Nonrelativistic multiple-scattering theory of a spin-polarized electron

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We present a nonrelativistic multiple-scattering theory of a spin-polarized electron including the spin-orbit interaction. It is generalized to the N-scatterer case and the scattering by an ordered layer. A proper design of the potential form and the radius of a quantum dot may enhance the electron spin polarization very effectively utilizing the spin-orbit interaction.

I. INTRODUCTION

It is known that an unpolarized electron beam can be polarized through a scattering process.[1] Two kinds of interactions are responsible for it. One is the exchange interaction; the other is the spin-orbit interaction. The exchange interaction is essentially a many-body effect between electrons. For example, it plays a key role in the scattering by magnetic impurities in metals, and it is well known as the Kondo problem. But the exchange effect may become smaller as the energy of the incident electron increases. In this paper, we study only the cases where the energy of the incident electron is sufficiently high to justify the neglect of the exchange interaction, namely, we study the potential scattering problem including the spin-orbit interaction. The theoretical basis for low-energy unpolarized electron diffraction (LEED) has been developed and many surface structures have been determined with it.[2–4] Feder and his co-researchers have also developed a relativistic version of the LEED theory including the spin polarization of an electron.[5–8] From their numerical analysis,[9] it is obvious that the spin-orbit interaction is not so effective in producing significant spin polarization; the functional form of the spin-orbit interaction is responsible for this. On the other hand, the recent rapid advance of microelectronics technology makes it possible to fabricate various kinds of artificial atoms known as quantum dots.[10] Then, the freedom to change the potential form and the radius of a quantum dot may provide a great opportunity to achieve high efficiency of spin polarization. Furthermore, a proper spatial distribution of quantum dots may lead to further enhancement. In order to proceed with the investigation of such systems, we need a nonrelativistic multiple-scattering theory of the spin-polarized electron for many scatterers, including the spin-orbit interaction. It is the main purpose of this paper to provide such a theoretical tool to investigate various scattering properties of the artificial atoms. It is a natural extension of our previous work for the spinless system[12] to the spin system. We hope that the present work helps further active use of the electron spin freedom in future microelectronic device design.

The outline of the present paper is as follows. First, we derive in Sec. II the T matrix of a spin-polarized electron for the individual scatterers. It is extended to the N-scatterer case, including scattering by an ordered layer, in Sec. III. Discussions are given in Sec. IV.

II. T MATRIX INCLUDING SPIN-ORBIT INTERACTION

We assume here that an electron is scattered by the following potential:[11]

$$V(\mathbf{r}) = V^1(\mathbf{r}) + V^2(\mathbf{r})\boldsymbol{l}\cdot\mathbf{s}, \tag{2.1}$$

where $V^2(\mathbf{r})\boldsymbol{l}\cdot\mathbf{s}$ is the spin-orbit interaction potential. Then the Lippmann-Schwinger equation becomes

$$\psi^{m_\sigma}(\mathbf{r}) = \chi_{\frac{1}{2}m_\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} + \int d^3\mathbf{r}' G_0(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi^{m_\sigma}(\mathbf{r}'), \tag{2.2}$$

using the spin wave function of an incident electron $\chi_{\frac{1}{2}m_\sigma}$, $m_\sigma = \pm\frac{1}{2}$. Substituting the following expansions of the wave functions[4,12]

$$\psi^{m_\sigma}(\mathbf{r}) \equiv \sum_{j_1L_1,j_2L_2} 4\pi i^{l_2} F_{j_1L_1j_2L_2}(r) \times Y_{j_1L_1\frac{1}{2}}(\hat{\mathbf{r}}) Y^{m_\sigma *}_{j_2L_2\frac{1}{2}}(\hat{\mathbf{k}}), \tag{2.3}$$

$$\chi^{m_\sigma}_{\frac{1}{2}} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{jL} 4\pi i^l j_l(kr) Y_{jL\frac{1}{2}}(\hat{\mathbf{r}}) Y^{m_\sigma *}_{jL\frac{1}{2}}(\hat{\mathbf{k}}), \tag{2.4}$$

