# Transport in quantum wells in the presence of interface roughness

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The effective Hamiltonian for two-dimensional quantum wells with rough interfaces is formally derived. Two terms are generated. The first term is identified with local energy-level fluctuations, and was introduced phenomenologically in the literature for interface roughness scattering, however, is now shown to be valid only for an infinite potential well or Hamiltonians with one single length scale. The other term is shown to modulate the wave function and cause fluctuations in the charge density. This will further reduce the electron mobility to a magnitude that is close to the experimental result.

The vast interest in the physics of charge transport in two-dimensional quantum wells stems from potential applications in devices and subsequent integration with Si-based chip technology. Experimentally, it is known that charge transport inside a quantum well is strongly affected by the quality of the well. In particular, it is believed that interface roughness is inherent to the quantum-well systems, and plays an important role for wells at low temperature with small well widths.[1] On the theoretical side, starting from the seminal work by Kardar, Parisi, and Zhang,[2] a large effort has been devoted to understanding the morphology of thin-film growth[3] during the past decade. Nevertheless, these works only characterize long-wavelength properties of the surface roughness; there has been no systematic attempt to investigate how electronic properties, such as charge transport, are affected by surface roughness.

The study of the effects of surface roughness on electronic transport properties has a long history, tracing back to the work by Prange and Nee[4] on magnetic surface states in metals. Later, a more complete model was reconsidered by Ando.[5] Quite often, these works are summarized phenomenologically by introducing a local energy-level fluctuation term in the potential, $(\partial E/\partial L)\Delta(\mathbf{r})$, where $E$ is the energy eigenvalue of the electron, $L$ is the averaged well width, and $\Delta(\mathbf{r})$ is the local change of the quantum-well width. Such a phenomenology finds its natural application in interpreting the photoluminescence data of GaAs/AlAs quantum wells.[1,6] In this case, it has been established that for temperatures less than 80 K, the linewidth of the photoluminescence is mainly determined by the local energy level fluctuations. Transport properties of two-dimensional (2D) carrier gases at $Si/SiO_2$ interfaces and in semiconductor quantum wells are also shown to be strongly affected by the interface roughness.[7,8,10] In these studies, theoretical mobility was also calculated based on the assumption that the local energy-level fluctuation is the dominant effect. It is known, however, that the experimentally observed mobility cannot be explained solely by the roughness. In some parameter regime one has to introduce, for example, a phenomenologically negative impurity charge to account for the extra reduction of the mobility observed in experiments.[10,12]

In this work, we shall systematically investigate the effects of surface roughness. Our starting point is an averaged version of the Hamiltonian specialized to the quantum well configuration. In an expansion in $\Delta(\mathbf{r})/L$, two lowest order terms are considered . The first term is identified to the local energy-level fluctuations $(\partial E/\partial L)\Delta(\mathbf{r})$. This term represents the mismatch effect of the energy band. It was introduced phenomenologically in the literature for interface roughness scattering, but is now shown to be valid only for an infinite potential well or Hamiltonians with one single length scale. The other term is shown to modulate the wave function and cause fluctuations in the charge density. This will further reduce the electron mobility.

Let us consider a generic quantum well specified by two interfaces at $z=z_+(\mathbf{r})$ and $z=z_-(\mathbf{r})$, where $\mathbf{r}=(x,y)$ is a two-dimensional vector. The average distance between the two surfaces is $L$ (see Fig. 1). For simplicity, we shall impose a hard wall condition on the interfaces. Our formulation is easily generalized to the case when the potential well is finite. To investigate effects that are due to the interface roughness, it is convenient to do a transformation that maps $z_+(\mathbf{r})$ to $L$ and $z_-(\mathbf{r})$ to 0. This transformation is easily implemented by $z'=L[z-z_-(\mathbf{r})]/[\Delta(\mathbf{r})+L]$, $\mathbf{r}'=\mathbf{r}$, where $\Delta(\mathbf{r})\equiv z_+(\mathbf{r})-z_-(\mathbf{r})-L$. After transformation, the wavefunction can be generically expressed by

$$\Psi_n=\psi_n(x,y)\sin\left(\frac{n\pi}{L}z'\right)\Big/\sqrt{\frac{L+\Delta(\mathbf{r})}{2}}.$$

