Friction coefficient of adatoms on metal surfaces at low temperatures

Ayao Okiji and Hideaki Kasai
Department of Applied Physics, Osaka University, Suita, Osaka 565, Japan
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The friction coefficient of adatoms on metal surfaces is investigated with the aid of the Newns-Anderson model. In particular, its temperature dependence is clarified on the basis of the local Fermi-liquid theory at low temperatures. It is shown that the friction coefficient strongly depends on the temperature as well as on the magnetic field.

I. INTRODUCTION

The friction coefficient is one of the fundamental quantities which characterize dynamical processes of particles on solid surfaces such as adsorption, desorption, scattering, diffusion, and catalysis. For instance, in Kramers's description[1] of chemical reactions as a Brownian motion of the reacting species, which can be applied to the desorption and the diffusion processes, it has been shown that the reaction rate strongly depends on the friction coefficient of the reacting species. In the process of adsorption the moving particle loses its kinetic energy, because it experiences a friction force, and is captured in the potential well near the surface if the energy loss exceeds the initial kinetic energy. In general, the friction force may result from the creation of phonons and the electronic fluctuation. At low temperatures, however, the friction force for adatoms on metal surfaces results mainly from the electronic fluctuation.[2]

With the aid of the Newns-Anderson model the friction coefficient of adatoms on metal surfaces has been investigated by several authors.[2-7] In particular, the case without the electron correlation has been discussed thoroughly by Nourtier[4] and subsequently with the use of an approximate method the electron correlation effect has been investigated by Yoshimori and Motchane.[6] In the previous paper[7] with the use of the Bethe-ansatz solution for the Anderson model[8] the friction coefficient has been calculated as a function of the magnetic field at the absolute zero of temperature. It has been shown that the friction coefficient strongly depends on the magnetic field.

The main purpose of the present paper is to investigate the temperature dependence of the friction coefficient on the basis of the local Fermi-liquid theory.[9-12] The analytic expression for the friction coefficient as a function of the magnetic field is also given at the absolute zero of temperature.

In the next section the model Hamiltonian and the expression for the friction coefficient are given. It is shown in Sec. III that the vertex part of the expression can be written in terms of the Green function of the adatom and its self-energy up to second order of the temperature. In light of the present understanding of the Green function and its self-energy the friction coefficient is evaluated in Sec. IV. Summary and discussions are given in the last section.

II. FRICTION COEFFICIENT

The Hamiltonian of the system we investigate is given by

$$H_A=\sum_{k,\sigma}\varepsilon_k n_{k\sigma}+\varepsilon_d\sum_{\sigma}n_{d\sigma}+\sum_{k,\sigma}(V_k C_{k\sigma}^\dagger C_{d\sigma}+\text{H.c.})+U n_{d\uparrow}n_{d\downarrow}\ , \tag{2.1}$$

where $C_{k\sigma}^\dagger$ ($C_{d\sigma}^\dagger$) is the electron creation operator for the state $|k\rangle$ with spin σ and energy ε_k of the conduction electron in the metal (for the orbital $|d\rangle$ of the adatom with spin σ and energy ε_d), $n=C^\dagger C$, and V_k is the matrix element of hybridization between the conduction electron and the electron on the adatom, which we assume to be real. The last term represents the intra-atomic Coulomb interaction for two electrons on the adatom.

The friction coefficient η is given in terms of the force correlation function as[2]

$$\eta=\frac{1}{MT}\text{Re}\int_0^\infty\langle\hat F\hat F(r)\rangle dt\ , \tag{2.2}$$

where M is the mass of the adatom, T the temperature in the unit of $k_B=1$, $\langle\ \rangle$ denotes the thermal average, and $\hat F$ is the fluctuating force defined by $\hat F=F-\langle F\rangle$. Here a one-dimensional system is assumed for the motion of the adatom. Following Bohnen *et al.*[3] we may take F as

$$F=\sum_{k,\sigma}W_k(C_{k\sigma}^\dagger C_{d\sigma}+C_{d\sigma}^\dagger C_{k\sigma}) \tag{2.3}$$

and

$$W_k=-\frac{\partial V_k}{\partial X}\ , \tag{2.4}$$

where X is the coordinate of the adatom. For simplicity we assume that ε_d and U are independent of X.

Using the Fourier transform of the two-particle temperature Green function and expressing it in terms of the one-particle Green functions and the vertex functions, we can express η as[6]

$$\eta=\eta_{(1,1)}+\eta_{(2,1)}+\eta_{(2,2)}\ , \tag{2.5}$$

$$\eta_{(l,j)}=-\frac{1}{M}\lim_{\nu\to 0+}\text{Im}\frac{\partial Q_{(l,j)}(i\nu)}{\partial i\nu}\ , \tag{2.6}$$

$$Q_{(1,1)}(i\nu)=T\sum_{\omega,\sigma}G^{\sigma}(i\omega)[\xi^{\sigma}(i\omega)+\xi^{\sigma}(i\omega+i\nu)] , \quad (2.7)$$

$$Q_{(2,1)}(i\nu)=T\sum_{\omega,\sigma}g^{\sigma}(i\omega+i\nu,i\omega)[A^{\sigma}(i\omega+i\nu,i\omega)]^2 , \quad (2.8)$$

and

$$Q_{(2,2)}(i\nu)=T\sum_{\omega,\sigma}A^{\sigma}(i\omega+i\nu,i\omega)g^{\sigma}(i\omega+i\nu,i\omega)\times L_1^{\sigma}(i\omega+i\nu,i\omega) . \quad (2.9)$$