and the free Green's function expanded in terms of $Y^{m_\sigma}_{jL\frac{1}{2}} \equiv C(l\tfrac{1}{2}j;m,m_\sigma)Y_L$ or $Y_{jL\frac{1}{2}} \equiv \sum_{m_\sigma} Y^{m_\sigma}_{jL\frac{1}{2}}\chi_{\frac{1}{2}m_\sigma}$,

$$G_0(\mathbf{r}-\mathbf{r}') \equiv -\frac{m_e}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = -\frac{2m_e ik}{\hbar^2}\sum_{jL} j_l(kr_<)h_l^{(1)}(kr_>) \times Y_{jL\frac{1}{2}}(\hat{\mathbf{r}})Y^*_{jL\frac{1}{2}}(\hat{\mathbf{r}}')\ , \tag{2.5}$$

into Eq. (2.2), we can obtain an integral equation

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$$F_{j_1L_1j_2L_2}(r) = j_{l_1}(kr)\delta_{j_1j_2}\delta_{L_1L_2} + \sum_{j_3L_3}\int_0^\infty dr' j_{l_1}(kr_<)h_{l_1}^{(1)}(kr_>) \times U_{j_1L_1j_3L_3}(r')F_{j_3L_3j_2L_2}(r') , \quad (2.6)$$

where

$$U_{j_1L_1j_3L_3}(r) \equiv -\frac{2m_e ik}{\hbar^2}A_{j_1L_1j_3L_3}\sum_{L_4}C_{L_3L_4}^{L_1}r^2 \times \left[V_{L_4}^1(r) + V_{L_4}2(r)\zeta(j_3,l_3)\right], \quad (2.7)$$

$$A_{j_1L_1j_3L_3} \equiv \sum_{m_\sigma} C(l_1\tfrac{1}{2}j_1;m_1,m_\sigma)C(l_3\tfrac{1}{2}j_3;m_3,m_\sigma), \quad (2.8)$$

and

$$C_{L_1L_2}^{L_3} \equiv \int d\Omega_r Y_{L_3}^*(\hat{\mathbf{r}})Y_{L_1}(\hat{\mathbf{r}})Y_{L_2}(\hat{\mathbf{r}}) \quad (2.9)$$

is the Gaunt number,[3] $C(l\frac{1}{2}j;m,m_\sigma)$ is the Clebsch-Gordan coefficient,[13] the energy of an incident electron is $E = \frac{\hbar^2k^2}{2m_e}$, $k = |\mathbf{k}|$, m_e is the electron mass, $\hbar$ is Planck's constant, $Y_L(\hat{\mathbf{r}})$ is spherical harmonics, $j_l(kr)$,$h_l^{(1)}(kr)$ are spherical Bessel and Hankel functions of the first kind, respectively, and $r_> = \max(r,r')$, $r_< = \min(r,r')$, $L = (l,m)$. Furthermore,

$$V^i(\mathbf{r}) = \sum_L V_L^i(r)Y_L(\hat{\mathbf{r}}), \quad i = 1,2,$$

$$\boldsymbol{l}\cdot\mathbf{s}Y_{jL\frac{1}{2}}(\hat{\mathbf{r}}) = \tfrac{1}{2}\left[j(j+1) - l(l+1) - \tfrac{1}{4}\right]Y_{jL\frac{1}{2}}(\hat{\mathbf{r}}) \equiv \xi(j,l)Y_{jL\frac{1}{2}}(\hat{\mathbf{r}}),$$

$$Y_L(\hat{\rho}_1)Y_L^*(\hat{\rho}_2) = \sum_j Y_{jL\frac{1}{2}}(\hat{\rho}_1)Y_{jL\frac{1}{2}}^*(\hat{\rho}_2),$$

$$Y_{L_1}(\hat{\rho}_1)Y_{L_2}^*(\hat{\rho}_2) = \frac{1}{A_{j_1L_1j_2L_2}}Y_{j_1L_1\frac{1}{2}}(\hat{\rho}_1)Y_{j_2L_2\frac{1}{2}}^*(\hat{\rho}_2),$$

and $j = l \pm \frac{1}{2} \equiv j_\pm$ are used. Since Eq. (2.6) is a one-dimensional integral equation of the Fredholm type, it can be easily solved numerically. It is also transformed to the Vorrtela type as[12,14]

