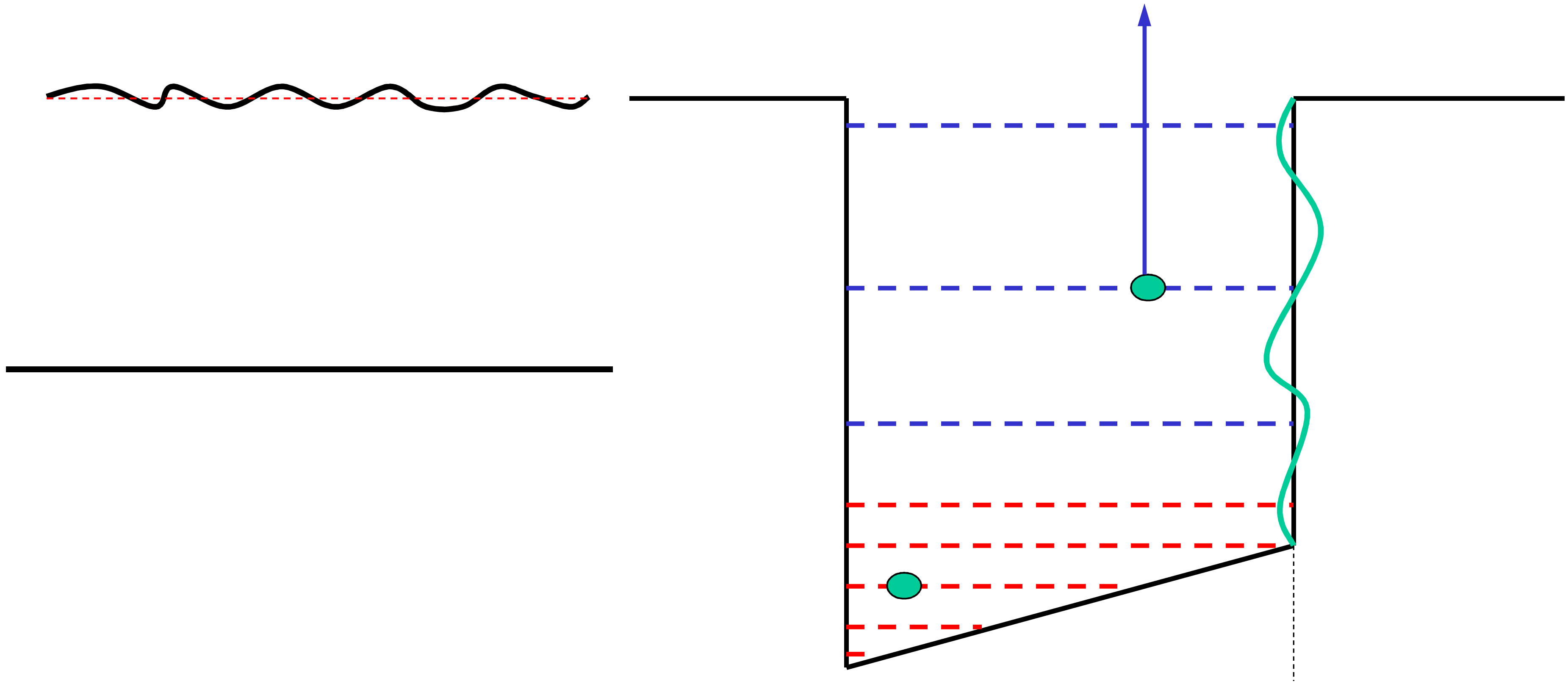


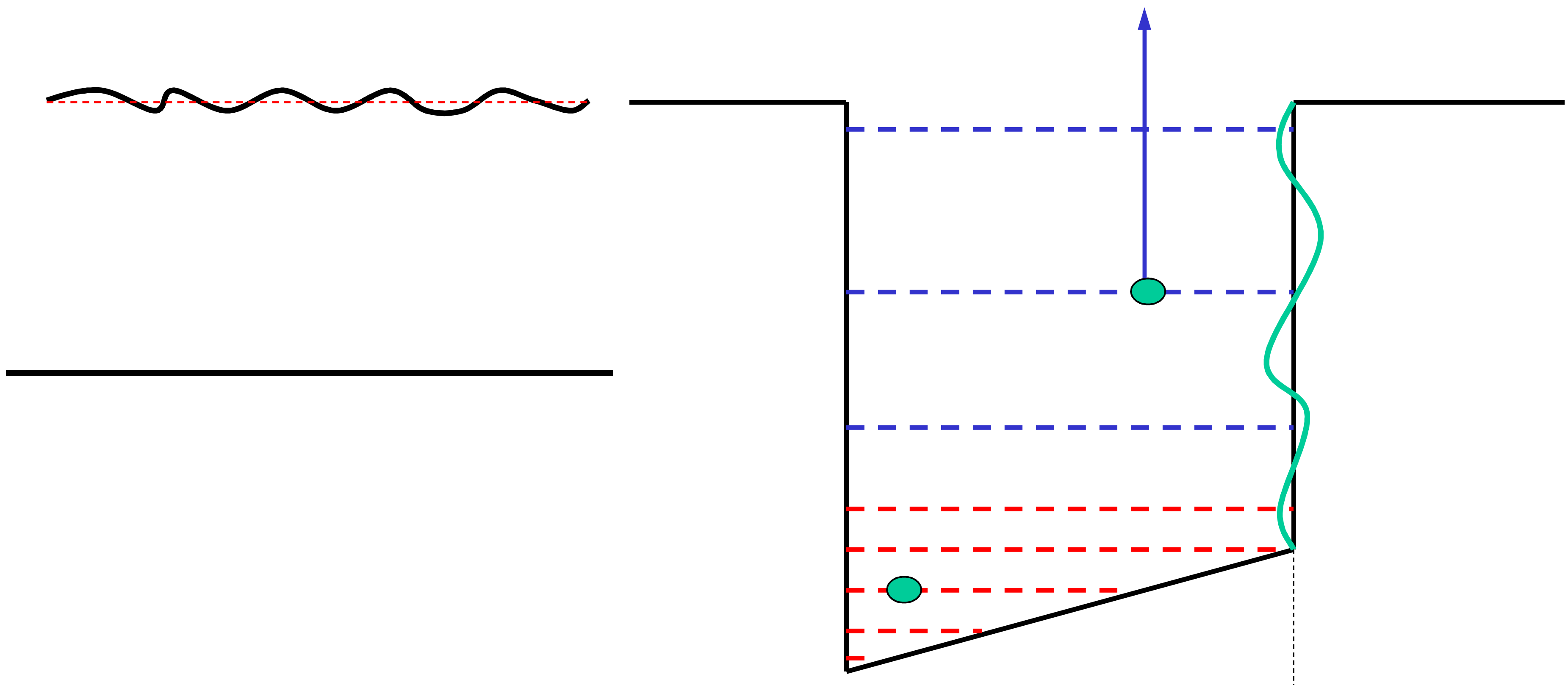
Scattering by a rough wall leads to transitions between quantized particle states (mode coupling)

Resolving the gravitational states: quantum language



After one or more collisions with the rough wall, particles go above the threshold and disappear.

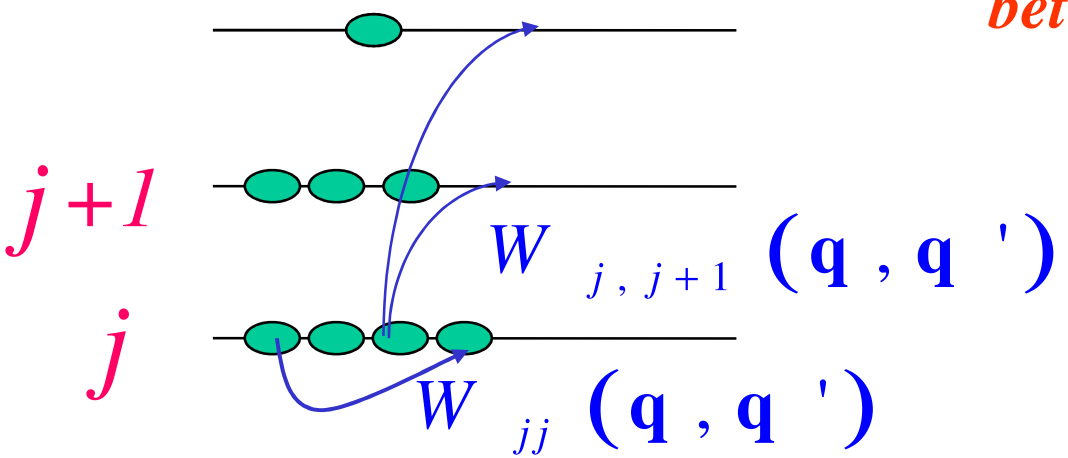
Resolving the gravitational states: quantum language



The wave functions for the upper levels reach the rough wall. After collisions, the particles can go above the threshold and disappear.
The wave functions for the lowest level particles do not reach the rough wall. Only these particles will survive the scattering!

