Many-body theory of indirect nuclear interactions

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We derive an expression for the indirect nuclear coupling tensor ($A_{jj'}^{\alpha\beta}$) including spin-orbit and many-body effects. We use a finite-temperature Green's-function method where the thermodynamic potential is expressed in terms of the exact one-particle propagator and the proper self-energy, and derive a general expression for $A_{jj'}^{\alpha\beta}$ in the Bloch representation. While the effects of spin-orbit interaction appear in our expression through the modification of the one-particle eigenvalues and eigenstates and through a change in the orbital hyperfine interaction via the modification of the electronic momentum operator, the many-body effects are more subtle. We find that the many-body corrections to $A_{jj'}^{\alpha\beta}$ in the quasiparticle approximation are cancelled in part by the inclusion of exchange and correlation effects. We also show, by making drastic assumptions while solving the matrix integral equations for the nuclear spin-dependent part of the self-energy, that the exchange enhancement effects in a band model on $A_{jj'}^{\alpha\beta}$ are different for different terms. The remarkability of the theory is that for the first time a systematic effort has been made to study the effects of electron-electron interaction on the various contributions to $A_{jj'}^{\alpha\beta}$. We also discuss the importance of relativistic and electron-electron interaction effects in the calculation of the coupling constant in real systems. The theory is general and can be applied to metals, semiconductors, and insulators.

I. INTRODUCTION

A first principles analysis of the indirect nuclear interactions[1,2] which were discovered independently by Hahn and Maxwell[3] and Gutowsky *et al.*[4] is of importance in solids, mainly for two reasons. First, since the indirect nuclear interactions depend rather sensitively on both the wave functions as well as features of the band structure and Fermi surface of the metal, they could provide a more detailed assessment of the applicability of band calculations than properties which depend only on the shape and dimensions of the Fermi surface. Second, they also depend on a variety of mechanisms involving both single-particle and many-particle effects connected with interactions among conduction electrons and between the conduction and core electrons. Thus a study of these interactions could sharpen our understanding not only of the electronic structure of solids, but also of electron-electron interaction effects. Furthermore, a detailed study of theoretically simpler nuclear exchange may serve to elucidate problems in magnetism related to electron spin exchange.

The basic mechanism contributing to the indirect nuclear interactions can be understood as follows. The nuclear moment at the lattice site R_j creates a local magnetic perturbation which induces an electronic magnetization varying in space, which in turn interacts with another nuclear moment at $\mathbf{R}_{j'}$. The net result of this effect may be described by a static coupling between the nuclear moments. In general, these interactions may be written as

$$H_{\rm int}=\sum_{\substack{jj',\alpha\beta\\ j\neq j'}} A_{jj'}^{\alpha\beta} I_j^{\alpha} I_{j'}^{\beta} , \tag{1.1}$$

where $A_{jj'}^{\alpha\beta}$ is a tensor. Its components are functions of distance $\mathbf{R}_{jj'}$ between the nuclei and also of the orientation of the unit vector $\hat{n}_{jj'}$ directed along the line joining the two nuclei with respect to the crystalline axis. The isotropic part of this coupling between the nuclei gives rise to the Ruderman-Kittel (RK) interaction[5]

$$H_{\rm RK}=\sum_{jj'}{}' A_{jj'} \mathbf{I}_j \cdot \mathbf{I}_{j'} , \tag{1.2}$$

which has the same form as the electrostatic exchange coupling. Since the physical origin is not an exchange interaction, it is often referred to as pseudoexchange coupling. In addition to the isotropic interaction there can be a dipolar-like coupling between the nuclei of the form[6]

$$H_{\rm PD}=\sum_{jj'}{}' B_{jj'}[\mathbf{I}_j\cdot\mathbf{I}_{j'} - 3(\mathbf{I}_j\cdot\mathbf{R}_{jj'}) \times(\mathbf{I}_{j'}\cdot\mathbf{R}_{jj'})R_{jj'}^{-2}] . \tag{1.3}$$

This interaction is referred to in the literature as the pseudo dipolar (PD) interaction, and the dominant contribution to $B_{jj'}$ arises (in the relativistic theory) from a combination of the contact and dipolar hyperfine interactions. There is an additional contribution to $B_{jj'}$ from second-order effects of the dipolar hyperfine interactions alone.

Besides this basic mechanism, the other mechanisms contributing to the indirect interactions are due to spin-orbit and other relativistic effects,[7] exchange-core-polarization effects,[8–10] and electron-electron interactions.[11] The one-electron description is inaccurate insofar as it disregards the spatial correlations between the electrons, as demonstrated for instance by the grossly incorrect results it yields for the magnetic susceptibility.[12–16] The importance of exchange-enhancement effects has also been emphasized in the case of the Knight shift.[17–19] Moriya[20] and, with improved numerical accuracy, Narath and Weaver[21] have shown that electron-electron interaction leads to an enhancement of the relaxation rate, which is different from the way the Knight shift is enhanced. Furthermore, up to now there has been no systematic effort to include the effects of orbital hyperfine interaction on $A_{jj'}^{\alpha\beta}$. This is particularly important for solids in which the electronic wave functions have appreciable p character. For example, in case of PbTe, which is a narrow-gap semiconductor with large spin-orbit interaction, the conduction bands transform like atomic p states about the Pb nucleus and the orbital hyperfine matrix elements are known to be comparable to the contact hyperfine matrix elements.[22,23] It is worthwhile to mention, further, that the earlier calculations have concentrated either on the RK or the pseudodipolar types of nuclear-spin interactions, but no attempt has been made to combine all three hyperfine interactions and study their mutual effects on the indirect coupling tensor. In addition, most of the previous theories are applicable to systems which are nearly-free-electron-like with a single occupied band.

It is clear, thus, from the foregoing remarks that, while the effects of electron-electron interaction on the magnetic susceptibility (χ), Knight shift (K), and relaxation rate (T_1^{-1}) have been fairly well understood, a theory of indirect nuclear interactions, starting from first principles, particularly for a many-band system including periodic potential, spin-orbit interaction, electron-electron interaction, and all the electron-nuclear hyperfine interactions, is still lacking in the literature. The present work was carried out as an attempt to fill this gap, and we believe that we have been able to derive a reasonably satisfactory theory for $A_{jj'}^{\alpha\beta}$, which analyzes all the contributions carefully.