$$f_{j_1L_1j_2L_2}(r) = j_{l_1}(kr)\delta_{j_1j_2}\delta_{L_1L_2} + \sum_{j_3L_3}\int_0^r dr'\left[j_{l_1}(kr')h_{l_1}^{(1)}(kr) - j_{l_1}(kr)h_{l_1}^{(1)}(kr')\right]U_{j_1L_1j_3L_3}(r')f_{j_3L_3j_2L_2}(r'), \quad (2.10)$$

and $F_{j_1L_1j_2L_2}(r) = (\tilde{F})_{j_1L_1j_2L_2}$ can be obtained from

$$\tilde{F} = \tilde{f}\tilde{C}, \qquad \tilde{C} = \left[\tilde{I} - \int_0^\infty dr'\tilde{H}(kr')\tilde{U}(r')\tilde{f}(r')\right]^{-1}, \quad (2.11)$$

where we have used the matrix representation; a tilde signifies a matrix, rows and columns of which are labeled (j,L), $\tilde{H}(kr) = h_{l_1}^{(1)}(kr)\delta_{j_1j_2}\delta_{L_1L_2}$, and $\tilde{I}$ is a unit matrix. In general, a T matrix is defined by

$$V(\mathbf{r}_1)\psi(\mathbf{r}_1) = \int t(\mathbf{r}_1,\mathbf{r}_2)\phi(\mathbf{r}_2)d\mathbf{r}_2 \ ; \quad (2.12)$$

then, expanding it in angular momentum space as

$$t(\mathbf{r}_1,\mathbf{r}_2) = \sum_{j_1L_1j_2L_2} t_{j_1L_1j_2L_2}(r_1r_2)Y_{j_1L_1\frac{1}{2}}(\hat{\mathbf{r}}_1)Y_{j_2L_2\frac{1}{2}}^*(\hat{\mathbf{r}}_2), \quad (2.13)$$

we can arrive at

$$t_{j_1L_1j_2L_2}(k) \equiv i^{-(l_1-l_2)}\int_0^\infty r_1^2dr_1\int_0^\infty r_2^2dr_2 j_{l_1}(kr_1)t_{j_1L_1j_2L_2}(r_1r_2)j_{l_2}(kr_2)$$

$$= \frac{\hbar^2}{2m_e}\frac{i^{-(l_1-l_2)}}{k}\int_0^\infty dr j_{l_1}(kr)\sum_{j_3L_3}U_{j_1L_1j_3L_3}(r)F_{j_3L_3j_2L_2}(r), \quad (2.14)$$

and the T matrix in $\mathbf{k}$ space is

$$\langle \mathbf{k}_f m_\sigma^f | t | \mathbf{k}_i m_\sigma^i \rangle \equiv (4\pi)^2 \sum_{j_1L_1j_2L_2} t_{j_1L_1j_2L_2}(k)Y_{j_1L_1\frac{1}{2}}^{m_\sigma^f}(\hat{\mathbf{k}}_f)Y_{j_2L_2\frac{1}{2}}^{m_\sigma^{i}*}(\hat{\mathbf{k}}_i). \quad (2.15)$$

Therefore, using solutions of one-dimensional integral equations of the Fredholm type or the Vorrtela type for $\tilde{F}$ or $\tilde{f}$, we can determine the scattering process of a spin-polarized electron exactly. In the next section let us extend it further to the N-scatterer problem.

III. N-SCATTERER PROBLEM

Similar to the spin-independent potential scattering case,[12] the total T matrix for N scatterers can be expanded as

$$T=\sum_{\mathbf{R}_i} t_{\mathbf{R}_i}+\sum_{\mathbf{R}_i\neq\mathbf{R}_j} t_{\mathbf{R}_i}G_0t_{\mathbf{R}_j} + \sum_{\mathbf{R}_i\neq\mathbf{R}_j}\sum_{\mathbf{R}_j\neq\mathbf{R}_k} t_{\mathbf{R}_i}G_0t_{\mathbf{R}_j}G_0t_{\mathbf{R}_k}+\cdots , \tag{3.1}$$