Randomly modulated surfaces: Particle dynamics & transition probabilities

Scattering by random surface inhomogeneities results in randomization of the lateral motion, momentum relaxation, and formation of the mean free path ***– and in diffusion of particles between the levels***



$$\frac{dn_j}{dt} = \sum_{j'} \int W_{jj'} \left[n_{j'} - n_j \right] \delta\left(\varepsilon_{j\mathbf{q}} - \varepsilon_{j'\mathbf{q}'} \right) \frac{d^2 q}{2\pi}$$

Dimensionless variables

Length scale: $\ell = \hbar^{2/3}\left(2m^2 g\right)^{-1/3} \simeq 5.87\ \mu m$ *- size of the lowest level*

Energy scale $e_0 = mg\ell \simeq 0.6\ peV \simeq 9.6\times10^{-32}\ J$

Threshold energy $u_c = U_c / e_0 \simeq 1.4\times10^5$

Total kinetic energy $1.4\times10^5 < E / e_0 < 8.7\times10^5$

Threshold ratio $0.15 < \chi \equiv U_c / E < 1$

Roughness correlation function

$$\zeta\left(\left|\vec{s}\right|\right) = \eta^2 \varphi\left(-s / r\right), \quad \eta = l_0 / \ell, \quad r = R / \ell$$

Energy levels $\lambda_j = \varepsilon_j / e_0$

Velocities $v_j = \beta_j v_0, \quad v_0 = \sqrt{2g\ell} \simeq 1.07\ cm / s$

Scattering rate scale $1/\tau_0 = \frac{\sqrt{2\pi}}{4m^2}\frac{\hbar^2}{\ell^3 v_0}\eta^2 \simeq 1.15\times10^3 \eta^2\ s^{-1}$

Neutron depletion: biased diffusion

Roughness-driven diffusion of particles over the states j has a strong upward bias. For illustration, for square well states,

$$W_{jj'} = \frac{2\pi^4 j^2 j'^2}{m^2 L^6} \zeta\left(\left|\vec{q}_j - \vec{q}_{j'}\right| r\right)$$

rapidly increases with growing j, j' and moderates only at $\delta q \sim 1/r$. As a result, the probability for a particle to return back to a lower state j is very small and the diffusion problem becomes simple.

Neutron depletion: biased diffusion

Because of a strongly biased nature of interlevel diffusion, the problem can be solved analytically. All parameters collapse into a single constant

$$\Phi \sim A \bullet \eta^2 / r^{1/2}$$

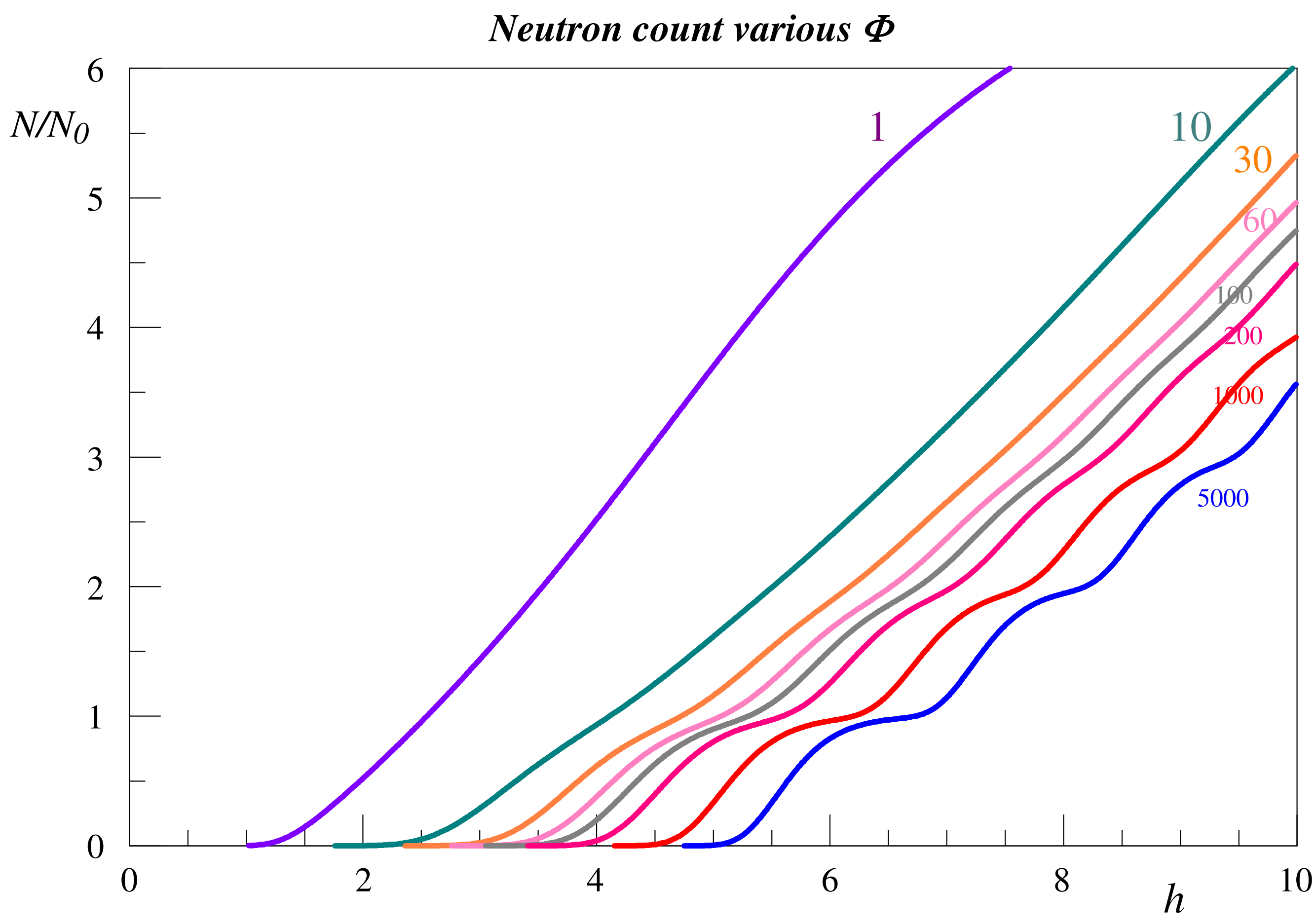
which is a complicated weighted integral of the roughness correlator and which determines the exit neutron count:

$$N_e = \sum N_j(0) exp\left[-\Phi b_j(h)\right]$$

where the constant A contains parameters of the beam and the cell, $b_j(h)$ describes the wave function of neutrons in state j on the (rough) ceiling and $N_j(0)$ are the numbers of neutrons entering the cell. The equation holds for both 1D and 2D surface roughness, though the expressions for and values of Φ are vastly different.

Neutron depletion

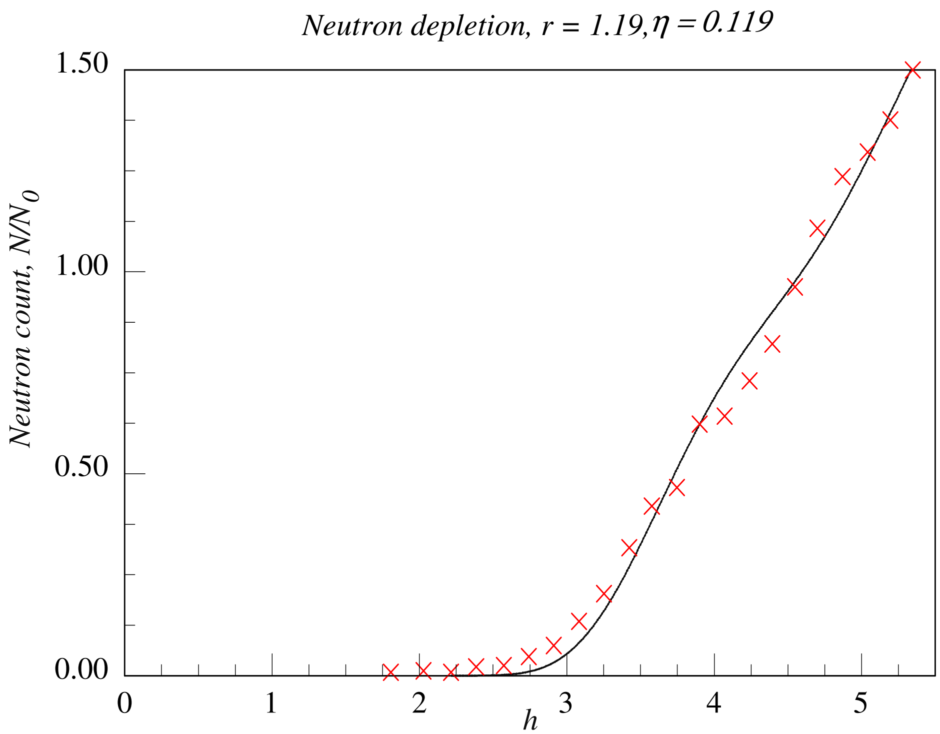
The value of Φ determines the shape of the curves for neutron count