Our approach is different from the earlier methods in the sense that we have used a finite-temperature Green's-function formalism, where the thermodynamic potential Ω for an interacting electron system in the presence of a periodic potential, spin-orbit interaction, and electron-nuclear hyperfine interaction is expressed in terms of the exact one-particle propagator G and the proper self-energy Σ. We have constructed in $\mathbf{k}$ space, using the Bloch representation, the equation of motion of the Green's function in the presence of electron-electron and hyperfine interactions and have evaluated Ω, and hence $A_{jj'}^{\alpha\beta}$. We have also shown that our theory reduces the Ruderman-Kittel result in appropriate limits.

The organization of the paper is as follows. In Sec. II we have constructed the effective equation of motion of the Green's function in the Bloch representation in the presence of a periodic potential, spin-orbit, electron-electron, and electron-nuclear hyperfine interactions. In Sec. III we derive a general expression for the indirect coupling tensor $A_{jj'}^{\alpha\beta}$. Finally, in Sec. IV we summarize and discuss the results. Further, in Appendix B we have discussed, in brief, the exchange-enhancement effects on the various constituent terms of $A_{jj'}^{\alpha\beta}$ and, in Appendix C, we have shown that our results reduce to the RK constant, if we ignore the orbital and dipolar hyperfine interactions.

II. EFFECTIVE EQUATION OF MOTION IN BLOCH REPRESENTATION

The exact one-particle propagator $G(\mathbf{r},\mathbf{r}',\zeta_l)$ for an interacting electron system in the presence of a periodic potential $V(\mathbf{r})$, spin-orbit interaction, and electron-nuclear hyperfine interactions satisfies the equation

$$(\zeta_l - H)G(\mathbf{r},\mathbf{r}',\mathbf{I},\zeta_1) + \int d\mathbf{r}''\Sigma(\mathbf{r},\mathbf{r}'',\mathbf{I},\zeta_l)G(\mathbf{r}'',\mathbf{r}',\mathbf{I},\zeta_l) = \delta(\mathbf{r}-\mathbf{r}') \ , \tag{2.1}$$

where Σ is the proper self-energy operator, ζ_l is the complex energy,

$$\zeta_l = \frac{(2l+1)i\pi}{\beta} + \mu, \quad l = 0, \pm 1, \pm 2, \ldots \tag{2.2}$$

μ being the chemical potential, and H is the one-particle Hamiltonian,

$$H = \frac{p^2}{2m} + V(\mathbf{r}) + \frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p} + \frac{\hbar}{8m^2c^2}\nabla^2 V + \sum_{j,\alpha}\mu_0\mu_{0N}g_{I_j}I_j^\alpha X_j^\alpha \ , \tag{2.3}$$

where summation over j includes all the nuclei. In Eq. (2.3), the first four terms are the well-known terms for a one-electron Hamiltonian in the presence of a periodic potential and spin-orbit interaction, where σ is the Pauli spin matrix, and the last term describes the electron-nuclear hyperfine interactions, where μ_0 and μ_{0N} are the electron and nuclear Bohr magnetons, respectively, g_{I_j} is the nuclear g factor for the jth nucleus with spin $\mathbf{I}_j$, and

$$X_j^\alpha = \frac{8\pi}{3}\sigma^\alpha\delta(\mathbf{r}-\mathbf{R}_j) + \left[-\frac{\sigma^\alpha}{|\mathbf{r}-\mathbf{R}_j|^3} + \frac{3[\sigma\cdot(\mathbf{r}-\mathbf{R}_j)](\mathbf{r}-\mathbf{R}_j)^\alpha}{|\mathbf{r}-\mathbf{R}_j|^5} \right] + 2\epsilon_{\alpha\beta\gamma}\frac{(\mathbf{r}-\mathbf{R}_j)^\beta\pi^\gamma}{\hbar|\mathbf{r}-\mathbf{R}_j|^3} \ . \tag{2.4}$$

In Eq. (2.4) the terms from left to right on the right-hand side form the parts of contact, dipolar, and orbital hyperfine interactions for the jth nucleus at $\mathbf{R}_j$. $\epsilon_{\alpha\beta\gamma}$ is an antisymmetric tensor of third rank and we follow the Einstein summation convention. π is the electronic momentum operator modified by the spin-orbit interaction and is defined as $\pi = \mathbf{p} + (\hbar/4mc^2)\sigma\times\nabla V$.

It is shown in Appendix A that Eq. (2.1) can be written in the Bloch representation, i.e., in terms of the basis functions

$$\psi_{n\mathbf{k}\rho} = e^{i\mathbf{k}\cdot\mathbf{r}}U_{n\mathbf{k}\rho}(\mathbf{r}) \ , \tag{2.5}$$

where $\psi_{n\mathbf{k}\rho}$ is a periodic two-component function, n is the band index, $\mathbf{k}$ is the reduced wave vector, and ρ is the spin index as

$$[\zeta_l - H(\mathbf{k},\mathbf{k}',\mathbf{I},\zeta_l)]G(\mathbf{k},\mathbf{k}',\mathbf{I},\zeta_l)=\delta_{\mathbf{k}\mathbf{k}'} . \quad (2.6)$$

We emphasize that, since large changes in $\mathbf{k}$ for conduction electrons between the initial and intermediate states may be involved, the hyperfine interaction cannot be treated in the effective-mass approximation[24] and must be taken with respect to Bloch states.

