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# Localization of Ultra-Cold Particles over Rough Substrates

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*Localization and diffusion parameters are calculated for particles adsorbed over inhomogeneous substrates for discrete and quasicontinuous spectra of the adsorbed states. The results are expressed via the angular harmonics of the correlation function of surface roughness. The problem is solved analytically in the limiting cases of longwave particles and large correlation radii of surface inhomogeneities. Elsewhere, the problem is solved numerically for Gaussian correlation of inhomogeneities. Applications to electrons on helium films, mobile adsorbed hydrogen atoms and molecules, ultra-cold neutrons in gravitational or magnetic field, etc., are discussed.*

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Scattering of $2D$ particles by random inhomogeneities, including the boundary ones, results in localization.[1–7] Often, instead of a random potential one encounters a problem with a random boundary condition, *e.g.*, $\Psi = 0$ on a wall $x = \xi(\mathbf{s})$ with random inhomogeneities $\xi(y, z)$, $\langle x \rangle = 0$. Though this problem is almost the same as for the random bulk potential, the explicit expressions for the localization parameters via the wall profile are unknown. This is especially important in a weak localization limit with an exponentially large localization length for which even a small uncertainty in the index may change the result by orders of magnitude. Another feature of this problem is that the correlation radius $R$ of surface inhomogeneities can be large while the analog of this parameter for bulk impurities is usually small. Recently we developed a formalism[8,9] for exact mapping of the problems with random boundaries onto problems with perfect boundaries and randomly distorted bulk by using a Migdal-like canonical transformation



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that flattens the boundary and, in the process, distorts the bulk.

Below this formalism is applied to a quantum ball $\epsilon = p^2/2m$ bouncing from a static random rough wall $x = \xi(\mathbf{s})$, $\langle x \rangle = 0$ in the field $mgx$. The motion in $x$ direction is finite with discrete spectrum $\epsilon_j$ and is continuous along the wall, $\epsilon_{j\mathbf{q}} = \epsilon_j + q^2/2m$. This formulation is typical for ultracold neutrons trapped in gravitational field[10] or electrons on helium surface in electric field. If the origin of adsorbed states $\epsilon_j$ is different, such as for hydrogen particles adsorbed on helium surface, the results require only minor modifications. Further modifications are required to account for interwall interference[9] in systems with two or more walls.

The problem is described by five parameters with dimensionality of length: the average height and correlation radius of surface inhomogeneities $\ell$ and $R$, size of the first bound state $L = \left(2m^2 g\right)^{-1/3}$ ($\widetilde{\epsilon}_j = \epsilon_j/mgL$), particle wavelength $\lambda$, and the amplitude $H \sim L^3/\lambda^2$ of jumps in the field $mg$. The quantum effects are characterized by $\alpha = \left(HR^2/L^3\right)^{1/2} = R/\lambda$ and by the number of minibands $S \sim (H/L)^{3/2}$ accessible for a particle with the energy $\epsilon_{j\mathbf{q}} = E$. Of course, in the quasiclassical regime $H \gg L$, $S \gg 1$ one cannot expect localization. The perturbative restriction on the results are $\ell \ll R, H$; the value of $\beta = R/L$ is arbitrary.

We start from the diffusion coefficient $D$ and mean free path $\mathcal{L} = 2D/v$ for particles with energy $E$, and then get the localization length $\mathcal{R}$[1,2]

$$\mathcal{R}(E) = \mathcal{L}(E) \exp\varphi, \;\; \varphi = \pi m S(E) D(E) \tag{1}$$

Among several feasible types of surface correlators,[11,12]

$$\zeta(|\mathbf{s}|) = \langle \xi(\mathbf{s}_1)\xi(\mathbf{s}_1 + \mathbf{s})\rangle \equiv \int \xi(\mathbf{s}_1)\xi(\mathbf{s}_1 + \mathbf{s}) d\mathbf{s}_1, \tag{2}$$

for numerical applications we assume that the correlations are Gaussian,

$$\zeta(\mathbf{s}) = \ell^2 \exp\left(-s^2/2R^2\right), \;\; \zeta(\mathbf{q}) = 2\pi\ell^2 R^2 \exp\left(-q^2R^2/2\right). \tag{3}$$