For typical quantum wells, the Fermi wavelength is about 400 Å. If $L$ is less than 340 Å, there will be no band crossing at low temperatures, and we can take the average along $z$ direction with respect to a given subband, i.e., average with respect to $\sin(n\pi/L)z'$ ($n$ will be taken to be 1). After

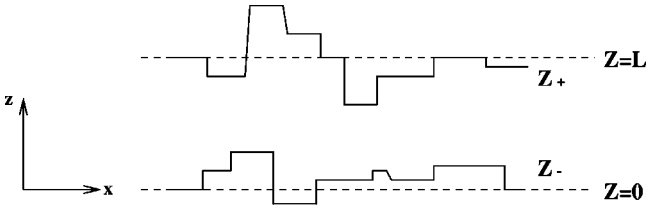


FIG. 1. A schematic plot of a 2D quantum well with rough interfaces.

 

the averaging, the effective Hamiltonian becomes $H_n = (-\hbar^2/2m)\nabla^2 + \delta V$, where the Laplacian is over the $(x,y)$ directions and

$$-\frac{2m}{\hbar^2}\delta V = \alpha_n \frac{(\nabla A)^2}{A^2} + \beta_n \frac{2}{A}\nabla A \cdot \left(\nabla B - \frac{B}{A}\nabla A\right) + \gamma_n\left[A^2 + \left(\nabla B - \frac{B}{A}\nabla A\right)^2\right] + \delta_n\left(\frac{2}{A}\nabla A\cdot\nabla + \frac{1}{A}\nabla^2 A\right). \quad (1)$$

Here $A \equiv L/[\Delta(\mathbf{r})+L]$, $B \equiv -[Lz_-(\mathbf{r})]/[\Delta(\mathbf{r})+L]$, $\alpha_n \equiv \langle z'^2(\partial^2/\partial z'^2)\rangle_n$, $\beta_n \equiv \langle z'(\partial^2/\partial z'^2)\rangle_n$, $\gamma_n \equiv \langle \partial^2/\partial z'^2\rangle_n$ and $\delta_n \equiv \langle z'(\partial/\partial z')\rangle_n$. It is easy to show that $\delta_n = -1/2$ is generally true.

If we expand $\delta V$ to the linear order of $\Delta/L$ and keep only up to $O(z_-)$, we obtain

$$\delta V = E_n - \frac{2E_n}{L}\Delta(\mathbf{r}) + \delta_n\frac{\hbar^2}{m}\left(\frac{1}{L}\nabla\Delta(\mathbf{r})\cdot\nabla + \frac{1}{2L}\nabla^2\Delta(\mathbf{r})\right) - \beta_n\frac{\hbar^2\nabla(z_+ - L)\cdot\nabla z_-}{mL}, \quad (2)$$

where we have identified $-\gamma_n\hbar^2/2m$ as $E_n$. Note that the resulting Hamiltonian is invariant under reflection: $L - z_- \to z_+$ and $L - z_+ \to z_-$. If $z_+(\mathbf{r})$ and $z_-(\mathbf{r})$ are uncorrelated, the last term is of higher order and can be neglected.

In general, the second term in Eq. (2) has no definite relation with $E_n$. Only when $L$ is the unique length scale in the Hamiltonian (e.g., an infinite potential well) will $E_n$ be proportional to $1/L^2$ and $-2E_n/L = \partial E_n/\partial L$. Equation (2) can then be written

$$\delta V = E_n + \frac{\partial E_n}{\partial L}\Delta(\mathbf{r}) - \frac{\hbar^2}{2m}\left[\frac{1}{L}\nabla\Delta(\mathbf{r})\cdot\nabla + \frac{1}{2L}\nabla^2\Delta(\mathbf{r})\right]. \quad (3)$$

Physically the second term in Eq. (3) describes the local energy-level fluctuation, which was introduced phenomenologically in the literature for interface roughness scattering.[8,10] The third term can be combined with the kinetic energy to become

$$H' = -\frac{\hbar^2}{2m}\left(\nabla + \frac{\nabla\Delta(\mathbf{r})}{2L}\right)^2 \quad (4)$$

(a second order term has been neglected). This has the effect of modulating the wave function for every particle by

$$\Psi(\mathbf{r}) \to \Psi(\mathbf{r})\exp\left(-\frac{\Delta(\mathbf{r})}{2L}\right). \quad (5)$$

Note that this result is *independent* of the depth of the well. We shall show later that this fluctuation in the electron density suppresses the mobility both from the screening effect and from the Landauer formula.[11]

