How many electrons are needed to flip a local spin?

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(Dated: October 31, 2004)

Considering the spin of a local magnetic atom as a quantum mechanical operator, we illustrate the dynamics of a local spin interacting with a ballistic electron represented by a wave packet. This approach improves the semi-classical approximation and provides a complete quantum mechanical understanding for spin transfer phenomena. Sending spin-polarized electrons towards a local magnetic atom one after another, we estimate the minimum number of electrons needed to flip a local spin.

PACS numbers: 72.25.-b, 73.23.Ad, 73.63.-b

arXiv:cond-mat/0410775 v1 29 Oct 2004

Electrons generally interact with magnetic atoms through a spin-flip interaction. For example, this is a fundamental mechanism for spin transfer [1, 2] from spin-polarized electrons to a magnetic moment in a ferromagnet [3, 4, 5]. Spin transfer results in a classical torque exerted on the magnetic moment and, thus, enables us to control a local structure in a ferromagnetic film. This picture is semi-classical and seems to work well n a practical sense [6, 7, 8, 9]. However, this view also causes some conceptual difficulties, and cannot answer fundamental questions associated with spin transfer. For example, it seems intuitive that the stronger the spin-flip interaction is, the easier it is to flip a local spin through the interaction. However, a more rigorous quantum mechanical treatment of the problem will illustrate that this intuition is incorrect.

The goals in this paper are following: (1) we scrutinize the physics of spin transfer between an incoming electron and a localized magnetic atom with spin S, *i.e.* we calculate the expectation value of the local spin operator as a function of time (t) and illustrate the physics in detail. (2) We provide an estimation of how many electrons are needed to flip the local spin by sending spin-polarized electrons one after another with an interval sufficiently long that no interference between two electrons occurs. For illustrative purposes, we consider spin values of $S = 1/2$, 1, and 3/2 to represent the local spin.

Imagine a magnetic atom residing at the origin of the X axis with spin pointing to the negative Z axis. Its spin state can be represented by $|-S\rangle$ at $t = 0$. We consider a normalized wave packet ϕ of an electron with spin along the positive Z direction away from the origin. Then, the total wave function is initially $\Psi = \phi|+\rangle|-S\rangle$, where $|+\rangle$ is the spin state of an incoming electron. Since the local atom is neutral, the Coulomb interaction will not be included. This problem can be set up in one dimension. The Hamiltonian we consider is

$$H = \frac{p^2}{2m} - 2J_0\sigma\cdot\mathbf{S}\delta(x) \tag{1}$$

where $p^2/2m$ is the kinetic energy of the incoming electron, σ is the electron spin operator, and J_0 (> 0) is the coupling of the spin-flip interaction. We use units such that $\hbar = c = 1$. Let us introduce $\lambda/a = 2mJ_0$, where a is a typical length scale in the problem and will be set to unity. The initial wave packet is normalized and given by $\phi(x) = (2\pi\alpha)^{-1/4}e^{ik_0(x+x_0)}e^{-(x+x_0)^2/4\alpha}$. Such a wave packet describes an "electron" with mean position $-x_0$ and mean momentum k_0. The uncertainties associated with the packet are $\Delta x_0 = \sqrt{2\alpha}$ and $\Delta k_0 = 1/\sqrt{2\alpha}$. In order to calculate the expectation value of the Z component of the local spin $\langle S_z(t)\rangle = \langle\Psi(x,t)|S_z|\Psi(x,t)\rangle$, where $\langle\cdots\rangle$ means an integration over x, we need to know the time evolution of the total wave function $\Psi(x,t)$. Since the initial state $\Psi(x,0)$ is not an eigenstate of the Hamiltonian because of the spin-flip coupling, $\Psi(x,0)$ should be decomposed into two channels depending on the total spin $j_\pm = S \pm 1/2$.

The Schrödinger equation to solve is

$$\partial_x^2\Psi(x) + 2mE\Psi(x) = \begin{cases} -S\lambda\delta(x)\Psi(x) & \text{for} \quad j_+ \\ (S+1)\lambda\delta(x)\Psi(x) & \text{for} \quad j_- \end{cases} \tag{2}$$

