IC/89/400
INTERNAL REPORT
(Limited Distribution)

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

NEW REAL SPACE CORRELATED–BASIS–FUNCTIONS APPROACH FOR THE ELECTRON CORRELATIONS OF THE SEMICONDUCTOR INVERSION LAYER

Wei–guo Feng *
International Centre for Theoretical Physics, Trieste, Italy,

Hong–Wei Wang
Department of Physics, Jiujiang Teachers Training College,
Jiujiang, Jiangxi, People's Republic of China

and

Xiang Wu *
Centre of Theoretical Physics, CCAST (World Laboratory),
P.O. Box 8730, Beijing, People's Republic of China
and
International Centre for Materials Physics, Academia Sinica,
People's Republic of China.

MIRAMARE – TRIESTE
December 1989

* Permanent address: Department of Physics, Tongji University, Shanghai, People's Republic of China.

ABSTRACT

Based on the real space Correlated–Basis–Functions theory and the collective oscillation behaviour of the electron gas with effective Coulomb interaction, the many–body wave function is obtained for the quasi–two–dimensional electron system in the semiconductor inversion layer. The pair–correlation function and the correlation energy of the system have been calculated by the integro–differential method in this paper. The comparison with the other previous theoretical results is also made. The new theoretical approach and its numerical results show that the pair–correlation functions are definitely positive and satisfy the normalization condition.

1 Introduction

In the past few years, many scientists have been much interested in the area of the physics of quasi-superlattice[1~5]. This is because since the experimental observation of icosahedral symmetry in quenched Al-Mn alloy[6], the wealthy fascinating physical information has been revealed both experimentally and theoretically for the quasiperiod systems. In our recent paper[7] (hereafter referred to as paper I), a newly transfer-matrix method, which was first presented by Xue and Tsai[8] and was later developed by Feng *et al.*[9,10], was used for the calculation of the reflectivity of TE waves off a metallic Fibonacci quasi-superlattice (MFQSL). The very interesting phenomenon we found is that for the case of the S-polarized soft X-rays and extreme ultraviolet, the reflecting spectrum pattern has the self-similar properties around the numerous scaling points with the increasing of the generation number. Besides, we found that due to the remodelling of the reflection curves as a function of frequency, some new peaks move to the higher frequency positions, which stimulate interest in the study and making of soft X-rays and extreme ultraviolet reflectors. The imperfection of paper I is that when the electron system in the MFQSL is considered as an ideal plasma liquid, the effect of retardation on the reflection has been neglected, therefore the numerical results could not predict the real case quantitatively. In this paper, we will prove the previous theory by including the retardation effect to the MFQSL system. For the details of the model structure of MFQSL system and relevant parameters, please refer to paper I and Ref. [2].

2 General formalism for the reflectivity

The system of MFQSL is generated by two elementary seeds, blocks L and B, mapping the mathematical rule in the Fibonacci sequence, i.e.,

$$S_1 = \{L\}, S_2 = \{LS\}, S_3 = \{LSL\}, \ldots, S_n = S_{n-1}S_{n-2}. \tag{1}$$

The Block L in this case is composed of metal A of thickness d_A and metal B of thickness d_{BL}, while for the block S, the only difference compared with the block L is that the metal B in block S is of the shorter thickness d_{BS}. As adopted in Paper I, the ratio of the thickness of the two elementary blocks

is just the inverse of the golden mean,

$$\Lambda \equiv \frac{d_A + d_{BS}}{d_A + d_{BL}} = \frac{\sqrt{5}-1}{2}. \tag{2}$$

To obtain the reflectivty for the S-polarized soft X-rays and extreme ultraviolet, we start from the general TE wave equation[7] for the MFQSL system,

$$\frac{d^2 E_y}{dz^2} + [(\omega/c)^2 \epsilon(\omega) - q^2] E_y = 0, \tag{3}$$

where q is a common x component wave vector, as a function of the incident angle θ, we have

$$q = (\omega/c)\sin\theta. \tag{4}$$

In paper I, the dielectric function $\epsilon(\omega)$ in Eq.(3) is approximated in the form for the ideal case,

$$\epsilon_I(\omega) = 1 - \frac{\omega_P^2}{\omega^2}. \tag{5}$$

To take account of the retardation effect on the reflection, we choose the model dielectric function in the form of Drude local dielectric function for the MFQSL system,

$$\epsilon_D(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\omega/\tau}. \tag{6}$$

where τ is the electric relaxation time in the metal layers.