Here $G^{\sigma}(i\omega)$ is the Fourier transform of the one-particle temperature Green function of the adatom with $\omega=(2n+1)\pi T$ (n integer) and $g^{\sigma}(i\omega+i\nu,i\omega)=G^{\sigma}(i\omega)G^{\sigma}(i\omega+i\nu)$ with $\nu=2n\pi T$. The quantities $\xi^{\sigma}(i\omega)$, $A^{\sigma}(i\omega+i\nu,i\omega)$, and $L_1^{\sigma}(i\omega+i\nu,i\omega)$ are defined by

$$\xi^{\sigma}(i\omega)=\sum_k \frac{W_k^2}{i\omega-\varepsilon_k^{\sigma}} , \quad (2.10)$$

$$A^{\sigma}(i\omega+i\nu,i\omega)=\zeta^{\sigma}(i\omega)+\zeta^{\sigma}(i\omega+i\nu) , \quad (2.11)$$

$$\zeta^{\sigma}(i\omega)=\sum_k \frac{V_k W_k}{i\omega-\varepsilon_k^{\sigma}} , \quad (2.12)$$

and

$$L_1^{\sigma}(i\omega+i\nu,i\omega)=T\sum_{\omega',\sigma'}\Gamma_{\sigma\sigma';\sigma'\sigma}(i\omega+i\nu,i\omega';i\omega'+i\nu,i\omega)\times g^{\sigma'}(i\omega'+i\nu,i\omega')\times A^{\sigma'}(i\omega'+i\nu,i\omega') , \quad (2.13)$$

where $\varepsilon_k^{\uparrow}=\varepsilon_k-g\mu_B H$, $\varepsilon_k^{\downarrow}=\varepsilon_k+g\mu_B H$ (H is the magnetic field) and $\Gamma_{\sigma\sigma';\sigma'\sigma}(i\omega+i\nu,i\omega';i\omega'+i\nu,i\omega)$ is the total vertex function.

Using the usual contour-integral method, we can obtain

$$\eta_{(1,1)}=\frac{2}{\pi M}\sum_{\sigma}\int_{-\infty}^{\infty}d\varepsilon\left[-\frac{df}{d\varepsilon}\right]\mathrm{Im}G^{\sigma}(\varepsilon+i0^+)\times\mathrm{Im}\xi^{\sigma}(\varepsilon+i0^+) \quad (2.14)$$

and

$$\eta_{(2,1)}=\frac{2}{\pi M}\sum_{\sigma}\int_{-\infty}^{\infty}d\varepsilon\left[-\frac{df}{d\varepsilon}\right](\mathrm{Im}G^{\sigma}(\varepsilon+i0^+)\mathrm{Im}[G^{\sigma}(\varepsilon+i0^+)\zeta^{\sigma}(\varepsilon+i0^+)^2]+\{\mathrm{Im}[G^{\sigma}(\varepsilon+i0^+)\zeta^{\sigma}(\varepsilon+i0^+)]\}^2) , \quad (2.15)$$

where

$$G^{\sigma}(\varepsilon+i0^+)=[\varepsilon+i0^+-\varepsilon_d^{\sigma}-B^{\sigma}(\varepsilon+i0^+)-\Sigma^{\sigma}(\varepsilon+i0^+)]^{-1} , \quad (2.16)$$

$$\xi^{\sigma}(\varepsilon+i0^+)=\int_{-\infty}^{\infty}d\varepsilon'\frac{\rho(\varepsilon')}{\varepsilon+i0^+-\varepsilon'}\langle W_k^2\rangle_{\varepsilon'}^{\sigma} , \quad (2.17)$$

$$\zeta^{\sigma}(\varepsilon+i0^+)=\int_{-\infty}^{\infty}d\varepsilon'\frac{\rho(\varepsilon')}{\varepsilon+i0^+-\varepsilon'}\langle V_k W_k\rangle_{\varepsilon'}^{\sigma} , \quad (2.18)$$

and

$$B^{\sigma}(\varepsilon+i0^+)=\int_{-\infty}^{\infty}d\varepsilon'\frac{\rho(\varepsilon')}{\varepsilon+i0^+-\varepsilon'}\langle V_k^2\rangle_{\varepsilon'}^{\sigma} . \quad (2.19)$$

