Weak Localization and Electron-Electron Interactions theories applied to the positive magnetoresistance in metallic $Si_{1-y}Ni_y$:H alloys

A. Narjis[1], A. El kaaouachi[1], S. Dlimi[1], A. Sybous[1], L. Limouny[1], R. Abdia[1], G. Biskupski [2]

[1] *Research Group ESNPS , Physics department, University Ibn Zohr, Faculty of Sciences, B.P 8106, Hay Dakhla, 80000 Agadir, Morocco.*

[2]*Laboratoire de Spectroscopie Hertzienne (CNRS), équipe des semiconducteurs, Université des Sciences et Technique de Lille I, F 59655 Villeneuve d'Ascq Cédex, France.*

Corresponding author: narjis78@gmail.com

Abstract: Electrical conductivity of hydrogenated amorphous silicon nickel alloys ($Si_{1-y}Ni_y$:H) is discussed on the metallic side of the metal insulator transition (MIT), at very low temperature, and in the presence of magnetic field up to *4.5T*. The experimental results are analyzed in the light of weak localization and electron-electron interaction theories in a strong spin-orbit case. The zero magnetic field conductivity is almost found to vary according to the formula $\sigma(B=0,T)=\sigma_0+m.T^{1/2}$. Physical interpretations of our results are given to understand the diffusion mechanism.

Keywords: Amorphous silicon-nickel alloys a-$Si_{1-y}Ni_y$: H; Transport phenomenon; Weak localization; Electron electron interaction; negative magnetoconductivity; Inelastic scattering time.

I- Introduction

In the last few decades, the magnetoconductivity (MC) has been an important physical property in various disordered systems such as amorphous alloys, granular metals, metallic glass… [1-5]. Much efforts, both theoretically and experimentally have been made to study the combined effects of weak localization (WL) and electron electron interaction (EEI). These effects assume more and more importance as the temperature is very low (near 0K).

The WL is a result of the constructive interference by partial travelling along time reversed electron path. Thouless [6] first studied this effect by applying the scaling theory, and found that it is dependent on the dimension of the system.

The EEI traduces the effect of the orbit and the spin on the energy of electrons during its scattering. This phenomenon has been studied theoretically by B. L. Altshuler [7] and A. Lee, and T. V. Ramakrishnan [8] by studying the influence of the temperature and the magnetic field on the electrical magnetotransport.

In this paper we are reporting the low-temperature properties transport in hydrogenated amorphous silicon nickel alloys ($Si_{1-y}Ni_y$:H) without and then within a magnetic field up to *4.5T*.

II- Experimental details

The samples were prepared by radio-frequency sputtering from silicon target. The substrates (Corning 7059 glass) were at room temperature during deposition and the sputtering gas was a 90% Ar and 10% H_2. The hydrogen was added to saturate silicon dangling bonds that might caused by the disorder.

Film thickness which were about 1µm, were measured to an accuracy of 0.1 µm using a Talysurf stylus. The amorphous nature was demonstrated by electron diffraction measurements in a transmission electron microscope.

The electrical resistivity was measured using standard four-terminal AC techniques.

We focus our study on the electrical transport in the amorphous alloy referenced 29% (where *y=0.29*).

III- Results and discussion:

3-a- Experimental data

The free mean path can be calculated from the conductivity at *T=0K*. $\sigma_0(T=0)$ is generally deduced from the Boltzmann conductivity:

$$\sigma_B = \frac{n.e^2.l_0}{m^*.V_F} \qquad (1)$$

Using equation (1), we found $l_0 = 0.24\,\mathring{A}$. This value is smaller than the Ni-Ni distance ($a \approx 3\,\mathring{A}$). However, the sample is from the metallic side of the MIT (detailed latter), thus l_0 have to be larger than *a*. Therefore we have to apply the perturbation theory [9]:

$$\sigma_0 = \sigma_B.(1 - C/(K_F l_0)) \qquad (2)$$

Where *C* is an integer constant between *1* and *3*.

Using this equation with *C=1* we obtain $l_0 = 7.8\,\mathring{A}$. and $K_F l_0 = 3.77$. This value is in agreement with Ioffe-Regel criterion $K_F l_0 = \pi$.

The diffusion constant *D* is calculated using the formula $D=D_0.(y- y_c)^{t-\beta}$ [10] where *t=1.9* in 3D [11] and $\beta=0.41$ [12]. D_0 is the diffusion constant in the metallic alloy $Si_{0,50}Ni_{0,50}$:H.

