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Motion of an impurity atom in a lattice of harmonically coupled atoms and the stationary generalized Langevin equation

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Abstract. The motion of an impurity atom imbedded in a harmonic lattice is investigated. It is a simple and exactly soluble example of a many-particle system in which diffusive motion may occur for the impurity atom. By the direct calculation of the Laplace transforms of the velocity autocorrelation function and the friction function $\Gamma(t)$, it is concluded that the fast decay of the friction function is necessary in order for diffusive motion to occur, and that this is the case when the stationary generalized Langevin equation describes the motion of the impurity atom.

1. Introduction

Mori (1965) investigated the Liouville equations of motion for a number of dynamical variables $X_1(t), X_2(t), \ldots, X_n(t)$, and showed that those equations can be expressed as the following generalized Langevin equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}X_j(t) - \sum_{k=1}^{n} \Omega_{jk}X_k(t) + \sum_{k=1}^{n} \int_{t_0}^{t} \mathrm{d}t' \Gamma_{jk}(t-t')X_k(t') = R_j^M(t). \tag{1.1}$$

He derived the second fluctuation–dissipation theorem for this equation

$$\sum_{k=1}^{n} \Gamma_{jk}(t-t')\langle X_k(0), X_l^*(0)\rangle = \langle R_j^M(t), R_l^{M*}(t')\rangle \tag{1.2}$$

where the bracket $\langle A, B\rangle$ of A and B denotes the canonical average of a suitably defined product of A and B.

Mori's equation is applicable after an initial time t_0, and the random force $R_j^M(t)$ depends on the arbitrarily chosen initial time t_0. Since the physical quantity 'random force' must be defined independently of such an arbitrary time, it is desirable to split the random force of this nature out of $R_j^M(t)$. In fact such a formulation has already been considered by Kubo (1966), who suggested that the second fluctuation–dissipation theorem (1.2) can also be extended to that case.

In a preceding paper (Fukui and Morita 1971), the present authors considered the Liouville equations for a number of variables $X_1(t), X_2(t), \ldots, X_n(t)$, and derived the stationary generalized Langevin equation in the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}X_j(t) - \sum_{k=1}^{n} \Omega_{jk}X_k(t) + \sum_{k=1}^{n} \int_{-\infty}^{t} \mathrm{d}t' \Gamma_{jk}(t-t')X_k(t') = R_j(t) \tag{1.3}$$

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where the friction function $\Gamma_{jk}(t-t')$ is expressed in terms of the correlation of the random forces through the second fluctuation–dissipation theorem

$$\sum_{k=1}^{n} \Gamma_{jk}(t-t')\langle X_k(0), X_l^*(0)\rangle = \langle R_j(t), R_l^*(t')\rangle. \tag{1.4}$$

As pointed out in the preceding paper, the assumption of fast decay is necessary for the friction function $\Gamma_{jk}(t)$ to derive the stationary generalized Langevin equation (1.3).

Rubin (1960, 1961) and others (eg Takeno and Hori 1962, Mazur 1965 and Nakazawa 1966) investigated harmonic lattices including an impurity atom as a model for brownian motion. If the model is appropriate, the position $\boldsymbol{x}_0(t)$ of the impurity atom follows the Langevin equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\dot{\boldsymbol{x}}_0(t)+\gamma\dot{\boldsymbol{x}}_0(t) = \boldsymbol{f}(t) \tag{1.5}$$

and the friction constant γ and the 'random force' $\boldsymbol{f}(t)$ occurring in this equation will satisfy the fluctuation–dissipation theorem

$$\langle f_\alpha(t), f_\beta(t')\rangle = \delta_{\alpha\beta}\gamma\delta(t-t') \tag{1.6}$$

where $\dot{\boldsymbol{x}}_0(t)$ is the time derivative of $\boldsymbol{x}_0(t)$, $f_\alpha(t)$ and $f_\beta(t)$ are the α and β components of $\boldsymbol{f}(t)$ and $\delta_{\alpha\beta}$ is the Kronecker delta. Most work in the past has been concentrated on finding out the limiting cases when the Langevin equation (1.5) with (1.6) can be used to describe the motion of the impurity atom. For instance, the impurity atom in the one dimensional lattice can be considered to follow the Langevin equation in the limit of infinite mass of the impurity atom, infinite coupling constant and infinitesimal lattice constant (Takeno and Hori 1962) or in the limit of infinite mass of the impurity atom and infinite time (eg Mazur 1965 and Nakazawa 1966).