Here $f(\varepsilon)$ is the Fermi distribution function, $\varepsilon_d^{\uparrow}=\varepsilon_d-g\mu_B H$ ($\varepsilon_d^{\downarrow}=\varepsilon_d+g\mu_B H$), and $\Sigma^{\sigma}(\varepsilon+i0^+)$ the self-energy. The quantities $\langle W_k^2\rangle_{\varepsilon}^{\sigma}$, $\langle V_k W_k\rangle_{\varepsilon}^{\sigma}$, and $\langle V_k^2\rangle_{\varepsilon}^{\sigma}$ denote the averages of W_k^2, $V_k W_k$, and V_k^2 on the energy contour $\varepsilon_k^{\sigma}=\varepsilon$, respectively, and $\rho(\varepsilon)$ is the density of states of the conduction electrons in the semi-infinite metal. Since $\eta_{(2,2)}$, contains the vertex functions, the separate treatments are necessary in order to derive the simple expression in terms of the self-energy and the Green function of the adatom (see the next section). The above expressions for $\eta_{(1,1)}$ and $\eta_{(2,1)}$ have been derived by Yoshimori and Motchane[6] and the temperature dependence of $\eta_{(1,1)}$ has been investigated in the absence of the magnetic field. The temperature dependences of $\eta_{(2,1)}$ and $\eta_{(2,2)}$ are investigated at low temperatures in Sec. IV, where it is shown that the main contribution to η is made by $\eta_{(2,2)}$ and that the value of $\eta_{(1,1)}$ is almost canceled out by that of $\eta_{(2,1)}$.

III. EXPRESSION FOR $\eta_{(2,2)}$ AT LOW TEMPERATURES

In this section it is shown that $\eta_{(2,2)}$ defined by (2.6) and (2.9) can be written in terms of the Green function of the adatom and its self-energy up to T^2 on the basis of the local Fermi-liquid theory.[9-12] In order to calculate (2.9) it is convenient to use the following expansion for a discrete sum of a function $S(i\omega+i\nu,i\omega)$ over $\omega=(2n+1)\pi T$ (n integer) which has singularities at $\omega=0$ and $\omega+\nu=0$:

$$T\sum_{\omega}S(i\omega+i\nu,i\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\,S(i\omega+i\nu,i\omega)+\frac{1}{2\pi}\frac{(\pi T)^2}{6}\times\left[\left[\frac{\partial}{\partial\omega}S(i\omega+i\nu,i\omega)\right]_{\omega=0^-}^{\omega=0^+}+\left[\frac{\partial}{\partial\omega}S(i\omega+i\nu,i\omega)\right]_{\omega=-\nu+0^-}^{\omega=-\nu+0^+}\right]+\cdots , \quad (3.1)$$

where

$$\left[\frac{\partial}{\partial\omega}S(i\omega+i\nu,i\omega)\right]_{\omega=0^-}^{\omega=0^+}=\left[\frac{\partial}{\partial\omega}S(i\omega+i\nu,i\omega)\right]_{\omega=0^+}-\left[\frac{\partial}{\partial\omega}S(i\omega+i\nu,i\omega)\right]_{\omega=0^-}. \tag{3.2}$$

Using the relation (3.1) we can write down the expression for $Q_{(2,2)}(i\nu)$ as follows:

$$\begin{aligned}Q_{(2,2)}(i\nu)=&\sum_{\sigma,\sigma'}\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}d\omega\int_{-\infty}^{\infty}d\omega'\,A^{\sigma}(i\omega+i\nu,i\omega)g^{\sigma}(i\omega+i\nu,i\omega)\Gamma_{\sigma\sigma'}(i\omega,i\omega';i\nu)g^{\sigma'}(i\omega'+i\nu,i\omega')A^{\sigma'}(i\omega'+i\nu,i\omega')\\&+\sum_{\sigma,\sigma'}\frac{1}{(2\pi)^2}\frac{(\pi T)^2}{6}\int_{-\infty}^{\infty}d\omega\,A^{\sigma}(i\omega+i\nu,i\omega)g^{\sigma}(i\omega+i\nu,i\omega)\\&\quad\times\left[\left[\frac{\partial}{\partial\omega'}\Gamma_{\sigma\sigma'}(i\omega,i\omega';i\nu)g^{\sigma}(i\omega'+i\nu,i\omega')A^{\sigma'}(i\omega'+i\nu,i\omega')\right]_{\omega'=0^-}^{\omega'=0^+}\right.\\&\quad\left.+\left[\frac{\partial}{\partial\omega'}\Gamma_{\sigma\sigma'}(i\omega,i\omega';i\nu)g^{\sigma'}(i\omega'+i\nu,i\omega')A^{\sigma'}(i\omega'+i\nu,i\omega')\right]_{\omega'=-\nu+0^-}^{\omega'=-\nu+0^+}\right]\\&+\sum_{\sigma,\sigma'}\frac{1}{(2\pi)^2}\frac{(\pi T)^2}{6}\int_{-\infty}^{\infty}d\omega'\,A^{\sigma'}(i\omega'+i\nu,i\omega')g^{\sigma'}(i\omega'+i\nu,i\omega')\\&\quad\times\left[\left[\frac{\partial}{\partial\omega}A^{\sigma}(i\omega+i\nu,i\omega)g^{\sigma}(i\omega+i\nu,i\omega)\Gamma_{\sigma\sigma'}(i\omega,i\omega';i\nu)\right]_{\omega=0^-}^{\omega=0^+}\right.\\&\quad\left.+\left[\frac{\partial}{\partial\omega}A^{\sigma}(i\omega+i\nu,i\omega)g^{\sigma}(i\omega+i\nu,i\omega)\Gamma_{\sigma\sigma'}(i\omega,i\omega';i\nu)\right]_{\omega=-\nu+0^-}^{\omega=-\nu+0^+}\right]+\cdots,\end{aligned} \tag{3.3}$$