In the following, we discuss the many-particle effect that is due to the wave-function modulation. We shall demonstrate its effect on the calculation of the electron mobility. The change of the wave function induces a local modulation in the density of electrons,

$$n(\mathbf{r},z') = n'(\mathbf{r})\frac{\sin^2\left(\frac{n\pi}{L}z'\right)}{[L+\Delta(\mathbf{r})]/2}\exp\left(-\frac{\Delta(\mathbf{r})}{L}\right),$$

with the understanding that the normalization is done with respect to $z$. Here $n'(\mathbf{r})$ is the 2D electron density after being perturbed by the local energy-level fluctuations, $(\partial E_n/\partial L)\Delta(\mathbf{r})$. It is easy to show that

$$n'(\mathbf{r}) = n_0\left\{1 + \frac{2m}{\pi\hbar^2 k_F^2}\frac{\partial E_n}{\partial L}\int_{k\le k_F} d^2\mathbf{k} \times \sum_{\mathbf{p}} \frac{[\Delta(\mathbf{k}-\mathbf{p})\cdot e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}} + \text{H.c.}]}{k^2 - p^2}\right\},$$

where $n_0 = k_F^2/2\pi$ is the equilibrium electron density at two dimensions, and H.c. denotes a Hermitian conjugate of the previous term. We shall assume that the density of positive charge background remains unchanged, so that the local charge modulation is entirely due to electrons. The change of charge density is

$$\delta\rho(\mathbf{r},z) = en(\mathbf{r},z')\theta(z-z_-)\theta(L+\Delta-z) - en_0\frac{\sin^2\left(\frac{n\pi}{L}z\right)}{L/2}\theta(z)\theta(L-z). \quad (6)$$

For convenience, we shall assume $z_- = 0$, and neglect the curvature effect due to the roughness (for instance, the special case when both interfaces fluctuate while their spacing remains $L$). To the first order in $\Delta(\mathbf{r})$, the total electric potential $\delta\phi$ satisfies

$$-\left(\nabla^2 + \frac{\partial^2}{\partial z^2}\right)\delta\phi(\mathbf{r},z) = 4\pi\rho_{ind} + 4\pi e n_0\frac{\sin^2\left(\frac{n\pi}{L}z\right)}{L/2}\left\{s - 2\left[1 + \frac{n\pi z}{L}\times\cot\left(\frac{n\pi}{L}z\right)\right]\frac{\Delta(\mathbf{r})}{L} + \frac{m}{\pi^2\hbar^2 n_0}\frac{\partial E_n}{\partial L}\int_{k\le k_F} d^2\mathbf{k} \times \sum_{\mathbf{p}}\frac{[\Delta(\mathbf{k}-\mathbf{p})\cdot e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}} + \text{H.c.}]}{k^2-p^2}\right\}\theta(z)\theta(L-z), \quad (7)$$

where $\rho_{ind}$ is the induced charge density. The associated scattering matrix within a given subband is given by

$$\delta M(\mathbf{q}) = \langle\mathbf{k}|\delta V|\mathbf{q}-\mathbf{k}\rangle_n = \frac{2e}{L}\int_0^L dz\,\delta\phi(\mathbf{q},z)\sin^2\left(\frac{n\pi}{L}z\right), \quad (8)$$

where $\delta\phi(\mathbf{q},z)$ is of the order of $\Delta$. We shall denote $\int_0^L dz\ \delta\phi(\mathbf{q},z)\sin^2[(n\pi/L)z]$ by $\delta\tilde{\phi}(\mathbf{q})$.

We now express the induced charge density in terms of $\delta\tilde{\phi}(\mathbf{q})$. This can be achieved in the conventional linear response theory by

$$\rho_{ind}(\mathbf{q},\omega=0,z)=\int dz'\,\mathrm{Re}\,\Pi(q,\omega=0,z,z')e^2\delta\phi(\mathbf{q},z'), \tag{9}$$

where $\Pi(q,\omega=0,z,z')$ is the polarization insertion.[13] If we focus on the $n$th subband, the one-loop contribution is

$$\mathrm{Re}\,\Pi(q,\omega=0,z,z') = \sin^2\left(\frac{n\pi}{L}z\right)\sin^2\left(\frac{n\pi}{L}z'\right)\frac{-16m}{\hbar^2L^2}\mathcal{P}\int\frac{d^2k}{(2\pi)^2} \times\theta(1-k)\frac{1}{qk(\cos\theta+x)}, \tag{10}$$

where $q$ and $k$ are measured in terms of $k_F$, $\theta(1-k)$ is the step function, $x\equiv q/2k$, and $\mathcal{P}$ denotes the Cauchy principle value. Since the momentum transfer $q$ is always less than $2k_F$, $x<1$ for the range of $k$ integration. We find that

$$\mathcal{P}\int\frac{d^2k}{(2\pi)^2}\theta(1-k)\frac{1}{qk(\cos\theta+x)}=\frac{1}{4\pi}. \tag{11}$$

