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Theory of dynamic conductivity and plasmon resonance in tunnelling superlattices

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Abstract. The theory of dynamic conductivity in a tunnelling superlattice which is composed of interacting electrons with both impurity and phonon scattering is presented using the memory-function approach and a newly developed matrix separation technique for the density correlation function. Taking into account the overlap of the wavefunctions between adjacent supercells, the memory function is explicitly expressed in terms of the matrix density correlation function. The contribution of plasmon resonance, which is dependent on the tunnelling, is estimated.

The dynamic conductivity of electrons in superlattices has recently attracted considerable interest [1, 2]. Previous studies of the electric conductivity in the x–y plane (where the superlattice axis is taken to be in the z direction), however, were carried out based on the assumption of complete confinement of carriers inside quantum wells. The electron tunnelling between adjacent wells, which, obviously, may play a role in systems with barriers of finite height and width, is neglected. The reason for the lack of a transport theory for tunnelling superlattices lay in the difficulty in obtaining a tractable expression for the density correlation function of the system. Recently, a new matrix separation technique has been developed [3, 4] for the density correlation function of a superlattice with wavefunction overlap. This technique has been applied to the investigation of the plasmon modes of tunnelling superlattice systems. In this paper, we would like to extend our study to linear dynamic transport of electrons using the memory function approach [5].

The superlattice we shall discuss consists of an infinite number of periodically arranged supercells of width d. The electrons are free to move within the x–y plane but are subject to a periodic potential $U(z)$ in the z direction. Limited to the lowest miniband, the single electron state is described by a wavevector $\boldsymbol{k} = (\boldsymbol{k}_\parallel, k_z)$ with $\boldsymbol{k}_\parallel = (k_x, k_y)$ and $-\pi/d < k_z \leqslant \pi/d$. The single-electron wavefunction can be written as $\psi_k(\boldsymbol{r}) = S^{-1/2}\exp(i\boldsymbol{k}_\parallel \cdot \boldsymbol{r}_\parallel)\varphi_{k_z}(z)$ with a band energy E_k. Here $\boldsymbol{r} = (\boldsymbol{r}_\parallel, z)$ with $\boldsymbol{r}_\parallel = (x, y)$ and S is the area of the x–y plane. We consider a many-body system composed of N electrons interacting with one another via a Coulomb potential, coupled with phonons and scattered by n_i randomly distributed impurities. The Hamiltonian of this system can be written as

$$H = H_e + H_p + H_{ep} + H_{ei} \tag{1}$$

$$H_e = \sum_k E_k c_k^\dagger c_k + \tfrac{1}{2}\sum_{q,k,k'} V(q, k_z, k_z') c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k \tag{2}$$

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$$H_{ei} = \sum_{k,q,a} u(\boldsymbol{q}, k_z, z_a) \exp(i\boldsymbol{q}_\parallel \cdot \boldsymbol{R}_{a\parallel}) c^+_{k+q} c_k \tag{3}$$

$$H_p = \sum_{q,\lambda} \Omega_{q\lambda} b^+_{q\lambda} b_{q\lambda} \tag{4}$$

$$H_{ep} = \sum_{q,\lambda} M(\boldsymbol{q}, \lambda)(b_{q\lambda} + b^+_{-q\lambda})\rho_q \tag{5}$$

where c^+_k and c_k are electron creation and annihilation operators corresponding to the single electron states ψ_k, ρ_q represents the Fourier transform of the electron density operator, $b^+_{q\lambda}$ and $b_{q\lambda}$ are the creation and annihilation operators for phonons with wavevector $\boldsymbol{q}$ in branch λ, R_a is the position of the ath impurity, $M(\boldsymbol{q}, \lambda)$ is the electron–phonon matrix element, $V(\boldsymbol{q}, k_z, k'_z)$ denotes the Coulomb potential between electrons, where

$$V(\boldsymbol{q}, k_z, k'_z) = \frac{2\pi e^2}{\varepsilon q_\parallel} \int dz_1\, dz_2 \varphi^*_{k_z+q_z}(z_1)\varphi^*_{k'_z-q_z}(z_2) \times \exp(-q_\parallel|z_1 - z_2|)\varphi_{k'_z}(z_2)\varphi_{k_z}(z_1) \tag{6}$$

and $u(\boldsymbol{q}, k_z, z_a)$ denotes the impurity potential

$$u(\boldsymbol{q}, k_z, z_a) = \frac{2\pi e^2}{\varepsilon q_\parallel} \int dz \exp(-q_\parallel|z - z_a|)\varphi^*_{k_z+q_z}(z)\varphi_{k_z}(z) \tag{7}$$

with ε being the background dielectric constant. The system we are discussing is an anisotropic one, such that the Coulomb and the impurity potential, as well as the density operator ρ_q, have more complicated expressions than those in isotropic three-dimensional (3D) or two-dimensional (2D) systems.