In the present paper we investigate in what situations the impurity atom follows the stationary generalized Langevin equation. Two cases are compared according to whether the atoms are coupled to their respective equilibrium positions or not. It is concluded that the stationary generalized Langevin equation is applicable only if these couplings do not exist. That equation is shown not to be applicable to the three dimensional case in any limit.

In § 2, the conditions to be satisfied for the friction function are discussed in the stationary generalized Langevin equation. Whether those conditions are satisfied or not is discussed in §§ 4 and 5 for the one, two and three dimensional infinite lattices. Solution of the problem for the one dimensional finite lattice is given and discussed in § 3.

2. The stationary generalized Langevin equation for the impurity atom

The stationary generalized Langevin equation (1.3) with (1.4) reads, for the impurity atom, as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}\dot{x}_0(t)+\int_{-\infty}^{t}\mathrm{d}t'\Gamma(t-t')\dot{x}_0(t') = R(t) \tag{2.1}$$

$$\Gamma(t-t')\langle\dot{x}_0(0), \dot{x}_0(0)\rangle = \langle R(t), R(t')\rangle = \langle R(t-t'), R(0)\rangle. \tag{2.2}$$

In the present paper, we investigate in which situations the impurity atom follows this equation (2.1) with conditions (2.2).

In order to show the applicability of (2.1) with (2.2), we recall that the condition that $\Gamma(t)$ decays fast to zero was used in deriving that equation (Fukui and Morita 1971). The condition that $\Gamma(t)$ decays to zero is written as

$$\lim_{t\to\infty} \Gamma(t) = 0. \tag{2.3}$$

If we denote the Laplace transform of $\Gamma(t)$ by

$$\Gamma_z = \int_0^\infty \mathrm{d}t \Gamma(t) \exp(-zt) \tag{2.4}$$

we have

$$\lim_{z\to 0^+} z\Gamma_z = 0 \tag{2.5}$$

from (2.3). It should be noted that (2.5) is necessary but not sufficient for (2.3). The rapidity of the decay of $\Gamma(t)$ required in deriving (2.1) depends on the property of $\dot{x}_0(t)$. It is natural to assume that $\dot{x}_0(t)$ is finite. Then it is sufficient to require that

$$|\Gamma_z| \leqslant \int_0^\infty |\Gamma(t)| \, \mathrm{d}t < \infty \qquad \text{for } \mathrm{Re}\, z \geqslant 0. \tag{2.6}$$

From these considerations, we observe that: (i) if (2.3) and (2.6) are satisfied, we can derive (2.1), and (ii) if (2.5) is not satisfied, we cannot derive (2.1). We shall check (ii) first, and when (2.5) is satisfied, (i) is also checked. By this procedure we investigate the applicability of (2.1) for the exactly soluble harmonically coupled atoms with one impurity atom.

Here we shall consider the velocity autocorrelation function of the impurity atom, $\langle \dot{x}_0(t), \dot{x}_0(0)\rangle$. We denote its Laplace transform by $\langle \dot{x}_0, \dot{x}_0\rangle_z$. According to the theory of the generalized Langevin equation developed by Mori (1965), Kubo (1966) and Fukui and Morita (1970), this Laplace transform $\langle \dot{x}_0, \dot{x}_0\rangle_z$ must be connected with Γ_z through the relation

$$\langle \dot{x}_0, \dot{x}_0\rangle_z = \frac{k_B T/M}{z+\Gamma_z} \tag{2.7}$$

where M is the mass of the impurity atom, k_B is the Boltzmann constant and T is the temperature of the system. Under a general assumption on the analytic properties of the function $\langle \dot{x}_0, \dot{x}_0\rangle_z$, one sees that this quantity reduces to the diffusion constant D in the limit of $z \to 0$ (eg Nakajima 1958 and Nakazawa 1966). As a result, one has

$$D = \lim_{z\to 0} \frac{k_B T}{M\Gamma_z}. \tag{2.8}$$

If (2.6) is satisfied, D is not zero and hence

$$D > 0. \tag{2.9}$$

This condition will be investigated in the following sections.