As a result, we obtain

$$\rho_{ind}(\mathbf{q},\omega=0,z)=-\frac{4me^2}{L^2\pi\hbar^2}\sin^2\left(\frac{n\pi}{L}z\right)\delta\tilde{\phi}(\mathbf{q}). \tag{12}$$

Substituting the above into Eq. (7) and performing Fourier transformations on both $\mathbf{r}$ and $z$, we find

$$(q^2+k_z^2)\delta\phi(\mathbf{q},k_z)=-\frac{16me^2}{L^2\hbar^2}v(k_z)\delta\tilde{\phi}(q)-\frac{16\pi en_0}{L^2} \times\Delta(\mathbf{q})[u(k_z)+v(k_z)]+\frac{16me}{\pi L\hbar^2}\frac{\partial E_n}{\partial L} \times\int_{k\le k_F}d^2\mathbf{k}\frac{\Delta(\mathbf{q})}{k^2-|\mathbf{k}-\mathbf{q}|^2}v(k_z), \tag{13}$$

where $u(k_z)=(n\pi/2L)\int_0^L e^{ik_zz}z\sin[(2n\pi/L)z]dz$ and $v(k_z)=\int_0^L e^{ik_zz}\sin^2[(n\pi/L)z]dz$. The $\mathbf{k}$ integration was done in Eq. (11). It is also easy to show that

$$\delta\tilde{\phi}(\mathbf{q})=\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}\delta\phi(\mathbf{q},k_z)v^*(k_z). \tag{14}$$

Substituting $\delta\phi(\mathbf{q},k_z)$ into the above equation, we obtain

$$\delta\tilde{\phi}(\mathbf{q})=\frac{\frac{16\pi en_0}{L^2}[I(q)+J(q)]-\frac{8me}{L\hbar^2}\frac{\partial E_n}{\partial L}I(q)}{1+\frac{16me^2}{L^2\hbar^2}I(q)}[-\Delta(\mathbf{q})], \tag{15}$$

where

$$I(q)\equiv\int\frac{dk_z}{2\pi}\frac{|v(k_z)|^2}{q^2+k_z^2}, \tag{16}$$

$$J(q)\equiv\int\frac{dk_z}{2\pi}\frac{v^*u}{q^2+k_z^2}. \tag{17}$$

For a narrow quantum well satisfying $qL\ll 2k_FL\ll 1$ (this requires $L\ll 33$ Å for $n_0\approx 2\times10^{15}$ m$^{-2}$ in quantum wells), $I(q)\approx L^2/8q$ and $J(q)\approx -L^2/16q$, and Eq. (15) reduces to the standard 2D screening form[9]

$$\delta\tilde{\phi}(\mathbf{q})=\frac{\alpha}{q+q_s}[-\Delta(\mathbf{q})] \tag{18}$$

[the second term in the denominator of Eq. (15) does not exist in two pure dimensions] where $q_s=2me^2/\hbar^2\simeq 1/(0.25\ \text{Å})$ and $\alpha=\pi en_0$.

However, if $qL\approx 1$, one shall have to use the full expression of $I(q)$ and $J(q)$. Since $(16me^2/L^2\hbar^2)\simeq 10^{30}$ m$^{-3}$ and $I(q)\simeq 10^{-27}$ m$^3$, the second term in the denominator of Eq. (19) dominates and $\delta\tilde{\phi}(\mathbf{q})\approx(\pi n_0\hbar^2/2em)\Delta(\mathbf{q})$. The resulting scattering matrix within a given subband is thus given by

$$|M(\mathbf{q})|^2=\langle|\delta V(\mathbf{q})|^2\rangle\approx\frac{1}{\aleph}\left(2\frac{\partial E_n}{\partial L}-\frac{2n_0\pi\hbar^2}{mL}\right)^2S(q), \tag{19}$$