The coordinate transformation $X = x - \xi(\mathbf{s})$, $Y = y$, $Z = z$ makes the wall flat, $X = 0$. In conjugate momentum variables, the Hamiltonian $\widehat{H}_0(\mathbf{p}, x) = \widehat{p}^2/2m + mgx$ acquires random inhomogeneous part

$$\widehat{H} = \widehat{H}_0(\mathbf{P}, X) + \widehat{V}, \;\; \widehat{V} = mg\xi(\mathbf{s}) - \frac{1}{2m}\widehat{P}_x\left[\widehat{\mathbf{P}}_s\frac{\partial\xi(\mathbf{s})}{\partial\mathbf{s}} + \frac{\partial\xi(\mathbf{s})}{\partial\mathbf{s}}\widehat{\mathbf{P}}_s\right] \tag{4}$$

The eigenvalues $\epsilon_j$ are given by the zeroes of the unperturbed Airy (wave) functions, $\Phi(-\widetilde{\epsilon}_j) = 0$. The transition probabilities between the states $\epsilon_{j\mathbf{q}}$ are given by the squares of the matrix elements of $\widehat{V}$ and, after averaging over the inhomogeneities $\xi$, are expressed via the surface correlator $\zeta(\mathbf{q}'-\mathbf{q})$. In the end, the transport equation for particle diffusion in density gradient $\nabla n_j^{(0)}(\mathbf{q})$ acquires a simple form applicable to a wide range of problems with scattering by rough boundaries:

$$\frac{\mathbf{q}}{m}\cdot\nabla n_j^{(0)}(\mathbf{q}) = 2\pi m^2 g^2 \sum_{j'} \int \frac{d\mathbf{q}}{(2\pi)^2}\zeta(\mathbf{q}'-\mathbf{q})\left(\delta n_{j'\mathbf{q}'} - \delta n_{j\mathbf{q}}\right)\delta\left(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'}\right).$$

The transport equation can be solved analytically in three limiting cases. If $1.53 < \alpha/\beta = qL < 2.02$, only the first miniband is accessible, $S = 1$, and

$$\varphi = \frac{8\pi L^6}{R^2}\frac{\alpha^2 - 2.34\beta^2}{\zeta^{(0)}(q_1) - \zeta^{(1)}(q_1)} \to \frac{2R^2}{\beta^6\ell^2}\frac{\alpha^2 - 2.34\beta^2}{{}_1F_1\left(\frac{3}{2};2;-2\left(\alpha^2 - 2.34\beta^2\right)\right)}. \quad (5)$$

(the last expression describes Gaussian correlations (3)). The localization can be observed for $\beta = R/L > (R/\ell)^{1/3}$. Together with the perturbation condition $\ell < L, R$ (in this case $H \sim L$), this requires $\ell/L < L/R$.

For long-wave particles $\alpha = R/\lambda \ll 1$ (quantum reflection), the transition probabilities are constants with the zero first harmonic, and

$$D\left(\alpha \ll 1, \beta\right) = \frac{2}{m^4 g^2 S^2 \zeta(0)}\sum_{j=1}^{S}\left(E - \epsilon_j\right) \to \frac{8}{5}\frac{HL^3}{mS\zeta(0)} \quad (6)$$

or, for Gaussian correlations (the last equations is quasiclassical),

$$D\left(\alpha \ll 1, \beta\right) = \frac{1}{\pi m^4 g^2 S^2 R^2 \ell^2}\sum_{j=1}^{S}\left(E - \epsilon_j\right) \to \frac{4}{5}\frac{HL^3}{\pi m S R^2 \ell^2} \quad (7)$$

If $\alpha/\beta^2 \sim L^2/R\lambda \ll 1$, the interband transitions are suppressed:

$$D\left(\alpha/\beta^2 \ll 1\right) = \frac{4}{m^4 g^2 S}\sum_{j=1}^{S}\frac{E - \epsilon_j}{\zeta^{(0)}\left(2q_j \sin\frac{\theta}{2}\right) - \zeta^{(1)}\left(2q_j \sin\frac{\theta}{2}\right)} \quad (8)$$

or, for Gaussian correlations,

$$D = \frac{1}{\pi m^4 g^2 R^2 \ell^2 S}\sum_{j=1}^{S}\frac{E - \epsilon_j}{{}_1F_1\left(\frac{3}{2};2;-2\left(\alpha^2 - \beta^2\tilde{\epsilon}_j\right)\right)} \to \frac{5RH^4}{16\sqrt{2\pi}mL^3\ell^2 S} \quad (9)$$

(quasiclassical expressions in (7),(9) correspond to $j$, $S$, $\alpha^2/\beta^3 \gg 1$ when $\tilde{\epsilon}_j = \left[(3\pi/2)(j + 1/2)\right]^{2/3}$ and $S = (2/3\pi)(\alpha/\beta)^3$). Elsewhere, the transport equation should be solved numerically.