A wave function with j_+ sees a potential well while a wave function with j_- feels a potential barrier. The time evolution of each channel is different because the eigenstates of each equation are different, and the overlap of the two wave functions determines the dynamics of the local spin as we will soon show. The time evolution of the wave function is a combination of the time evolutions of the two channels of $j_\pm$:

$$\Psi(x,t) = \phi_+(x,t)\frac{1}{\sqrt{2S+1}}|j_+, -S+1/2\rangle + \phi_-(x,t)\sqrt{\frac{2S}{2S+1}}|j_-, -S+1/2\rangle \tag{3}$$

where $\phi_\pm(x,t)$ is the time evolution of the wave packet in the presence of the well/barrier, and $\phi_\pm(x,0)=\phi(x)$. The Z component of the total spin is conserved to be $-S+1/2$. The expectation value of the Z component of the local spin as a function of time is calculated to be

$$\langle S_z(t)\rangle = -\frac{S}{(2S+1)^2}\left\{4S^2+4S+4\mathrm{Re}\left[\langle\phi_+|\phi_-\rangle\right]-3\right\} . \tag{4}$$

Using the Schwartz inequality: $|\langle\phi_+|\phi_-\rangle|^2\le 1$, we find a constraint of $\langle S_z(t)\rangle$ as follows: $-S\le\langle S_z(t)\rangle\le -S\left[4S^2+4S-7\right]/(2S+1)^2$. This constraint is more restrictive than the obvious one that requires a maximum change in the spin to be unity since the spin of the incoming electron is 1/2. Note that there always exists a probability that the state of the local spin remains unchanged even after the interaction; therefore, actual values of $\langle S_z(t)\rangle$ should be evaluated quantum mechanically. We can also determine the local spin state from the total wave function $\Psi(t)$. The spin state is written as $a_1|-S\rangle+b_1|-S+1\rangle$, where $|a_1|^2 = \left\{1+4S^2+4S\mathrm{Re}\left[\langle\phi_+|\phi_-\rangle\right]\right\}/(2S+1)^2$ and $|b_1|^2=4S\left\{1-\mathrm{Re}\left[\langle\phi_+|\phi_-\rangle\right]\right\}/(2S+1)^2$. It is straightforward to show that $\langle S_z(t)\rangle=-S+|b_1|^2$. Without loss of generality we can assume that a_1 and b_1 are real.

As mentioned for $\langle S_z(t)\rangle$, we need to solve Eq. (2) because the time evolution of the wave packet $\phi_\pm$ will be governed by the solutions of this equation. Let us consider a Hamiltonian $H_\pm=p^2/2m+(\lambda_\pm/2m)\delta(x)$, where $\lambda_+=-S\lambda$ for the j_+ channel while $\lambda_-=(S+1)\lambda$ for the other channel. This Hamiltonian could be treated as a scattering problem for $E>0$ to obtain an asymptotic solution which is plane wave-like. Note that the asymptotic solution does not describe the detailed dynamics of the local spin. However, it implies important physics associated with the problem. The asymptotic solution is $\eta_k(x)=\left[e^{ikx}+R_\pm e^{-ikx}\right]\Theta(-x)+T_\pm e^{ikx}\Theta(x)$, where $\Theta(x)$ is a step function. The momentum is well-defined while the position cannot be; namely, $\Delta k=0$ but $\Delta x=\infty$. The transmittance and the reflectance are determined by the boundary condition at $x=0$, and they are $|T_\pm|^2=4/\left[4+(\lambda_\pm/k)^2\right]$ and $|R_\pm|^2=(\lambda_\pm/k)^2/\left[4+(\lambda_\pm/k)^2\right]$. It is worth mentioning that $|T_\pm|^2$ and $|R_\pm|^2$ depend only on $(\lambda_\pm/k)^2$; furthermore, for large $\lambda_\pm/k$ both channels give unit reflectance and almost zero transmission. As we showed in Eq. (4), the dynamics of the local spin depends on the overlap of the two wave functions $\phi_+(x,t)$ and $\phi_-(x,t)$. The above exercise indicates that for a large λ, $\phi_\pm$ would not differ significantly from each other. In this instance, $\mathrm{Re}\left[\langle\phi_+|\phi_-\rangle\right]\approx 1$; consequently, $\langle S_z\rangle\approx -S$. In other words, if the spin-flip coupling is very large, it becomes more difficult to flip a local spin. This seems to oppose the semi-classical understanding but we will show that this is the case. We should mention that the $\lambda_\pm/k$ scaling in $|T_\pm|^2$ and $|R_\pm|^2$ takes place because of zero uncertainty in the momentum ($\Delta k=0$) for a plane wave. Rigorously speaking, however, one cannot expect such a perfect scaling when a wave packet with $\Delta k\neq 0$ is used instead of a plane wave.

