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Hopping rate of charged particles in a superlattice

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Abstract. The hopping rate ν of heavy, positively charged particles (e.g. positive muons) in a type-I superlattice is calculated. The electron–electron and electron–charged-particle interactions are treated in the random-phase approximation. It is assumed that the charged particle is confined to the barrier regions between the quantum wells where there are no electrons, and hops between nearest-neighbour lattice sites $\boldsymbol{R}_1$, $\boldsymbol{R}_2$ only. It is shown that ν is an anisotropic function of $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$. The contribution to ν due to particle–hole modes and plasmon excitations is obtained.

1. Introduction

The presence of electrically charged defects in solids (e.g. muons or protons in metals or semiconductors) presents an interesting problem in condensed matter physics [1–5]. Whenever these charged particles hop from one lattice site to another they may excite either electronic excitations or phonons. For example, a slowly moving heavy charged particle within a degenerate Fermi gas can excite electron–hole pairs with small excitation energy. In this case, electrons of low energy may not be able to rearrange their wavefunctions to be centred around the new lattice site to which the charged particle hops. As a consequence, the hopping bandwidth can be reduced. This result, referred to as the '*Anderson orthogonality catastrophe*' [6], is produced when a large number of electron–hole pairs of low excitation energy must be accounted for within the structure of the many-particle wavefunction for the basis of electronic eigenstates. By assuming a screened-electron–charged-particle interaction V_0, a constant density of states ρ for conduction electrons, Kondo has shown that the hopping rate for metals is proportional to T^{2K-1}, where $K \equiv V_0^2\rho^2[1-\sin^2(k_\mathrm{F}a)/(k_\mathrm{F}a)^2]$. Here, a is the nearest-neighbour hopping distance and k_F is the Fermi wavenumber. This power law can be understood as follows: the factor of T^{2K} is due to electronic screening whereas T^{-1} is due to level broadening proportional to T. Kadono *et al* [7,8] were the first to observe this power law behaviour for Cu.

In recent work [9], we have shown that the reduction of the hopping bandwidth is due not only to electron wavefunction overlap but to all possible virtual excitations as well. As a matter of fact, by treating the dynamically screened fields due to electron–electron interaction self-consistently, we have demonstrated that plasmon excitations

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may contribute a normalization factor as large as one or two orders of magnitude in bulk materials.

Whereas the motion of heavy charged particles in bulk materials has been extensively studied both theoretically and experimentally, very little attention has been given to their effects on the dynamical properties of lower-dimensional structures. To the best of our knowledge, no work has been carried out on this subject. It is the purpose of this paper to analyse the hopping rate of heavy charged particles when the dimensionality of their environment (represented by the conduction electrons here) is reduced. We show that the T^{2K-1} power law behaviour of the hopping rate will be changed as a result of the distinctive collective nature of the plasmon excitations in the long-wavelength limit. It is well known that the frequency of the collective excitation of a type-I superlattice tends to zero as the in-plane wavenumber decreases, unlike the bulk three-dimensional system. The motion of a heavy charged particle in superlattices will not only provide us with information about the nature of the particle but will help us understand the electronic and transport properties of the conduction electrons.

The system used in our study to represent the low-dimensional environment is a superlattice structure consisting of a periodic arrangement of two-dimensional (2D) electron gases. Such an arrangement is an appropriate model for layered semiconducting superlattices such as GaAs/$Al_xGa_{1-x}As$ intentionally doped with Si donors during the molecular beam epitaxy (MBE) growth of the $Al_xGa_{1-x}As$ layers [10]. In our calculations, we assume that electrons are located only on the 2D planes and the charged particle is confined to the region between these planes. In this way, we are able to study the interaction between a 2D gas and a point defect. This interaction, together with the screening properties of the electrons, essentially control the motion of the particle in these structures. We shall calculate the hopping rate of charged particles in superlattices by treating the particle–electron interaction and electron–electron interaction self-consistently. Our result for the hopping rate ν shows two new features: firstly, due to the wavenumber dependence of the collective excitation, the temperature dependence of ν is no longer simply a power law. Secondly, due to the anisotropic nature of the system, ν is an anisotropic function of the lattice site vectors $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, depending on the difference $\boldsymbol{R}_\| = \boldsymbol{R}_{1\|} - \boldsymbol{R}_{2\|}$ but on z_1 and z_2 separately, where the superlattice growth direction is along the z axis. (Here, we write $\boldsymbol{R} = (\boldsymbol{R}_\|, z)$). The reason for this is that, the interaction strength being site-dependent, the charged particle hops to a neighbouring lattice site where the electron–particle interaction is lower.

An outline of the remainder of this paper is as follows. In section 2, we derive the site-dependent hopping rate ν for a charged particle in a superlattice. The contribution to ν due to particle–hole modes is derived in section 3. In section 4, the plasmon contribution is obtained. Section 5 contains explicit results for the hopping rate in a superlattice in the limit when the period d of the superlattice is short. Section 6 is devoted to concluding remarks and discussion of our numerical results.

2. General formulation of the problem

The problem of calculating the hopping rate of a positively charged particle in a superlattice is relevant for an understanding of the transport properties of microstructures. The transition probability per unit time for a particle in eigenstate $|i\rangle$ hopping from lattice site 1 to lattice site 2 in eigenstate $|f\rangle$ within a solid is, to lowest order in the transfer integral Δ, given by [11]

$$\nu = \Delta^2 \int_{-\infty}^{\infty} \mathrm{d}t \, \langle \mathrm{e}^{\mathrm{i}H_i t/\hbar} \mathrm{e}^{-\mathrm{i}H_f t/\hbar} \rangle_1$$

where the average is carried out over all possible initial states. This definition for ν assumes that the energy levels for a particle at lattice sites 1 and 2 are virtually the same, i.e. we ignore the energy difference ΔE between corresponding energy levels at the two lattice sites. This is justified as long as $T > \Delta E$. The case $\Delta E > T$ can be obtained in a straightforward way.