3. The velocity autocorrelation function

We consider a one dimensional harmonic lattice including an impurity atom. The Hamiltonian of our system is given by

$$H = \sum_{j=0}^{N} \left(\frac{p_j^2}{2m_j} + \frac{1}{2} k'_j x_j^2 \right) + \sum_{j=0}^{N} \frac{k}{2} (x_{j+1} - x_j)^2 \tag{3.1}$$

where x_j and p_j are the displacement and the canonical conjugate momentum of the jth atom, respectively. The impurity atom is labelled by $j = 0$. We require the periodic boundary condition and assume that $x_{N+1} \equiv x_0$ and $x_{-1} \equiv x_N$. We denote the masses of the impurity and the host atoms by M and m: $m_0 = M$, $m_1 = m_2 = \ldots = m_N = m$, and the coupling constants of the impurity and the host atoms to their respective equilibrium positions by K' and k': $k'_0 = K'$, $k'_1 = k'_2 = \ldots = k'_N = k'$. The parameters K' and k' are real and non-negative. The coupling constant k between the neighbouring atoms is a positive constant. The equation of motion for the jth atom is written as

$$m_j \ddot{x}_j(t) = k x_{j+1}(t) - (2k + k'_j) x_j(t) + k x_{j-1}(t) \tag{3.2}$$

where $x_{-1}(t)$ appearing in the equation for $j = 0$ represents $x_N(t)$ as noticed above.

Since we are interested in the velocity autocorrelation function for the impurity atom, the product of equation (3.2) with $\dot{x}_0(0)$ is averaged in the canonical ensemble:

$$\begin{aligned} m_j \langle \ddot{x}_j(t), \dot{x}_0(0) \rangle = {} & k \langle x_{j+1}(t), \dot{x}_0(0) \rangle - (2k + k'_j) \langle x_j(t), \dot{x}_0(0) \rangle \\ & + k \langle x_{j-1}(t), \dot{x}_0(0) \rangle. \end{aligned} \tag{3.3}$$

Here and in the following, the correlation function $\langle A, B \rangle$ represents the canonical average of the product AB. By taking the Laplace transform, one obtains the following set of linear equations:

$$\begin{aligned} & m_j z \langle \dot{x}_j, \dot{x}_0 \rangle_z + (2k + k'_j) \frac{1}{z} \langle \dot{x}_j, \dot{x}_0 \rangle_z - \frac{k}{z} \langle \dot{x}_{j+1}, \dot{x}_0 \rangle_z - \frac{k}{z} \langle \dot{x}_{j-1}, \dot{x}_0 \rangle_z \\ & \quad = k_B T \delta_{j0} \qquad j = 0, 1, 2, \ldots, N. \end{aligned} \tag{3.4}$$

In the matrix form, this set of equations is written as

$$\mathbf{M}_N(z; M, K') \begin{pmatrix} \langle \dot{x}_0, \dot{x}_0 \rangle_z \\ \langle \dot{x}_1, \dot{x}_0 \rangle_z \\ \langle \dot{x}_2, \dot{x}_0 \rangle_z \\ \vdots \\ \langle \dot{x}_N, \dot{x}_0 \rangle_z \end{pmatrix} = \begin{pmatrix} z k_B T / m \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{3.5}$$

where $\mathbf{M}_N(z; M, K')$ is the following matrix of order $N+1$:

$$\mathbf{M}_N(z;M,K') = \begin{pmatrix} \frac{M}{m}z^2+\frac{2k+K'}{m} & -\frac{k}{m} & 0 & \cdots & 0 & -\frac{k}{m} \\ -\frac{k}{m} & z^2+\frac{2k+k'}{m} & -\frac{k}{m} & \cdots & 0 & 0 \\ 0 & -\frac{k}{m} & z^2+\frac{2k+k'}{m} & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -\frac{k}{m} & 0 & 0 & \cdots & -\frac{k}{m} & z^2+\frac{2k+k'}{m} \end{pmatrix}. \tag{3.6}$$