The larger is the value of $\Phi \propto \eta^2 / r^{1/2}$ *, the more pronounced are the steps*

Calculation for different rough mirrors

We performed calculations for different cells and mirrors with 1D *and* 2D *roughness*



"Old" GRANIT cell. The roughness is assumed to be 1D with Gaussian correlations; $r = 1.19$, $\eta = 0.119$. The value of $\Phi = 23.5$

Φ for the exponential correlation function

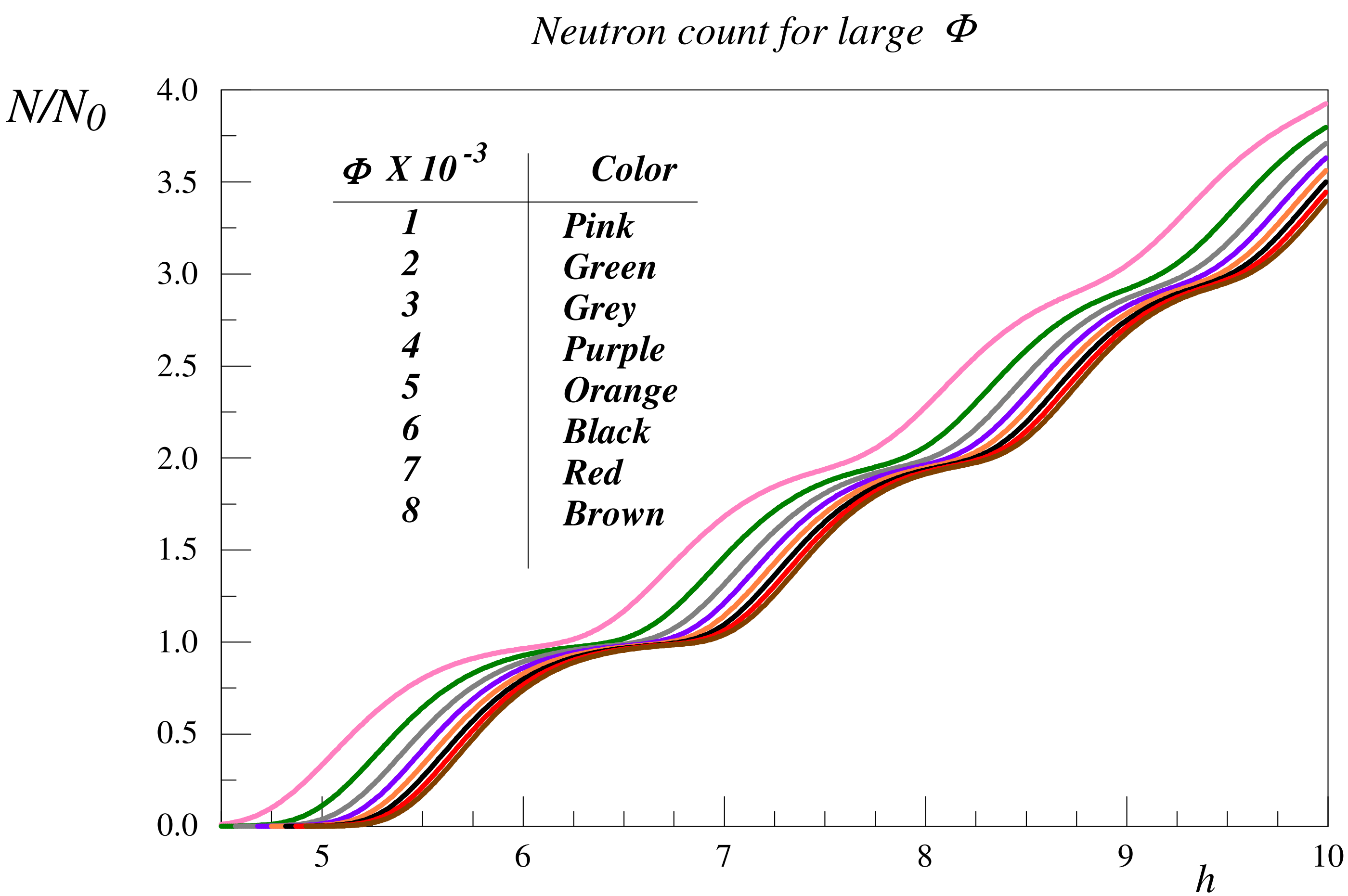
In the case of 1D *exponential correlation function one can calculate the value of Φ analytically:*

$$\Phi_1 = \frac{1}{3} A_1 \eta^2 r \; {}_2F_1\left(\frac{3}{4}, \frac{3}{2}, \frac{7}{4}, -r^2 u_c / 4\chi\right) \approx \frac{A_1 \eta^2}{r^{1/2}} \frac{(4\chi)^{3/4}}{3 u_c^{\;3/4}} \frac{\Gamma(3/4)}{\Gamma(3/2)},$$

$$A_1 = 4 \times 10^{-5} t_L u_c^{\;2} / \tau_0 \pi \chi$$

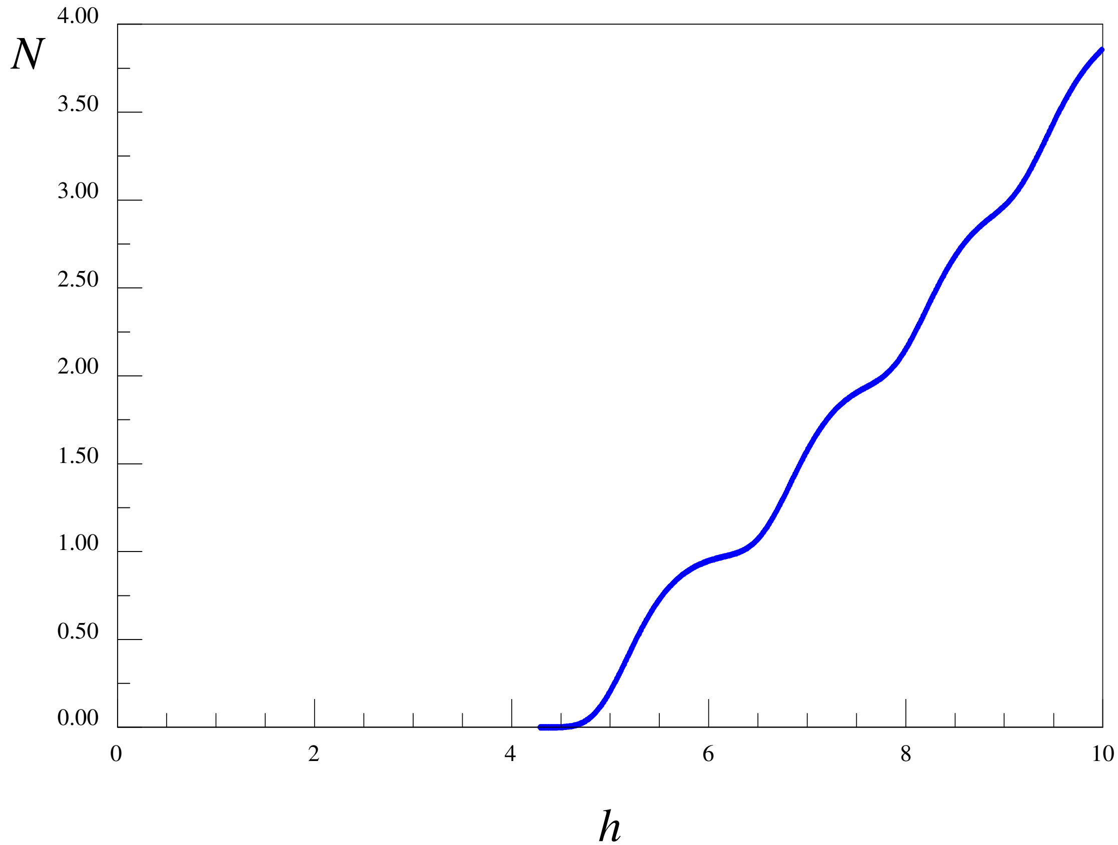
In 2D *the calculation can be done only numerically*

Neutron depletion: large Φ



We are lucky: at Φ around 5,000 the depletion curve is not very sensitive to Φ!

