The effective Hamiltonian H^, describing the motion of a spin σ electron in the static self-consistent approximation is (E.N. Economou, P. Mihas 1977)

$$\hat{H} = \sum_{i\sigma} (\epsilon_0 + \epsilon_{I\sigma})\hat{n}_{i\sigma} + \sum_{ij} V_{ij}\, \alpha_i^+ a_j$$

where the site energy $\varepsilon_0 + \varepsilon_{i\sigma}$ is

$$\varepsilon_0 + \varepsilon_{i\sigma} = \varepsilon_0 + \frac{U}{2} \pm \frac{U\mu}{2} \qquad (2.2)$$

For simplicity we choose $\varepsilon_Q$+ U/2 = 0; then the siteener-

gies for a spin up electron ($\sigma$ = +1) are as shown in Figure lb, where x = Uμ/2

$$\boldsymbol{\mu} = \langle \hat{n}_{i\uparrow} \rangle_{\iota-\theta} - \langle \hat{n}_{i\downarrow} \rangle_{\iota-\theta} \qquad (1.3)$$

The corresponding site DOS $\rho_A$, $\rho_g$ are given by

$$\rho_\alpha = -\frac{I}{\pi} \operatorname{Im} G_a(E^+), \qquad a = A, \ B \qquad (2.7)$$

where $E^+$ denotes the limit of $G_a(E + is)$ as $s \to 0^+$. The self-consistency Eq. (1.3) for the size of the moment u becomes

$$\mu = \int_{-\infty}^{0} [\rho_B(E) - \rho_A(E)]\delta E$$

$$G_A(iy) = 2K(iy + x)((K-1)(-y^2 - x^2) + (K+1)(-y^2 - x^2)^{1/2}(-y^2 - x^2 - B^2)^{1/2})^{-1}$$

$$G_A(iy) = 2K(iy + x)(-(K-1)(y^2 + x^2) - (K+1)(y^2 + x^2)^{1/2}(y^2 + x^2 + B^2)^{1/2})^{-1}$$

$$\mu = \frac{1}{\pi} Im \int_0^\infty \frac{2K(x - iy)}{D} + \frac{2K(x + iy)}{D} dy = \frac{1}{\pi} Im \int_0^\infty \frac{4Kx}{D} diy = \frac{1}{\pi} \int_0^\infty \frac{4Kx}{D} dy =$$

$$= \frac{1}{\pi} \int_0^\infty \frac{4Kx}{(K-1)(x^2 + y^2) + (K+1)\sqrt{(x^2 + y^2)(x^2 + y^2 + B^2)}} dy =$$

$$= \frac{1}{\pi} \int_0^{\pi/2} \frac{4Kx}{(K-1)(x^2 + x^2 \tan^2\vartheta) + (K+1)\sqrt{(x^2 + x^2 \tan^2\vartheta)(x^2 + x^2 \tan^2\vartheta + B^2)}} dx\tan\theta =$$

$$= \frac{1}{\pi} \int_0^{\pi/2} \frac{4K}{(K-1) + (K+1)\sqrt{(1 + (B/x)^2 cos^2\theta)}} d\theta =$$

$$= \frac{1}{\pi} \int_0^{\pi/2} \frac{4K}{(K-1) + (K+1)\sqrt{\left(1 + \left(\frac{B}{x}\right)^2 - \left(\frac{B}{x}\right)^2 sin^2\theta\right)}} d\theta =$$

$$\gamma = \frac{\left(\frac{B}{x}\right)}{\sqrt{1+\left(\frac{B}{x}\right)^2}} \quad |\gamma| \leq 1$$

$$\mu = \frac{1}{\pi}\int_0^{\pi/2} \frac{4K}{(K-1)+\delta\sqrt{(1-\gamma^2 sin^2\theta)}}d\theta =$$

$$\delta = (K+1)\sqrt{\left(1+\left(\frac{B}{x}\right)^2\right)} \quad so\ \delta > 1$$

$$\mu = \frac{1}{\pi}\int_0^{\pi/2} \frac{4K\left[(K-1)-\delta\sqrt{(1-\gamma^2 sin^2\theta)}\right]}{(K-1)^2-\delta^2(1-\gamma^2 sin^2\theta)}d\theta =$$

$$= \frac{1}{\pi}\int_0^{\pi/2} \frac{4K\left[(K-1)-\delta\sqrt{(1-\gamma^2 sin^2\theta)}\right]}{(K-1)^2-\delta^2+\delta^2\gamma^2 sin^2\theta}d\theta =$$

$$= \frac{4K}{\pi}\int_0^{\pi/2} \frac{\left[(K-1)-\delta\sqrt{(1-\gamma^2 sin^2\theta)}\right]}{((K-1)^2-\delta^2)(1+\lambda sin^2\theta)}d\theta =$$

$$\lambda = \frac{\delta^2\gamma^2}{((K-1)^2 \ \ -\delta^2)} = \frac{(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)}{\left((K-1)^2 \ \ -(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)\right)}\frac{\left(\frac{B}{x}\right)^2}{\left(1+\left(\frac{B}{x}\right)^2\right)} = \frac{(K+1)^2}{\left((K-1)^2 \ \ -(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)\right)}\left(\frac{B}{x}\right)^2 < 0$$

$$\mu = \frac{4K(K-1)}{\pi((K-1)^2-\delta^2)}\int_0^{\pi/2} \frac{1}{(1+\lambda sin^2\theta)}d\theta - \frac{4K\delta}{\pi((K-1)^2-\delta^2)}\int_0^{\pi/2} d\theta\frac{(1-\gamma^2 sin^2\theta)}{(1+\lambda sin^2\theta)\sqrt{1-\gamma^2 sin^2\theta}} =$$