In fig. 1, we plotted the variation of the conductivity versus temperature at *B=0* for the amorphous alloys $Si_{1-y}Ni_y$:H (*y=0.23; 0.26; 0.29*; 0.*50*; and *0.52*). The curves can be fitted to the following formula used for doped crystalline and amorphous semiconductors [13-15]:

$$\sigma = \sigma_0(y) + m(y).T^Z \qquad (3)$$

Where $\sigma_0(y)$ is the residual *T=0* term. We obtain the best linear fits with an exponent *z* close to *0.5 (z=0.42* for *y=0.23*, z=*0.45* for *y=0.26*, and *z=0.64* for *y=0.29)*. Our results are obtained with better accuracy by using the percentage deviation method. We adjusted the parameters $\sigma_0(y)$ and *m(y)* in equation (3) for each value of the exponent z varying between *0* and *1* by a step of 0.01, and calculate the percentage deviation defined as:

$$Dev(\%) = \left[\frac{1}{n} \sum_{i=1}^{n} \left(\frac{100}{\sigma_i} \left([\sigma_0(y) + m(y).T^Z] - \sigma_i \right) \right)^2 \right]^{1/2} \qquad (4)$$

The minimum deviation correspond to the best value of the exponent *z*. the plot of *Dev(%)* versus exponent *z* is shown in fig. 2 for each alloy. The exponents close to *0.5* suggest that the EEI is the main correction to the conduction phenomenon in absence of magnetic field.

In a previous study, Biskupski et al. [16] observed a transition from *z=1/2* to *z=1/3* in n-InP with decreasing magnetic field, and suggested that this crossover is due to the competition between two length scales: the correlation length and the interaction length. This is not the case here even if *B=0*.

We observe also that the alloy referenced 23% (where *y=0.23)* is an insulator since σ_0 is "negative". In contrast, for *y=0.26* and *0.29*, the conductivity is positive at *T=0*, thus the alloys referenced 26% and 29% are in the metallic side and near the MIT. The alloys referenced 50% and 52% (where *y=0.50* and *0.52*, respectively) are clearly metallic because y>>0.24.

By considering the function *w(T, x) = dLn(σ)/dLn(T)* for $Si_{1-x}Ni_x$, Rosenbaum et al. [1] found the exponent *z* to be close to *0.5 (z=O.79)* for *x=0.248*.

The positive value of the factor *m>0* presents other reason to refer that the electron-electron interaction is dominant over the WL at zero magnetic field. We have shown this property in n-GaAs [17], in $Si_{1-x}Ni_x$ close to the MIT [18], and in doped conducting polymers [19].

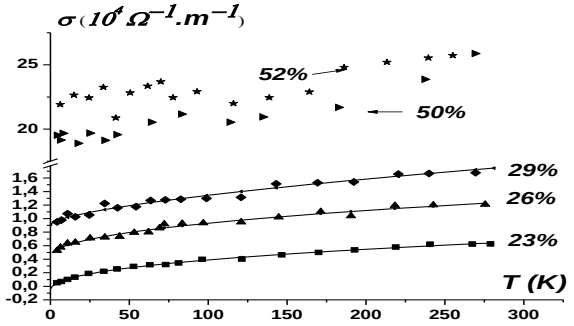

Figure 1. Zero magnetic field conductivity versus temperature for various nickel compositions.

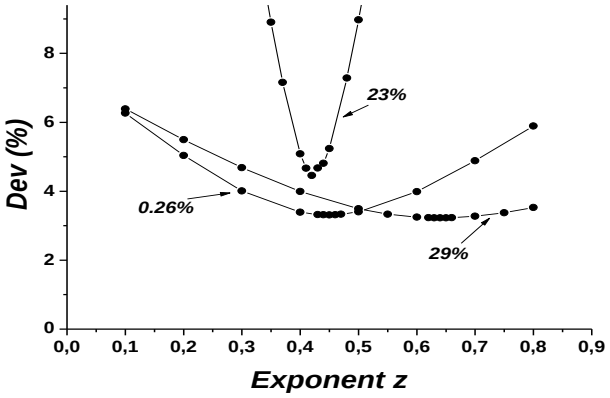

Figure 2. Pourcentage deviation versus exponent *z* in equation (3) for various nickel compositions.