In Eq. (2.6),

$$H(\mathbf{k},\mathbf{k}',\zeta_l)=\frac{p^2}{2m}+V(\mathbf{r})+\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}+\frac{\hbar^2}{8m^2c^2}\nabla^2 V+\mu_0\mu_{0N}\sum_{j,\alpha} g_{I_j} I_j^\alpha X^\alpha(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}+\Sigma(\mathbf{k},\mathbf{k}',\mathbf{I},\zeta_l) . \quad (2.7)$$

It should be pointed out that Σ is a 2×2 matrix, an operator in $\mathbf{k}$ space, and has implicit dependence on nuclear spin. We can, therefore, expand $\Sigma(\mathbf{k},\mathbf{k}',\mathbf{I},\zeta_l)$ as

$$\Sigma(\mathbf{k},\mathbf{k}',\mathbf{I},\zeta_l)=\Sigma^0(\mathbf{k},\mathbf{k}',\zeta_l)+\sum_{j,\alpha} I_j^\alpha \Sigma_j^{1,\alpha}(\mathbf{k},\mathbf{k}',\zeta_l)+\sum_{jj',\alpha\beta}{}' I_j^\alpha I_{j'}^\beta \Sigma_{jj'}^{2,\alpha\beta}+\cdots , \quad (2.8)$$

where the prime over the summation sign in the third term implies $j\neq j'$.

From Eqs. (2.7) and (2.8), we write

$$H(\mathbf{k},\mathbf{k}',\zeta_l)=H_0(\mathbf{k},\zeta_l)+H'(\mathbf{k},\mathbf{k}',\zeta_l) , \quad (2.9)$$

where

$$H_0=\frac{p^2}{2m}+V(\mathbf{r})+\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}+\frac{\hbar^2}{8m^2c^2}\nabla^2 V+\Sigma^0(\mathbf{k},\zeta_l) \quad (2.10)$$

and

$$H'=\sum_{j,\alpha} I_j^\alpha (P_j^\alpha e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}+\Sigma_j^{1,\alpha})+\sum_{jj',\alpha\beta}{}' I_j^\alpha I_{j'}^\beta \Sigma_{jj'}^{2,\alpha\beta}(\mathbf{k},\mathbf{k}') . \quad (2.11)$$

In Eq. (2.11)

$$P_j^\alpha=\mu_0\mu_{0N}g_{I_j}X^\alpha(\mathbf{r}) . \quad (2.12)$$

Further, in obtaining Eq. (2.10), we have approximated

$$\Sigma^0(\mathbf{k},\mathbf{k}',\zeta_l)=\Sigma^0(\mathbf{k},\zeta_l)\delta_{\mathbf{k}\mathbf{k}'} . \quad (2.13)$$

For nontrivial solutions, Eq. (2.6) can be solved by a perturbation expansion

$$G(\mathbf{k},\mathbf{k}',\zeta_l)=G_0(\mathbf{k},\zeta_l)+G_0(\mathbf{k},\zeta_l)H'G_0(\mathbf{k},\zeta_l)+G_0(\mathbf{k},\zeta_l)H'G_0(\mathbf{k},\zeta_l)H'G_0(\mathbf{k},\zeta_l)+\cdots , \quad (2.14)$$

where

$$G_0^{-1}(\mathbf{k},\zeta_l)=[\zeta_l-H_0(\mathbf{k},\zeta_l)] \quad (2.15)$$

and is diagonal in the basis $\psi_{n\mathbf{k}\rho}$. In the expansion equation (2.14), we have retained terms up to the second order in H'. From Eqs. (2.11) and (2.14), we obtain

$$\begin{aligned}G(\mathbf{k},\mathbf{k}',\zeta_l)= {}& G_0(\mathbf{k},\zeta_l)+\sum_{j,\alpha} I_j^\alpha G_0(\mathbf{k},\zeta_l)(P_j^\alpha e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}+\Sigma_j^{1,\alpha})G_0(\mathbf{k},\zeta_l)\\ &+\sum_{jj',\alpha\beta}{}' I_j^\alpha I_{j'}^\beta [G_0(\mathbf{k},\zeta_l)\Sigma_{jj'}^{2,\alpha\beta}(\mathbf{k},\mathbf{k}')G_0(\mathbf{k},\zeta_l)+G_0(\mathbf{k},\zeta_l)(P_j^\alpha e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}+\Sigma_j^{1,\alpha})G_0(\mathbf{k},\zeta_l)\\ &\times(P_{j'}^\beta e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta})G_0(\mathbf{k},\zeta_l)] ,\end{aligned} \quad (2.16)$$

where we have retained terms up to second order in the nuclear spin $\mathbf{I}$.

III. DERIVATION OF $A_{jj'}^{\alpha\beta}$

We shall now derive an expression for $A_{jj'}^{\alpha\beta}$ from the expression

$$A_{jj'}^{\alpha\beta}=\lim_{\substack{\mathbf{I}_j\to 0\\ \mathbf{I}_{j'}\to 0}}\frac{\partial^2\Omega}{\partial I_j^\alpha \partial I_{j'}^\beta} , \quad (3.1)$$

where $\Omega(T,V,\mu,\mathbf{I})$ is the thermodynamic potential for an interacting electron system in the presence of a periodic potential $V(\mathbf{r})$, spin-orbit interaction, and electron-nuclear hyperfine interaction. Ω can be evaluated from the Luttinger and Ward expression[25,26]

$$\Omega=\frac{1}{\beta}[\operatorname{Tr}\ln(-G_{\zeta_l})-\operatorname{Tr}\Sigma_{\zeta_l}G_{\zeta_l}+\phi(G_{\zeta_l})] . \quad (3.2)$$

In Eq. (3.2), G_{ζ_l} and Σ_{ζ_l} are the abbreviated notations for the exact one-particle Green's function and proper self-energy defined earlier. Tr is defined as $\sum_l \mathrm{Tr}$, where Tr refers to summation over a complete one-particle set, and the functional $\phi(G_{\zeta_l})$ is defined as[26]

$$\phi(G_{\zeta_l})=\lim_{\lambda\to 1}\operatorname{Tr}\Sigma_n\frac{\lambda^n}{2n}\Sigma_{\zeta_l}^{(n)}G_{\zeta_l} . \quad (3.3)$$