$$\frac{(1-\gamma^2 sin^2\theta)}{(1+\lambda sin^2\theta)} = \frac{1-\gamma^2 sin^2\theta}{(1+\lambda sin^2\theta)} = \frac{1-\gamma^2(1+\lambda sin^2\theta - 1)/\lambda}{(1+\lambda sin^2\theta)} =$$

$$= \frac{1+\frac{\gamma^2}{\lambda}-\frac{\gamma^2}{\lambda}(1+\lambda sin^2\theta)}{(1+\lambda sin^2\theta)} = \frac{1+\frac{\gamma^2}{\lambda}}{(1+\lambda sin^2\theta)} - \frac{\frac{\gamma^2}{\lambda}(1+\lambda sin^2\theta)}{(1+\lambda sin^2\theta)} =$$

$$= \frac{1+\frac{\gamma^2}{\lambda}}{(1+\lambda sin^2\theta)} - \frac{\gamma^2}{\lambda}$$

$$\mu = \left(\frac{4K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\int_0^{\pi/2} \frac{1}{(1+\lambda sin^2\theta)}d\theta - \frac{4K\delta}{\pi((K-1)^2-\delta^2)}\int_0^{\pi/2} d\theta\frac{(1-\gamma^2 sin^2\theta)}{(1+\lambda sin^2\theta)\sqrt{1-\gamma^2 sin^2\theta}}$$

$$\mu_1 = \frac{4K\delta}{\pi((K-1)^2-\delta^2)}\int_0^{\pi/2} d\theta\frac{(1-\gamma^2 sin^2\theta)}{(1+\lambda sin^2\theta)\sqrt{1-\gamma^2 sin^2\theta}}$$

$$= \frac{4K\delta}{\pi((K-1)^2-\delta^2)}\left[\int_0^{\frac{\pi}{2}} d\theta\frac{1+\frac{\gamma^2}{\lambda}}{(1+\lambda sin^2\theta)\sqrt{1-\gamma^2 sin^2\theta}} - \frac{\gamma^2}{\lambda}\int_0^{\frac{\pi}{2}}\frac{d\theta}{\sqrt{1-\gamma^2 sin^2\theta}}\right]$$

$$\boldsymbol{\mu_1 = \frac{4K\delta}{\pi((K-1)^2-\delta^2)}\left[\left(1+\frac{\gamma^2}{\lambda}\right)\Pi\left(\gamma,\lambda,\frac{\pi}{2}\right) - \frac{\gamma^2}{\lambda}K(\gamma)\right]}$$

$$\mu_2 = \left(\frac{4K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\int_0^{\pi/2} \frac{1}{(1+\lambda sin^2\theta)}d\theta = \left(\frac{4K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\int_0^{\pi/2} \frac{1}{(1+\lambda/2(1-cos2\theta)}d\theta$$

$$= \left(\frac{2K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\int_0^{\pi/2} \frac{1}{(1+\lambda/2)-\lambda/2cos2\theta)}d2\theta =$$

$$\mu_2 = \left(\frac{2K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\int_0^{\pi} \frac{2}{(2+\lambda)-\lambda cos\varphi)}d\varphi =$$

$$(2+\lambda)^2-(\lambda)^2 = 2(1+\lambda) = 2\frac{(K-1)^2 \quad -(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)+(K+1)^2\left(\frac{B}{x}\right)^2}{\left((K-1)^2 \quad -(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)\right)}$$

$$= 2\frac{(K-1)^2 \quad -(K+1)^2}{\left((K-1)^2 \quad -(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)\right)} = -2\frac{4K}{\left((K-1)^2 \quad -(K+1)^2\left(1+\left(\frac{B}{x}\right)^2\right)\right)}$$

$$= \frac{8K}{\left(4K+\left((K+1)^2\left(\frac{B}{x}\right)^2\right)\right)} > 0$$

$$\boldsymbol{\mu_2 = \left(\frac{2K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\int_0^{\pi} \frac{2}{(2+\lambda)-\lambda cos\varphi)}d\varphi = \left(\frac{2K(K-1)}{\pi((K-1)^2-\delta^2)}\right)\frac{4}{2\sqrt{1+\lambda}}\tan^{-1}\left(\sqrt{1+\lambda}\tan(\frac{\varphi}{2})\right)}$$

$$\boldsymbol{= \left(\frac{K(K-1)}{((K-1)^2-\delta^2)}\right)\frac{2}{\sqrt{1+\lambda}} = \left(\frac{\sqrt{K}}{(K-1)}\right)\sqrt{\left(4K+\left((K+1)^2\left(\frac{B}{x}\right)^2\right)\right)}}$$

$$\boldsymbol{\mu = \mu_2 - \mu_1}$$

***For the calculation of the elliptic integrals the method employed by*** Norman Derby and Stanislaw Olbert (2010). In their appendix the Basic program for Elliptic Integrals is presented. This was employed for a Visual Basic for Applications program used in the excel file "Magnetic moments
The excel fil is located in the site www.kyriakosxolio.gr (moment by elliptic function Microsoft Excel Macro Enabled Worksheet)


E N Economou and Paul Mihas (1977) Random one-body approximation to the Hubbard model: magnetic interactions **J. Phys. C: Solid State Phys., Vol. 10,1977. Printed in Great Britain. © 1977**

N. Derby, S. Olbert (2010) Cylindrical Magnets and Ideal Solenoids
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