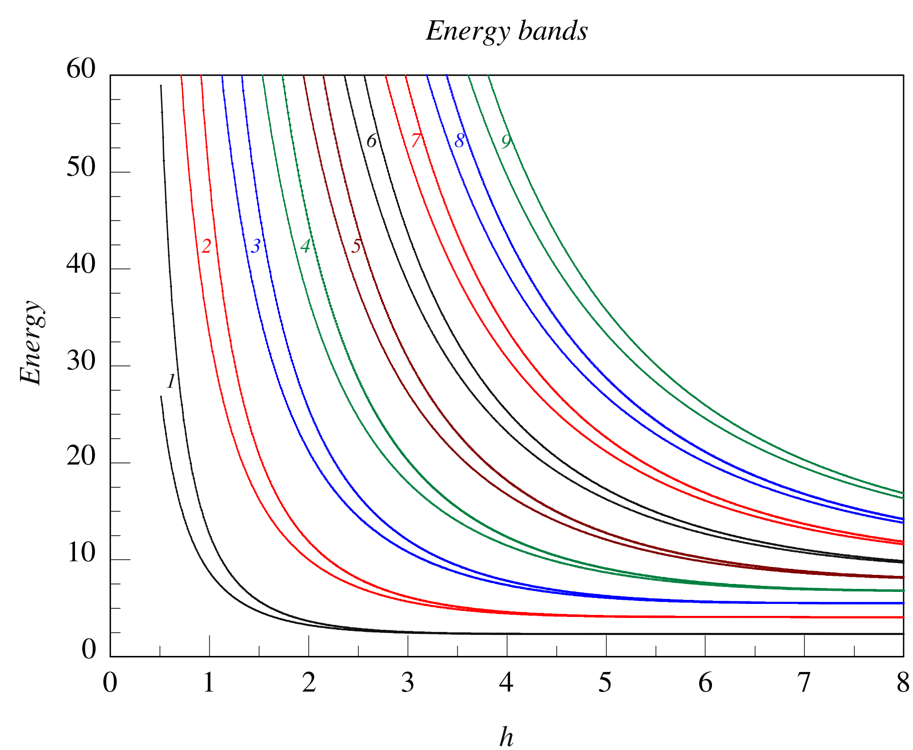
Calculation for the exponential correlation function



Predictions for the "new" GRANIT cell. 2D roughness with the exponential correlation function with $r = 0.65$, $\eta = 1.02$. The correlation function was extracted from the experimental data on the surface profile.

Broadening of levels

Large amplitude of roughness results not only in more rapid neutron depletion from upper levels, but also in broadening of energy levels and, by extension, in smearing of steps in neutron count.



Accuracy of prediction

Theoretical concerns:

- *Roughness amplitude is too large,* $\eta > r$
- *Accuracy of the roughness correlation function*
- *Distribution of particles in front of the cell is unknown and*

is not necessarily uniform

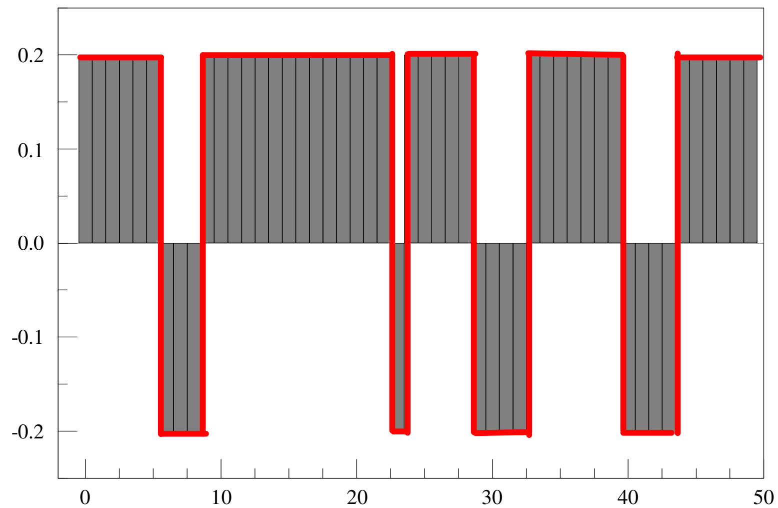
Potential experimental issues:

- *Roughness amplitude is too large; difficult to measure spacing*
- *The overall accuracy of roughness measurements*
- *Effect of sideway scattering for 2D roughness*
- *Distribution of particles in front of the cell is largely unknown*
- *Broadening of levels and potential smearing of the steps*

Most of this issues disappear if a future rough mirror is designed on the basis of Monte Carlo simulations for 1D *Ising model!*

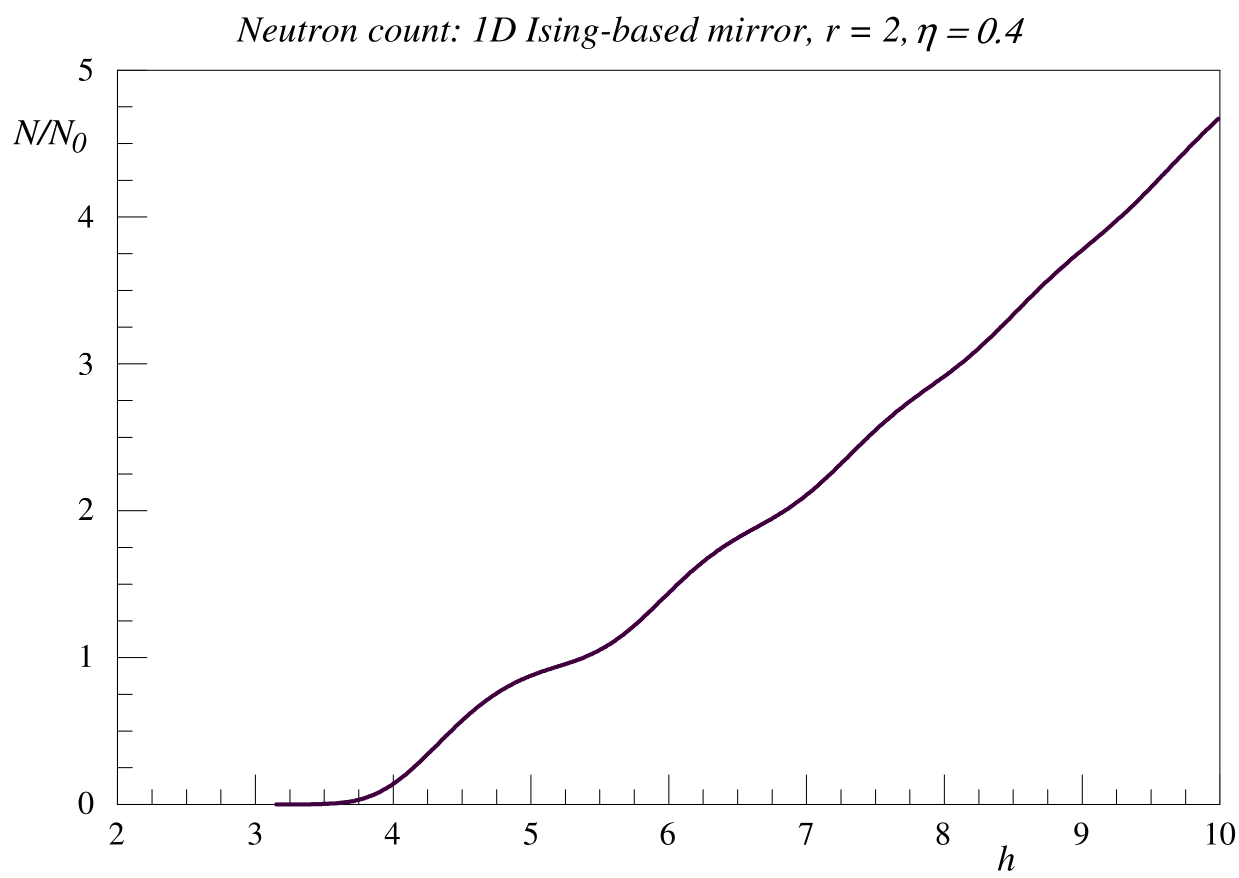
Advantages of the Ising-based mirror

- *The environment is much better controlled*
- *The shape of the correlation function is known and its parameters can be extracted with a very high accuracy*
- *The spacing between the mirrors can be easily measured*
- 1D *geometry: minimal sideway scattering and neutron loss*



Element of an "Ising" mirror: red lines- mirror surface,
grey bars – Ising "spins" (~ 6 μ wide)

Predicted neutron count for the Ising-based mirror



Conclusions

- *We developed a theoretical framework for an accurate description of GRANIT experiments*
- *The approach is based on our theory of transport along rough surfaces*
- *Strong upward bias in interstate diffusion allows for analytical solution*
- *The results express the neutron count explicitly via the mirror (roughness0 parameters*
- *Calculations are performed for both* 1D *and* 2D *roughness*
- *Our prediction for the neutron count is based on analysis of a new rough mirror looks quite promising*
- *We carefully analyzed the accuracy of our results for the neutron count*
- *We proposed a new design for a neutron mirror with roughness based on Monte Carlo simulations for* 1D *Ising model*
- *If such a mirror can be fabricated, it could greatly improve the quality of measurements and theory by providing a much better controlled environment!*

Thank you!