where $\Gamma_{\sigma\sigma'}(i\omega,i\omega',i\nu)$ is the abbreviation of $\Gamma_{\sigma\sigma';\sigma'\sigma}(i\omega+i\nu,i\omega';i\omega'+i\nu,i\omega)$. The derivative of the above expression with respect to ν, whose imaginary part gives $\eta_{(2,2)}$ in the limit of $\nu\to 0+$, can be calculated in the following way. First we express the total vertex function $\Gamma_{\sigma\sigma'}(i\omega,i\omega';i\nu)$ included in (3.3) in terms of the proper vertex function $\Gamma^0_{\sigma\sigma'}(i\omega,i\omega',i\nu)$ and the one-particle Green function using the Dyson equation

$$\Gamma_{\sigma\sigma'}(i\omega,i\omega',i\nu)=\Gamma^0_{\sigma\sigma'}(i\omega,i\omega';i\nu)+T\sum_{\omega'',\sigma''}\Gamma^0_{\sigma\sigma''}(i\omega,i\omega'';i\nu)g^{\sigma''}(i\omega''+i\nu,i\omega'')\Gamma_{\sigma''\sigma'}(i\omega'',i\omega',i\nu). \tag{3.4}$$

Secondly with regards to the positions of singularities, we expand the discrete sum over ω'', ω''', and so on appearing in the expression up to T^2 using the relation (3.1). Then taking the derivative of the obtained expression with respect to ν,[13] we can derive the following expression up to T^2:

$$\begin{aligned}\frac{\partial Q_{(2,2)}(i\nu)}{\partial i\nu}=&\sum_{\sigma}\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\,G^{\sigma}(i\omega)\left[\frac{\partial G^{\sigma}(i\omega+i\nu)\zeta^{\sigma}(i\omega+i\nu)}{\partial i\nu}+\zeta^{\sigma}(i\omega)\frac{G^{\sigma}(i\omega+i\nu)}{\partial i\nu}\right]\\&\quad\times[L_1^{\sigma}(i\omega+i\nu,i\omega)+L_2^{\sigma}(i\omega+i\nu,i\omega)]\\&+\sum_{\sigma}\frac{1}{2\pi}\frac{(\pi T)^2}{6}\left\{\left[\frac{\partial}{\partial\omega}G^{\sigma}(i\omega)\left[\frac{\partial G^{\sigma}(i\omega+i\nu)\zeta^{\sigma}(i\omega+i\nu)}{\partial i\nu}+\zeta^{\sigma}(i\omega)\frac{\partial G^{\sigma}(i\omega+i\nu)}{\partial i\nu}\right]\right.\right.\\&\quad\left.\times[L_1^{\sigma}(i\omega+i\nu,i\omega)+L_2^{\sigma}(i\omega+i\nu,i\omega)]\right]_{\omega=0^-}^{\omega=0^+}\\&\quad+\left[\frac{\partial}{\partial\omega}G^{\sigma}(i\omega)\left[\frac{\partial G^{\sigma}(i\omega+i\nu)\zeta^{\sigma}(i\omega+i\nu)}{\partial i\nu}+\zeta^{\sigma}(i\omega)\frac{\partial G^{\sigma}(i\omega+i\nu)}{\partial i\nu}\right]\right.\\&\quad\left.\times[L_1^{\sigma}(i\omega+i\nu,i\omega)+L_2^{\sigma}(i\omega+i\nu,i\omega)]\right]_{\omega=-\nu+0^-}^{\omega=-\nu+0^+}\\&\quad+\left[i\frac{\partial^2}{\partial\omega^2}A^{\sigma}(i\omega+i\nu,i\omega)g^{\sigma}(i\omega+i\nu,i\omega)\right.\\&\quad\left.\left.\times[L_1^{\sigma}(i\omega+i\nu,i\omega)+L_2^{\sigma}(i\omega+i\nu,i\omega)]\right]_{\omega=-\nu+0^-}^{\omega=-\nu+0^+}\right\}\end{aligned}$$

$$+\sum_\sigma \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, L_2^\sigma(i\omega+i\nu,i\omega)G^\sigma(i\omega)\frac{\partial G^\sigma(i\omega+i\nu)}{\partial i\nu}L_1^\sigma(i\omega+i\nu,i\omega)$$
$$+\sum_\sigma \frac{1}{2\pi}\frac{(\pi T)^2}{6}\left[\left[\frac{\partial}{\partial\omega}L_2^\sigma(i\omega+i\nu,i\omega)G^\sigma(i\omega)\frac{\partial G^\sigma(i\omega+i\nu)}{\partial i\nu}L_1^\sigma(i\omega+i\nu,i\omega)\right]_{\omega=0^-}^{\omega=0^+}\right.$$
$$+\left[\frac{\partial}{\partial\omega}L_2^\sigma(i\omega+i\nu,i\omega)G^\sigma(i\omega)\frac{\partial G^\sigma(i\omega+i\nu)}{\partial i\nu}L_1^\sigma(i\omega+i\nu,i\omega)\right]_{\omega=-\nu+0^-}^{\omega=-\nu+0^+}$$
$$\left.+\left[i\frac{\partial^2}{\partial\omega^2}L_2^\sigma(i\omega+i\nu,i\omega)g^\sigma(i\omega+i\nu,i\omega)L_1^\sigma(i\omega+i\nu,i\omega)\right]_{\omega=-\nu+0^-}^{\omega=-\nu+0^+}\right]+\cdots\,, \tag{3.5}$$