In fig. 3, we plotted the variation of the conductivity as a function of magnetic field. The negatives values of the magnetoconductivity are produced by the strong spin-orbit scattering. The magnetoconductivity increases rapidly with the temperature, most likely due to the effect of the thermal energy and the field splitting in the interval of the temperature *1.7K < T <4.2K*.

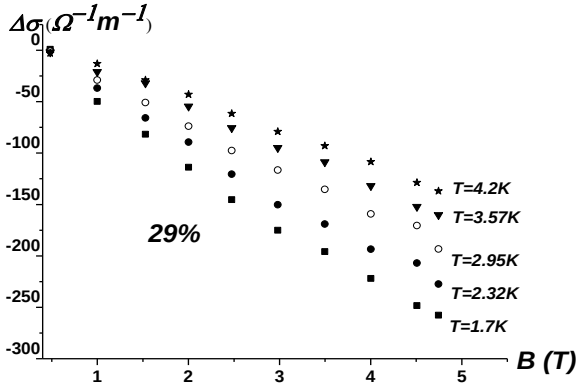

Figure 3. Conductivity versus magnetic field for the alloy referenced 29%.

3- b- Weak localization

The transport mechanism, either in absence or with magnetic field, has been interpreted by two distinct contributions , the weak localization (WL) and the electon electron interactions (EEI) phenomenon so that :

$$\Delta\sigma = \Delta\sigma(WL) + \Delta\sigma(EEI) \tag{5}$$

The expression of the first contribution (i.e. the WL) was given by Baxter et al. [20] as:

$$\Delta\sigma_{WL}(B,T) = \left(\frac{e^2}{2\hbar^2}\right)\sqrt{\frac{eB}{\hbar}}\left[\frac{3}{2} f_3\left(\frac{B}{B_{in}(T)+\frac{4}{3}B_{so}+\frac{2}{3}B_s}\right) - \frac{1}{2} f_3\left(\frac{B}{B_{in}(T)+2B_s}\right)\right] \tag{6}$$

In this expression B_x=h/8π.D.e.B.τ_x where x=*so* for the spin-orbit scattering calculated from the value of the elastic scattering time τ_0 using the formula $\tau_{so} = \tau_0(137/Z)^4$ as it was proceeded by Resombaum et al. [1] ($Z=28$ is the atomic number of nickel). In the same reference and to simplify the calculations, the magnetic scattering was taking to be very weak- that $B_s=0$ (i.e. $\tau_s=0$). The variations of the inelastic scattering time τ_{in} with the temperature allow to identify which the mechanism of the scattering that dominates in the sample.

The function $f_3(x)$ was given numerically approached by an error of *0.1%* by Baxter et al. [20] as the following:

$$f_3(x) = 2\left[\sqrt{2+x} - \sqrt{x}\right] - \left[\left(\frac{1}{2}+x\right)^{-1/2} + \left(\frac{3}{2}+x\right)^{-1/2}\right] + \frac{1}{48}(2.03+x)^{-3/2} \tag{7}$$

3- c- Electron electron interaction

3- c- 1- Orbital contribution

The second term in equation (5) is also written as a sum of two contributions, the first one is the orbital contribution, and was expressed by B. L. Altshuler [7]:

$$\Delta\sigma_{CO}(B,T) = -\frac{e^2}{2\pi^2\hbar} g(B,T)\sqrt{\frac{eB}{\hbar}}\varphi_3\left(\frac{2DeB}{\pi k_B T}\right) \tag{8}$$

Where $g(B,T)$ is the renormalized coupling constant, expressed by A. Lee And T. V. Ramakrishnan [8] as:

$$g(B,T) = \frac{F/2}{1+(F/2).\ln(E_F/E_0)} \tag{9}$$

Where

$$E_0 = \max(D.e.B, 1.7464.K_B.T) \tag{10}$$

The Hartree Fock constant F is between *0* and *1*, it is an adjustable parameter in our work. Nevertheless we have calculated it using two theoretical methods: the Thomas-Fermi approximation "$F_{T\text{-}F}$", and the Kleinman-Langreth dielectric function [21-22] "$F_{T\text{-}F}$ ".

$$F_{T-F} = \frac{\ln(1+x)}{x} \tag{11}$$

Where $x = \left(\frac{2k_F}{K_{T-F}}\right)^2$

K_F is the Fermi vector and $F_{T\text{-}F}$ is the Thomas-Fermi scattering vector.

