Brief Reports

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Trapping in the presence of anisotropic diffusion

D. L. Huber
Department of Physics, University of Wisconsin, Madison Wisconsin 53706
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The asympotic limit of the rate of decay of excitation in the presence of a low concentration of trapping centers is investigated with the assumption that transfer of excitation is governed by an anisotropic diffusion equation. An effective isotropic diffusion constant is introduced which in the appropriate limit leads to results similar to those obtained recently by Richards using variational methods.

Recently, attention has been directed to the calculation of the decay of the excitation in the presence of a random distribution of trapping centers.[1–3] An important limiting case of the general problem occurs when the transfer of excitation among the donors is governed by a diffusion equation. In this case the (asymptotic) decay rate can be written[2]

$$\Gamma = n_A \int d\vec{r}\, T(\vec{r},0) \ , \tag{1}$$

where n_A is the trap concentration and $T(\vec{r},0)$ is a solution of the integral equation

$$T(\vec{r},0) = v(r) - v(r) \int d\vec{r}\,' g(\vec{r}-\vec{r}\,',0)T(\vec{r}\,',0) \ . \tag{2}$$

Here $v(r)$ is the donor-trap transfer rate at separation r and $g(\vec{r},0)$ is the Fourier transform of the diffusion propagator which can be written

$$g(\vec{r},0) = \frac{1}{(2\pi)^3} \int \frac{d\vec{k}\, e^{i\vec{k}\cdot\vec{r}}}{Dk^2} \ , \tag{3}$$

assuming isotropic diffusion.

The purpose of this Brief Report is to discuss the trapping when the diffusion is anisotropic. Our interest in this problem was stimulated by a recent paper by Richards[4] who calculated the asymptotic decay rate appropriate to a quasi-one-dimensional system using variational techniques. In this paper we propose a simple approximation which reproduces Richard's results in the appropriate limit and which provides a straightforward generalization of his findings to arbitrarily anisotropic situations.

In the presence of anisotropic diffusion Eqs. (1) and (2) still apply. However, the propagator is given by

$$g(\vec{r},0) = \frac{1}{(2\pi)^3} \int \frac{d\vec{k}\, e^{i\vec{k}\cdot\vec{r}}}{D_x k_x^2 + D_y k_y^2 + D_z k_z^2} \ . \tag{4}$$

The essential step in the approximation is to replace (4) with an effective propagator

$$g_{\text{eff}}(\vec{r},0) = \frac{1}{(2\pi)^3} \int \frac{d\vec{k}\, e^{i\vec{k}\cdot\vec{r}}}{D_{\text{eff}} k^2} \ , \tag{5}$$

where the effective diffusion constant is given by an angular average of the denominator in (4):

$$\frac{1}{D_{\text{eff}} k^2} = \frac{1}{4\pi} \int \frac{d\Omega_k}{D_x k_x^2 + D_y k_y^2 + D_z k_z^2} \ . \tag{6}$$

The resulting expression for the decay rate is then obtained from the rate for the corresponding isotropic problem by making the replacement $D \rightarrow D_{\text{eff}}$.

The integral in (6) can be evaluated in terms of an incomplete elliptic integral of the first kind[5] $F(\phi\backslash\alpha)$ with the result

$$D_{\text{eff}} = \frac{D_2^{1/2}(D_3 - D_1)^{1/2}}{F(\phi\backslash\alpha)} \ , \tag{7}$$

where

$$\phi = \tan^{-1}(D_3/D_1 - 1)^{1/2} \ ,$$

and

$$\alpha = \cos^{-1}\left[\frac{(D_3/D_2 - 1)^{1/2}}{(D_3/D_1 - 1)^{1/2}}\right] \ . \tag{8}$$

Here D_3 is the largest and D_1 the smallest of the three diffusion constants, D_x, D_y, and D_z.

In a quasi-on-dimensionl system $D_3 \equiv D_\parallel > D_2 = D_1 = D_\perp$, Eq. (7) reduces to

$$D_{\rm eff} = \frac{D_\perp^{1/2}(D_\parallel - D_\perp)^{1/2}}{\tan^{-1}(D_\parallel/D_\perp - 1)^{1/2}} , \tag{9}$$

whereas in a quasi-two-dimensional system $D_3 = D_2 \equiv D_\perp > D_1 = D_\parallel$, we obtain

$$D_{\rm eff} = \frac{(D_\perp - D_\parallel)^{1/2} D_\perp^{1/2}}{\tanh^{-1}(1 - D_\parallel/D_\perp)^{1/2}} . \tag{10}$$

In the problem investigated in Ref. 4 $v(r)$ was equal to α/r^6 and $D_\parallel >> D_\perp$. In the case of isotropic diffusion we have[1]

$$\Gamma = 8.5 n_A \alpha^{1/2} D^{3/4} , \tag{11}$$

so that with the effective diffusion constant we obtain

$$\Gamma = 6.1 n_A \alpha^{1/4} (D_\perp D_\parallel)^{3/8} . \tag{12}$$

Equation (12) gives a value for Γ which is 15% less than the result obtained by variational methods[4]:

$$\Gamma = 7.2 n_A \alpha^{1/4} (D_\perp D_\parallel)^{3/8} . \tag{13}$$

For comparison we note that in the isotropic limit the variational method gives a value for Γ which is 12% larger than the exact result.[4]

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