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Diffusion in overlayers in the presence of dipolar interactions

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Abstract. The diffusion of a tracer particle with dipolar moment in the paramagnetic or para-electric overlayer is considered. The dependence of the diffusion on the direction of dipolar moments and on the strength of dipolar interactions is discussed.

Consider the random walk of a tracer particle with a dipolar moment in the two-dimensional paramagnetic or para-electric overlayer with a simple square lattice. The dipolar moment of the particle interacts with dipolar moments in the overlayer by dipolar interactions. The results that we have obtained in this paper apply to different problems [1], e.g. they describe the diffusion of thermalised positrons trapped in the paramagnetic or para-electric overlayer on the metal surface [2]. We denote by $|P_n(x, y)|$ the probability that the particle starting at the point $(0, 0)$ is at the point (x, y) after n units of time; $R^2(n)$ and $D(n)$ are the mean-square displacement and the diffusion coefficient after n units of time respectively.

Let us first assume that the dipolar moments are in a direction parallel to the plane of the overlayer. The quantity $P_n(x, y)$ can be written in the following form [3, 4]:

$$P_n(x,y) = C_n \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \exp(-\mathrm{i}\kappa_x x) \exp(-\mathrm{i}\kappa_y y) \left[(\cos \kappa_x + \cos \kappa_y) \times \exp\left(\frac{\delta(1 - \cos \kappa_x)}{\cos \kappa_x + \cos \kappa_y - 3} \right) \right]^n \mathrm{d}\kappa_x \, \mathrm{d}\kappa_y \qquad (1)$$

where the parameter δ expresses the strength of dipolar interactions. When δ increases, the modes with $\kappa_x \neq 0$ are increasingly damped; so the mode with $\kappa_x = 0$ becomes more and more favoured. This causes $R^2(n)$ and $D(n)$ to increase when δ increases.

Let us now assume that the dipolar moments are in the direction perpendicular to the plane of the overlayer. The quantity $P_n(x, y)$ can be written in the form [3, 4]

$$P_n(x,y) = C_n \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \exp(-\mathrm{i}\kappa_x x) \exp(-\mathrm{i}\kappa_y y) \times \left[(\cos \kappa_x + \cos \kappa_y) \exp\left(\frac{\delta}{\cos \kappa_x + \cos \kappa_y - 3} \right) \right]^n \mathrm{d}\kappa_x \, \mathrm{d}\kappa_y . \qquad (2)$$

For $\delta < 4$ the modes with κ_x, $\kappa_y = 0, \pm\pi$ are dominant. When δ increases, the damping of the mode with $\kappa_x = \kappa_y = 0$ increases. On the contrary the factor $\cos \kappa_x + \cos \kappa_y$ is largest for $\kappa_x = \kappa_y = 0$. The dominant modes thus become the modes with κ_x, $\kappa_y = \kappa_c \neq 0, \pm\pi$. For $n \to \infty$ one can write

$$P_n(x, y) = C_n \cos(\pi x) \cos(\pi y) \exp[(-x^2 - y^2)/nD]. \tag{3}$$

When δ increases, the modes with $\kappa_x \neq \pm\pi$ and $\kappa_y \neq \kappa_c$ are increasingly damped, so $R^2(n)$ and D increase.

We conclude that for $n \to \infty$ and for dipolar moments parallel to the plane of the overlayer the probability $|P_n(x, y)|$ is Gaussian with D increasing for increasing δ. For $n \to \infty$ and dipolar moments perpendicular to the plane of the overlayer the quantity $P_n(x, y)$ has spatial oscillations (the dipolar moment of the particle may reverse) with Gaussian damping and D increasing for increasing δ.

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