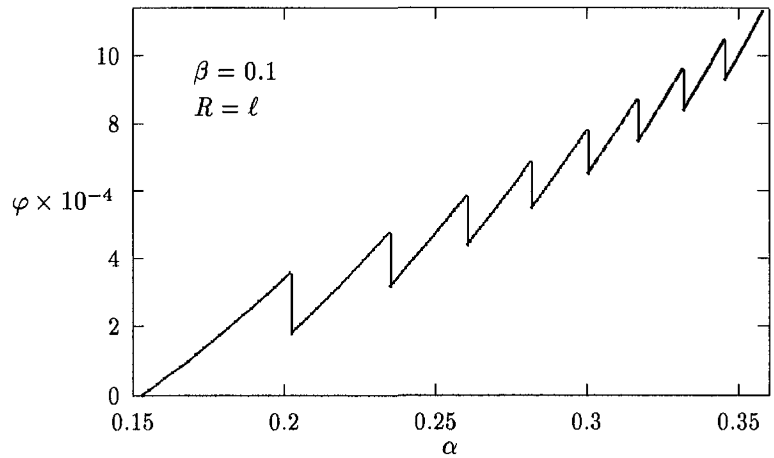


Fig. 1. The localization exponent $\phi$ (1) as a function of $\alpha = R/\lambda$ at $\ell = R$, $\beta = R/L = 0.1$

To have reasonable localization lengths, the exponent $\varphi$ in Eq.(1) should not be large, $\varphi \leq 20$. $\varphi$ grows with growing $\alpha = (HR^2/L^3)^{1/2}$ and decreasing $\beta = R/L$. Thus, one should decrease the particle energy $E = mgH$ and the correlation radius $R$, and increase the amplitude of inhomogeneities $\ell$ and the force $mg$. If $\beta = R/L < H/L$, the minimal localization length requires $\ell \sim R < H$, while for $\beta > H/L$ the best regime is $\ell \sim H < R$. Relatively small values of $\varphi$ often correspond to the range $\alpha/\beta^2 \ll 1$ (8), (9) in which the quasiclassical expression $\varphi\,(\alpha/\beta^2 \ll 1) \simeq 24.4 S^{8/3} RL/\ell^2$ is the most convenient one for a crude estimate of $D$ and $\varphi$. If $H \gg L$, it gives $\varphi \gg 1$ and the localization is not feasible. To observe localization, one should cool particles into the lowest miniband $\epsilon_{1\mathrm{q}}$ (5).

The singularities in transport in the points when the number of accessible minibands $S$ changes by 1 are distinct at small $\beta$ as in Figure 1 for $\beta = 0.1$. The appearance and acuteness of singularities are similar to those for transport in rough films.[8,9]

One of the most interesting applications is the trapped system of ultracold neutrons[13] bouncing in gravitational field for which $L = 5.86 \times 10^{-4}$ $cm$, $\alpha = 1.6 \times 10^3 Rv$ ($R$ in $cm$, $v = \sqrt{2E/m}$ - in $cm/s$). The neutrons can be cooled down to velocity $v = 100$ $cm/s$ ($H \sim 5$ $cm$) when $H \gg \ell, R \gg L$, and $S \gg 1$. Thus the anomalies in neutron count in experiment[13] cannot be explained by Anderson localization of neutrons. As it is clear from Figure 2, the localization can be observed only when the neutrons are condensed into the lowest miniband with velocities $v < 2$ $cm/s$ (or $H < 2 \times 10^{-3}$ $cm$)