One can easily show that the Laplace transform of the velocity autocorrelation function $\langle \dot{x}_0, \dot{x}_0 \rangle_z$ is solved in the following form:

$$\langle \dot{x}_0, \dot{x}_0 \rangle_z = \frac{2k_BT}{m} D_N \left\{ \left(\frac{M}{m}z^2+\frac{2k+K'}{m} \right) D_N - 2\left(\frac{k}{m}\right)^2 D_{N-1} - 2\left(\frac{k}{m}\right)^{N+1} \right\}^{-1} \tag{3.7}$$

where D_n is the determinant of order n defined by

$$D_n = \begin{vmatrix} z^2+\frac{2k+k'}{m} & -\frac{k}{m} & 0 & \cdots & 0 & 0 \\ -\frac{k}{m} & z^2+\frac{2k+k'}{m} & -\frac{k}{m} & \cdots & 0 & 0 \\ 0 & -\frac{k}{m} & z^2+\frac{2k+k'}{m} & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & z^2+\frac{2k+k'}{m} & -\frac{k}{m} \\ 0 & 0 & 0 & \cdots & -\frac{k}{m} & z^2+\frac{2k+k'}{m} \end{vmatrix}. \tag{3.8}$$

We shall introduce the resolvent matrix $\mathbf{R}_N(z)$ for the uniform system by

$$\mathbf{M}_N(z;m,k')\mathbf{R}_N(z) = \mathbf{1} \tag{3.9}$$

where $\mathbf{1}$ on the right hand side is the unit matrix. Since $\mathbf{M}_N(z;m,k')$ is a cyclic matrix, so is $\mathbf{R}_N(z)$. We denote the (i,j) element of $\mathbf{R}_N(z)$ as $R_N(z,i-j)$. The $(0,0)$ element is readily obtained by comparing equations (3.5) and (3.9). In place of (3.7), one has

$$R_N(z,0) = D_N \left\{ \left(z^2+\frac{2k+k'}{m} \right) D_N - 2\left(\frac{k}{m}\right)^2 D_{N-1} - 2\left(\frac{k}{m}\right)^{N+1} \right\}^{-1}. \tag{3.10}$$

In terms of this element of the resolvent, (3.7) is expressed as follows:

$$\langle \dot{x}_0, \dot{x}_0 \rangle_z = \frac{zk_BT}{m}\left\{\left(\frac{M}{m}-1\right)z^2+\frac{K'-k'}{m}+\frac{1}{R_N(z,0)}\right\}^{-1}. \tag{3.11}$$

Comparison of (3.7) and (3.11) with equation (2.7) leads to the result that Γ_z must be given by

$$\Gamma_z = -\frac{m}{M}z+\frac{K'-k'}{M}\frac{1}{z}+\frac{m}{MzR_N(z,0)}. \tag{3.12}$$

The elements of the resolvent $\mathbf{R}_N(z)$ of the cyclic matrix $\mathbf{M}_N(z; m, k')$ are well known to have the form:

$$R_N(z,l) = \frac{1}{N+1}\sum_{n=0}^{N}\cos\left(\frac{nl}{N+1}2\pi\right)\left\{z^2+\frac{2k+k'}{m}-\frac{2k}{m}\cos\left(\frac{n}{N+1}2\pi\right)\right\}^{-1}. \tag{3.13}$$

We check the condition (2.5) for (3.12), and then we find that

$$\lim_{z\to 0^+} z\Gamma_z \begin{cases} > 0 & \text{if } k' > 0 \text{ or } K' > 0 \\ = 0 & \text{if } k' = K' = 0. \end{cases} \tag{3.14}$$

Thus if $k' > 0$ or $K' > 0$, (2.5) is not satisfied and hence (2.1) is not derived for the one dimensional lattice of finite length. For this case, $\Gamma_z \to \infty$ as $z \to 0$ and hence D given by (2.8) is zero. This shows that if the impurity atom or the other particles are coupled to fixed points, the impurity atom cannot diffuse.

If $k' = K' = 0$, $\Gamma_z \sim Nmz/M \to 0$ $(z \to 0)$ and hence $D = \infty$. This behaviour is a consequence of the zero frequency mode which occurs when the periodic boundary condition is adopted. That mode represents the free rotation of the ring of coupled atoms. When one adopted the fixed boundary condition and assumed

$$x_{N/2}(t) = x_{-N/2}(t) \equiv 0$$

one would have no zero frequency mode and $\lim_{z\to 0^+} z\Gamma_z > 0$ and $D = 0$.