In Eq. (3.3), $\Sigma_{\zeta_l}^{(n)}$ is the nth-order self-energy part, where the interaction parameter λ occurring explicitly in Eq. (3.3) is used to determine the order. In fact $\phi(G_{\zeta_l})$ is defined through the decomposition of $\Sigma_{\zeta_l}^{(n)}$ into skeleton diagrams. There are $2nG_{\zeta_l}$ lines for the nth-order diagrams in $\phi(G_{\zeta_l})$. Differentiating $\phi(G_{\zeta_l})$ with respect to G_{ζ_l} has the effect of "opening" any of the $2n$ lines of the nth-order diagram, and each will give the same contribution when Tr is taken. Using Eqs. (3.2) and (3.3) in Eq. (3.1), we have

$$A_{jj'}^{\alpha\beta}=\frac{1}{\beta}\frac{\partial^2}{\partial I_j^\alpha \partial I_{j'}^\beta}\operatorname{Tr}\ln(-G_{\zeta_l}) -\frac{1}{\beta}\operatorname{Tr}\left[\frac{\partial^2\Sigma_{\zeta_l}}{\partial I_j^\alpha\partial I_{j'}^\beta}G_{\zeta_l}+\frac{\partial\Sigma_{\zeta_l}}{\partial I_j^\alpha}\frac{\partial G_{\zeta_l}}{\partial I_{j'}^\beta}\right] . \quad (3.4)$$

The first term in the right-hand side of Eq. (3.4), which has exactly the same form as that for the noninteracting Fermi system, except for the replacement of the noninteracting G_{ζ_l} by the exact G_{ζ_l}, is the quasiparticle contribution, and the second term is the contribution due to exchange and correlation effects. Thus Eq. (3.4) can be written as

$$A_{jj'}^{\alpha\beta}=A_{jj'\mathrm{qp}}^{\alpha\beta}+A_{jj'\mathrm{corr}}^{\alpha\beta} , \quad (3.5)$$

where

$$A_{jj'\mathrm{qp}}^{\alpha\beta}=\frac{1}{\beta}\frac{\partial^2}{\partial I_j^\alpha\partial I_{j'}^\beta}\operatorname{Tr}\ln(-G_{\zeta_l}) \quad (3.6)$$

and

$$A_{jj'\mathrm{corr}}^{\alpha\beta}=-\frac{1}{\beta}\operatorname{Tr}\left[\frac{\partial^2\Sigma_{\zeta_l}}{\partial I_j^\alpha\partial I_{j'}^\beta}G_{\zeta_l}+\frac{\partial\Sigma_{\zeta_l}}{\partial I_{j'}^\beta}\frac{\partial G_{\zeta_1}}{\partial I_{j'}^\beta}\right] . \quad (3.7)$$

We now proceed to derive an expression for $A_{jj'\mathrm{qp}}^{\alpha\beta}$ by assuming the self-energy to be independent of frequency, which is valid in a static screening approximation.[27] We use, in order to carry out the frequency sums appearing in $A_{jj'\mathrm{qp}}^{\alpha\beta}$, the identity[25]

$$\frac{1}{\beta}\operatorname{Tr}\ln(-G_{\zeta_l})=-\frac{1}{2\pi i}\operatorname{Tr}\int_c\phi(\zeta)G(\zeta)d\zeta , \quad (3.8)$$

where

$$\phi(\zeta)=-\frac{1}{\beta}\ln(1+e^{-\beta(\zeta-\mu)}) \quad (3.9)$$

and the contour c encircles the imaginary axis in an anticlockwise direction. The advantage of using Eq. (3.8) is that after substituting the perturbation expansion $G(\zeta)$ [Eq. (2.16)], the free energy can be easily evaluated. The one-particle trace is evaluated over $\psi_{n\mathbf{k}\rho}$ which are eigenfunctions of H_0. In this basis G_0 is diagonal and is given by

$$G_0^{-1}=(\zeta-E_{n\mathbf{k}}) , \quad (3.10)$$

where $E_{n\mathbf{k}}$ is the eigenvalue corresponding to H_0. After performing the trace, we perform the contour integration to obtain

$$\begin{aligned}\frac{1}{\beta}\operatorname{Tr}\ln(-G_{\zeta_l})=&\sum_{\mathbf{k}}\phi(E_{n\mathbf{k}})+\sum_{\substack{j,\alpha\\ n,\mathbf{k},\rho}}I_j^\alpha\langle n\mathbf{k}\rho\,|\,P_j^\alpha+\Sigma_j^{1,\alpha}\,|\,n\mathbf{k}\rho\rangle f(E_{n\mathbf{k}})\\ &+\sum_{\substack{jj',\alpha\beta\\ n,n',\mathbf{k},\mathbf{k}',\rho,\rho'\\ n\neq n',\mathbf{k}\neq\mathbf{k}'}}{}' I_j^\alpha I_{j'}^\beta\Bigg[\tfrac{1}{2}\langle n\mathbf{k}\rho\,|\,P_j^\alpha+\Sigma_j^{1,\alpha}\,|\,n\mathbf{k}\rho'\rangle\langle n\mathbf{k}\rho'\,|\,P_{j'}^\beta+\Sigma_{j'}^{1,\beta}\,|\,n\mathbf{k}\rho\rangle f'(E_{n\mathbf{k}})\\ &+\frac{\langle n\mathbf{k}\rho\,|\,P_j^\alpha+\Sigma_j^{1,\alpha}\,|\,n'\mathbf{k}\rho'\rangle\langle n'\mathbf{k}\rho'\,|\,P_{j'}^\beta+\Sigma_{j'}^{1,\beta}\,|\,n\mathbf{k}\rho\rangle}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}}f(E_{n\mathbf{k}})\\ &+(\langle n\mathbf{k}\rho\,|\,P_j^\alpha e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}+\Sigma_j^{1,\alpha}\,|\,n\mathbf{k}'\rho'\rangle\\ &\times\langle n\mathbf{k}'\rho'\,|\,P_{j'}^\beta e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta}\,|\,n\mathbf{k}\rho\rangle)\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}\\ &+(\langle n\mathbf{k}\rho\,|\,P_j^\alpha e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}+\Sigma_j^{1,\alpha}\,|\,n'\mathbf{k}'\rho'\rangle\\ &\times\langle n'\mathbf{k}'\rho'\,|\,P_{j'}^\beta e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta}\,|\,n\mathbf{k}\rho\rangle)\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}\end{aligned}$$