We obtain the eigenstates and the corresponding eigenvalues of $H_\pm$ introducing a box of the length $2L$ ($-L\le x\le L$) with a periodic boundary condition: $\psi(-L)=\psi(L)$ and $\partial_x\psi(-L)=\partial_x\psi(L)$, where $\psi(x)$ is an eigenstate of $H_\pm$ with an eigenvalue $E_\pm$. Since the potential is symmetric about $x=0$, the eigenstates are either even or odd; $\psi_{e,k_\pm}(x)$ or $\psi_{o,p_\pm}(x)$. We found [10] for the even solution

$$\psi_{e,k_\pm}(x)=\frac{1}{\sqrt{N_{k_\pm}}}\left[\cos(k_\pm x)+\frac{\lambda_\pm}{2k_\pm}\sin(k_\pm|x|)\right] \tag{5}$$

where $N_{k_\pm}=L\left[1+(\lambda_\pm/2k_\pm)^2\right]+\lambda_\pm/2k_\pm^2$, and for the odd solutions $\psi_{o,p_\pm}(x)=\sin(p_\pm x)/\sqrt{L}$. The corresponding eigenvalues are $E_{k_\pm}=k_\pm^2/2m$, where $k_\pm$ is a solution of $\tan(k_\pm L)=\lambda_\pm/2k_\pm$, while $E_{p_\pm}=p_\pm^2/2m$ with $p_\pm=n_\pm\pi/L$ ($n_\pm$ is an integer). Since the potentials do not affect the odd solutions, the dynamics of the local spin is determined only by the even solutions. For λ_+ (<0), the number of the even states decreases by one and a single bound state occurs for $E<0$ to keep the total number of eigenstates unchanged. As long as we initially put a wave packet far away from $x=0$, the bound state does not participate in the time evolution of the wave packet [11]. Now the time evolution of $\phi_\pm(x,t)$ for both channels can be written as

$$\phi_\pm(x,t)=\sum_{k_\pm}e^{-iE_{k_\pm}t}C_{k_\pm}\psi_{e,k_\pm}(x)+\sum_{p_\pm}e^{-iE_{p_\pm}t}C_{p_\pm}\psi_{o,p_\pm}(x) \tag{6}$$

where $C_{k_\pm}=\langle\psi_{e,k_\pm}|\phi\rangle$ and $C_{p_\pm}=\langle\psi_{o,p_\pm}|\phi\rangle$. Using these expressions we obtain the overlap between ϕ_+ and ϕ_- as follows:

$$\begin{aligned}\langle\phi_+|\phi_-\rangle &= (2S+1)\lambda\sum_{k_\pm}\frac{e^{i(E_{k_+}-E_{k_-})t}}{k_-^2-k_+^2}\frac{\langle\phi|\psi_{e,k_+}\rangle}{\sqrt{N_{k_+}}}\frac{\langle\psi_{e,k_-}|\phi\rangle}{\sqrt{N_{k_-}}}\\ &+\frac{1}{2}\left[1-e^{-(k_0/\Delta k_0)^2-(x_0/\Delta x_0)^2}\right] ,\end{aligned} \tag{7}$$

where Δk_0 and Δx_0 are the uncertainties associated with the initial wave packet. Note that the time dependence of $\langle\phi_+|\phi_-\rangle$ is determined only by the even solutions while the odd solutions contribute to a constant, which would be close to 1/2 if the momentum or the position is well defined and finite initially. Since we consider a wave packet far away from the origin with a finite mean position at $t=0$, the second term in Eq. (7) is approximately 1/2 to high precision.

Fig. 1 illustrates the time evolution of the wave packet for the j_- channel away from a local spin of $S=1/2$. We introduce a dimensionless time $\tau=t/2ma^2$. Initially the wave packet is located at $x=-x_0$ ($x_0=100$) with a mean momentum $k_0=1$. We choose α to be 10 and L

to be $10^3 \sim 10^4$. As long as $L \gg x_0$, L is not important. The wave packet does not interact with the potential with $\lambda_- = (S+1)\lambda = 3.45$ until $\tau \simeq 30$. At $\tau = 50$, the potential strongly scatters the wave packet and a part of the packet is transmitted to the other side of the potential. After $\tau = 150$, the reflected and transmitted parts of the packets freely move away from the potential in the opposite direction as indicated by the arrows. The time evolution for j_+ is similar and not shown in this figure. In the insert, we show $\langle S_z(\tau)\rangle$ as a function of τ. It increases from $\langle S_z(0)\rangle = -0.5$ to $\langle S_z(150)\rangle \simeq -0.01$, and then becomes saturated. The saturation is expected because after $\tau = 150$ the wave packet does not interact with the potential any more. In fact, the mean momentum determines when $\langle S_z\rangle$ becomes saturated. We define the saturation value of $\langle S_z\rangle$ as S_1, which depends on k_0 and λ. It is this value that we use to estimate how many spin-polarized electrons are needed to flip a local spin as we will show later.