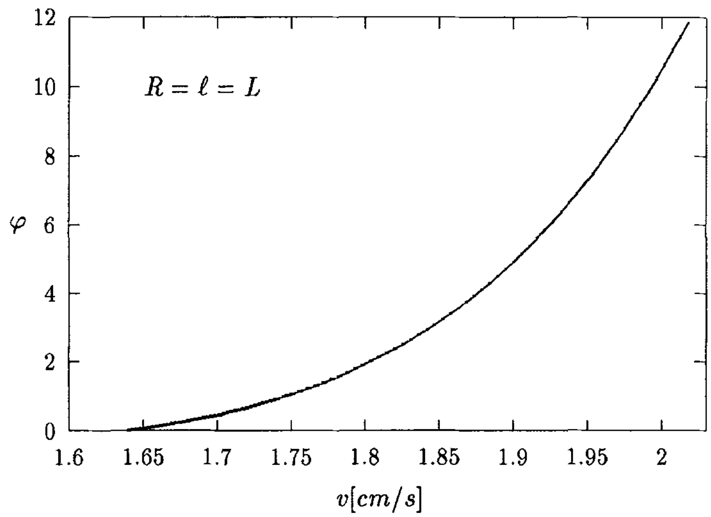


Fig. 2. The localization exponent $\phi(v)$ (1) for neutrons at $\ell = L = R$

while the parameters of inhomogeneities $\ell$, $R$ are comparable to $L$. Another option is to use the gradient of the magnetic field $g\mu\nabla B$ instead of gravity [1 $T/cm$ is equivalent to $g^* = 58g$]. This raises the threshold velocity $v$ by the factor $(g^*/g)^{1/3} \sim 4$, but results in decrease of $L$ and requires scaling down of inhomogeneities.

Electrons over helium in electric field $\mathcal{E}$ are different in two aspects.[14,15] First, the ripplon-induced inhomogeneities are not static (for ripplons at $T \sim 1$ $K$ the values $R \sim 20$ Å, $\ell \sim 0.8$ Å). A better choice is the electron system over the helium film on the surface of inhomogeneous substrate similar to the quasi-1$D$ electron-helium system in.[16] The second difference is that the electron in strong field $\mathcal{E}$ creates a dimple on helium. This makes the effective mass dependent on $\mathcal{E}$ and leads, in large fields, to auto-localization of electrons in ripplonic polarons thus restricting the application of our equations to relatively low fields. If $\mathcal{E} = 10^3$ $V/cm$, $mg$ should be replaced by $e\mathcal{E} = 1.6\times10^{-9}$ $erg/cm$, $L = (2me\mathcal{E})^{-1/3} = 1.4\times10^{-6}$ $cm$, while the scale of inhomogeneities in setup[16] is large, $\ell \sim R \sim 1$ $\mu m$. Then the 2$D$ localization of electrons requires either a decrease in scale of inhomogeneities or a decrease in field with a corresponding decrease in electron velocity to $v < 10^6$ $cm/s$ . It is not clear whether this is feasible.

More promising are the hydrogen atoms or molecules adsorbed on helium surface ($\epsilon_0 \sim 1$ $K$, $L \sim 5$ Å) at temperatures above condensation[17,18] for which one can use the same transport equation. The exponent $\varphi$,

$$\varphi = \pi m D = 2\left(L^6/R^4\ell^2\right) q^2R^2/{}_1F_1\left(3/2; 2; -2q^2R^2\right), \qquad (10)$$

(*cf.* Eq.(5)) depends on momentum $\mathbf{q}$ in the same way as $\varphi(v)$ in Figure 2 for neutrons with $mv^2/2 = \epsilon_0 + q^2/2m$. At $T \sim 1\ K$, the average amplitude and wavelength of capillary waves $\omega^2 = \sigma k^3/\rho + gk$ with $\sigma/\rho \sim 2.5\ cm^3/s^2$ provide $\ell \sim 0.8$ Å and $R \sim 20$ Å. The coefficient in Eq.(10) is approximately 0.3, and localization can be observed for particles with $qR \leq 1.5$.

Ripplon-induced localization is different from the static estimates in one important aspect. The collision operator contains the perturbation as $\left\langle |V_{jj'}(\mathbf{q},\mathbf{q}')|^2 \right\rangle_\xi \delta\left(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'}\right)$. The energy $\delta$-function is, to a large extent, the key to the simplicity of the transport equation. In a non-static case, the $\delta$-function is different, $\delta\left(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'} - \omega\right)$, and the transport equation for a quantum bouncing ball problem with a dynamic wall becomes extremely complicated[9] when $\omega$ is comparable to the transition probability $W_{jj'}(\mathbf{q},\mathbf{q}')$.

In summary, we calculated diffusion and localization parameters for a quantum bouncing ball with static random rough wall. In three limiting cases the results are analytical an can be applied to any surface correlator. Elsewhere, we performed numerical calculations for Gaussian correlations. This work was supported by NSF grants DMR-9412769 and DMR-9705304.

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