$$+\langle n\mathbf{k}\rho\,|\,\Sigma_{jj'}^{2,\alpha\beta}\,|\,n\mathbf{k}\rho\rangle f(E_{n\mathbf{k}})$$

$$+(\,\langle n\mathbf{k}\rho\,|\,P_{j'}^{\beta}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta}\,|\,n'\mathbf{k}'\rho'\rangle$$

$$\times\langle n'\mathbf{k}'\rho'\,|\,P_{j}^{\alpha}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j}^{1,\alpha}\,|\,n\mathbf{k}\rho\rangle$$

$$-\langle n\mathbf{k}\rho\,|\,P_{j}^{\alpha}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j}^{1,\alpha}\,|\,n'\mathbf{k}'\rho'\rangle$$

$$\times\langle n'\mathbf{k}'\rho'\,|\,P_{j'}^{\beta}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta}\,|\,n\mathbf{k}\rho\rangle)\frac{\phi(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}\Bigg], \tag{3.11}$$

where f is the Fermi function. From Eqs. (3.6) and (3.11), we obtain

$$A_{jj'qp}^{\alpha\beta}=\sum_{\substack{\mathbf{k},\mathbf{k}',n,n',\rho,\rho'\\ n\neq n',\mathbf{k}\neq\mathbf{k}'}}\Bigg[(P_{j}^{\alpha}+\Sigma_{j}^{1,\alpha})_{n\mathbf{k}\rho,n\mathbf{k}\rho'}(P_{j'}^{\beta}+\Sigma_{j'}^{1,\beta})_{n\mathbf{k}\rho',n\mathbf{k}\rho}f'(E_{n\mathbf{k}})$$

$$+\left[\frac{(P_{j}^{\alpha}+\Sigma_{j}^{1,\alpha})_{n\mathbf{k}\rho,n'\mathbf{k}\rho'}(P_{j'}^{\beta}+\Sigma_{j'}^{1,\beta})_{n'\mathbf{k}\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}}+\frac{(P_{j'}^{\beta}+\Sigma_{j'}^{1,\beta})_{n\mathbf{k}\rho,n'\mathbf{k}\rho'}(P_{j}^{\alpha}+\Sigma_{j}^{1,\alpha})_{n'\mathbf{k}\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}}\right]f(E_{n\mathbf{k}})$$

$$+[(\,P_{j}^{\alpha}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j}^{1,\alpha})_{n\mathbf{k}\rho,n\mathbf{k}'\rho'}(P_{j'}^{\beta}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta})_{n\mathbf{k}'\rho',n\mathbf{k}\rho}$$

$$+\,(P_{j'}^{\beta}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j'}^{1,\beta})_{n\mathbf{k}\rho,n\mathbf{k}'\rho'}(P_{j}^{\alpha}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j}^{1,\alpha})_{n\mathbf{k}'\rho',n\mathbf{k}\rho}]\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}$$

$$+[\,(P_{j}^{\alpha}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j}^{1,\alpha})_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(P_{j'}^{\beta}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta})_{n'\mathbf{k}'\rho',n\mathbf{k}\rho}$$

$$+\,(P_{j'}^{\beta}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma_{j'}^{1,\beta})_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}$$

$$\times\,(P_{j}^{\alpha}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j}}+\Sigma_{j}^{1,\alpha})_{n'\mathbf{k}'\rho',n\mathbf{k}\rho}]\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}+\Sigma_{jj'n\mathbf{k}\rho,n\mathbf{k}\rho}^{2,\alpha\beta}f(E_{n\mathbf{k}})\Bigg]. \tag{3.12}$$

We note that in the absence of electron-electron interaction the Σ terms become zero and $E_{n\mathbf{k}}$ reduces to the corresponding value for the noninteracting Bloch electron.

In order to derive an expression for $A_{jj'\mathrm{corr}}^{\alpha\beta}$ we obtain from Eqs. (2.8), (2.16), and (3.7)

$$A_{jj'\mathrm{corr}}^{\alpha\beta}=-\frac{1}{\beta}\mathrm{Tr}(\Sigma_{jj'}^{2,\alpha\beta}G_0+\Sigma_{j}^{1,\alpha}G_0P_{j'}^{\beta}G_0)\;. \tag{3.13}$$

Assuming, as before, the self-energy to be independent of frequency and following the prescription[25]

$$\frac{1}{\beta}\sum_{\zeta_l}\frac{1}{(\zeta_l-E_n)^m}=\frac{1}{2\pi i}\int_{\Gamma_0}\frac{f(\zeta)}{(\zeta-E_n)^m}d\zeta\;, \tag{3.14}$$

we obtain from Eq. (3.13)

$$
\begin{aligned}
A^{\alpha\beta}_{jj'\mathrm{corr}} = -\sum_{\substack{n,n',\mathbf{k},\mathbf{k}',\rho,\rho' \\ \mathbf{k}\neq\mathbf{k}',n\neq n'}} \Bigg[& \Sigma^{1,\alpha}_{jn\mathbf{k}\rho,n\mathbf{k}\rho'}(P^{\beta}_{j'}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho',n\mathbf{k}\rho} f'(E_{n\mathbf{k}}) \\
& + \frac{\Sigma^{1,\alpha}_{jn\mathbf{k}\rho,n'\mathbf{k}\rho'}(P^{\beta}_{j'}+\Sigma^{1,\beta}_{j'})_{n'\mathbf{k}\rho',n\mathbf{k}\rho} + (P^{\beta}_{j'}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho,n'\mathbf{k}\rho'}\Sigma^{1,\alpha}_{jn'\mathbf{k}\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}} f(E_{n\mathbf{k}}) \\
& + \left\{ \frac{\Sigma^{1,\alpha}_{jn\mathbf{k}\rho,n\mathbf{k}'\rho'}(P^{\beta}_{j'}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}'\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}} + \frac{(P^{\beta}_{j'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho,n\mathbf{k}'\rho'}\Sigma^{1,\alpha}_{jn\mathbf{k}'\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}} \right\} f(E_{n\mathbf{k}}) \\
& + \left\{ \frac{\Sigma^{1,\alpha}_{jn\mathbf{k}\rho,n'\mathbf{k}'\rho'}(P^{\beta}_{j'}e^{-(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n'\mathbf{k}'\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}} \right. \\
& \left. + \frac{(P^{\beta}_{j'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}\Sigma^{1,\alpha}_{jn'\mathbf{k}'\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}} \right\} f(E_{n\mathbf{k}}) + \Sigma^{2,\alpha\beta}_{jj'n\mathbf{k}\rho,n\mathbf{k}\rho} f(E_{n\mathbf{k}}) \Bigg] .
\end{aligned} \tag{3.15}
$$