It is possible to control the mean momentum reasonably well while the spin-flip coupling is uncontrollable and even not well known experimentally. In this sense, it does not seem possible to pinpoint how many electrons are needed to flip a specific local spin. Nevertheless, it is theoretically feasible to estimate the minimum number of electrons to flip a local spin by calculating the maximum value of S_1 denoted as S_1^{max}. To this end, we evaluate S_1 as a function of k_0 and λ because a scaling relation is not expected to hold for the wave packet with the momentum uncertainty $(1/\sqrt{2\alpha})$. We choose the same value of α as before. Fig. 2 is a contour plot of S_1 in the $(\lambda,\ k_0)$ plane. Interestingly, we found a λ/k_0 scaling holds fairly well in this case as well. Moreover, S_1^{max} of a local spin $S = 1/2$ is approximately zero for $\lambda \simeq 2.3k_0$; for example, $\lambda = 6.9$ with $k_0 = 3$. We obtained the same scaling behavior for other values of α. Note that this value of S_1^{max} is smaller than the mathematical upper bound based on the Schwartz inequality, which is a half for $S = 1/2$. Looking in particular at the lower part of Fig. 2, we know that for a given k_0, S_1 decreases with increasing λ. This clearly indicates that if the coupling is too large, it becomes more and more difficult to flip the local spin, which is consistent with our early analysis. We plot S_1 for the local spin $S = 1$ and $S = 3/2$ in Fig. 3 as a function of λ/k_0 with $\alpha = 10$. There is also a similar scaling behavior in S_1 while different values of λ/k_0 give S_1^{max}. For $S = 1$, the maximum value is $S_1^{max} \simeq -0.556$ $(< -1/9)$ along $\lambda \simeq 1.4k_0$, and $S_1^{max} \simeq -1.126$ $(< -3/4)$ along $\lambda \simeq k_0$ for $S = 3/2$, where $-1/9$ and $-3/4$ are the mathematical upper bounds for $S = 1$ and $S = 3/2$, respectively.

Now consider the spin-polarized electrons sent towards the local spin one after another over an interval τ_0 which is sufficiently long so as to prevent any interference between two electrons. That is, we wait long enough before sending the second electron so that the first has cleared away from the region of interest, and left the local spin in a state $a_1|-S\rangle + b_1|-S+1\rangle$, where a_1 and b_1 have acquired saturated values after a time $\tau_0 \approx 200$ (see Fig. 1). Note that this time can be shorter if we increase the mean momentum, for example. At $\tau = \tau_0$, the total wave function is $\phi|+\rangle\Big[a_1(\tau_0)|-S\rangle + b_1(\tau_0)|-S+1\rangle\Big]$. Since $|+\rangle|-S\rangle$ and $|+\rangle|-S+1\rangle$ are not eigenstates of the Hamiltonian in general, we need to decompose each state into two channels for $j_\pm$ with appropriate Clebsch-Gordan coefficients [12]. Later the spin state of the local spin will be $a_2|-S\rangle + b_2|-S+1\rangle + c_2|-S+2\rangle$. The coefficients a_2, b_2, and c_2 can be determined from the total wave function, and they turn out to be functions of a_1 and b_1. Repeating this procedure we can calculate the expectation value of the local spin after sending the n-th electron.