The *total* Hamiltonian for a particle of positive charge Ze hopping between nearest-neighbour lattice sites within the barrier of a superlattice of period d is

$$H = H_{\mathrm{T}} + H_{\mathrm{el}} + H_{\mathrm{int}} \tag{1}$$

where

$$H_{\mathrm{T}} = \Delta \left(c_1^\dagger c_2 + c_2^\dagger c_1 \right) \tag{2a}$$

is the transfer Hamiltonian with $c_s^\dagger$ and c_s the creation and destruction operator for a charged particle at lattice site s,

$$H_{\mathrm{el}} = \sum_{\boldsymbol{k},l} \epsilon_{\boldsymbol{k}} a_{\boldsymbol{k},l}^\dagger a_{\boldsymbol{k},l} + \sum_{\boldsymbol{k},l} \sum_{\boldsymbol{k}',l'} \sum_{\boldsymbol{q}} v_q \mathrm{e}^{-q|l-l'|d} a_{\boldsymbol{k}+\boldsymbol{q},l}^\dagger a_{\boldsymbol{k}'-\boldsymbol{q},l'}^\dagger a_{\boldsymbol{k}',l'} a_{\boldsymbol{k},l} \tag{2b}$$

$$H_{\mathrm{int}} = Z \sum_{\boldsymbol{k},\boldsymbol{q},l} v_q \mathrm{e}^{-q|ld-z|} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_\parallel} a_{\boldsymbol{k},l}^\dagger a_{\boldsymbol{k}-\boldsymbol{q},l}. \tag{2c}$$

Here, Δ is the tunnelling matrix for electrons hopping between nearest-neighbour lattice sites. $a_{\boldsymbol{k},l}^\dagger a_{\boldsymbol{k},l}$ are creation and destruction operators for an electron with wavevector $\boldsymbol{k}$ at lattice site l. $\boldsymbol{k}$, $\boldsymbol{q}$, $\boldsymbol{R}_\parallel$ are in the xy plane perpendicular to the direction of growth (the z axis) of the superlattice, $v_q \equiv 2\pi e^2/\epsilon_\infty q$ is the two-dimensional Fourier transform of the Coulomb interaction, (with $q = |\boldsymbol{q}|$); ϵ_∞ is the high-frequency background dielectric constant, $l, l' = -\infty, \ldots, -1, 0, 1, \ldots, \infty$ label the 2D layers of the superlattice.

The hopping rate for electrons between lattice sites $\boldsymbol{R}_1 = (0, z_1)$ and $\boldsymbol{R}_2 = (\boldsymbol{R}_\parallel, z_2)$ is

$$\nu = \Delta^2 \int_{-\infty}^{\infty} \mathrm{d}t \, \phi(t) \tag{3}$$

where

$$\phi(t) = \mathrm{e}^{-F(t)} \qquad F(t) \equiv \frac{1}{\hbar} \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \, \langle V(t_1) V^\dagger(t_2) \rangle \tag{4}$$

with

$$V(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar} \hat{V} \mathrm{e}^{-\mathrm{i}Ht/\hbar} \tag{5}$$

and

$$\hat{V} = Z \sum_{k,q,l} v_q \left(e^{-q|ld-z_2|} e^{iq \cdot R_{\|}} - e^{-q|ld-z_1|} \right) a^{\dagger}_{k,l} a_{k-q,l}. \tag{6}$$

We have

$$\langle V(t_1) V^{\dagger}(t_2) \rangle = Z^2 \sum_{k,l} \sum_{k',l} \sum_{q,q'} v_q v_{q'} \langle a^{\dagger}_{k+q,l}(t_1) a_{k,l}(t_1) a^{\dagger}_{k'-q',l'}(t_2) a_{k',l'}(t_2) \rangle \\ \times \left(e^{-q|ld-z_2|} e^{iq \cdot R_{\|}} - e^{-q|ld-z_1|} \right) \left(e^{-q'|l'd-z_2|} e^{-iq' \cdot R_{\|}} - e^{-q'|l'd-z_1|} \right). \tag{7}$$

Now, the density–density correlation function is

$$\sum_{k,k'} \langle a^{\dagger}_{k+q,l}(t_1) a_{k,l}(t_1) a^{\dagger}_{k'-q',l'}(t_2) a_{k',l'}(t_2) \rangle \equiv \langle \hat{n}^{\dagger}_{q,l}(t_1) \hat{n}_{q',l'}(t_2) \rangle \\ = \delta(q - q') \sum_{k_z,(l-l')} \int_{-\infty}^{\infty} d\omega \, \frac{e^{i\omega(t_1-t_2)}}{e^{\beta\hbar\omega} - 1} e^{ik_z d(l-l')} \Im [\Pi(q,\omega)] \tag{8}$$

where $1/\beta$ is the thermal energy $k_B T$ and $\Pi(q,\omega)$ is the proper polarization. The frequency ω has a small positive imaginary part and the sum over k_z is to be carried out from $-\pi/d$ to π/d. In the random-phase approximation, we have

$$\Pi(q,\omega) = \frac{\Pi^0(q,\omega)}{\varepsilon_{q,k_z}(\omega)} \tag{9}$$

where the single-particle density–density response function is

$$\Pi^0(q,\omega) = 2 \sum_{k} \frac{f_{k+q} - f_k}{\epsilon_{k+q} - \epsilon_k - \hbar\omega - i0^+} \tag{10}$$