$A^{\alpha\beta}_{jj'\mathrm{corr}}$ vanishes in the absence of electron-electron interaction, as it should. From Eqs. (3.5), (3.12), and (3.15), we obtain

$$
\begin{aligned}
A^{\alpha\beta}_{jj'} = \sum_{\substack{\mathbf{k},\mathbf{k}',n,n',\rho,\rho' \\ \mathbf{k}\neq\mathbf{k}',n\neq n'}} \Bigg[& P^{\alpha}_{jn\mathbf{k}\rho,n\mathbf{k}\rho'}(P^{\beta}_{j'}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho',n\mathbf{k}\rho} f'(E_{n\mathbf{k}}) \\
& + \left\{ \frac{P^{\alpha}_{jn\mathbf{k}\rho,n'\mathbf{k}\rho'}(P^{\beta}_{j'}+\Sigma^{1,\beta}_{j'})_{n'\mathbf{k}\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}} + \frac{(P^{\beta}_{j'}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho,n'\mathbf{k}\rho'}P^{\alpha}_{jn'\mathbf{k}\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}} \right\} f(E_{n\mathbf{k}}) \\
& + [e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j} P^{\alpha}_{jn\mathbf{k}\rho,n\mathbf{k}'\rho'}(P^{\beta}_{j'}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}'\rho',n\mathbf{k}\rho} \\
& + (P^{\beta}_{j'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho,n\mathbf{k}'\rho'}P^{\alpha}_{jn\mathbf{k}'\rho',n\mathbf{k}\rho}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}] \frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}} \\
& + [e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j} P^{\alpha}_{jn\mathbf{k}\rho,n'\mathbf{k}'\rho'}(P^{\beta}_{j'}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n'\mathbf{k}'\rho',n\mathbf{k}\rho} \\
& + (P^{\beta}_{j'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'})_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}P^{\alpha}_{jn'\mathbf{k}'p',n\mathbf{k}}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}] \frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}} \Bigg] .
\end{aligned} \tag{3.16}
$$

In Eq. (3.16) we have obtained a general expression for the indirect nuclear coupling tensor in the presence of a periodic potential, spin-orbit interaction, and electron-electron interaction. Furthermore, it includes all three hyperfine interactions. Had we considered only the quasiparticle contribution, we would have obtained exactly the same expression as in Eq. (3.16), except for the replacement of P^{α}_{j} by $P^{\alpha}_{j}+\Sigma^{1,\alpha}_{j}$. Thus, while in the quasiparticle approximation both the hyperfine vertices become renormalized, the effect of exchange and correlation is to cancel precisely the many-body corrections to one of the hyperfine vertices and keep the renormalization of the other vertex intact. The source of this apparent asymmetry between the two hyperfine vertices is in Eq. (3.4). If we would have interchanged I^{α}_{j} and $I^{\beta}_{j'}$ in the last term of Eq. (3.4), we would have obtained in the final expression the renormalization of P^{α}_{j} instead of $P^{\beta}_{j'}$. But, as can be seen later, our final result would be independent of these renormalizations. Thus one has to consider both the quasiparticle and correlation contributions in order to obtain physically meaningful results. Furthermore, unlike the case of the Knight shift (K),[18,19] where we obtain an additional contribution due to spin-orbit interaction, its effect in the present case manifests through the modification of one-particle eigenvalues and eigenfunctions and through a change in the orbital hyperfine interaction via the modification of the electronic momentum operator. It may be noted that the spin-orbit interaction, due to its dependence on the magnetic field, has a profound effect on both the magnetic susceptibility[15] and the Knight shift.[19] In addition to modifying the free-electron g factor, which is due to the effect of spin-orbit interaction on the spin of the Bloch electron, the spin-orbit interaction gives rise to extra contributions to both the magnetic susceptibility and the Knight shift, which we attribute to the effect of spin-orbit interaction on the orbital motion of Bloch electrons. Although such effects do not occur in $A_{jj'}^{\alpha\beta}$, the mere modifications of one-particle eigenvalues and eigenfunctions are expected to be important for heavy metals, semimetals, and narrow-gap semiconductors.

It is also interesting to note that, while the first two terms in the expression for $A_{jj'}^{\alpha\beta}$, do not show any oscillatory behavior, the last two terms do. Thus whether or not the coupling constant is oscillatory depends on the competition between these two types. The expression for $A_{jj'}^{\alpha\beta}$, obtained in Eq. (3.16), is not in a form from which computations can be done. In order to make the formula tractable, we need to express the matrix elements of the self-energy operator in physically meaningful quantities. Since these matrix elements are different in different terms, they require markedly different methods of theoretical treatment. However, once we obtain an expression for the most general matrix element $\Sigma^{1,\beta}_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}$, we can obtain the other matrix elements from this in appropriate limits. In Appendix B we have shown that $\Sigma^{1,\beta}_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}$ can be expressed in the following form:

$$\Sigma^{1,\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}'\rho'}=\frac{\alpha_{nn'}(\mathbf{k},\mathbf{k}')}{1-\alpha_{nn'}(\mathbf{k},\mathbf{k}')}P^{\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}'\rho'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}\ , \tag{3.17}$$

where

$$\alpha_{nn'}(\mathbf{k},\mathbf{k}')=-\sum_{\mathbf{k}'',\mathbf{k}'''}\bar{v}_{nn'}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\frac{f(E_{n\mathbf{k}''})-f(E_{n'\mathbf{k}'''})}{E_{n\mathbf{k}''}-E_{n'\mathbf{k}'''}}\ , \tag{3.18}$$

$\bar{v}$ being the average interparticle interaction.