$$F_{K-L} = \frac{\ln(1+\alpha)}{\alpha} \tag{12}$$

where $\alpha = \left(\frac{K_S}{2k_F}\right)^2$

where K_S is the scattering parameter given by:

$$K_S = K_F\left(\frac{2}{1+0.158\left(\frac{k_{TF}}{2k_F}\right)^2} - 1\right)^{1/2} \tag{13}$$

and $k_{TF} = \left(\frac{12\pi m^* n e^2}{4\pi\varepsilon\varepsilon_0\hbar^2 K_F^2}\right)^{1/2}$

We have obtained for our sample: $F_{T\text{-}F}$ *=0,072* and $F_{K\text{-}L}$*= 0,892*.

The function $\varphi_3(x)$ is defined for long phase coherence time by:

$$\varphi_3(x) = \sqrt{\frac{\pi}{2x}}\int_0^\infty \frac{\sqrt{t}}{sh^2(t)} \times \left(1 - \frac{xt}{sh(xt)}\right)dt \tag{14}$$

and was approached with an accuracy of $2{,}5.10^{-4}$ [20,23]:

- for $x \le 0.7$

$$\varphi_3(x) = 0.32925x^{3/2} - 0.11894x^{7/2} + 0.10753x^{11/2} - 0.0636x^{6.63}$$

- for $0.7 \le x \le 2.4$

$$\varphi_3(x) = -0.03043 + 0.22616x + 0.14104x^2 - 0.10293x^3 + 0.02759x^4 - 0.0028x^5$$

- for $x \ge 2.4$

$$\varphi_3(x) = 1.900344 - \frac{2.29392}{\sqrt{x}} + \frac{1.2266}{x^2} - \frac{0.826}{x^{7/2}}$$

3- c- 2- Zeeman effect

The spin splitting in the diffusion channel has been considered by Lee and Ramakrishan [8] who assumed that the Hartree interaction between opposite spins is alone sensitive to the magnetic field B. The exchange term implies a correlation between electrons of the identical spin and is constant when B varies. Thus the correction to the conductivity caused by Zeeman effect is:

$$\Delta\sigma_{ZE}(B,T) = \frac{-e^2}{4\pi^2\hbar} F\left(\frac{k_B T}{2\hbar D}\right)^{1/2} g_3(h) \quad (15)$$

Where $h = \frac{g_e \mu_B B}{k_B T}$; g_e is the Landé factor, and μ_B the Bohr magneton.

The function g_3 has the following form:

$$g_3(h) = \int_0^\infty d\Omega . \frac{d^2\left[\Omega(1/e^\Omega - 1)\right]}{d^2\Omega} \times \left(\sqrt{\Omega + h} + \sqrt{|\Omega - h|} - 2\sqrt{\Omega}\right) \quad (16)$$

and was approached with an accuracy of $2{,}5.10^{-4}$ [23]:

- for $h \le 3$

$$g_3(h) = 5.646410^{-2} h^2 - 1.475910^{-3} h^4 + 4.274710^{-5} h^6 - 1.535110^{-6} h^8 + 610^{-8} h^{10}$$

- for $3 \le h \le 8$

$$g_3(h) = 0.64548 + 0.235(h-4) - 7.4510^{-4}(h-4)^2 - 2.9410^{-3}(h-4)^3 + 6.3210^{-4}(h-4)^4 - 5.2210^{-5}(h-4)^5$$

- for $h \ge 8$

$$g_3(h) = \sqrt{h} - 1.2942 - \frac{\pi^2}{12h^{3/2}} - \frac{\pi^4}{16h^{7/2}} - \frac{5\pi^6}{32h^{11/2}}$$

In fig. 4 we tentatively fitted the experimental magnetoconductivity to the equation (5) through theories and approximations described above. The adjustable parameters are τ_{in} and F.

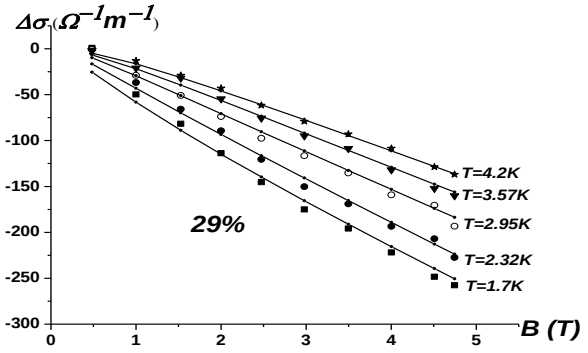

Figure 4. Conductivity versus magnetic field for sample referenced 29%. The solid curves correspond to the theoretical predictions detailed in text.