where $\aleph$ is the normalization and $S(q)$ is the power spectrum of $\Delta(\mathbf{q})$, given[10] by $\langle|\Delta(\mathbf{q})|^2\rangle$. Given the scattering matrix, we can calculate the relaxation time via the relation

$$\frac{1}{\tau(\mathbf{k})}=\frac{1}{2\pi\hbar}\int d^2k'|M(\mathbf{k}-\mathbf{k}')|^2(1-\cos\Phi) \times\delta[E(\mathbf{k})-E(\mathbf{k}')], \tag{20}$$

where $\Phi$ denotes the angle between the initial and final wave vectors $\mathbf{k}$ and $\mathbf{k}'$. The mobility of the electron can then be solved by

$$\mu=e\int dE\frac{\rho(E)v_x^2(E)\tau(E)}{4nk_BT\cosh^2[(E-E_F)/2k_BT]}. \tag{21}$$

We see that the interparticle interaction reduces the electron mobility estimated by the energy-level fluctuations by at least three quarters. Since $\partial E_n/\partial L<0$, the second term in Eq. (19) due to wave-function modulation increases the scattering matrix and further reduces the mobility. The overall reduction of the mobility in comparison to previous approach is about one-fourth.

We note in passing that in general, in addition to the above Coulomb interaction, the density modulation induced by the surface roughness also affects any interactions that depend on the electron density. If, in the absence of surface roughness, the interaction is described by $\int d\mathbf{r}\int d\mathbf{r}'\hat{n}(\mathbf{r})V_0(\mathbf{r},\mathbf{r}')\hat{n}(\mathbf{r}')$, then formally the effect of surface roughness can be simply included by replacing $V_0$ by

$$V(\mathbf{r},\mathbf{r}')\approx V_0(\mathbf{r},\mathbf{r}')\left(1-\frac{\Delta(\mathbf{r})+\Delta(\mathbf{r}')}{L}\right). \tag{22}$$

The validity of this effective Hamiltonian can be checked by solving the Schrödinger equation for a simple step, i.e., $z_+ = L\,\theta(-x) + (L+\Delta)\,\theta(x)$ and $z_- = 0$. We find that the fluctuations in both the energy level and the electron density are indeed reproduced by calculating the transmission amplitude.[14] Let us now briefly re-examine the effect due to the change of the single-particle state in the ballistic regime. For a single step, according to the Landauer formula,[11] the conductance due to the step is given by

$$G = \frac{e^2}{\pi\hbar}\,\frac{T}{R}, \tag{23}$$

where $T$ and $R$ are transmission and reflection probabilities. A simple analysis shows that the mobility is given by

$$\mu = \frac{|e|}{\pi\hbar n_0}\,\frac{T}{R} \simeq \frac{|e|}{\pi\hbar n_0}\left[\frac{L(1+\pi^2/k_F^2L^2)}{\Delta} - 1\right]$$
$$\simeq 4836\left[\frac{L(1+\pi^2/k_F^2L^2)}{\Delta} - 1\right]\ \mathrm{cm^2/V\,sec}. \tag{24}$$

For many steps, $\Delta$ needs to be replaced by $\Sigma\Delta_i$. But since $\Delta_i$ can be either positive or negative, $\Sigma\Delta_i \approx \Delta \approx 3$–$4$ Å. The mobility is then about $10^4 - 10^5$ $\mathrm{cm^2/V\,sec}$ for $L = 100$ Å. This number when combined with the contribution from Eq. (21) ($\sim 10^5$ $\mathrm{cm^2/V\,sec}$) predicts that the mobility is at the order of $10^4$ $\mathrm{cm^2/V\,sec}$, close to the experimental result.[15]

In conclusion, we have derived an effective Hamiltonian for two-dimensional quantum wells with rough interfaces. Two terms are generated. The first term is identified with the local energy-level fluctuations, which were introduced phenomenologically in the literature, but the previous form is now shown to be valid only when the Hamiltonian has one single length scale. The effect of this term on the electron mobility has been discussed before. The other term is a new finding, to our knowledge, which is shown to modulate the wave function and cause fluctuations in the charge density. We discuss its effects on the reduction of the electron mobility both at the level of the single-particle state and by including the many-particle interactions. An estimate of the electron mobility is made, and gives rise to the correct order in comparison to experimental data.

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