We note that all the self-contained equations and the transfer-matrices driven by paper I are still available for the present calculation except for the wave vector in the metallic layers is changed to the complex form,

$$k_\mu = \alpha_\mu + i\beta_\mu, \tag{7}$$

$$\alpha_\mu = \sqrt{A_\mu}\{\frac{1}{2}[(1 + (\frac{B_\mu}{A_\mu})^2)^{1/2} + 1]\}^{1/2}, \tag{8}$$

$$\beta_\mu = \sqrt{A_\mu}\{\frac{1}{2}[(1 + (\frac{B_\mu}{A_\mu})^2)^{1/2} - 1]\}^{1/2}, \tag{9}$$

$$A_\mu = k_0^2 - \frac{(\omega_{P\mu}/c)^2}{1 + \frac{1}{\omega^2\tau^2}}, \tag{10}$$

$$B_\mu = \frac{(\omega_{P\mu}/c)^2}{\omega\tau(1 + \frac{1}{\omega^2\tau^2})}, \tag{11}$$

where

$$k_0 = (\omega/c)\cos\theta \qquad \omega_{r\mu} = \sqrt{4\pi n_\mu e^2/m}, \tag{12}$$

and μ runs from A to B for the two different electron densities n_A and n_B in the metallic multilayers. The transfer-matrices of the MFQSL system, as a consequence, also become the complex ones. Following the way presented in Paper I and through directly mathematical calculation, we finally obtain the reflectivity for the nth generation MFQSL as follows,

$$R = |r|^2, \tag{13}$$

$$r = \frac{\eta_1(k_A + k_0) - \eta_2(k_A - k_0)}{\eta_2(k_A + k_0) - \eta_1(k_A - k_0)}, \tag{14}$$

$$\eta_1 = exp(i2k_A d_A)[w_{21}(k_B + k_0) + w_{22}(k_B - k_0)], \tag{15}$$

$$\eta_2 = w_{11}(k_B + k_0) + w_{12}(k_B - k_0), \tag{16}$$

where w_{ij} denotes the element of the matrix W, which is defined as

$$W \equiv \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \equiv \begin{cases} X_A^{-1} C_n C_1 \tilde{X}_{BL} & \text{when } n = \text{odd number} \\ X_A^{-1} C_n C_0 \tilde{X}_{BS} & \text{when } n = \text{even number.} \end{cases} \tag{17}$$

Here

$$X_\mu \equiv \begin{bmatrix} 1 & 1 \\ ik_\mu & -ik_\mu \end{bmatrix}, \tag{18}$$

$$\tilde{X}_\mu \equiv \begin{bmatrix} exp(-ik_\mu d_\mu) & exp(ik_\mu d_\mu) \\ ik_\mu exp(-ik_\mu d_\mu) & -ik_\mu exp(ik_\mu d_\mu), \end{bmatrix} \qquad \mu = A, BL, BS, \tag{19}$$

and the nth order transfer-matrix C_n is generated in the manner of the Fibonacci sequence,

$$C_n = C_{n-1} C_{n-2}, \tag{20}$$

with the two initial generating seeds, which is corresponding to the two elementary units of the metallic multilayers, as defined in paper I,

$$C_0 = M_{BS} M_A \qquad C_1 = M_{BL} M_A, \tag{21}$$

$$M_\mu \equiv \begin{bmatrix} \cos k_\mu d_\mu & -\sin k_\mu d_\mu / k_\mu \\ k_\mu \sin k_\mu d_\mu & \cos k_\mu d_\mu \end{bmatrix} \qquad \mu = A, BL, BS. \tag{22}$$

3 Numerical results and conclusions

In order to compare with the previous theoretical results, we take the same relevant parameters as in paper I. We still choose the thicknesses of the metal layers as $d_A = 100\text{Å}$, and $d_{BL} = 200\text{Å}$. For the metallic electron densities, we take $n_A = 8.63 \times 10^{23} cm^{-3}$ and $n_B = 18.1 \times 10^{23} cm^{-3}$. In the frequency range from $0.75\omega_{PB}$ to $2.75\omega_{PB}$, we plotted the two calculated reflectance curves for the normal incidence as shown in Fig. 1. The curve (b) for the case of $\tau = 100/\omega_P$, and the curve (a) is for the limiting case, in which the effect of the retardation is neglected, which is just the same as the case of Paper I.