where

$$L_2^\sigma(i\omega+i\nu,i\omega)=T\sum_{\omega',\sigma'}\Gamma_{\sigma'\sigma}(i\omega',i\omega;i\nu)g^{\sigma'}(i\omega'+i\nu,i\omega')A^{\sigma'}(i\omega'+i\nu,i\omega')\,. \tag{3.6}$$

Finally we can write $\eta_{(2,2)}$ in terms of the Green function of the adatom and its self-energy as

$$\eta_{(2,2)}=-\frac{2}{\pi M}\sum_\sigma\left[\mathrm{Im}G^\sigma(i0^+)\frac{\partial\Sigma^\sigma(i0^+)}{\partial X}\mathrm{Im}G^\sigma(i0^+)\zeta^\sigma(i0^+)+\mathrm{Im}G^\sigma(i0^+)\zeta^\sigma(i0^+)\frac{\partial\Sigma^\sigma(i0^+)}{\partial X}\mathrm{Im}G^\sigma(i0^+)\right]$$
$$+\frac{1}{\pi M}\sum_\sigma \mathrm{Im}G^\sigma(i0^+)\mathrm{Im}G^\sigma(i0^+)\left[\frac{\partial\Sigma^\sigma(i0^+)}{\partial X}\right]^2$$
$$+\frac{1}{\pi M}\frac{(\pi T)^2}{6}\sum_\sigma\left[-\mathrm{Re}\left[\frac{\partial^2}{\partial\varepsilon^2}[\zeta^\sigma(\varepsilon+i0^+)+\zeta^\sigma(\varepsilon+i0^-)]G^\sigma(\varepsilon+i0^+)G^\sigma(\varepsilon+i0^-)\frac{\partial\Sigma^\sigma(\varepsilon+i0^-)}{\partial X}\right]_{\varepsilon=0}\right.$$
$$\left.+\mathrm{Re}\left[\frac{\partial^2}{\partial\varepsilon^2}[\zeta^\sigma(\varepsilon+i0^-)+\zeta^\sigma(\varepsilon+i0^-)]G^\sigma(\varepsilon+i0^-)G^\sigma(\varepsilon+i0^-)\frac{\partial\Sigma^\sigma(\varepsilon+i0^-)}{\partial X}\right]_{\varepsilon=0}\right]$$
$$+\frac{1}{2\pi M}\frac{(\pi T)^2}{6}\sum_\sigma\left\{\mathrm{Re}\left[\frac{\partial^2}{\partial\varepsilon^2}G^\sigma(\varepsilon+i0^+)G^\sigma(\varepsilon+i0^-)\left[\frac{\partial\Sigma^\sigma(\varepsilon+i0^-)}{\partial X}\right]^2\right]_{\varepsilon=0}\right.$$
$$\left.-\mathrm{Re}\left[\frac{\partial^2}{\partial\varepsilon^2}G^\sigma(\varepsilon+i0^-)G^\sigma(\varepsilon+i0^-)\left[\frac{\partial\Sigma^\sigma(\varepsilon+i0^-)}{\partial X}\right]^2\right]_{\varepsilon=0}\right\}\,. \tag{3.7}$$

Here we have used the Ward identity,[6]

$$L_1^\sigma(i\omega,i\omega)=L_2^\sigma(i\omega,i\omega)=-\frac{\partial\Sigma^\sigma(i\omega)}{\partial X} \tag{3.8}$$

and the following manipulations:

$$\lim_{\nu\to0+}\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\,G^\sigma(i\omega)\left[\frac{\partial G^\sigma(i\omega+i\nu)\zeta^\sigma(i\omega+i\nu)}{\partial i\nu}+\zeta^\sigma(i\omega)\frac{\partial G^\sigma(i\omega+i\nu)}{\partial i\nu}\right][L_1^\sigma(i\omega+i\nu,i\omega)+L_2^\sigma(i\omega+i\nu,i\omega)]$$
$$=-\frac{1}{\pi}\int_{-\infty}^{0}d\varepsilon\,\mathrm{Im}\left[4[G^\sigma(\varepsilon+i0^+)]^3\zeta^\sigma(\varepsilon+i0^+)\left[1-\frac{\partial B^\sigma(\varepsilon+i0^+)}{\partial\varepsilon}-\frac{\partial\Sigma^\sigma(\varepsilon+i0^+)}{\partial\varepsilon}\right]\frac{\partial\Sigma^\sigma(\varepsilon+i0^+)}{\partial X}\right.$$
$$\left.+2[G^\sigma(\varepsilon+i0^+)]^2\frac{\partial\zeta^\sigma(\varepsilon+i0^+)}{\partial\varepsilon}\frac{\partial\Sigma^\sigma(\varepsilon+i0^+)}{\partial X}\right]$$
$$-\frac{1}{\pi}\frac{\delta G^\sigma\zeta^\sigma}{i}G^\sigma(i0^-)\frac{\partial\Sigma^\sigma(i0^-)}{\partial X}-\frac{1}{\pi}\frac{\delta G^\sigma}{i}G^\sigma(i0^-)\zeta^\sigma(i0^-)\frac{\partial\Sigma^\sigma(i0^-)}{\partial X} \tag{3.9}$$