4. Limit as $N \to \infty$

In the limit when $N \to \infty$, the resolvent tends to the value at the origin of the lattice Green function $G_1(\omega; 0)$ as follows:

$$\lim_{N\to\infty} R_N(z,0) = G_1\left(z^2+\frac{2k+k'}{m}; 0\right) \tag{4.1}$$

where

$$G_1(\omega;0) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx\left(\omega-\frac{2k}{m}\cos x\right)^{-1} = \left\{\omega^2-4\left(\frac{k}{m}\right)^2\right\}^{-1/2}. \tag{4.2}$$

Substituting (4.1) with (4.2) into (3.11) and (3.12), one derives the following limiting

forms for the Laplace transforms of the velocity autocorrelation function and the friction function:

$$\langle \dot{x}_0, \dot{x}_0 \rangle_z = \frac{zk_BT}{m}\left[\left(\frac{M}{m}-1\right)z^2+\frac{K'-k'}{m}+\left\{\left(z^2+\frac{2k+k'}{m}\right)^2-\frac{4k^2}{m^2}\right\}^{1/2}\right]^{-1} \tag{4.3}$$

$$\Gamma_z = \frac{K'-k'}{zM}+\frac{m}{zM}\left[\left\{\left(z^2+\frac{2k+k'}{m}\right)^2-\frac{4k^2}{m^2}\right\}^{1/2}-z^2\right]. \tag{4.4}$$

We check (2.5) for the present case:

$$\lim_{z\to 0^+} z\Gamma_z \begin{cases} > 0 & \text{if } k' > 0 \text{ or } K' > 0 \\ = 0 & \text{if } k' = K' = 0. \end{cases} \tag{4.5}$$

This shows that if $k' > 0$ or $K' > 0$, (2.1) is not derived. If $k' = K' = 0$, we have to check (2.3) and (2.6). From (4.4) we see that (2.6) is satisfied and hence the Laplace inverse transform $\Gamma(t)$ of (4.4) must decay to zero as $t \to \infty$. In fact, it is given by

$$\Gamma(t) = \frac{2k}{M}\frac{J_1(2t\sqrt{(k/m)})}{t\sqrt{(k/m)}}. \tag{4.6}$$

Thus we confirm that (2.1) is derived for this system as $N \to \infty$.

If $k' > 0$ or $K' > 0$, D given by (2.8) is zero. This result corresponds to the physical situation that the diffusive motion cannot occur when the particles are bound to some fixed point.

If $k' = K' = 0$, Γ_z at $z = 0$ is finite and the diffusion constant D is given by

$$D = \frac{k_BT}{2\sqrt{(km)}}. \tag{4.7}$$

It should be noted that the free rotational mode which results in $D = \infty$ for the finite system is not serious for the infinite system and we obtain a finite value of D. The Laplace inverse transform of (4.3) for this case was given by Rubin (1961) and Nakazawa (1966) for the cases of $M/m = 1$ and 2 in a closed form. These authors gave the following asymptotic behaviour for the general case:

$$\langle \dot{x}_0(t), \dot{x}_0(0) \rangle = \frac{k_BT}{M}\left\{\frac{1-r}{1-2r}\exp(-\alpha t)-\frac{r}{(1-r)^2}\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{(\omega_0 t)^{3/2}}\right.$$
$$\left.\times \sin\left(\omega_0 t-\frac{\pi}{4}\right)+rO\left(\frac{1}{(\omega_0 t)^{5/2}}\right)\right\} \qquad t \gg \frac{1}{\omega_0} \tag{4.8}$$

where $r = m/M$, $\alpha = \omega_0 r/(1-2r)^{1/2}$ and $\omega_0 = 2(k/m)^{1/2}$.