From our numerical results, we find that when the retardation is taken into consideration, the maxima of the reflection are reduced monotonously. The self-similar pattern of the curves is thus restrained strongly with the increasing of the generation number in the low frequency range. This can be easily understood, for we know that when let the electric relaxation time τ approach infinity, which means there is no damping in the system, all of the metal layers will give the contributions to the phase superposition in the manner of reflection, which enhances the self-similarity. But when τ is introduced into the dielectric function, the consequent damping effect restricts the reflecting contribution from the metal layers far from the surface of the MFQSL. So while we increase the generation number, which means adding more metal layers, the fine structure of the self-similar pattern of the reflectivity will gradually disappear at the ideal scaling points due to the limiting contribution from the extra-layers.

Fortunately, we find that for the high frequency region or for the grazing incidence, the effect of retardation can be ignored due to the form of dielectric function we choose. This is also true in the real experiments. Fig. 2 shows the rescaled reflectance curves for the three generation number, n =9, 12 and 15 around an incident angle 80.35°, which shows that the self-similarity still exists for the large incident angles. From our present theoretical calculations, we find that for the finite generation numbers ($n \leq 18$), the six-circle property[3,4] around the fixed points for the reflectivities is approximately of the following form,

$$R_{n+6}[\Lambda^6(\theta - \theta_0)] = R_n(\theta - \theta_0). \tag{23}$$

This equation suggests a simple way to test the predicted scaling results.

As the reflectivity for the grazing incidence of higher frequency will be only slightly affected by the effect of the retardation, the aperiodic design of MFQSL is a stimulating way to enhance the reflectivities for the soft X-rays and extreme ultraviolet.

ACKNOWLEDGMENTS

The authors gratefully acknowledge many helpful discussions with Drs. Hong Chen, Deng-ping Xue, and they also thank Professor Zhong-xiu Fan for suggesting and encouraging this work. One of the authors (W.F.) would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste. Part of this work was supported by the Chinese National Advanced Technology Foundation through grant No.144-05-085.

References

[1] P. J. Steinhardt and S. Ostlund, *The Physics of of Quasicrystals*, (World Scientific, Singapore, 1987).

[2] R. Merlin, K. Bajema, R. Clarke, F. Y. Juang and P. K. Bhattacharya, Phys. Rev. Lett. **55**, 1768 (1985).

[3] M. Kohmoto and J. R. Banavar, Phys. Rev. **B34**, 563 (1986).

[4] M. Kohmoto, B. Sutherland and C. Tang, Phys. Rev. **B35**, 1020 (1987).

[5] D. Levine and P. J. Steinhardt, Phys. Rev. Lett. **53**, 2477 (1984).

[6] D. Shechtman, I. Blech, D. Gratias and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).

[7] Wei-guo Feng, Wen-zhong He, Deng-ping Xue, Yi-bing Xu and Xiang Wu, J. Phys.: Condensed Matter **1**, in press (1989).

[8] Deng-ping Xue and C. H. Tsai, Commun. Theor. Phys. (China) **9**, 279 (1988).

[9] Wei-guo Feng, Yan-ping He and Xiang Wu, *Proc. Workshop on the Physics of Superlattice and Quantum Well* (World Scientific, Singapore, 1988).

[10] Wei-guo Feng, Yan-ping He and Xiang Wu, Acta Optics Sin., in press (1989) .