Correlation function of surface inhomogeneities

$$\zeta(\mathbf{s}) = \langle \xi(\mathbf{s}_1)\xi(\mathbf{s}_1+\mathbf{s})\rangle_{surface}$$

$$\zeta(\mathbf{q}) = \int d^2s\, e^{i\mathbf{q}\mathbf{s}}\zeta(\mathbf{s}) \quad - \textit{power spectrum}$$

#		$\zeta(\mathbf{s})$	$\zeta(\mathbf{q})$
1	*Gaussian*	$\ell^2 \exp\left(-s^2/2R^2\right)$	$\sim \exp\left(-q^2R^2/2\right)$
2	*power-law correlators*	$2\mu\ell^2\left(\frac{R^2}{s^2+R^2}\right)^{1+\mu}$	$\sim \frac{(qR)^\mu}{2^{\mu-1}\Gamma(\mu)}K_\mu(qR)$
3	*power-law power spectrum*	$\frac{\ell^2\left(s/R\right)^\lambda}{2^\lambda\Gamma(1+\lambda)}K_\mu\left(s/R\right)$	$\sim \frac{1}{\left(1+q^2R^2\right)^{1+\lambda}}$

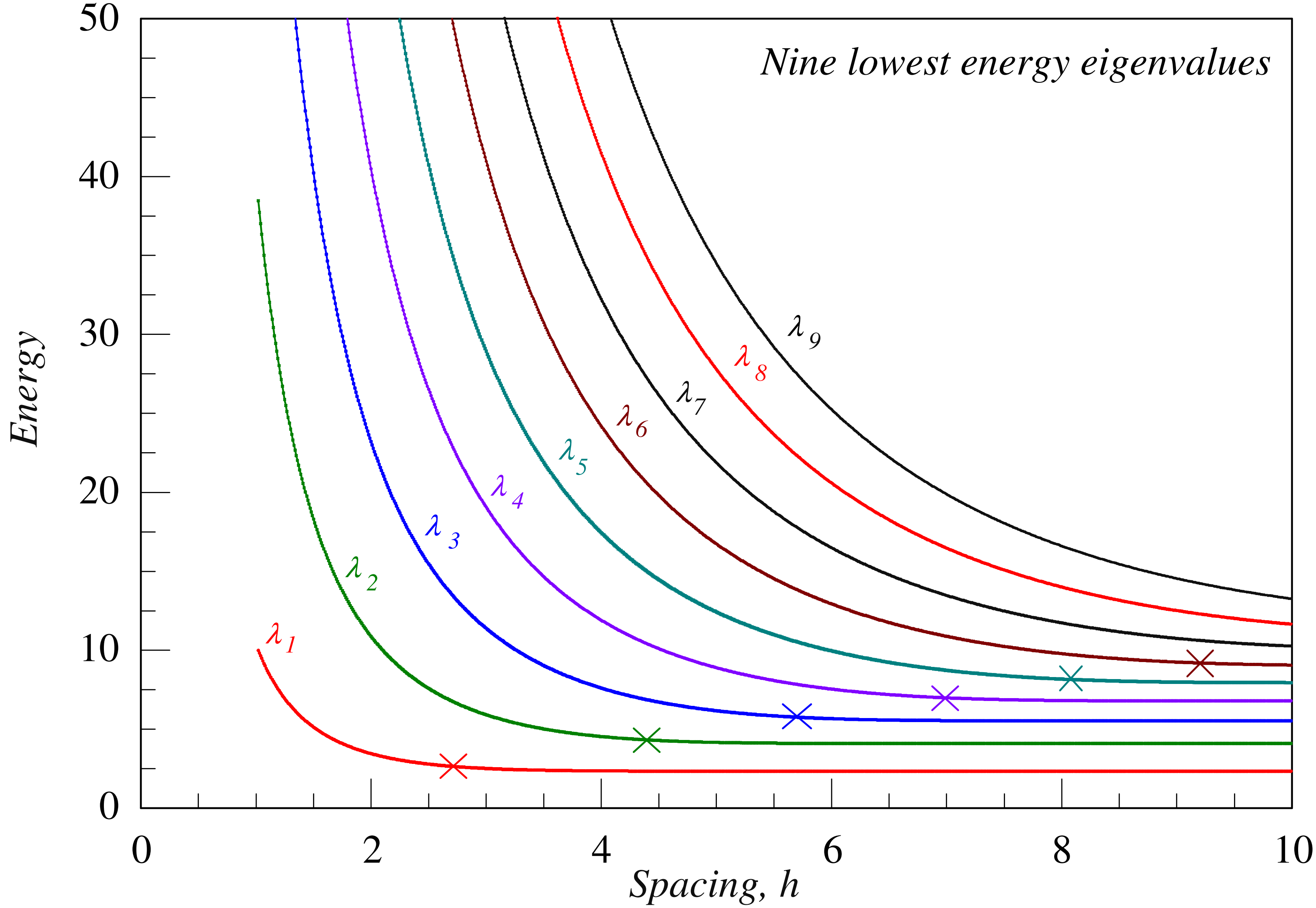
We will use the Gaussian correlations. However, for small-size inhomogeneities, R << L, the exact shape of the correlation function is not important!

Results: Absorption rate

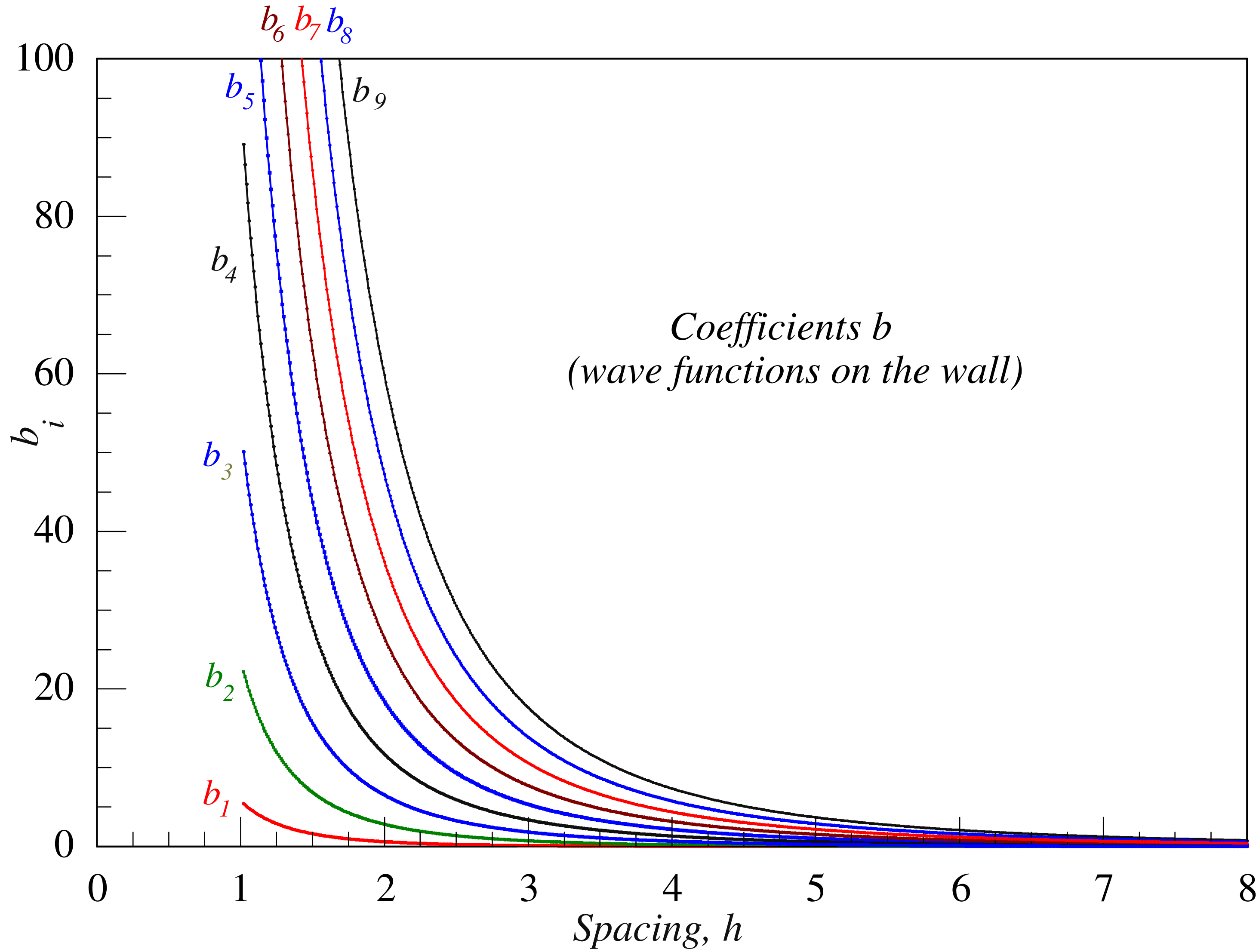
$$\frac{\tau_0}{\tau_j} = \frac{u_c^2 \ell r \psi_j^{\,2}(h)}{\pi\beta_j} \int_0^{e-u_c} \frac{d\lambda}{\sqrt{\lambda+u_c}} \frac{\exp\left[-\left(\sqrt{e-\lambda_j}-\sqrt{e-u_c-\lambda}\right)^2 r^2/2\right]}{1+\left(1+u_c/\lambda\right)\cos^2\left(h\sqrt{\lambda+u_c}\right)}$$

Change of momentum in a collision $\delta p \sim 1/r$ *and effective collisions require small* r *and large* η. *On the other hand, the condition of weak roughness requires* $\eta \ll r$.