$f_k = \{\exp[\beta(\epsilon_k - E_F)] + 1\}^{-1}$ is the Fermi–Dirac function, with E_F equal to the Fermi energy and ϵ_k equal to the single-particle electron energy. We also have introduced the dielectric function defined by

$$\varepsilon_{q,k_z}(\omega) \equiv 1 - v_q S_q(k_z) \Pi^0(q,\omega) \tag{11}$$

where the geometric structure factor

$$S_q(k_z) \equiv \frac{\sinh(qd)}{\cosh(qd) - \cos(k_z d)}. \tag{12}$$

Combining these results, (7) becomes

$$\langle V(t_1) V^{\dagger}(t_2) \rangle = Z^2 \sum_{q,k_z} \frac{v_q}{S_q(k_z)} \left| \sum_l (e^{-q|ld-z_2|} e^{-iq \cdot R_{\|}} - e^{-q|ld-z_1|}) e^{ik_z ld} \right|^2 \\ \times \int_{-\infty}^{\infty} d\omega \, \left(\frac{e^{i\omega(t_1-t_2)}}{e^{\beta\hbar\omega} - 1} \right) \Im \left[\frac{1}{\varepsilon_{q,k_z}(\omega)} \right]. \tag{13}$$

Substituting (13) into (4) for $F(t)$ and carrying out the integrals over t_1 and t_2, our calculation shows that the term linear in t cancels the first-order term $\langle V(t)\rangle$ and we obtain

$$F(t)=\frac{Z^2}{\hbar}\sum_{q,k_z}A\left(q,k_z,R_{\|};z_1,z_2\right)\frac{v_q}{S_q\left(k_z\right)}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega^2\left(\mathrm{e}^{\beta\hbar\omega}-1\right)}\left(1-\mathrm{e}^{\mathrm{i}\omega t}\right)\Im\left[\frac{1}{\varepsilon_{q,k_z}(\omega)}\right] \tag{14}$$

where

$$\begin{aligned}A\left(q,k_z,R_{\|};z_1,z_2\right)&\equiv\left|\sum_l\left(\mathrm{e}^{-q|ld-z_2|}\mathrm{e}^{-\mathrm{i}q\cdot R_{\|}}-\mathrm{e}^{-q|ld-z_1|}\right)\mathrm{e}^{\mathrm{i}k_z ld}\right|^2\\&=\left|G_{q,k_z}\left(z_2\right)\mathrm{e}^{-\mathrm{i}q\cdot R_{\|}}-G_{q,k_z}\left(z_1\right)\right|^2\end{aligned} \tag{15a}$$

where

$$G_{q,k_z}\left(z\right)\equiv\frac{\sinh\left[q\left(d-z\right)\right]+\mathrm{e}^{\mathrm{i}k_z d}\sinh\left(qz\right)}{\cosh(qd)-\cos\left(k_z d\right)}. \tag{15b}$$

Noting that the imaginary part ($\Im(x)$) of the inverse dielectric function is given by ($\Re(x)$ denotes the real part)

$$\Im\left[\frac{1}{\varepsilon_{q,k_z}(\omega)}\right]=-\left[\frac{\Im\varepsilon_{q,k_z}(\omega)}{|\varepsilon_{q,k_z}(\omega)|^2}+\pi\delta(\Re\varepsilon_{q,k_z}(\omega))\right] \tag{16}$$

we separate the contributions to $F(t)$ due to plasmons (pl) and particle–hole modes (ph). We write $F(t)=F_{\mathrm{ph}}(t)+F_{\mathrm{pl}}(t)$ where

$$F_{\mathrm{ph}}(t)=\frac{Z^2}{\hbar}\sum_{q,k_z}\left|v_q\right|^2A\left(q,k_z,R_{\|};z_1,z_2\right)\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega^2\left(\mathrm{e}^{\beta\hbar\omega}-1\right)}\left(\mathrm{e}^{\mathrm{i}\omega t}-1\right)\frac{\Im\left[\Pi^0(q,\omega)\right]}{\left|\varepsilon_{q,k_z}(\omega)\right|^2}. \tag{17a}$$

$$F_{\mathrm{pl}}(t)=\frac{\pi Z^2}{\hbar}\sum_{q,k_z}\frac{v_q}{S_q\left(k_z\right)}A\left(q,k_z,R_{\|};z_1,z_2\right)\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega^2\left(\mathrm{e}^{\beta\hbar\omega}-1\right)}\left(\mathrm{e}^{\mathrm{i}\omega t}-1\right)\delta\left[\Re\varepsilon_{q,k_z}(\omega)\right]. \tag{17b}$$

At $T=0$, the real and imaginary parts of the single-particle polarization function are

$$\begin{aligned}\Re[\Pi^0(q,\omega)]=-\frac{m}{2\pi\hbar^2\tilde{q}}\Bigg\{&2\tilde{q}-\operatorname{sgn}\left(\tilde{q}+\frac{\Omega}{4\tilde{q}}\right)\left[\left(\tilde{q}+\frac{\Omega}{4\tilde{q}}\right)^2-1\right]^{1/2}\eta_+\left(\left(\tilde{q}-\frac{\Omega}{4\tilde{q}}\right)^2-1\right)\\&-\operatorname{sgn}\left(\tilde{q}-\frac{\Omega}{4\tilde{q}}\right)\left[\left(\tilde{q}-\frac{\Omega}{4\tilde{q}}\right)^2-1\right]^{1/2}\eta_+\left(\left(\tilde{q}-\frac{\Omega}{4\tilde{q}}\right)^2-1\right)\Bigg\}\end{aligned} \tag{18a}$$