Using $S = 1/2$, 1 and $3/2$ we illustrate the procedure and estimate the minimum number of electrons to flip a local spin. The expansion for an arbitrary spin can be done systematically. For a local spin $S = 1/2$, $j_+ = 1$ and $j_- = 0$. After the first electron interacts with the local spin, the total wave function is $\Psi = \frac{1}{\sqrt{2}}\phi_1|10\rangle + \frac{1}{\sqrt{2}}\phi_0|00\rangle$. The spin state of the atom is $a_1|-1/2\rangle + b_1|1/2\rangle$, where $a_1^2 = 1/2 - S_1$ and $b_1^2 = 1/2 + S_1$, and $\langle S_z\rangle = S_1$. When we send the second electron, $\Psi = \frac{1}{\sqrt{2}}a_1\phi_1|10\rangle + \frac{1}{\sqrt{2}}a_1\phi_0|00\rangle + b_1\phi_1|11\rangle$. The local state becomes $a_2|-1/2\rangle + b_2|1/2\rangle$, where $a_2^2 = a_1^4$ and $b_2^2 = \left(a_1^2+1\right)b_1^2$, and $S_2 = 1/4 + S_1 - S_1^2$, where S_n is $\langle S_z\rangle$ after the n-th electron. The third electron gives $S_3 = 1/4 + (S_1+S_2)/2 - S_1S_2$, and the n-th electron leaves $S_n = 1/4 + (S_1 + S_{n-1})/2 - S_1S_{n-1}$. We can express S_n in terms of S_1 as follows:

$$S_n = \frac{1}{2} - \left(\frac{1}{2} - S_1\right)^n . \tag{8}$$

Using a similar procedure we obtain S_n for $S = 1$ and $S = 3/2$

$$\begin{aligned} S_n &= 1 - n\left(-S_1\right)^{n-1} + (n-2)\left(-S_1\right)^n \quad \text{for} \quad S = 1 \\ S_n &= \frac{3}{2} - \left(-S_1 - 1/2\right)^{n-1}\Big[(3+4n)S_1 + 3(1+4n)/2\Big] \\ &- 6\left(-4S_1/3 - 1\right)^n \quad \text{for} \quad S = 3/2 \end{aligned} \tag{9}$$

Note that $S_0 = -S$, which means that initially the local spin state is $|-S\rangle$ while $S_n \to S$ as n increases for a given S_1; in other words, the local spin becomes flipped. Mathematically speaking, $S_n = S$ only when $n = \infty$. This is because there always exists a quantum mechanical possibility that the spin state remains unchanged even after the spin-flip interaction. Nevertheless, when S_n becomes sufficiently close to S, we can claim that the local spin has flipped. When $S_1 = S_1^{max}$, we can approximate $S_n^{max} \simeq S - 2S\ e^{-\beta_S n}$, where $\beta_{1/2} \simeq 0.7$, $\beta_1 \simeq 0.35$, and $\beta_{3/2} \simeq 0.23$. Let us define the minimum number N_S to be the number which satisfies, for example, $2S\ e^{-\beta_S N_S} = 10^{-5}$. Then we evaluate $N_S = \left[5\ln(10) + \ln(2S)\right]/\beta_S$. Our estimation shows that the minimum number of the spin-polarized electrons to

flip a local spin of 1/2 is about 16; namely, $N_{1/2} \simeq 16$. For $S = 1$, $N_1 \simeq 35$ while $N_{3/2} \simeq 55$ for the local spin of 3/2. Therefore, less electrons are needed to flip a smaller spin as one might expect.

In summary, using straightforward quantum mechanics, we have studied the time evolution of the spin of a local magnetic atom under a spin-flip interaction with an incoming electron. This treatment goes beyond the semi-classical approximation, which considers the local moment as a classical vector. The expectation value of the spin operator has been evaluated using the wave function of the electron, which is the solution of the time dependent Schrödinger equation. Sending spin-polarized electrons towards a local magnetic atom one after another, we also provide an estimate of how many electrons are needed to flip a local spin. For an experimental realization of our estimate, we suggest a setup where a magnetic atom is fixed at the hub of a wheel, while spin-polarized electrons are sent towards the atom along orthogonal spokes in the wheel.

One of us (W.K.) thanks H.K. Lee and M. Revzen for discussions. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC), by ICORE (Alberta), and by the Canadian Institute for Advanced Research (CIAR).

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[10] As far as we know, these eigenstates and the corresponding eigenvalues have never been presented in literature.
[11] Mathematically speaking, a wave function $\phi(x,t)$ is expanded in terms of eigenstates $u_n(x)$ with eigenvalues E_n; $\phi(x,t) = \sum_n C_n(t) u_n(x)$, where $C_n(t) = C_n(0) e^{-iE_n t}$. Therefore, if $C_{n'}(0) = 0$, then $C_{n'}(t) = 0$.
[12] See, for example, L. Schiff, *Quantum mechanics* (McGraw-Hill, New York, 1968).