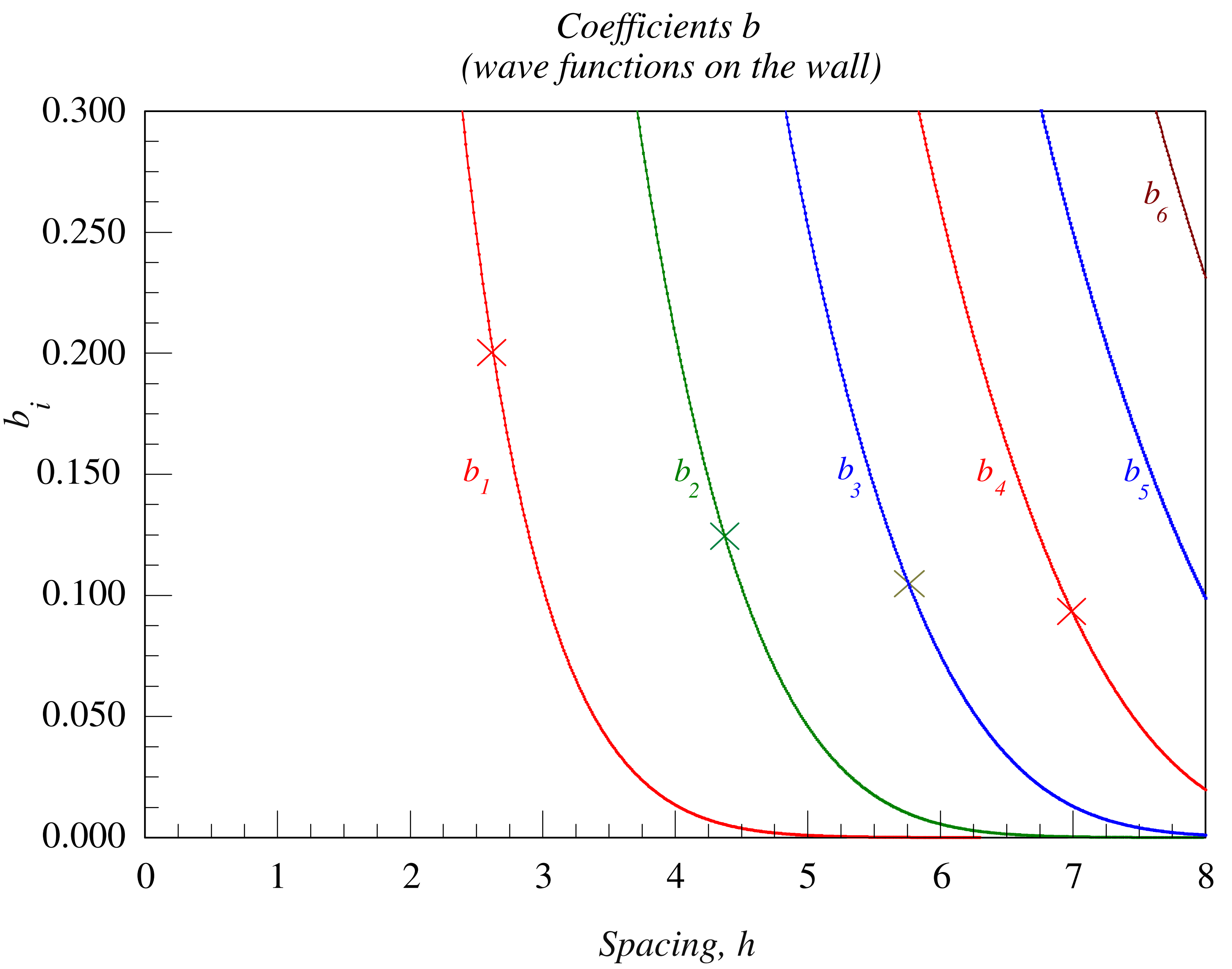
Results: Energy levels



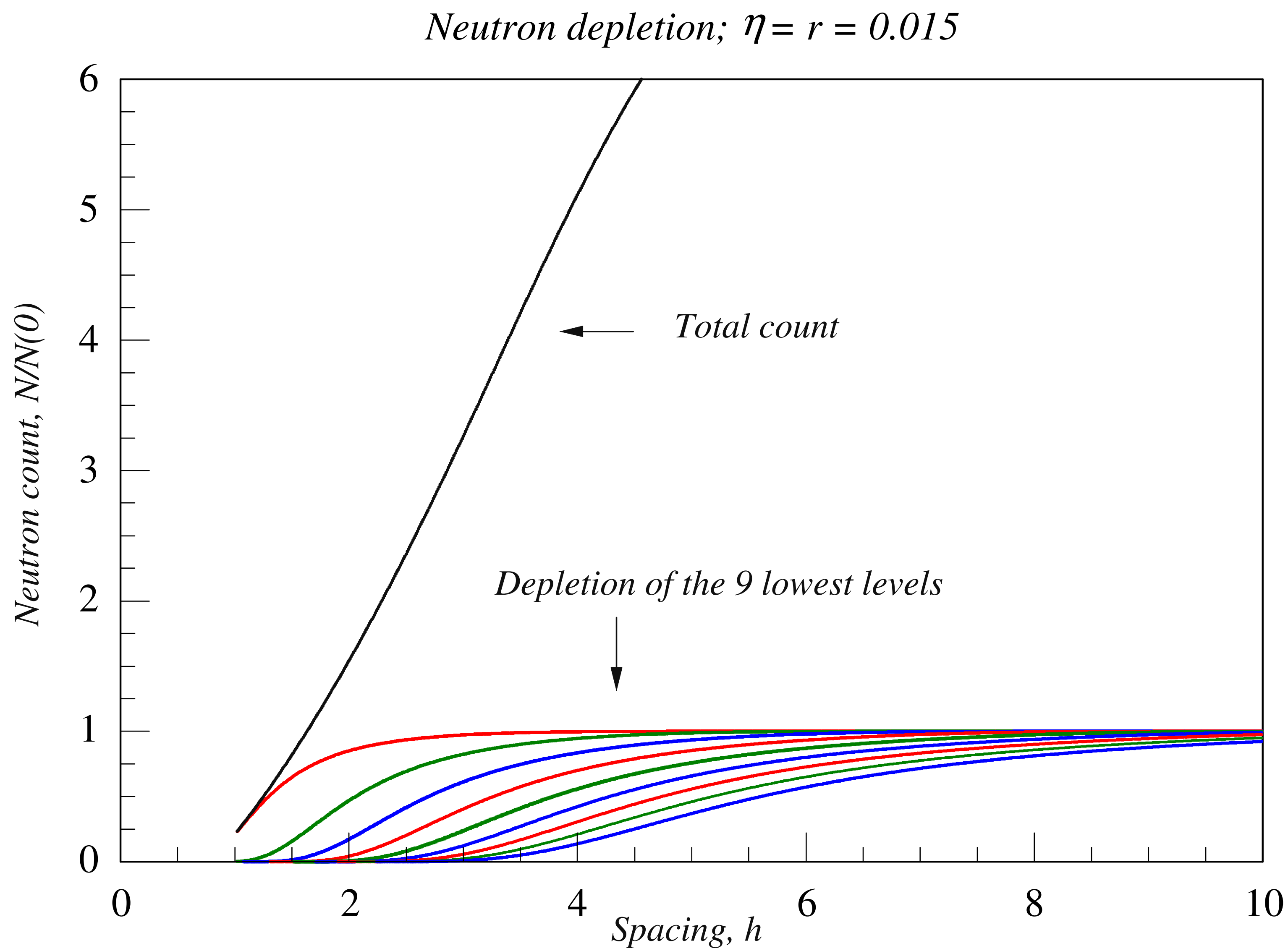
Results: Wave functions on the wall



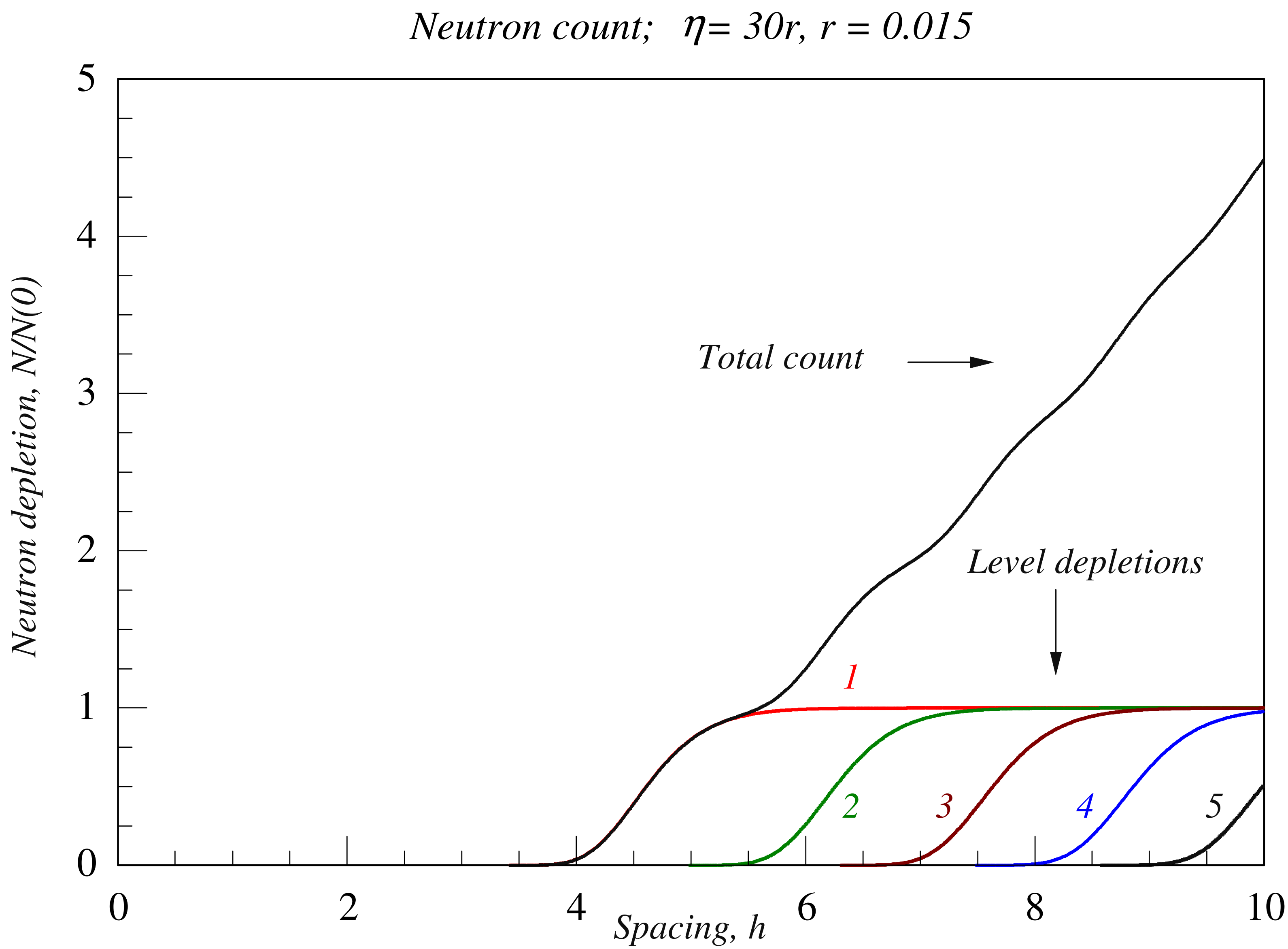