$$\begin{aligned}\Im\left[\Pi^0(q,\omega)\right]=-\frac{m}{2\pi\hbar^2\tilde{q}}\Bigg\{&\left[1-\left(\tilde{q}-\frac{\Omega}{4\tilde{q}}\right)^2\right]^{1/2}\eta_+\left(1-\left(\tilde{q}-\frac{\Omega}{4\tilde{q}}\right)^2\right)\\&-\left[1-\left(\tilde{q}+\frac{\Omega}{4\tilde{q}}\right)^2\right]^{1/2}\eta_+\left(1-\left(\tilde{q}+\frac{\Omega}{4\tilde{q}}\right)^2\right)\Bigg\}\end{aligned} \tag{18b}$$

where $\eta_+(x)$ is the Heaviside unit step function, $\tilde{q} \equiv q/2k_F$ and $\Omega \equiv \hbar\omega/E_F$; k_F is the Fermi wavenumber.

In the low-frequency ($\Omega \ll 1$) and long-wavelength ($\tilde{q} \ll 1$) limits, we obtain

$$\Re\left[\varepsilon_{q,k_z}(\omega)\right] = 1 - \left(\frac{\omega_p(q,k_z)}{\omega}\right)^2 \tag{19a}$$

$$\Im\left[\Pi^0(q,\omega)\right] \approx -\frac{m\Omega}{4\pi\hbar^2\tilde{q}\sqrt{1-\tilde{q}^2}} \tag{19b}$$

where the plasma frequency is given by

$$\omega_p(q,k_z) \equiv \left(\frac{2\pi e^2 n_s q}{m\epsilon_\infty} S_q(k_z)\right)^{1/2}. \tag{20}$$

Here, n_s is the electron density per unit area, with $k_F = (2\pi n_s)^{1/2}$. We use these results to calculate (a) the particle–hole and (b) the plasmon contributions to the transition probability.

3. Particle–hole contribution

Assuming that the dielectric screening is static, we obtain, making use of (19b) in (17a) and carrying out the frequency integration (see appendix A)

$$\begin{aligned} F_{ph}(t) = Z^2\left(\frac{d}{2\pi}\right)\int_{-\pi/d}^{\pi/d} dk_z \int_0^{2k_F} \frac{dq\, q}{(2\pi)^2}\left|\frac{v_q}{\varepsilon_{q,k_z}(\omega=0)}\right|^2 \tilde{A}(q,k_z,R_\parallel;z_1,z_2) \\ \times \frac{m}{4\pi E_F\hbar^2\tilde{q}\sqrt{1-\tilde{q}^2}}\left[\ln\left(\frac{\sinh(\pi k_B T t/\hbar)}{\pi k_B T t/\hbar}\sqrt{1+\xi_q^2 t^2}\right) + \mathrm{i}\tan^{-1}(\xi_q t)\right] \end{aligned} \tag{21}$$

where ξ_q is a cut-off frequency which determines the range of validity of the low-frequency approximation in (19b) for $\Im\,\Pi^0(q,\omega) \sim \omega$. Here, we have integrated over the angle θ between the wavevector $\boldsymbol{q}$ and the relative position vector $\boldsymbol{R}_\parallel$, separating nearest neighbours, in the xy plane:

$$\begin{aligned} \tilde{A}(q,k_z,R_\parallel;z_1,z_2) &\equiv \int_0^{2\pi} d\theta\, A(q,k_z,\boldsymbol{R}_\parallel;z_1,z_2) \\ &= 2\pi\left\{\left|G_{q,k_z}(z_1)\right|^2 + \left|G_{q,k_z}(z_2)\right|^2 - 2J_0\left(qR_\parallel\right)\Re\left[G_{q,k_z}(z_1)\,G_{q,k_z}(z_2)\right]\right\} \end{aligned} \tag{22}$$

where $J_0(x)$ is a Bessel function of the first kind. Referring to (18b), we find that, if we assume that $\Omega \ll 1$, we must have $1-\tilde{q}^2 > \pm\Omega/2$ for $\Im\,\Pi^0 \neq 0$. Thus, we choose $\xi_q = 2\left(1-\tilde{q}^2\right) > 0$. In the limit of large $|t|$, we obtain

$$\ln\left(\frac{\sinh(\pi k_B T t/\hbar)}{\pi k_B T t/\hbar}\sqrt{1+\xi_q^2 t^2}\right) \approx \ln\left(\frac{\xi_q}{\omega_F}\right) - \ln\left(\frac{\pi k_B T}{E_F}\right) + \frac{\pi k_B T|t|}{\hbar} \tag{23}$$

where $\omega_F \equiv E_F/\hbar$. Therefore,

$$\mathrm{e}^{-F_{\mathrm{ph}}(t)} \approx \left(\frac{\pi k_B T}{E_F}\right)^{2K} \mathrm{e}^{-2\pi k_B T K|t|/\hbar}\mathrm{e}^{-B}\mathrm{e}^{-i\pi K\,\mathrm{sgn}(t)} \tag{24}$$

where

$$K \equiv Z^2\left(\frac{d}{2\pi}\right)\int_{-\pi/d}^{\pi/d}\mathrm{d}k_z\int_0^{2k_F}\frac{\mathrm{d}q\,q}{(2\pi)^2}\left|\frac{v_q}{\varepsilon_{q,k_z}(\omega=0)}\right|^2 \times \tilde{A}(q,k_z,R_\|;z_1,z_2)\frac{m}{8\pi E_F\hbar^2\tilde{q}\sqrt{1-\tilde{q}^2}} \tag{25}$$

is *independent* of the choice for ξ_q. Also, B is given by

$$B \equiv Z^2\left(\frac{d}{2\pi}\right)\int_{-\pi/d}^{\pi/d}\mathrm{d}k_z\int_0^{2k_F}\frac{\mathrm{d}q\,q}{(2\pi)^2}\left|\frac{v_q}{\varepsilon_{q,k_z}(\omega=0)}\right|^2\tilde{A}(q,k_z,R_\|;z_1,z_2) \times\frac{m}{4\pi E_F\hbar^2\tilde{q}\sqrt{1-\tilde{q}^2}}\ln\left(\frac{\xi_q}{\omega_F}\right) \tag{26}$$

showing that *both* K and B depend on z_1 and z_2 separately. Unlike K, we find that B depends on ξ_q.