where $\mathbf{R}_i$ are the positions of the scatterers. Using

$$G_0(\rho_1+\mathbf{R}_s-\rho_2-\mathbf{R}_t) \equiv \sum_{j_1L_1j_2L_2} G^{st}_{j_1L_1j_2L_2} i^{l_1-l_2} j_{l_1}(k\rho_1)j_{l_2}(k\rho_2) \times Y_{j_1L_1\frac{1}{2}}(\hat{\rho}_1)Y^*_{j_2L_2\frac{1}{2}}(\hat{\rho}_2) \tag{3.2}$$

and

$$G^{st}_{j_1L_1j_2L_2}=-\frac{8\pi m_e ik}{\hbar^2}\frac{1}{A_{j_1L_1j_2L_2}}\sum_{L_3} i^{l_3}(-1)^{m_3}C^{L_1}_{L_2\bar{L}_3} \times h^{(1)}_{l_3}(k\,|\mathbf{R}_s-\mathbf{R}_t|)Y^*_{L_3}(\mathbf{R}_s\hat{-}\mathbf{R}_t), \tag{3.3}$$

we can obtain the following total T matrix in $\mathbf{k}$ space:

$$T(\mathbf{k}_f m^f_\sigma,\mathbf{k}_i m^i_\sigma)\equiv\langle \mathbf{k}_f m^f_\sigma\,|T|\,\mathbf{k}_i m^i_\sigma\rangle = (4\pi)^2\sum_{j_1L_1j_2L_2}\left[K_fT_t\left(\mathcal{I}-GT_t\right)K^+_i\right]_{j_1L_1j_2L_2} Y^{m^f_\sigma}_{j_1L_1\frac{1}{2}}(\hat{\mathbf{k}}_f)Y^{m^i_\sigma *}_{j_2L_2\frac{1}{2}}(\hat{\mathbf{k}}_i), \tag{3.4}$$

where $\bar{L}=(l,-m)$,

$$T_t=\begin{bmatrix} \tilde{t}^1 & \tilde{0} & \tilde{0} & \tilde{0} & \tilde{0}\\ \tilde{0} & \tilde{t}^2 & \tilde{0} & \tilde{0} & \tilde{0}\\ \tilde{0} & \tilde{0} & \ddots & \tilde{0} & \vdots\\ \vdots & \tilde{0} & \tilde{0} & \ddots & \tilde{0}\\ \tilde{0} & \tilde{0} & \cdots & \tilde{0} & \tilde{t}^N \end{bmatrix}, \tag{3.5}$$

$$G=\begin{bmatrix} \tilde{0} & \tilde{G}^{12} & \cdots & \cdots & \tilde{G}^{1N}\\ \tilde{G}^{21} & \tilde{0} & \ddots & \ddots & \tilde{G}^{2N}\\ \vdots & \ddots & \ddots & \ddots & \vdots\\ \vdots & \ddots & \ddots & \ddots & \tilde{G}^{N-1N}\\ \tilde{G}^{N1} & \tilde{G}^{N2} & \cdots & \tilde{G}^{NN-1} & \tilde{0} \end{bmatrix}, \tag{3.6}$$

$$K_f=\left(\, e^{-i\mathbf{k}_f\cdot\mathbf{R}_1}\tilde{I} \;\cdots\; \cdots \;\cdots\; e^{-i\mathbf{k}_f\cdot\mathbf{R}_N}\tilde{I}\,\right), \tag{3.7}$$

$$K^+_i=\begin{pmatrix} e^{i\mathbf{k}_i\cdot\mathbf{R}_1}\tilde{I}\\ \vdots\\ \vdots\\ \vdots\\ e^{i\mathbf{k}_i\cdot\mathbf{R}_N}\tilde{I} \end{pmatrix}, \tag{3.8}$$

and

$$\mathcal{I}=\begin{bmatrix} \tilde{I} & \tilde{0} & \cdots & \cdots & \tilde{0}\\ \tilde{0} & \tilde{I} & \ddots & \ddots & \vdots\\ \vdots & \ddots & \ddots & \ddots & \vdots\\ \vdots & \ddots & \ddots & \ddots & \tilde{0}\\ \tilde{0} & \cdots & \cdots & \tilde{0} & \tilde{I} \end{bmatrix}. \tag{3.9}$$