and

$$\lim_{\nu\to 0+}\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\, L_2^{\sigma}(i\omega+i\nu,i\omega)G^{\sigma}(i\omega)\frac{\partial G^{\sigma}(i\omega+i\nu)}{\partial i\nu}L_1^{\sigma}(i\omega+i\nu,i\omega)$$
$$=\frac{1}{2\pi}\frac{\delta G^{\sigma}}{i}G^{\sigma}(i0^-)\left[\frac{\partial\Sigma^{\sigma}(i0^-)}{\partial X}\right]^2$$
$$-\frac{1}{\pi}\int_{-\infty}^{0}d\varepsilon\,\mathrm{Im}\left[[G^{\sigma}(\varepsilon+i0^+)]^3\left[1-\frac{\partial B^{\sigma}(\varepsilon+i0^+)}{\partial\varepsilon}-\frac{\partial\Sigma^{\sigma}(\varepsilon+i0^+)}{\partial\varepsilon}\right]\left[\frac{\partial\Sigma^{\sigma}(\varepsilon+i0^+)}{\partial X}\right]^2\right], \tag{3.10}$$

where δG is defined by $\delta G=G(i0^+)-G(i0^-)$. The main results of the present section are the expression (3.7) for $\eta_{(2,2)}$ up to T^2. In the next section we evaluate $\eta_{(2,2)}$ together with $\eta_{(1,1)}$ and $\eta_{(2,1)}$ in light of the present understanding of the self-energy and the Green function of the adatom[11] and clarify the temperature dependence of η at low temperatures.

IV. TEMPERATURE DEPENDENCE OF η

When the k dependence of V_k is dropped and the density of states of the conduction electron is assumed to be constant, the quantities $B^{\sigma}(\varepsilon+i0^+)$, $\xi^{\sigma}(\varepsilon+i0^+)$ and $\zeta^{\sigma}(\varepsilon+i0^+)$ are independent of ε and are written by $-i\Delta$, $-i\xi$, and $-i\zeta$, respectively. Furthermore the self-energy around the Fermi level (chosen as the origin of energy) is known as[11]

$$\Sigma(\varepsilon+i0^+)=\frac{U}{2}-[\pi\Delta(\chi_s+\chi_c)-1]\varepsilon$$
$$-i\frac{\Delta}{2}\pi^2(\chi_s-\chi_c)^2(\varepsilon^2+\pi^2T^2)\ , \tag{4.1}$$

where $\Delta=\pi\rho V^2$ and χ_s (χ_c) is the magnetic (charge) susceptibility at $T=0$. Here we consider the symmetric case ($\varepsilon_d+U/2=0$) in the absence of the magnetic field. In this case we can use the analytic expressions for χ_s and χ_c which have been derived with the use of the exact solution for the Anderson model.[8] Substituting (4.1) into (3.7) we can derive $\eta_{(2,2)}$ as

$$\eta_{(2,2)}=\frac{4}{\pi M}\frac{\zeta^2}{\Delta^2}\left[\frac{2}{3}\left[\Delta\frac{\partial\chi_s}{\partial\Delta}+\Delta\frac{\partial\chi_c}{\partial\Delta}\right]^2-\tfrac{8}{3}(\chi_s-\chi_c)\left[\Delta\frac{\partial\chi_s}{\partial\Delta}-\Delta\frac{\partial\chi_c}{\partial\Delta}\right]+\tfrac{4}{3}\chi_s\chi_c-2\chi_s^2-2\chi_c^2\right]\pi^4T^2\ . \tag{4.2}$$

Similarly up to T^2, $\eta_{(1,1)}$ and $\eta_{(2,1)}$ are given by

$$\eta_{(1,1)}=\frac{4}{\pi M}\frac{\xi}{\Delta}[1-(\chi_s^2+\chi_c^2-\tfrac{2}{3}\chi_s\chi_c)\pi^4T^2] \tag{4.3}$$

and

$$\eta_{(2,1)}=\frac{4}{\pi M}\frac{\zeta^2}{\Delta^2}[-1+(\tfrac{7}{3}\chi_s^2+\tfrac{7}{3}\chi_c^2-\tfrac{2}{3}\chi_s\chi_c)\pi^4T^2]\ . \tag{4.4}$$