The formulation is amenable to further analysis in the *close-packed limit* ($d \to 0$). In this limit †, we obtain in a straightforward way after replacing $1-\cos(k_z d)$ by the parabolic approximation $(k_z d)^2/2$

$$S_q(k_z) \approx \frac{2q}{(q^2+k_z^2)\,d} \qquad G_{q,k_z}(z) \approx \frac{2q}{(q^2+k_z^2)\,d}\cosh(qz) \tag{27}$$

and

$$\varepsilon_{q,k_z}(\omega=0) \approx 1 + r_s^2\left(\frac{a_0}{2d}\right)\frac{\tilde{q}}{\tilde{q}^2+(k_z/2k_F)^2} \tag{28}$$

where, in this notation, $a_0 \equiv \hbar^2\epsilon_\infty/me^2$ is the effective Bohr radius, where m is the effective band mass for an electron, and $r_s \equiv (\pi n_s)^{-1/2}/a_0$ is a measure of the electron density per unit area, n_s. Making use of these results in (25), it can be shown after some algebra that for $d \to 0$

$$K \approx \frac{1}{8}\left(\frac{Ze^2}{\epsilon_\infty E_F d}\right)^2\int_0^1\mathrm{d}\tilde{q}\,\frac{1}{\sqrt{1-\tilde{q}^2}}\Phi(\tilde{q},d) \times\left\{\cosh^2(\tilde{q}\tilde{z}_1)+\cosh^2(\tilde{q}\tilde{z}_2)-2J_0(\tilde{q}\tilde{R})\cosh(\tilde{q}\tilde{z}_1)\cosh(\tilde{q}\tilde{z}_2)\right\} \tag{29}$$

† The k_z variable would be integrated over the interval $-\pi/d < k_z < \pi/d$. Changing the variable of integration to $k = k_z d$, one has, for example, a factor $\cosh(qd) - \cos k$ in the denominator of the geometric structure factors $S_q(k_z)$ and G_{q,k_z}. By approximating the hyperbolic cosine function by $1 + (qd)^2/2$, in the limit as $d \to 0$, one finds that the dominant contributions to the integrals come from the vicinity of $k = 0$. Therefore, from this point of view the cos function could be approximated by its first two terms only.

where

$$\Phi(\tilde{q}, d) \equiv \frac{1}{\pi a^3}\left[\int_0^{\cosh^{-1}[(\pi^2+a^2)^{1/2}/a]} \mathrm{d}\phi \frac{1}{\cosh^3\phi + b^2/a^3} - \frac{1}{a}\left(\frac{b}{a}\right)^2 \int_0^{\cosh^{-1}[(\pi^2+a^2)^{1/2}/a]} \mathrm{d}\phi \frac{1}{[\cosh^3\phi + b^2/a^3]^2}\right]. \tag{30a}$$

Here $\tilde{z} \equiv 2k_{\mathrm{F}}z$, $\tilde{R} \equiv 2k_{\mathrm{F}}R_{\parallel}$, and

$$a \equiv 2k_{\mathrm{F}}d\tilde{q} \qquad b \equiv 2r_s d\left(k_{\mathrm{F}}^3 a_0 \tilde{q}\right)^{1/2}. \tag{30b}$$

For a fixed nearest-neighbour hopping length R_0, our calculations show that K is fairly sensitive to the direction of motion of the particle as well as z_1 and z_2. The polar angle θ is chosen in such a way that $R_{\parallel} = R_0 \sin\theta$ and $z_2 = z_1 + R_0\cos\theta$. In these calculations, we retained the cosine trigonometric function in the structure factors. However, the same conclusions for the spatial dependence of the function K are obtained for the parabolic approximation.

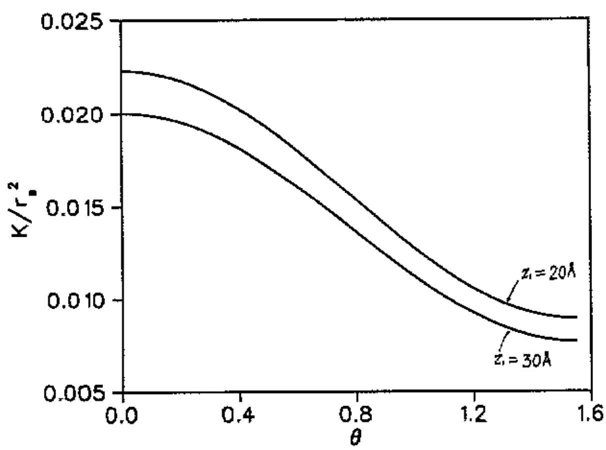

Figure 1. Plot of K/r_s^2 given by (25), in the static approximation, as a function of $\theta = \tan^{-1}[R_{\parallel}/(z_2 - z_1)]$ for two different values of z_1. The particle is chosen to be singly charged with $Z = 1$. The other parameters are: $d = 100$ Å, $R_0 = 4$ Å.