When a uniform AC electric field of frequency ω is applied parallel to the layer plane, the steady-state linear conductivity $\sigma(\omega)$ for this system can be expressed by means of the memory function $M(\omega)$ [5] as

$$\sigma(\omega) = i(Ne^2/m)\, 1/(\omega + M(\omega)) \tag{8}$$

where N as the 3D density equals the 2D density divided by d. The expression for $M(\omega)$ can be derived as the linear limit of a frequency-dependent generalisation of the non-linear balance-equation theory of transport [2, 6]. The derivation involves the analysis of the correlation function $\langle\langle c^+_{k+q} c_k | c^+_{k'-q} c_{k'} \rangle\rangle_\omega$ and an average over impurity sites. Generally, $M(\omega)$ can be expressed as the sum of two terms:

$$M(\omega) = M^i(\omega) + M^p(\omega) \tag{9}$$

where $M^i(\omega)$ is the impurity contribution to the memory function and $M^p(\omega)$ is the phonon contribution to the memory function. To illustrate we give the expression of $M^i(\omega)$:

$$M^i(\omega) = \frac{n_i}{2\pi N m \omega} \sum_{q,k,k'} q_x^2 g(q_z) u(\boldsymbol{q}, k_z) u(-\boldsymbol{q}, k'_z)(\langle\langle c^+_{k+q} c_k | c^+_{k'-q} c_{k'} \rangle\rangle_\omega |^0_\omega) \tag{10}$$

where $g(q_z)$ is an impurity correlation function [2, 6], which is defined in coordinate space

$$g(z'_a - z_a) = \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dq'_z g(q_z) \exp(iq'_z(z'_a - z_a)) = \left\langle \sum_{R_{a\parallel}} \exp(i\boldsymbol{q}_\parallel \cdot (\boldsymbol{R}'_{a\parallel} - \boldsymbol{R}_{a\parallel})) \right\rangle \tag{11}$$

and $u(q, k_z)$ denotes the effective impurity potential

$$u(\boldsymbol{q}, k_z) = \int_{-d/2}^{d/2} \mathrm{d}z_a P(z_a) \exp(\mathrm{i}q_z z_a) u(\boldsymbol{q}, k_z, z_a). \tag{12}$$

Here we have introduced an impurity distribution function $P(z_a)$ satisfying the normalisation condition

$$\int_{-d/2}^{d/2} \mathrm{d}z_a P(z_a) = 1. \tag{13}$$

A similar expression can be obtained for the phonon contribution to the memory function $M^{\mathrm{p}}(\omega)$. We omit this here to save space.

To proceed we have to calculate the Greens functions such as $\langle\langle c^+_{k+q} c_k | c^+_{k'-q} c_{k'} \rangle\rangle_\omega$ involved in the expression of the memory function $M(\omega)$. In an anisotropic many-body system such as a tunnelling superlattice, the k_z-dependence in $V(\boldsymbol{q}, k_z, k_z')$, $u(\boldsymbol{q}, k_z)$ and ρ_q makes it difficult to solve the RPA equation for the correlation function $\langle\langle c^+_{k+q} c_k | c^+_{k'-q} c_{k'} \rangle\rangle_\omega$ in contrast to the case of an isotropic system. This difficulty has been surmounted in weak tunnelling cases by the newly developed matrix separation technique [3, 4] for the density correlation function. By means of the tight-binding wavefunction and the nearest-neighbour overlap approximation, the electron–electron interaction and the density operator can be written as a series of separable factors in matrix form [3, 4]. In the same way, the impurity potential can also be expressed as

$$u(\boldsymbol{q}, k_z) = \hat{u}(\boldsymbol{q}) \hat{T}'(k_z) A_{k_z+q_z} A_{k_z} = \hat{T}(k_z) \hat{u}'(\boldsymbol{q}) A_{k_z+q_z} A_{k_z} \tag{14}$$

where we have defined two one-low matrices: $\hat{T}(k_z) \equiv (1, \cos k_z d, \sin k_z d)$ and