Fig. 1 (Kim et al)

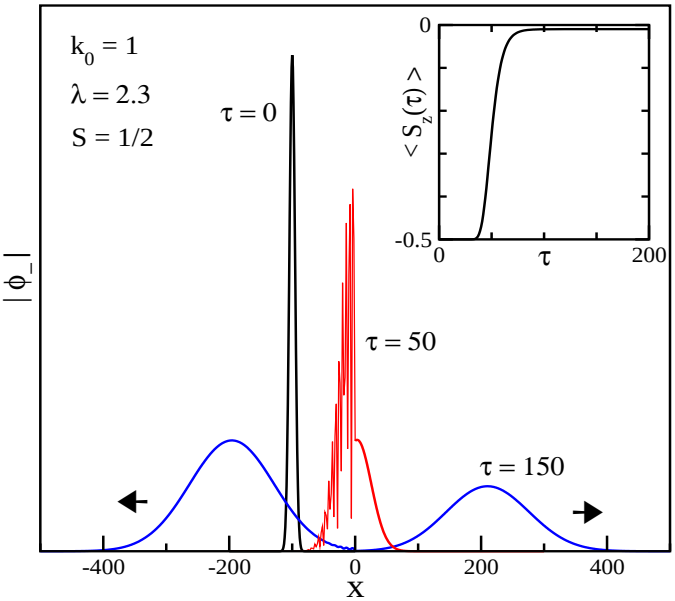

FIG. 1: (Color online) The time evolution of the wave packet for the j_- channel. The other channel shows similar behavior and is not plotted. The local spin is 1/2. The inset describes dynamics of the local spin. After $\tau = 150$, $\langle S_z \rangle$ becomes saturated.

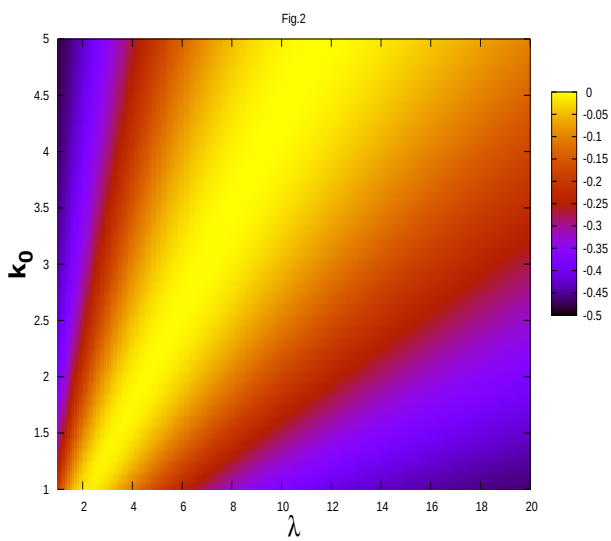

FIG. 2: (Color online) Contour plot of S_1 for $S = 1/2$ in the (λ, k_0) plane. Note a (λ/k_0) scaling behavior with a maximum value of S_1 along $\lambda = 2.3k_0$.

Fig.3 (Kim et al)

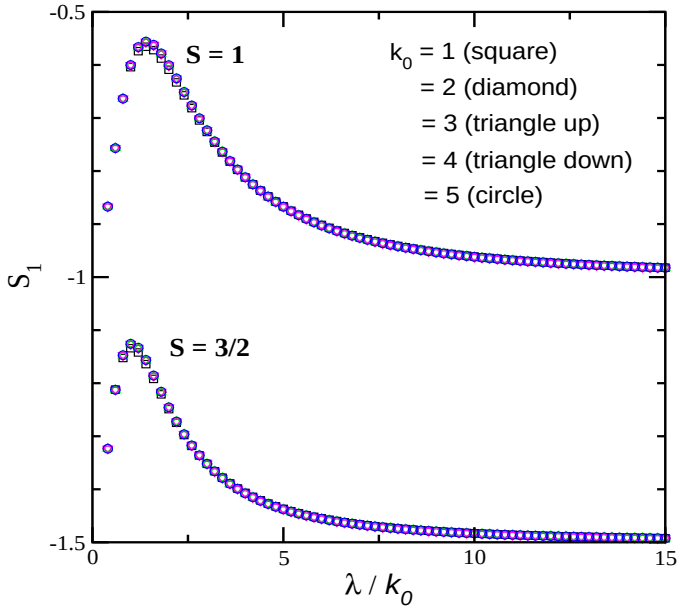

FIG. 3: (Color online) S_1 as a function of λ/k_0 for $S = 1$ and $S = 3/2$, for various values of k_0. The maximum value of S_1 is about -0.556 and -1.126 for $S = 1$ and $S = 3/2$, respectively.