Results: Wave functions on the wall



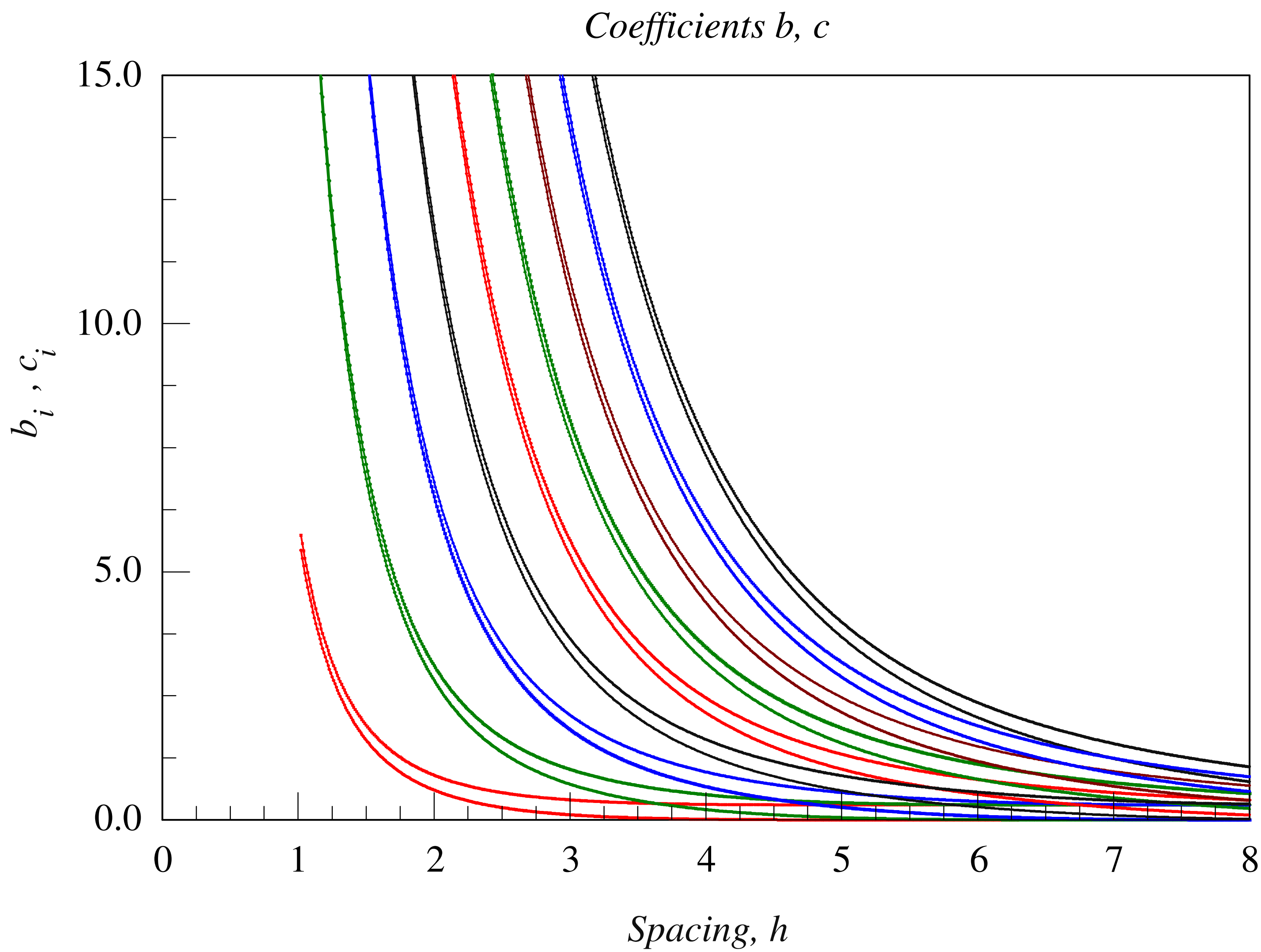
Results: Neutron count with “optimal” weak roughness



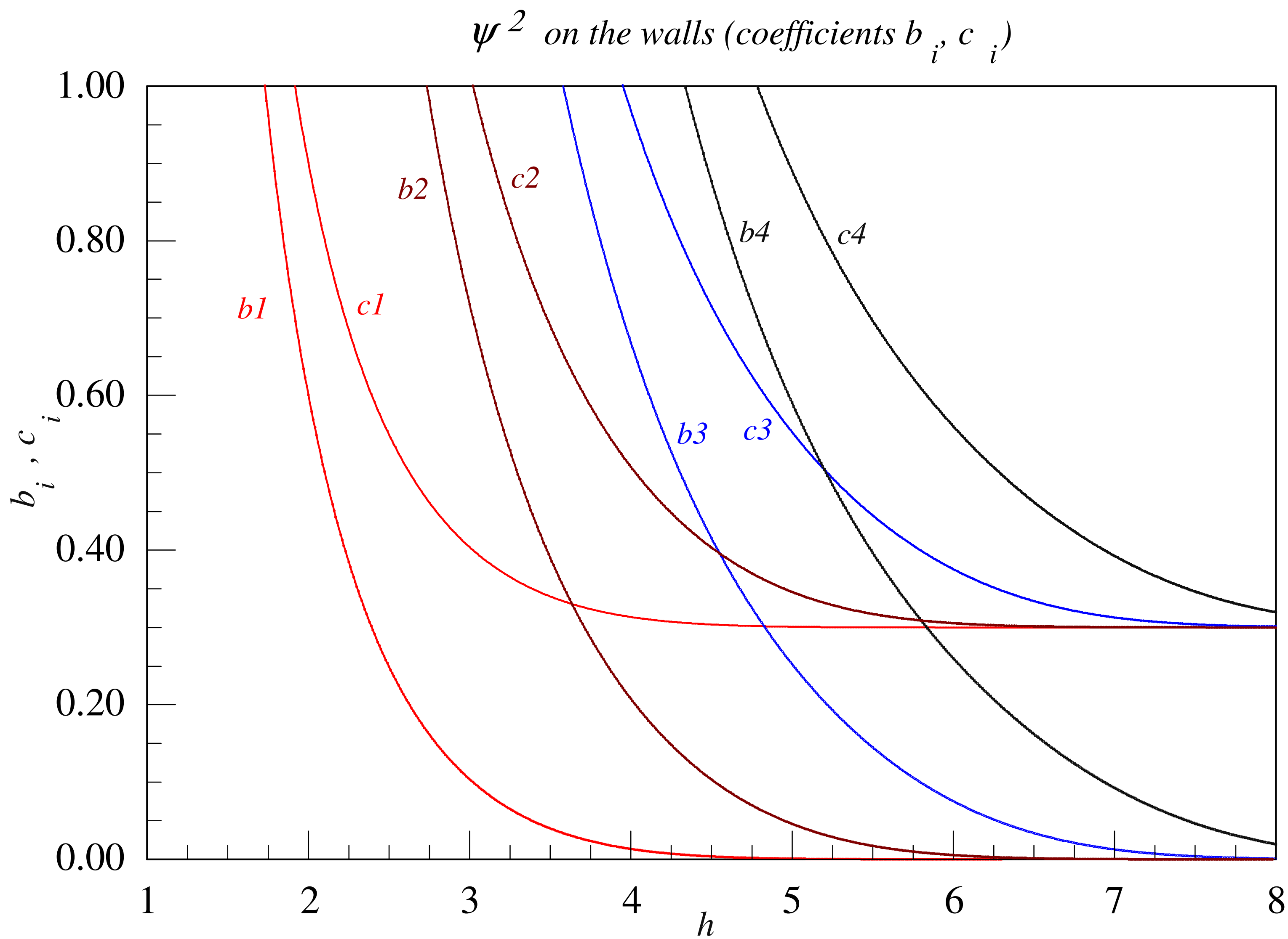
Neutron count for high-aperture roughness