$$\hat{u}(\boldsymbol{q}) = (\hat{u}_1(\boldsymbol{q}), \hat{u}_2(\boldsymbol{q}), \hat{u}_3(\boldsymbol{q})) \tag{15}$$

with their transpositions $\hat{T}'(k_z)$ and $\hat{u}'(\boldsymbol{q})$. Here, $A_{k_z} = (1 + 2\alpha \cos k_z d)^{-1/2}$ with $\alpha = \int \phi(z)\phi(z-d)\,\mathrm{d}z$, where $\phi(z)$ is a 'single-well wavefunction', which is chosen to be real and normalised by $\int \phi(z)^2 \,\mathrm{d}z = 1$, and

$$\hat{u}_i(q) = \frac{2\pi e^2}{\varepsilon q_\parallel} \int_{-d/2}^{d/2} P(z_a)\,\mathrm{d}z_a \int_{-d/2}^{d/2} \exp(\mathrm{i}q_z - z_a) S(z - z_a, q) f_i(z, q_z)\,\mathrm{d}z \tag{16}$$

$(i = 1, 2, 3)$ in which

$$\begin{aligned}
f_1(z, q_z) &= \phi(z)^2 + [\phi(z+d)^2 + \phi(z-d)^2] \cos q_z d \\
&\quad + \mathrm{i}[\phi(z+d)^2 - \phi(z-d)^2] \sin q_z d \\
f_2(z, q_z) &= \phi(z)[\phi(z+d) + \phi(z-d)](\cos q_z d + 1) \\
&\quad + \mathrm{i}\phi(z)[\phi(z+d) - \phi(z-d)] \sin q_z d \\
f_3(z, q_z) &= \mathrm{i}\phi(z)[\phi(z+d) - \phi(z-d)](\cos q_z d - 1) \\
&\quad - \phi(z)[\phi(z+d) + \phi(z-d)] \sin q_z d
\end{aligned} \tag{17}$$

$$S(z - z', q) = \exp(-q_\parallel |z - z'|) + \frac{(\cos q_z d - \exp(-q_\parallel d)) \cosh q_\parallel (z - z') + \mathrm{i} \sin q_z d \sinh q_\parallel (z - z')}{\cosh q_\parallel d - \cos q_z d}.$$

By means of these matrices the memory functions $M^{\mathrm{i}}(\omega)$ and $M^{\mathrm{p}}(\omega)$ can be explicitly expressed as

$$M^{\mathrm{i}}(\omega) = \frac{n_{\mathrm{i}}}{2\pi N m \omega} \sum_q q_x^2 g(q_z) \hat{u}(\boldsymbol{q}) (\hat{\pi}(\boldsymbol{q}, 0) - \hat{\pi}(\boldsymbol{q}, \omega)) \hat{u}'(-\boldsymbol{q}) \tag{18}$$

$$M^{\mathrm{P}}(\omega) = \frac{1}{mN\omega} \sum_{q,\lambda} |M(q, \lambda)|^2 q_x^2 (\Lambda(q, \lambda, 0) - \Lambda(q, \lambda, \omega)) \tag{19}$$

where the imaginary part of Λ is

$$\Lambda_2(q, \lambda, \omega) = \Pi_2(q, \omega - \Omega_{q\lambda}) \left[n\left(\frac{\Omega_{q\lambda}}{k_B T}\right) - n\left(\frac{\Omega_{q\lambda} - \omega}{k_B T}\right) \right]$$

$$+ \Pi_2(q, \omega + \Omega_{q\lambda}) \left[n\left(\frac{\Omega_{q\lambda}}{k_B T}\right) - n\left(\frac{\Omega_{q\lambda} + \omega}{k_B T}\right) \right]. \tag{20}$$

Here $n(x/T) = 1/(e^{x/T} - 1)$ is the Bose function and Π_2 is the imaginary part of the electron density correlation function $\Pi(q, \omega)$ which can be obtained from the relation [3, 4]

$$\Pi(q, \omega) = \hat{p}(q_z) \tilde{\pi}(q, \omega) \hat{p}'(-q_z) \tag{21}$$

where we have defined a one-row matrix $\hat{p}(q_z) = (p_1(q_z), p_2(q_z), p_3(q_z))$ with its transposition $\hat{p}'(q_z)$, elements of which can be expressed as

$$p_i(q_z) = \int_{-d/2}^{d/2} \exp(\mathrm{i} q_z z) f_i(z, q_z)\, \mathrm{d}z \qquad i = 1, 2, 3 \tag{22}$$

and $\tilde{\pi}(q, \omega)$ is the matrix density correlation function which can be expressed in the RPA as [3, 4]

$$\tilde{\pi}(q, \omega) = (1 - \tilde{\pi}^0(q, \omega) \hat{V}(q))^{-1} \tilde{\pi}^0(q, \omega). \tag{23}$$