The summing up $\eta_{(l,j)}$ over l and j, we obtain the friction coefficient η as

$$\eta=\frac{4}{\pi M}\frac{\zeta^2}{\Delta^2}\left[\frac{2}{3}\left[\Delta\frac{2\chi_s}{\partial\Delta}+\frac{\partial\chi_c}{\partial\Delta}\right]^2-\tfrac{8}{3}(\chi_s-\chi_c)\left[\Delta\frac{\partial\chi_s}{\partial\Delta}-\Delta\frac{\partial\chi_c}{\partial\Delta}\right]-\tfrac{2}{3}(\chi_s-\chi_c)^2\right]\pi^4T^2\ , \tag{4.5}$$

where the relation $\xi/\Delta=\zeta^2/\Delta^2$ has been used. It is noted that the main contribution to η is made by $\eta_{(2,2)}$, which contains the derivatives of χ_s and χ_c with respect to Δ and brings a strong temperature dependence. The value of $\eta_{(1,1)}$ is almost canceled out by that of $\eta_{(2,1)}$ and hence they give a small contribution to η. In Fig. 1 we show the T^2 dependence of η. As the value of $U/2\Delta$ increases, the slope of η as a function of T^2 becomes steeper. In the so-called s-d limit ($\varepsilon_a+U/2=0$, U being large, $\chi_s\simeq 1/2\pi T_K$, and $\chi_c\simeq 0$), η can be written as

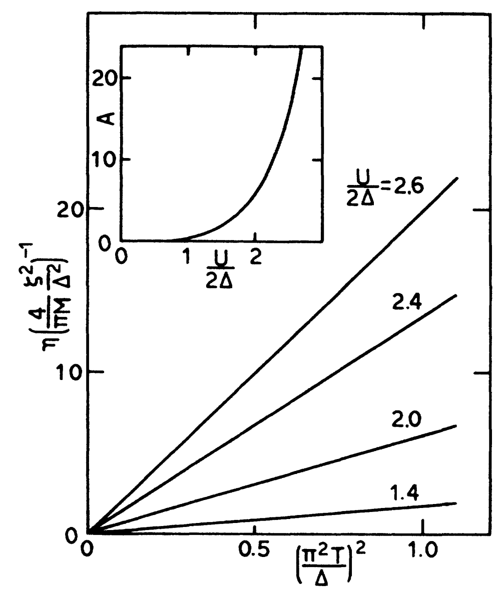

FIG. 1. The temperature dependence of the friction coefficient η at low temperatures for $U/2\Delta=1.4$, 2.0, 2.4, and 2.6. The inset shows A as a function of $U/2\Delta$, where A is defined by $\eta=(4/\pi M)(\zeta^2/\Delta^2)A(\pi^2T/\Delta)^2$. The value of A at $U/2\Delta=0$ is $2/3\pi^2$.

$$\eta=\frac{4}{\pi M}\frac{\zeta^2}{\Delta^2}\left[\frac{2}{3}\pi^2\left[\frac{\Delta}{T_K}\frac{dT_K}{d\Delta}\right]^2+\tfrac{8}{3}\pi^2\left[\frac{\Delta}{T_K}\frac{dT_K}{d\Delta}\right]-\tfrac{2}{3}\pi^2\right]\times\left[\frac{T}{2T_K}\right]^2, \quad (4.6)$$

where T_K is the Kondo temperature[8] defined by $T_K=(\sqrt{2U\Delta}/\pi)\exp(-\pi U/8\Delta)$. One can see that the main contribution to η comes from the first term in the bracket of the above expression, in this case.

As for the magnetic-field dependence of η at $T=0$ the numerical calculations have been made in the previous paper.[7] Using the exact solution[8] for the Anderson model we can also derive the analytic expression for η in the high as well as in the low magnetic field:

$$\eta=\frac{8}{\pi M}\frac{\zeta^2}{\Delta^2}\left[\frac{\Delta}{T_K}\frac{dT_K}{d\Delta}\right]^2\left[\frac{H}{2T_K}\right]^2 \quad \text{for } H \ll T_K \quad (4.7)$$

and

$$\eta=\frac{4}{\pi M}\frac{\zeta^2}{\Delta^2}\frac{\pi^2}{8}\left[\frac{\Delta}{T_K}\frac{dT_K}{d\Delta}\right]^2\left[\ln\frac{H}{T_H}\right]^{-4} \quad \text{for } H > T_H\ , \quad (4.8)$$

where T_H is defined by $T_H=\sqrt{2\pi/e}\,T_K$. It can be seen from the above expressions in addition to the previous results[7] that, as a function of H, η increases with H^2 dependence for $H \ll T_K$, reaches a maximum, and then decreases with $\ln H$ dependence for $H > T_H$.