It was worth notice during our calculations that the negative magnetoconductivity is dominated by the WL effect. In fact, by introducing the magnetic field, we suppress this effect.

In fig. 5, we plot the inelastic scattering time versus temperature as derived from the adjustments in fig. 4 using the above theories. It is found to vary as:

$$\tau_{in} = 1{,}05.10^{-10}.T^{-1,86}$$

Where T is in Kelvin and τ_{in} is in second.

The exponent is close to 2. This quadratic temperature dependence ($\tau_{in} \alpha T^{-2}$) indicates that the electron phonon scattering dominates the electrical transport [24, 26]. This property has been observed in disordered three-dimensional alloys [26-28].

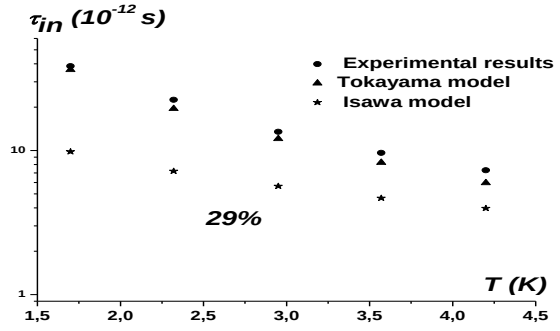

Figure 5. Inelastic scattering time for sample referenced 29% versus temperature obtained by using the complete model (WL + EEI), and by applying theories explained in the text.

Our results have to be compared to some theories that treat the low temperature scattering. The inelastic scattering time is written:

$$\tau_{in}^{-1} = \tau_{e-ph}^{-1} + \tau_{e-e}^{-1} \qquad (17)$$

As the electron phonon scattering dominates in our sample, we can eliminate the second term.
Tokayama [29] studied the scattering caused by phonons and give the following equation:

$$\tau_{e-ph}^{-1} = C'^2 . \frac{2\pi^2}{K_F . l} . \frac{k_B^2}{\hbar^2 . \omega_D} . T^2 \qquad (18)$$

Where $\omega_D = q_D . v_s$ is the Debye frequency (temperature) and $v_s = \tau_0 . m^* V_F^2 / 3.M$, and M is the ion mass. And C' a constant that depends on τ_0 , the valence Z, and the ions density n_i and given by: $C' = (2/Z)^{2/3} K_F^2 / 6\pi^2 . Z . n_i$.
Isawa [30] studied the inelastic scattering phenomenon in 3D systems, and found two terms in the total rate:

$$\tau_{in}^{-1} = 1.710^{11} (\hbar / E_F \tau_0)^2 T + 3.189 (\hbar \tau_0)^{1/2} (k_B T)^{3/2} / (E_F \tau_0)^2 \qquad (19)$$

However for $T < 0.166.h/2\pi.K_B.\tau_0$, only the first term is taken into account i[30].
Our results are in good agreement with Tokayama prediction, but slightly three times larger than the values found using Isawa approach. The discrepancy is most likely due to the fact that the temperature is too low. In fact, the ratio becomes more and more large with decreasing temperature. This disagreement was also observed in a previous study in amorphous $Si_{1-x}Ni_x$ alloy with $x=0.282$ below $4K$ [1].
The Hartree factor is found to be close to 0.9 at all temperatures. This value is slightly the same calculated under the Kleinman and Langreth approximation [21, 22] ($F_{K-L}=0.892$).

IV. Conclusion:

Either in absence or with magnetic field, the experimental results are consistent with the theoretical predictions considering the effects of the weak localization and the electron-electron interactions.
It is observed that the electrical conductivity increases with increasing temperature and decreases with increasing magnetic field. This observation suggests that WL effects dominates the electrical transport mechanism within magnetic field in hydrogenated amorphous silicon nickel alloys and indicates the strength of the spin-orbit coupling. However, the positive value of the slope m in the equation $\sigma(B=0,T)=\sigma_0+mT^Z$ (where z is close to $1/2$) allows us to infer that the EEI effect is dominant over the WL effect at $B=0$.
The quadratic low temperature behaviour of the inelastic scattering time suggests that the electrical transport is dominated by electron-phonons scattering. Our results are well consistent with theoretical model proposed by Tokayama. Whereas, Isawa model is not observed probably because the temperature is very low.
The Hartree factor is consistent with Kleinman and Langreth approximation.