Here $\hat{V}(q)$ is a 3×3 matrix effective Coulomb potential having the elements ($i, j = 1, 2, 3$)

$$\hat{V}_{ij}(q) = \frac{2\pi d e^2}{\varepsilon q_\parallel} \int_{-d/2}^{d/2} \mathrm{d}z \int_{-d/2}^{d/2} \mathrm{d}z' S(z - z', q) f_i(z, -q_z) f_j(z', q_z) \tag{24}$$

and $\tilde{\pi}^0(q, \omega)$ is a 3×3 matrix density correlation bubble given by

$$\tilde{\pi}^0(q, \omega) = 2 \sum_k \hat{T}'(k_z) \hat{T}(k_z + q_z) \frac{n_{\mathrm{F}}(E_{k+q}) - n_{\mathrm{F}}(E_k)}{\omega + E_{k+q} - E_k + \mathrm{i}0^+} A_{k_z+q_z}^2 A_{k_z}^2 \tag{25}$$

where $n_{\mathrm{F}}(E)$ is the Fermi function.

Now, the memory function $M(\omega)$ can be calculated directly as long as the single-well wavefunction is given. Here, we pay attention to the contribution of plasmon pole to $M_2^{\mathrm{i}}(\omega)$ the imaginary part of the memory function due to impurity scattering, which has been focused upon by many authors [2, 7]. For a quasi-2D superlattice system in which the tunnelling was neglected, Lei *et al* [2] showed a strong resonance around the plasmon frequency, and for a 3D bulk system, Ron and Tzoar [7] found a relatively weak (15%) effect from the contribution of plasmon poles. In the tunnelling superlattices, how electron tunnelling affects the contribution of plasmon poles to $M_2^{\mathrm{i}}(\omega)$ is interesting.

For a completely uncorrelated distribution of impurities $g(q_z) = 2\pi\delta(q_z d)$, the enhancement of $M_2^{\mathrm{i}}(\omega)$ comes from the long-wavelength ($q_\parallel \sim 0$ and $q_z = 0$) plasmon contribution at $\omega \approx \omega_{\mathrm{p}} = (4\pi e^2 N/\varepsilon m)^{1/2}$ (at zero temperature). In the limit, the density correlation function bubble can be solved as

$$\Pi^0(q, \omega) = (N/m)(q_\parallel^2/\omega^2) + (3\pi N^2 d/2m^3 C_t)(q_\parallel^4/\omega^4) \qquad (q_z = 0) \tag{26}$$

where

$$c_t = \begin{cases} \left(\dfrac{(x^2 + 1/2)\cos^{-1}x - (3/2)x(1\,s\,x^2)^{1/2}}{(1-x^2)^{1/2} - x\cos^{-1}x}\,\pi \right)^{-1} & |x| \leqslant 1 \qquad (27a) \\ (1 + x^{-2}/2)^{-1} & x < -1. \qquad (27b) \end{cases}$$

Here, $x = (t - E_F)/t$, t is the half-width of the miniband and E_F is the Fermi energy which is determined by the electron density N. The jump of $M_2^i(\omega_p)$ due to the plasmon pole can be obtained from the behaviour of $\Pi^0(q, \omega)$ at small $q_\parallel$ as

$$\Delta M_2^i(\omega_p) = C_t \tfrac{2}{3} n_i (e^2/\varepsilon)^{3/2} (m\pi)^{1/2}/N^{3/2}d^2. \qquad (28)$$

If electron tunnelling was neglected, $t = 0$ and $C_t = 1$, equation (28) reduces to the results of Lei *et al* [2]. We show

$$\Delta M_2^i(\omega_p)/\Delta M_2^i(\omega_p)|_{t=0} = C_t$$

as the function of t/E_F in figure 1. $\Delta M_2^i(\omega_p)|_{t=0}$ is the value of $\Delta M_2^i(\omega_p)$ calculated by neglecting the tunnelling. From equation (27), we know $C_t < 1$. In figure 1, it can be seen that the contribution of the plasmon oscillation to $M_2^i(\omega_p)$ is obviously diminished due to the electron tunnelling.