In figure 1, K is plotted as a function of θ for fixed z_1 and R_0. The following parameters have been used in our numerical calculations, $m = 0.067m_0$, where m_0 is the free electron mass and $\epsilon_\infty = 10.94$. For these values of m and ϵ_∞, $a_0 \approx 86$ Å, a value of $r_s \approx 1$ corresponds to an areal density of $\sim 10^{12}$ cm^{-2} which is typical for this material. Our results show that the particle motion parallel to the 2D plane is more favoured if the nearest-neighbour lattice sites along different direction are originally equivalent in the host material. This can also be understood from another point of view: when the particle hops from one lattice site to a neighbouring one, it is easier to rearrange the electronic wave function if the particle hops within a plane. The decrease of K when z_1 increases is a direct consequence of a reduction in the coupling strength between the particle and the electrons located in an adjacent plane.

4. Plasmon contribution

We now turn to a calculation of the long-wavelength plasmon contribution to the hopping rate. Substituting (19*a*) into (17*b*), we obtain in a straightforward way

$$F_{\rm pl}(t) = Z^2\left(\frac{d}{4}\right)\int_{-\pi/d}^{\pi/d}\mathrm{d}k_z\int_0^\infty \frac{\mathrm{d}q\,q}{(2\pi)^2}\tilde{A}(q,k_z,R_\parallel;z_1,z_2) \times\left(\frac{1}{\hbar\omega_{\rm p}(q,k_z)}\right)\left(\frac{2\pi e^2}{\epsilon_\infty q}\right)\left(\frac{\cosh(qd)-\cos(k_z d)}{\sinh(qd)}\right) \times\left[\frac{1-\mathrm{e}^{-\mathrm{i}\omega_{\rm p}(q,k_z)t}}{1-\mathrm{e}^{-\beta\hbar\omega_{\rm p}(q,k_z)}}+\frac{1-\mathrm{e}^{\mathrm{i}\omega_{\rm p}(q,k_z)t}}{1-\mathrm{e}^{\beta\hbar\omega_{\rm p}(q,k_z)}}\right]. \tag{31}$$

In the *close-packed limit* ($d\to 0$), we make use of (27) and obtain

$$F_{\rm pl}(t)\approx\frac{(Ze)^2}{\epsilon_\infty}\int_0^\pi \mathrm{d}k\int_0^{q_c}\mathrm{d}q\,\frac{1}{[(qd)^2+k^2]^{1/2}}\frac{1}{\hbar\omega_{\rm p}^{\rm B}} \times\left\{\cosh^2(qz_1)+\cosh^2(qz_2)-2J_0(qR_\parallel)\cosh(qz_1)\cosh(qz_2)\right\} \times\left[\frac{1-\mathrm{e}^{-\mathrm{i}\omega_{\rm p}(q,k_z)t}}{1-\mathrm{e}^{-\beta\hbar\omega_{\rm p}(q,k_z)}}+\frac{1-\mathrm{e}^{\mathrm{i}\omega_{\rm p}(q,k_z)t}}{1-\mathrm{e}^{\beta\hbar\omega_{\rm p}(q,k_z)}}\right]. \tag{32}$$

Here, $q_{\rm c}$ is a cut-off wavenumber which has been introduced to ensure the convergence of the q integral and

$$\omega_{\rm p}^{\rm B}\equiv\left(\frac{4\pi e^2 n_s}{\epsilon_\infty md}\right)^{1/2}. \tag{33}$$

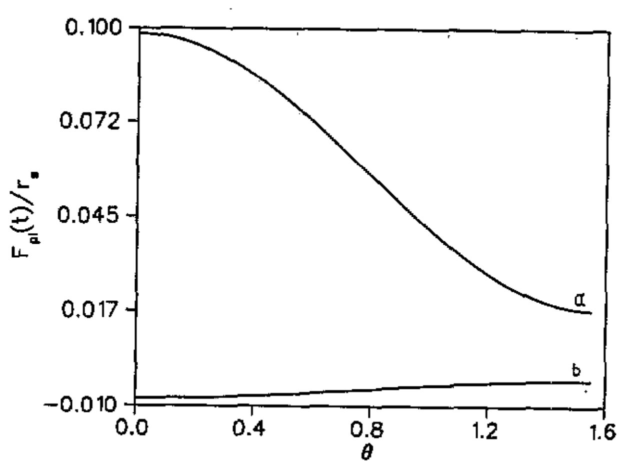

Figure 2. Plot of the real part (upper curve) and imaginary part (lower curve) of $F_{\rm pl}(t)/r_s$ given by (31), as functions of θ (defined in the caption for figure 1) for $z_1 = 20$ Å and $R_0 = 4$ Å at time $t = 0.5$ ps. The values used for m, ϵ_∞, d, n_s, T and $q_{\rm c}$ are given in the text.

In figure 2, the real and imaginary parts of $F_{\rm pl}$ are plotted as functions of θ for fixed z_1 and R_0. In these calculations, we chose the electron effective mass $m = 0.067m_0$ (m_0 is the free electron mass) and $\epsilon_\infty = 10.94$. The lattice period $d = 100$ Åand the areal density $n_s = 10^{12}$ cm^{-2} so that $\hbar\omega_{\rm p}^{\rm B} = 474.05$ meV. We chose the temperature as $T = 170$ K and the cut-off wavenumber $q_{\rm c} = a_0^{-1} \sim k_{\rm F}$. The real part of $F_{\rm pl}(t)$ is, of course, temperature independent. As one can see, the real part of $F_{\rm pl}$ which determines the renormalization of the hopping bandwidth is strongly angle dependent. It is easier to excite collective excitations in such structures when the motion of the particle is along the superlattice axis. The imaginary part has a relatively weak angular dependence. The temperature dependence of $F_{\rm pl}$ is weaker compared to that of $F_{\rm ph}$.