5. Two and three dimensional lattices

The problems of the two and three dimensional lattice with one impurity atom are also solved without difficulty (see eg Rubin 1960, 1961). The result for Γ_z is

$$\Gamma_z = \frac{K'-k'}{zM}+\frac{m}{zM}\left(G_d\left(z^2+\frac{2dk+k'}{m};0\right)^{-1}-z^2\right) \tag{5.1}$$

where $G_2(\omega;0)$ and $G_3(\omega;0)$ are the values at the origin of the lattice Green functions for the square and cubic lattices:

$$G_2(\omega;0) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \left(\omega - \frac{2k}{m}(\cos x + \cos y)\right)^{-1}$$
$$= \frac{2}{\pi\omega} K\left(\frac{4k/m}{\omega}\right) \tag{5.2}$$

$$G_3(\omega;0) = \frac{1}{(2\pi)^3}\int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \int_{-\pi}^{\pi} dz \left(\omega - \frac{2k}{m}(\cos x + \cos y + \cos z)\right)^{-1}$$
$$= \frac{1}{\pi^2}\int_0^{\pi} dx\, 2\left(\omega - \frac{2k}{m}\cos x\right)^{-1} K\left(\frac{4k/m}{\omega - (2k\cos x/m)}\right) \tag{5.3}$$

where $K(k)$ is the complete elliptic integral of the first kind:

$$K(k) = \int_0^{\pi/2} \frac{d\theta}{(1-k^2\sin^2\theta)^{1/2}}.$$

From the behaviour of $G_d(\omega;0)$ at $\omega \simeq 2dk/m$, we know that

$$G_d\left(z^2 + \frac{2dk+k'}{m};0\right) \simeq \begin{cases} \left(z^2 + \dfrac{k'}{m}\right)^{-1/2} & d = 1 \\ \ln\left(z^2 + \dfrac{k'}{m}\right) & d = 2 \\ \text{finite constant} & d = 3. \end{cases} \tag{5.4}$$

In all the cases, if $k' > 0$ or $K' > 0$

$$\lim_{z\to 0+} z\Gamma_z > 0 \tag{5.5}$$

and

$$D = 0. \tag{5.6}$$

If $k' = K' = 0$

$$\lim_{z\to 0+} z\Gamma_z = \begin{cases} 0 & d = 2 \\ \text{finite constant} & d = 3 \end{cases} \tag{5.7}$$

and

$$D = 0 \qquad \text{for } d = 2 \text{ or } d = 3. \tag{5.8}$$

For $k' = K' = 0$, $d = 2$, $\Gamma(t)$ is given by

$$\Gamma(t) \sim \frac{ke\sqrt{(2\pi)}}{M \ln t} \qquad \text{as } t \to \infty. \tag{5.9}$$

Equation (5.5) shows that condition (2.5) is not satisfied if $k' > 0$ or $K' > 0$ both for the two and the three dimensional lattices. Equation (5.7) shows that the condition (2.6) is not satisfied even when $k' = K' = 0$ for the three dimensional lattice. For the two dimensional lattice, if $k' = K' = 0$, (5.4) shows that Γ_z diverges as $z \to 0$ and condition (2.6) is not satisfied; this is a consequence of the very slow decay of $\Gamma(t)$ as given by

(5.9). Because of this behaviour of $\Gamma(t)$, we cannot conclude that the integral on the right hand side of (2.1) is meaningful, and hence the stationary generalized Langevin equation will not be applicable to this case.

6. Conclusions

A harmonic lattice including an impurity atom is considered and the behaviour of the impurity atom is investigated in the framework of the generalized Langevin equation. With the aid of the exact expressions for the Laplace transforms of the velocity autocorrelation function and the friction function for the impurity atom, we conclude that diffusive motion can occur only for the impurity atom in the one dimensional lattice when atoms are not bound to fixed points. For this case, the friction function $\Gamma(t)$ decays rapidly to zero in the limit of $t \to \infty$, and the stationary generalized Langevin equation is seen to be applicable. In the two dimensional lattice, if the atoms are not bound to fixed points, $\Gamma(t)$ decays to zero but the decay is so slow that the stationary generalized Langevin equation is considered not to be applicable; the diffusion constant D for the impurity atom is zero for this system. In the three dimensional case, $\Gamma(t)$ does not decay and $D = 0$, and the stationary generalized Langevin equation cannot be applicable. The simple model gives an example for which the fast decay of the friction function $\Gamma(t)$ is physically significant in describing the diffusive motion of a variable.

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