V. SUMMARY AND DISCUSSIONS

The electronic contribution to the friction coefficient η of adatoms on metal surfaces is discussed along the approach by Bohnen *et al.*[3] On the basis of the local Fermi-liquid theory[9–12] the expression for η is derived at low temperatures. It turns out that η can be expressed in terms of the self-energy around the Fermi level, its derivative with respect to the coordinate of an adatom and the one-particle Green function of the adatom. It is shown that η increases strongly with T^2 dependence as T increases. The coefficient contains, in addition to χ_s and χ_c, their derivatives with respect to Δ and becomes very large when U is large as compared with Δ. At the absolute zero of temperature the localized electron on the adatom tightly couples with the conduction electrons. Hence the fluctuation of the force defined by the expression (2.3) scarcely occurs and η is practically zero. As the temperature increases, however, the coupling is relaxed. Then the fluctuation of the force may appear. Hence η takes finite values and increases rapidly due to the electron-correlation effect as the temperature increases. As for the behavior of η at high temperatures $(T > T_K)$ it seems to be difficult to investigate its temperature dependence. It may be necessary to introduce some kinds of approximations. We may, however, make the following conjecture. Since the temperature dependences of physical quantities such as the susceptibility and the electronic resistivity due to a magnetic impurity in dilute alloys described by the Anderson model are quite similar to their magnetic field dependences if the value of U is fairly large, and since it may be considered to be the case for η [see (4.6) and (4.7)], it may be said that η has a maximum and decreases with $\ln T$ dependence as the temperature increases at $T > T_K$.

As for the position dependence of η it can be considered as follows. When adatoms are moving in the surface layers (surface diffusion), a periodic X dependence may appear to η through a periodic X dependence of $V(X)$. If we take $V(X)=V_0\{1+\beta\cos[(2\pi/a)X]\}$, for instance, η shows the periodic behavior as shown in Fig. 2, where the quantities a and β are related to the lattice constant and the corrugation of the surface layer. The value of η becomes zero where $V(X)$ takes maximum as well as minimum values, and takes a maximum value in between.

On the other hand, when adatoms are moving along

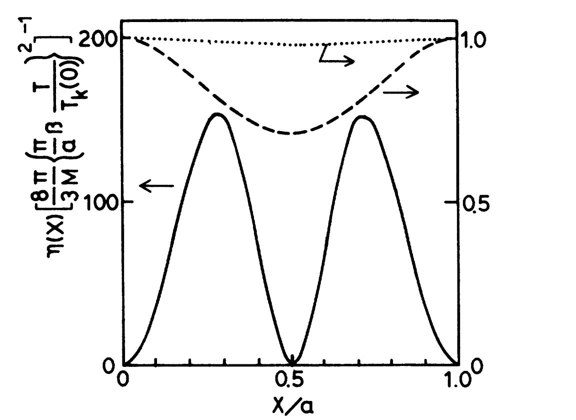

FIG. 2. The friction coefficient η as a function of the coordinate of an adatom X at low temperatures for the symmetric case of $\varepsilon_d/2\Delta(0)=-5$ and $U/2\Delta(0)=10$ (——). The case of surface diffusion is considered and the X dependence of $V(X)$ is taken as $V(X)=V_0\{1+\beta\cos[(2\pi/a)X]\}$ and $\beta=0.01$. Also X dependences of $\Delta(X)/\Delta(0)$ ($\cdots$) and $T_K(X)/T_K(0)$ (— — —) are drawn in the figure.

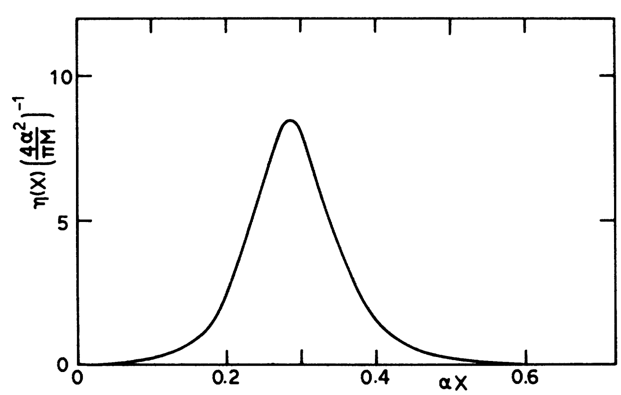

FIG. 3. The friction coefficient η as a function of the coordinate of an adatom X in the magnetic field at the absolute zero of temperature. The X dependence of $V(X)$ is taken as $V(X)=V_0\exp(-\alpha X)$. Used parameters are $U/2\Delta(0)=5$ and $H/2\Delta(0)=1.0\times10^{-3}$.

normal to surfaces, $V(X)$ may be an exponentially decreasing function of X, $V(X)=V_0\exp(-\alpha X)$. In Fig. 3 we show the position dependence of η in the magnetic field at $T=0$. As one can see from the figure, η has a peak structure as a function of X. It can also be shown that the peak position comes nearer to the surface as the magnetic field gets higher. It can be considered that the position dependence of η at low temperatures show similar behavior to that in the magnetic field and has a peak structure. For simplicity only the symmetric case has been considered in the present paper. It can be said[7] that the feature of η in the asymmetric case is qualitatively the same as that in the symmetric case.

In the present calculation we have dropped the k dependence of V_k. The feature of η described by the present calculation may suffer little modifications quantitatively if we taken into account the k dependence of V_k, although the qualitative feature of η may be the same.[14] From the results of the present investigation it can be suggested that the dynamical processes of adatoms such as hydrogen on metal surfaces strongly depend on the temperature and on the magnetic field through the temperature and the magnetic-field dependences of the friction coefficient.

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[14]It is noted that if the k dependence of V_k is taken into account, the Bethe-ansatz method cannot be applied to this model.