In the limit when the 2D planes are spread out ($d \to \infty$), it can be shown in a straightforward way that

$$F_{\rm pl}(t) \approx \frac{\pi Z^2 e^2}{\epsilon_\infty} \int_0^\infty {\rm d}q \left[1 - J_0(qR_\|)\right] \left(\frac{1}{\hbar\omega_{\rm p}^{2D}(q)}\right) \times \left\{1 - \cos\left(\omega_{\rm p}^{\rm 2D}(q)t\right) + {\rm i}\sin\left(\omega_{\rm p}^{\rm 2D}(q)t\right)\left[2n_{\rm B}\left(\omega_{\rm p}^{\rm 2D}(q)\right) + 1\right]\right\} \tag{34}$$

where $\omega_{\rm p}^{2D}(q)$ in (34) is the 2D plasmon frequency given by (20) with $S_q(k_z)$ replaced by unity and $n_{\rm B}(\omega)$ is the Bose distribution function defined by $n_{\rm B}(\omega) = 1/({\rm e}^{\beta\hbar\omega} - 1)$. Clearly, $F_{\rm pl}(t)$ is independent of z_1 and z_2 and only the imaginary part is temperature dependent. The dependence of $\Im F_{\rm pl}$ on temperature is appreciable in the 2D limit. We now make use of these results to calculate the hopping rate for a charged particle in a superlattice.

5. Hopping rate for a superlattice

We now apply (3) to calculate the hopping rate which, in general, is given by

$$\nu = \Delta^2 \int_{-\infty}^{\infty} {\rm d}t\, {\rm e}^{-F_{\rm ph}(t)} {\rm e}^{-F_{\rm pl}(t)}. \tag{35}$$

Making use of (24) and (31) in (35), we obtain

$$\nu = 2\Delta^2 \left(\frac{\pi k_{\rm B}T}{E_{\rm F}}\right)^{2K} {\rm e}^{-B} {\rm e}^{-F_{\rm pl}^0} \Re\left\{{\rm e}^{-{\rm i}\pi K} \int_0^\infty {\rm d}t\, {\rm e}^{-2\pi k_{\rm B}TKt/\hbar} {\rm e}^{-F_{\rm pl}^1(t)}\right\} \tag{36}$$

where $F_{\rm pl}(t) = F_{\rm pl}^0 + F_{\rm pl}^1(t)$ is the sum of a time-independent part $F_{\rm pl}^0$ and a time-dependent part $F_{\rm pl}^1(t)$, with

$$F_{\rm pl}^0 \equiv Z^2 \left(\frac{d}{4}\right) \int_{-\pi/d}^{\pi/d} {\rm d}k_z \int_0^\infty \frac{{\rm d}q\, q}{(2\pi)^2} \tilde{A}(q, k_z, R_\|; z_1, z_2) \times \left(\frac{1}{\hbar\omega_{\rm p}(q, k_z)}\right) \left(\frac{2\pi e^2}{\epsilon_\infty q}\right) \left(\frac{\cosh(qd) - \cos(k_z d)}{\sinh(qd)}\right) \tag{37}$$

and

$$F^{1}_{\mathrm{pl}}(t) \equiv -Z^2 \left(\frac{d}{4}\right) \int_{-\pi/d}^{\pi/d} \mathrm{d}k_z \int_0^{\infty} \frac{\mathrm{d}q\, q}{(2\pi)^2}\, \tilde{A}(q, k_z, R_{\parallel}; z_1, z_2) \times \left(\frac{1}{\hbar\omega_{\mathrm{p}}(q, k_z)}\right) \left(\frac{2\pi e^2}{\epsilon_{\infty} q}\right) \left(\frac{\cosh(qd) - \cos(k_z d)}{\sinh(qd)}\right) \times \left[\frac{\mathrm{e}^{-\mathrm{i}\omega_{\mathrm{p}}(q,k_z)t}}{1 - \mathrm{e}^{-\beta\hbar\omega_{\mathrm{p}}(q,k_z)}} + \frac{\mathrm{e}^{\mathrm{i}\omega_{\mathrm{p}}(q,k_z)t}}{1 - \mathrm{e}^{\beta\hbar\omega_{\mathrm{p}}(q,k_z)}}\right]. \tag{38}$$

Since the energy of the plasmon excitation is wavenumber dependent the plasmon contribution to the hopping rate, in general, depends on temperature.

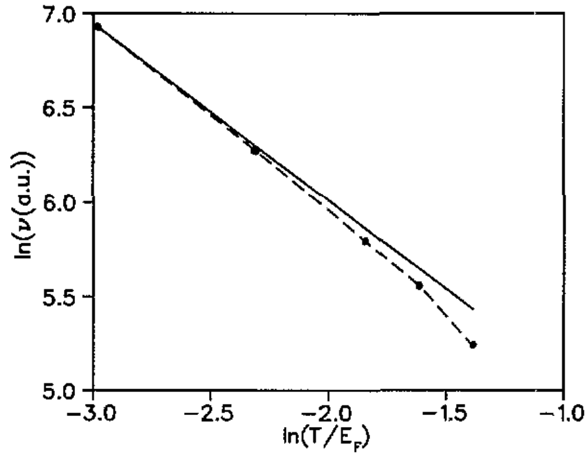

Figure 3. Plot of the hopping rate of a charged particle ($Z = 1$) in a superlattice. The parameters used here are the same as those used for the upper curve of figure 1 with $\theta = 0.4$. The full circles are the calculated values. The broken line is a guide for viewing. The full line is the power law behaviour which is presented for comparison.