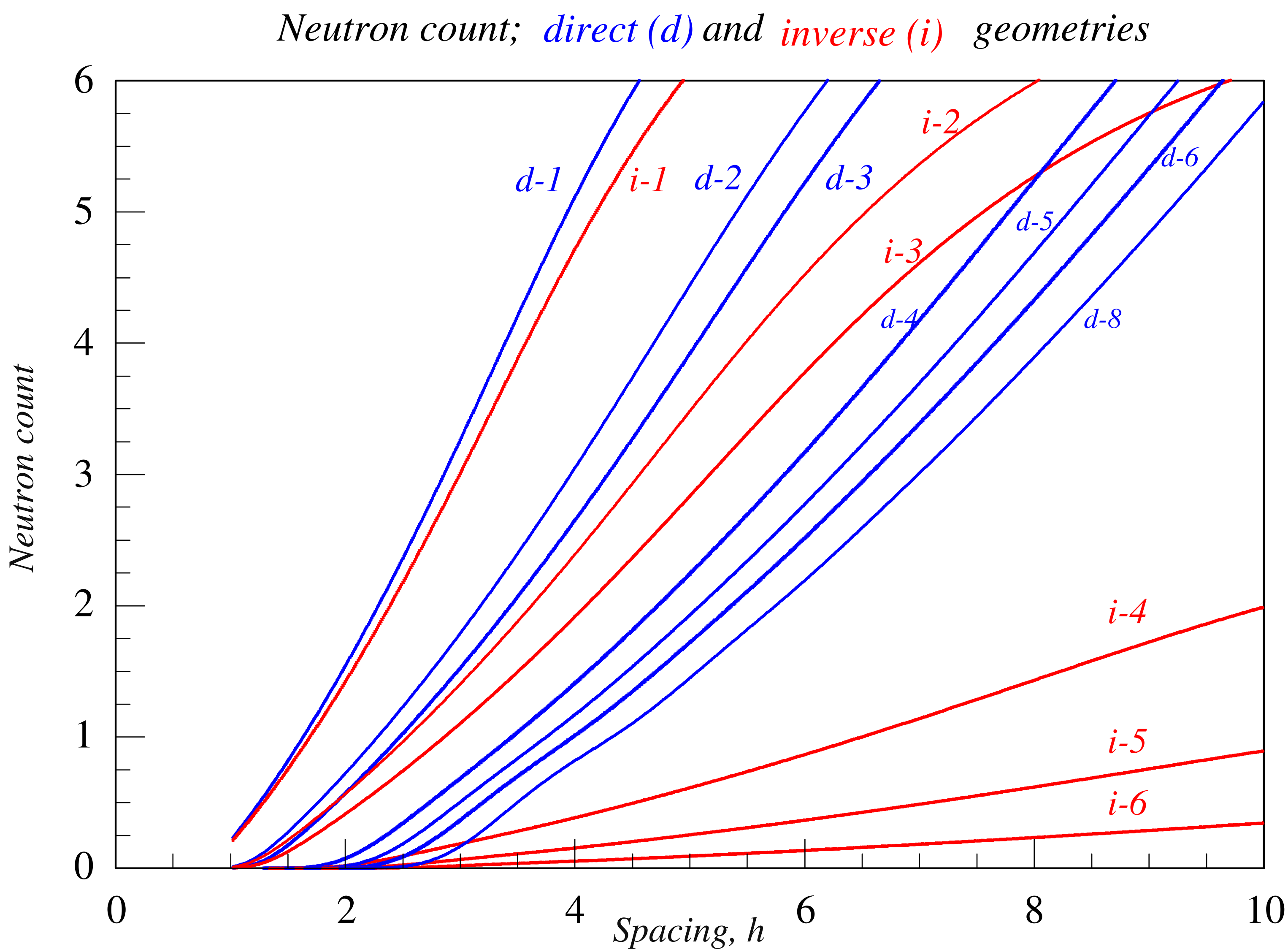
Inverse geometry: wave functions on the rough wall



Inverse geometry: wave functions on the rough wall

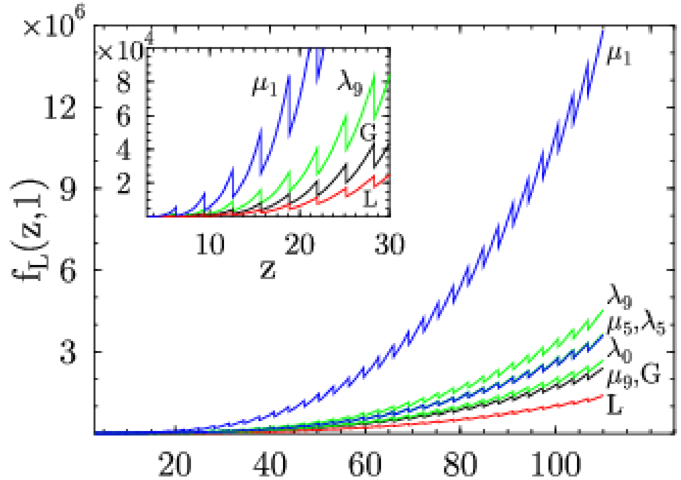


Neutron count: direct & inverse geometries



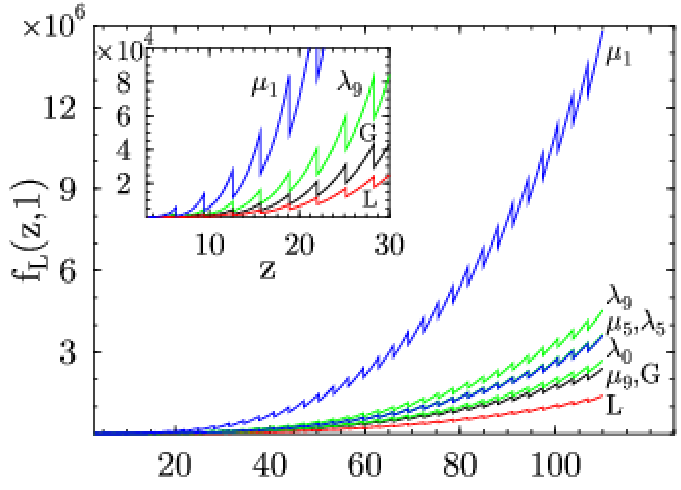
Thank you!

Conductivity & single-particle diffusion; small-scale inhomogeneities

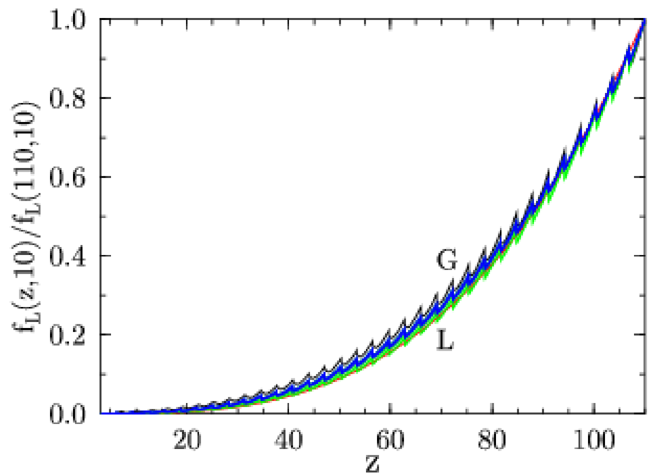


Conductivity (in units of $\frac{2e^2}{\hbar}\frac{R^2}{\ell^2}$ *)*
as a function of the film thickness
(in units of Fermi wavelength)

Conductivity & single-particle diffusion; small-scale inhomogeneities



Conductivity (in units of $\frac{2e^2}{\hbar}\frac{R^2}{\ell^2}$ *) as a function of the film thickness (in units of Fermi wavelength)*



Normalized conductivity as a function of the film thickness (in units of Fermi wavelength)

*The **shapes** of the curves are indistinguishable!*