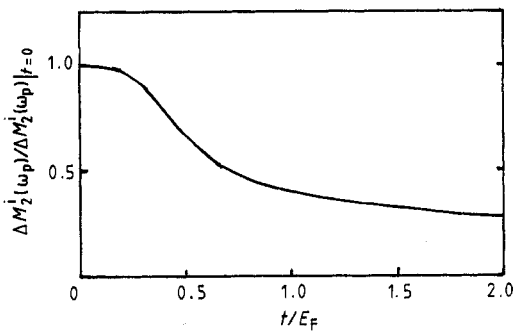

Figure 1. Calculated $\Delta M_2^i(\omega_p)/\Delta M_2^i(\omega_p)|_{t=0}$ shown as a function of t/E_F.

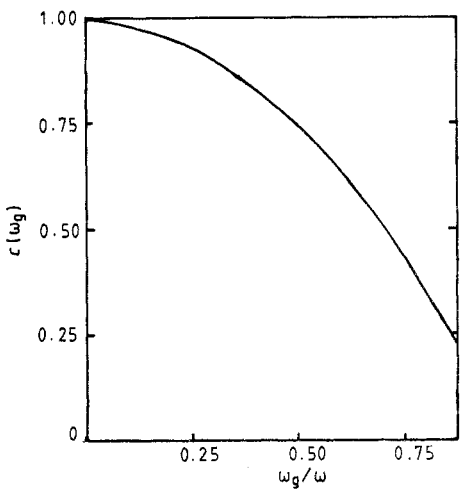

Figure 2. Plot of the function $c(\omega_g)$.

In the general case, the impurity distribution has some correlation $g(q_z) \neq 2\pi\delta(q_z d)$, and the plasmon modes of $q_z \neq 0$ will contribute to the $M_2^i(\omega)$. For an anisotropic 3D system similar to the tunnelling superlattice, the plasmon frequency $\omega_p(q)$ is given as [3, 4, 8–10]

$$\omega_p^2 = (\omega_B^2 q_\parallel^2 + \omega_g^2 q_z^2)/(q_\parallel^2 + q_z^2) \qquad (29)$$

where $\omega_B^2 = 4\pi Ne^2/\varepsilon m$, ω_g^2 is the contribution due to the electron tunnelling which is given by

$$\omega_g^2 = \begin{cases} 2e^2mdt^2/\varepsilon\hbar^2 & E_F > 2t \\ \dfrac{2e^2mdt^2}{\varepsilon\pi\hbar^2}\{\cos^{-1}(1 - E_F/t) + (E_F/t - 1)[1 - (E_F/t - 1)^2]^{1/2}\} & E_F < 2t. \end{cases} \tag{30}$$

$\omega_g (< \omega_B)$ is a gap in the plasmon spectrum [3, 4, 8–10], with magnitude directly proportional to the half-width of the miniband t. The plasmon contributions begins at lower frequency ω_g. The contribution of plasmon poles from long-wavelength range to $M_2^i(\omega)$ for $\omega_g < \omega < \omega_B$ can be estimated from

$$\Delta M_2^i(\omega) = \frac{n_i e^2}{N\varepsilon md}\int dq_z \frac{\omega(\omega^2 - \omega_g^2)}{(\omega_B^2 - \omega^2)^2} q_z^2 g(q_z) \qquad \omega_g < \omega < \omega_B. \tag{31}$$

Since the range of q_z limited by the plasmon becomes small when the tunnelling increases, the $\Delta M_2^i(\omega)/\Delta M_2^i(\omega)|_{t=0}$ is not larger than $c(\omega_g) = 1 - \omega_g^2/\omega^2$. We plot the function $c(\omega_g)$ in figure 2, which shows that the electron tunnelling will greatly weaken the contribution of plasmon oscillation to the $M_2^i(\omega)$.

In summary, we have presented a theory of dynamic transport of electrons in the tunnelling superlattices, and estimate the contribution of plasmon poles. We show that the contribution of plasmon oscillation, to the $M_2^i(\omega)$ decreases from the strong resonance of the quasi-2D superlattice system to a relatively weak effect of the 3D bulk system with the increase of the electron tunnelling. This behaviour is a characteristic of the crossover between 2D and 3D for the tunnelling superlattice systems.

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