As an example, we have calculated the temperature-dependent hopping rate for the same sample parameters used in figure 1. The hopping direction is chosen as $\theta = 0.4$ and $z_1 = 20$ Å. Our calculations show that except for very low temperature (note $E_{\mathrm{F}} \approx 400$ K), the hopping rate deviates from the power behaviour due to the inclusion of low-energy collective excitations. We should note that this temperature dependence may be further altered if the dynamical screening is taken into account.

6. Concluding remarks

The basic physical quantity that we are concerned with in this paper is the hopping rate ν for a charged particle in the barrier region of a superlattice. Our results show that the hopping rate ν is a function of z_1 and z_2 separately, which are the z coordinates of the lattice sites between which the charged particle hops but ν depends on the difference $\boldsymbol{R}_{\parallel}$ for the lattice translation vector perpendicular to the axis of the superlattice. In general, the temperature dependence of ν for layered materials is not of the form T^{2K-1} which is the behaviour for bulk three-dimensional systems. This difference is due to the fact that the collective normal modes for quasi-2D samples are wavenumber dependent in the long-wavelength limit.

We believe that the results presented here could be verified experimentally with the use of muons or protons. We suggest that muon spin-relaxation experiments be carried out in layered materials. By observing the decay of the muon spin, the hopping rate of muons can be deduced. When muons are separated from the metallic/conducting electron plane, the effective muon–electron interaction is reduced. Therefore we expect that a fast spin relaxation will be observed. On the other hand, one can use the muon as a local probe to study the properties of the structure. From measured hopping rates, one can deduce the value of the effective mass of electrons which is usually determined through optical and transport experiments.

In conclusion, we have presented a study of the motion of charged particles in a superlattice. A quite different temperature dependence of ν is predicted. The relevance to experiment has been discussed.

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Appendix A. Notes on a frequency integral

In this appendix, we evaluate the integral

$$I \equiv \int_{-D}^{D} \frac{d\omega}{\omega} \frac{1-e^{-i\omega t}}{1-e^{-\beta\hbar\omega}} = I_1 + I_2 \tag{A1}$$

where

$$I_1 \equiv \int_{0}^{D} \frac{d\omega}{\omega} \frac{1-e^{-i\omega t}}{1-e^{-\beta\hbar\omega}} \tag{A2}$$

$$I_2 \equiv \int_{-D}^{0} \frac{d\omega}{\omega} \frac{1-e^{-i\omega t}}{1-e^{-\beta\hbar\omega}} = \int_{0}^{D} \frac{d\omega}{\omega} \frac{1-e^{i\omega t}}{e^{\beta\hbar\omega}-1}. \tag{A3}$$

Clearly, we have

$$I_1 \equiv I' + I''$$

where

$$I' \equiv \int_{0}^{D} \frac{d\omega}{\omega} (1-e^{-i\omega t}) \tag{A4}$$

$$I'' \equiv \int_{0}^{D} \frac{d\omega}{\omega} \frac{1-e^{-i\omega t}}{e^{\beta\hbar\omega}-1}. \tag{A5}$$

Expanding the integrand in (A4) in a Taylor series, we obtain

$$I' = \int_0^1 \frac{\mathrm{d}x}{x}(1 - \mathrm{e}^{-\mathrm{i}Dtx}) = -\int_0^1 \frac{\mathrm{d}x}{x}\sum_{n=1}^{\infty}\frac{(-\mathrm{i}Dtx)^n}{n!}$$

$$= -\sum_{n=1}^{\infty}\frac{(-\mathrm{i}Dt)^n}{n!}\frac{1}{n} \approx \ln(1 + \mathrm{i}Dt) \tag{A6}$$

where the approximation is valid in the limit of large t.

We now turn our attention to the evaluation of the remaining integrals given by

$$I'' + I_2 = 2\int_0^D \frac{\mathrm{d}\omega}{\omega}\frac{1 - \cos(\omega t)}{\mathrm{e}^{\beta\hbar\omega} - 1}. \tag{A7}$$

Replacing the upper limit of integration in (A7) by infinity (since the integrand quickly approaches zero at high frequency) and expanding the integrand, we obtain

$$I'' + I_2 = 2\sum_{n=1}^{\infty}\frac{(-1)^{n+1}\tau^{2n}}{(2n)!}\int_0^{\infty}\mathrm{d}x\frac{x^{2n-1}}{\mathrm{e}^x - 1} \tag{A8}$$

where $\tau \equiv k_{\mathrm{B}}Tt/\hbar$. The integral over x in (A8) can be calculated by expanding $1/(\mathrm{e}^x - 1)$ in powers of $\mathrm{e}^{-x} < 1$. Calculation shows that

$$I'' + I_2 = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\frac{\tau}{m}\right)^{2n} = \sum_{m=1}^{\infty}\ln\left[1 + \left(\frac{\tau}{m}\right)^2\right]. \tag{A9}$$

Our evaluation of $I'' + I_2$ is completed by observing that (A9) can be rewritten as

$$I'' + I_2 = \ln\left[\prod_{m=1}^{\infty}\left(1 + \left(\frac{\tau}{m}\right)^2\right)\right] = \ln\left[\frac{\sinh(\pi\tau)}{\pi\tau}\right] \tag{A10}$$

where the infinite product has been evaluated using 1.431#2 of Gradshteyn and Ryzhik [12]. Combining (A6) and (A10), we obtain ($\tau \equiv k_{\mathrm{B}}Tt/\hbar$)

$$I = I' + I'' + I_2 = \ln\left[\frac{\sinh(\pi k_{\mathrm{B}}Tt/\hbar)}{\pi k_{\mathrm{B}}Tt/\hbar}\sqrt{1 + D^2t^2}\right] + \mathrm{i}\tan^{-1}(Dt). \tag{A11}$$

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