If we introduce the two-dimensional translational invariance and assume that all the scatterers are identical, the T matrix in $\mathbf{k}$ space becomes

$$T(\mathbf{k}_f m^f_\sigma,\mathbf{k}_i m^i_\sigma)=(4\pi)^2\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha} \times\sum_{j_1L_1j_2L_2}\left\{\tilde{t}[\tilde{I}-\tilde{B}(\mathbf{k}_i)\tilde{t}]^{-1}\right\}_{j_1L_1j_2L_2} \times Y^{m^f_\sigma}_{j_1L_1\frac{1}{2}}(\hat{\mathbf{k}}_f)Y^{m^i_\sigma *}_{j_2L_2\frac{1}{2}}(\hat{\mathbf{k}}_i), \tag{3.10}$$

and then the following scattered wave function can be obtained:

$$\psi_{\text{scatt}}(\mathbf{r})=-\frac{m_e i}{\hbar^2}\sum_{\mathbf{g}}\frac{e^{i\mathbf{k}_g\cdot\mathbf{r}}}{k_z(\mathbf{g})}\langle \mathbf{k}_g m^{\mathbf{g}}_\sigma\,|T|\,\mathbf{k}_i m^i_\sigma\rangle, \tag{3.11}$$

where

$$\left[\tilde{B}(\mathbf{k}_i)\right]_{j_1L_1j_2L_2}\equiv B_{j_1L_1j_2L_2}(\mathbf{k}_i) =\sum_{\mathbf{R}_\beta\neq0} G_{j_1L_1j_2L_2}(\mathbf{R}_\beta)e^{-i\mathbf{k}_i\cdot\mathbf{R}_\beta}, \tag{3.12}$$

$$\mathbf{k}_{\mathbf{g}}=\left[\mathbf{k}_{i\|}+\mathbf{g},k_z(\mathbf{g})\right],$$

$$k_z(\mathbf{g})=\text{sgn}(z)\left[k^2-(\mathbf{k}_{i\|}+\mathbf{g})^2\right]^{1/2},$$

$\mathbf{g}$ is the two-dimensional reciprocal-lattice vector, $\text{sgn}(z)=1$ for $z\geq 0$ and -1 for $z<0$, and $\mathbf{k}_{i\|}$ is the parallel component of the incident wave (see Appendix A of Ref. 12 for the details). The electron wave function

given by Eq. (3.11) corresponds to that of the dynamical theory for nonrelativistic polarized low-energy electron diffraction (PLEED) analysis. If we choose forward scattering, it can be applied to transport problems,[15] too.

IV. DISCUSSIONS

Although a relativistic version of the LEED theory has been developed by Feder *et al.* before[6] using a different approach from ours, the scope of the application of spin-polarized electron scattering looks relatively limited until now. We may find several reasons for this. For example, for a surface structure analysis we need highly spin-polarized electron beams, but it is a relatively difficult task to get them since the efficiency of the spin polarization is not so great in general. Besides, an extra process of the separation of spin up and down electrons is required in order to utilize the spin polarization. The functional form of the spin-orbit interaction is responsible for the low efficiency of the spin polarization. However, in the case of artificial atoms such as quantum dots we can obtain the freedom to change the potential form and the radius by choosing the constituent materials properly.[10] Thus it may be natural to expect more active use of the spin polarization in future quantum devices. In this paper, we have generalized the nonrelativistic elastic electron multiple scattering theory[12] further, including the spin-orbit interaction, hoping that it helps to design such a new type of quantum device and to find the proper spatial distribution of quantum dots for high spin polarization. We have, however, neglected many-body effects during the scattering process in this paper. Consideration of the confined electrons in the quantum dot in the scattering process makes this problem quite analogous to that of electron-atom scattering, but with a different balance of the electron correlation and the spin-orbit interaction. Such a study is also in progress. Unlike in the atomic cases, the balance is variable in the case of quantum dots; thus we can expect many more interesting physical phenomena which originate in the spin polarization than in the electron-atom scattering.

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