Similarly, one can obtain

$$\Sigma^{1,\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}\rho'}=\frac{\alpha_{nn'}(\mathbf{k})}{1-\alpha_{nn'}(\mathbf{k})}P^{\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}\rho'}\ , \tag{3.19}$$

$$\Sigma^{1,\beta}_{j'n\mathbf{k}\rho,n\mathbf{k}'\rho'}=\frac{\alpha_{nn}(\mathbf{k},\mathbf{k}')}{1-\alpha_{nn}(\mathbf{k},\mathbf{k}')}P^{\beta}_{j'n\mathbf{k}\rho,n\mathbf{k}'\rho'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}\ , \tag{3.20}$$

and

$$\Sigma^{1,\beta}_{j'n\mathbf{k}\rho,n\mathbf{k}\rho}=\frac{\alpha_{n}(\mathbf{k})}{1-\alpha_{n}(\mathbf{k})}P^{\beta}_{j'n\mathbf{k}\rho,n\mathbf{k}\rho}\ , \tag{3.21}$$

where

$$\alpha_{nn'}(\mathbf{k})=-\sum_{\mathbf{k}'}\bar{v}_{nn'}(\mathbf{k},\mathbf{k}')\frac{f(E_{n\mathbf{k}'})-f(E_{n'\mathbf{k}'})}{E_{n\mathbf{k}'}-E_{n'\mathbf{k}'}}\ , \tag{3.22}$$

$$\alpha_{nn}(\mathbf{k},\mathbf{k}')=-\sum_{\mathbf{k}'',\mathbf{k}'''}\bar{v}_{nn}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\frac{f(E_{n\mathbf{k}''})-f(E_{n\mathbf{k}'''})}{E_{n\mathbf{k}''}-E_{n\mathbf{k}'''}}\ , \tag{3.23}$$

and

$$\alpha_{n}(\mathbf{k})=-\sum_{k'}\bar{v}_{nn}(\mathbf{k},\mathbf{k}')f'(E_{n\mathbf{k}'})\ . \tag{3.24}$$

Using Eqs. (3.17), (3.19), (3.20), and (3.21) in Eq. (3.16), we obtain

$$\begin{aligned}A_{jj'}^{\alpha\beta}=\sum_{\substack{n,n',\mathbf{k},\mathbf{k}',\rho,\rho'\\ n\neq n',\mathbf{k}\neq\mathbf{k}'}}\Bigg[&\frac{1}{1-\alpha_n(\mathbf{k})}P^{1,\alpha}_{jn\mathbf{k}\rho,n\mathbf{k}\rho'}P^{1,\beta}_{j'n\mathbf{k}\rho',n\mathbf{k}\rho}f'(E_{n\mathbf{k}})+\frac{1}{1-\alpha_{nn'}(\mathbf{k})}\frac{P^{\alpha}_{jn\mathbf{k}\rho,n'\mathbf{k}\rho'}P^{\beta}_{j'n'\mathbf{k}\rho',n\mathbf{k}\rho}+P^{\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}\rho'}P^{\alpha}_{jn'\mathbf{k}\rho',n\mathbf{k}\rho}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}}f(E_{n\mathbf{k}})\\&+\frac{1}{1-\alpha_{nn}(\mathbf{k},\mathbf{k}')}(P^{\alpha}_{jn\mathbf{k}\rho,n\mathbf{k}'\rho'}P^{\beta}_{j'n\mathbf{k}'\rho',n\mathbf{k}\rho}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}+P^{\beta}_{j'n\mathbf{k}\rho,n\mathbf{k}'\rho'}P^{\alpha}_{jn\mathbf{k}'\rho',n\mathbf{k}\rho}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}})\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}\\&+\frac{1}{1-\alpha_{nn'}(\mathbf{k},\mathbf{k}')}(P^{\alpha}_{jn\mathbf{k}\rho,n'\mathbf{k}'\rho'}P^{\beta}_{j'n'\mathbf{k}'\rho',n\mathbf{k}\rho}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}+P^{\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}'\rho'}P^{\alpha}_{jn'\mathbf{k}'\rho',n\mathbf{k}\rho}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}})\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}\Bigg]\ .\end{aligned} \tag{3.25}$$

Thus different terms in $A_{jj'}^{\alpha\beta}$ are exchange-enhanced in different ways. We use Eq. (2.12) and, combining all four terms, we write

$$A_{jj'}^{\alpha\beta}=\mu_0\mu_{0N}g_{I_j}g_{I'_j}\sum_{n,n',\mathbf{k},\mathbf{k}'}\frac{1}{1-\alpha_{nn'}(\mathbf{k},\mathbf{k}')}(X^{\alpha}_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}X^{\beta}_{n'\mathbf{k}'\rho',n\mathbf{k}\rho}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}+X^{\beta}_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}X^{\alpha}_{n'\mathbf{k}'\rho',n\mathbf{k}\rho}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}})\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}\ . \tag{3.26}$$

This is a reasonably complete expression for the indirect nuclear coupling tensor including spin-orbit interaction, electron-electron interaction, and all the three electron-nuclear hyperfine interactions. We shall show in Appendix C that our coupling constant reduces to the Ruderman-Kittel constant in appropriate limits.

IV. SUMMARY AND CONCLUSION

In this paper we have presented what we believe to be a reasonably complete theory of the indirect nuclear interactions for a many-band system including the effects of electron-electron and spin-orbit interactions. While the effect of spin-orbit interaction on $A_{jj'}^{\alpha\beta}$ appears in our expression via the modification of one-particle eigenvalues and eigenfunctions, and through a change in the orbital hyperfine interactions, the many-body effects are more subtle. We have shown that, due to significant cancellation effects, one has to consider both the quasiparticle contribution and the contributions due to exchange-correlation effects for obtaining physically meaningful results. It has also been emphasized in our theory that one cannot interpret the exchange-enhancement effects on $A_{jj'}^{\alpha\beta}$ in an intuitive way, because they are different for different terms. Moreover, the present attempt is the first of its kind involving the finite-temperature Green's function technique to derive a tractable expression for the indirect coupling tensor $A_{jj'}^{\alpha\beta}$ including spin-orbit and many-body effects.