References

[1] R. Rosenbaum, A. Heinesy and A. Palevskiy, J. Phys.: Condens. Matter **9** (1997) 5395–5411.
[2] A. El kaaouachi, A. Moudden, A. Nafidi and G. Biskupski Physica B **304** (2001) 377–381.
[3] S. Shekhar , V. Prasad and S.V. Subramanyam Physics Letters A, **361** (2007) 500–503.
[4] A.K. Majumdar Journal of Magnetism and Magnetic Materials, **263** (2003) 26–31.
[5] C. Biagini, T. Caneva, V. Tognetti and A. A. Varlamov Phys. Rev. B, **72** (2005) 041102 (R).
[6] D.J. Thouless, Physi. Rev. Lett. **39** (1977) 116.
[7] B. L. Altshuler., A. G. Aronov, A. I. Larkin and D. E. Khmelmitskii, Sov.Phys-JETP, **54** (1981) 4111.
[8] A. Lee and T. V. Ramakrishnan, Rev. Modern Phys, **57** (1985) 287.
[9] Mott N F and Kaveh M Adv. Phys, **34** (1985) 329.
[10] Entin-Wohlman O, Kapitulnik A, Alexander S and Deutscher G Phys. Rev. B, **30** (1984) 2617.
[11] Derrida B, Stauffer D, Herrmann H J and Vannimenus J J. Physique Lett, **44** (1983) L701.
[12] Alexander S Phys. Rev. B, **27** (1983) 1541.
[13] F. Hellman, M. Q. Tran, A. E. Gebala, E. M. Wilcox, and R. C. Dynes, Phys. Rev. Lett, **77** (1996) 4652.
[14] C. Leighton, I. Terry, and P. Becla, Phys. Rev. B, **58** (1998) 9773.
[15] G. A. Thomas, A. Kawabata, Y. Ootuka, S. Katsumoto, S. Kobayashi, and W. Sasaki, Phys. Rev., B **26** (1982) 2113.
[16] G. Biskupski, A. El kaaouachi, and A. Briggs J. Phys. Condens. Matter, vol. **3** (1991) pp. 8417-8424.
[17] A. Sybous, A. Elkaaouachi, N. AitBenAmeur, B. Capoen, J. Hemine, R. Abdia, A. Narjis, H. Sahsah, G. Biskupski, Physica B, **406** (2011) 3489–3492
[18] A. Mobius, C. Frenzel, R. Thielsch, R. Rosenbaum, C.J. Adkins, M. Schreiber, H.-D. Bauer, R. Grotzsche, V. Hoffmann, T. Krieg, N. Matz, H. Vinzelberg, and M. Witcomb, Phys. Rev. B**, 60** (1999) 14209–14223.
[19] M. Ahlskog and R. Menon, J. Phys.: Condens. Matter, **10** (1998) 7171.
[20] D. V. Baxter, R. Richter, M. L. Trudeau, R. W. Cochrane, J. O. Strom-Olsen, J. Phys. France, **50** (1989) 1673.
[21] L. Kleinman, Phys . Rev., **160** (1967) 585.
[22] D. Langreth, Phys . Rev., **181** (1969) 753.
[23] Ousset J C, Askenazy S, Rakoto H and Broto J M J. Physique, **46** (1985) 2145.

[24] A. Sergeev, V. Mitin, Phys. Rev. B, **61** (2000) 6041.
[25] A. Sergeev and V. Mitin, Superlattices Microstruct., **27** (2000) 499;
[26] J. Rammer and A. Schmid, Phys. Rev. B **34** (1986) 1352.
[27] G. Bergmann, W. Wei, Y. Zou and R.M. Mueller, Phys. Rev. B **41** (1990) 7386.
[28] Y. K. Kuo and K. M. Sivakumar C. A. Su, C. N. Ku, and S. T. Lin A. B. Kaiser J. B. Qiang, Q. Wang, and Dong Physical Review B, **74** (2006) 014208.
[29] H. Z Tokayama, Phys, **263** (1973) 329.
[30] Y. Isawa, J. Phys. Soc. Japan **53** (1984) 2865.