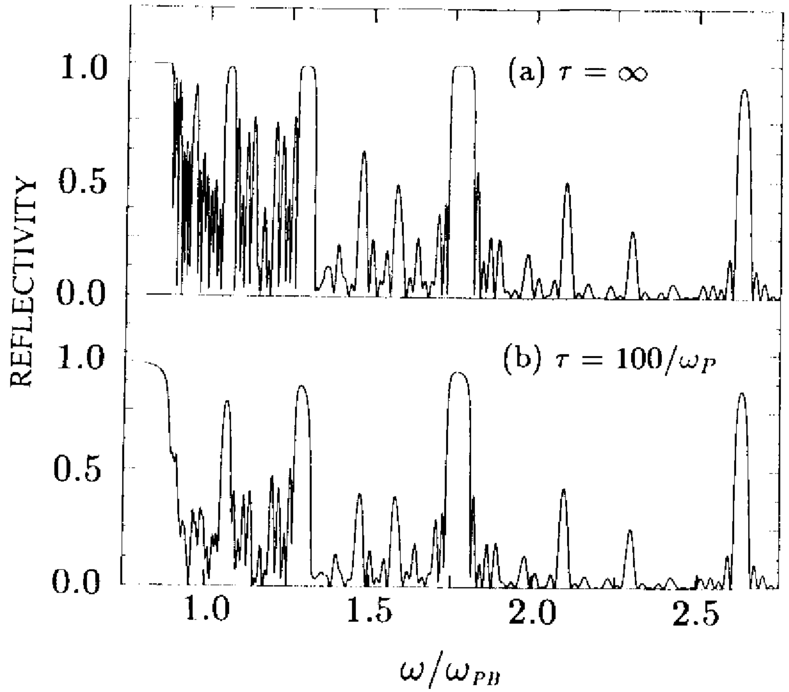

Fig.1. Reflectivities for normal incidence on the 9th generation MFQSL with 110 metal layers. $\omega_{PB} = 2.4 \times 10^{16} s^{-1}, d_A = 100 Å$ and $d_{BL} = 200 Å$. The upper figure demonstrates the ideal case without the retardation effect.

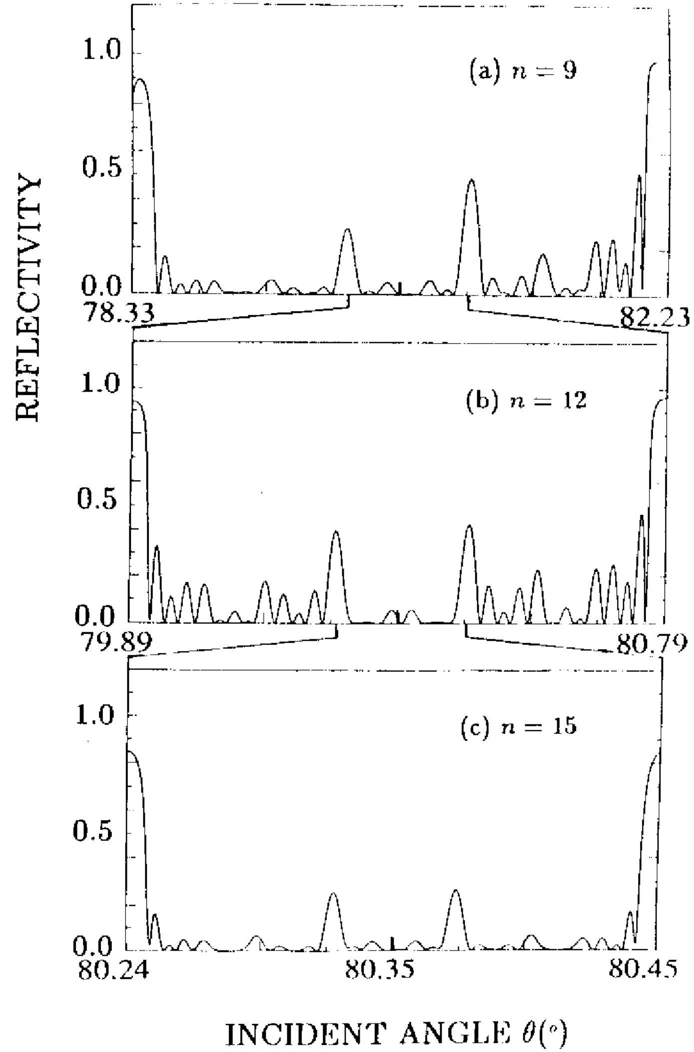

Fig.2. Reflectivities of the grazing incidence on the three generation MFQSL systems S_0, S_{12} and S_{15} for the incident wave length $\lambda = 60 Å$. The other relevant parameters are the same as in Fig.1.