The theory is general and can be applied to metals, semiconductors, and diamagnetic solids. For dielectrics, however, the first term is zero and the coupling constant is accounted for by the other three terms. We have also considered the effect of orbital hyperfine interaction on the electron-coupled nuclear-spin interaction. This effect is particularly important for solids whose wave functions have appreciable p character. The theory, in view of rigorous treatment of spin-orbit and many-body effects, could be applied to heavy metals. For example, while the previous theories which deal with a single occupied band are quite good for nearly-free-electron systems, the present theory would be more suitable in the analysis of $A_{jj'}^{\alpha\beta}$ of polyvalent metals such as lead, platinum, and thallium. It is also expected to work equally well for semiconductors like the lead salts which are many-band systems having multiple conduction and valence bands, large spin-orbit interactions, and appreciable p character, since the conduction bands in these systems transform like atomic p states around the lead nucleus. We note that we have not considered the electron core-polarization effect but it can be incorporated in the application of this theory to any real system through the use of one-electron procedures available in the literature.[8,9] The other mechanism which we have also not considered is the core-conduction correlation effects. A quantitative analysis of core-conduction correlation effects would be rather difficult. However, in view of the dynamic independence of core and conduction electrons, its effect may be expected to be small.[28]

Before we conclude, we would like to discuss the experimental situation vis-à-vis theoretical calculations of the indirect nuclear coupling constants. Although the indirect exchange coupling between nuclear spins exists in all metals with finite nuclear spin, its magnitude is large enough to be experimentally detectable only in the case of relatively heavy metals. The various metals where the coupling has been measured so far are rubidium,[29] cesium,[29] platinum,[30] silver,[6] tin,[5] and thallium,[5] and in these systems the effects of spin-orbit interaction are expected to be important. Moreover, the importance of relativistic effects on the indirect nuclear spin-spin interactions can further be understood from the fact that a nonrelativistic calculation[7] of A_{12} in case of Rb and Cs shows a poor agreement with experiment. Furthermore, while a relativistic calculation of A_{12} compares well with experiment in case of Cs, there is no marked improvement in case of Rb. The calculation also shows that in the calculation of B_{12} the overall situation both for Rb and Cs is far from satisfactory, even after inclusion of relativistic effects. One of the reasons for this discrepancy may be attributed to the fact that, since the B_{12} values are rather small in alkali metals, there might be inaccuracies in the measurement of these parameters. There have also been calculations[31] of A_{12} and B_{12} for lead and a near exact agreement with experiment has been reported. However, the agreement is fortuitous and is due, as pointed out by the authors, to the use of arbitrary weighting factors in utilizing a superposition of results from radial integrations in the symmetry directions ΓX and ΓL, and to the neglect of correlation and core-polarization effects. Thus the mechanisms contributing to the indirect nuclear interactions necessitate a fresh treatment with regard, first, to the development of a suitable theory including relativistic and electron-electron interaction effects and, second, to the incorporation of suitable electronic structure calculations as appropriate to the system under study. The present work, we believe, takes care of the first aspect of this treatment and we are planning at present to apply this theory, as a test, to the alkali metals. It may be noted, in this connection, that we have recently calculated the Knight shift of alkali metals,[32] using a nonlocal pseudopotential formalism and degenerate perturbation theory, which shows excellent agreement with experiment for all the alkali metals including Rb and Cs. We have also found out from the calculations that electron-electron interaction effects contribute about 20% to the result. We are of the opinion, therefore, that the effects of electron-electron interaction on the coupling constants would be equally important.

In conclusion, we note that we have derived a general expression for the indirect nuclear coupling tensor, where the effects of electron-electron interaction have been carefully analyzed on each of the constituent terms. It is also pointed out that the effects of spin-orbit interaction are important insofar as they modify the one-electron eigenvalues and eigenfunctions and change the orbital hyperfine interaction through modifications of the momentum operator for the electron. Finally, in contrast to previous theories, where efforts have been made to concentrate only on particular types of indirect nuclear interactions, our attempt is general and could be more useful in studying the electron-coupled nuclear-spin interactions in solids.

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APPENDIX A

The Bloch functions [Eq. (2.5)] form a complete set and have the properties

$$\sum_{n,\mathbf{k},\rho} \psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})\psi_{n\mathbf{k}\rho}(\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}') \tag{A1}$$

and

$$\int d\mathbf{r}\, \psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})\psi_{n'\mathbf{k}'\rho'}(\mathbf{r})=\delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\rho\rho'} \ . \tag{A2}$$

In the Bloch representation, Eq. (2.1) can be written as

$$\int d\mathbf{r}\, d\mathbf{r}'\psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})(\zeta_1-H)G(\mathbf{r},\mathbf{r}',\mathbf{I},\zeta_1)\psi_{n'\mathbf{k}'\rho'}(\mathbf{r}')+\int d\mathbf{r}\, d\mathbf{r}'\, d\mathbf{r}''\psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})\Sigma(\mathbf{r},\mathbf{r}'',\mathbf{I},\zeta_l)G(\mathbf{r}'',\mathbf{r}',\mathbf{I},\zeta_l)\psi_{n'\mathbf{k}'\rho'}(\mathbf{r}')=\delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\rho\rho'} \ . \tag{A3}$$

Denoting the first term as T_1 and the second as T_2 in Eq. (A3), we have

$$T_1=\int d\mathbf{r}\, d\mathbf{r}'\psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})\left[\zeta_l-\frac{p^2}{2m}-V(\mathbf{r})-\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}-\frac{\hbar^2}{8m^2c^2}\nabla^2V-\mu_0\mu_{0N}\sum_{j,\alpha} g_{I_j}I_j^\alpha X^\alpha(\mathbf{r}-\mathbf{R}_j)\right]$$
$$\times G(\mathbf{r},\mathbf{r}',\mathbf{I},\zeta_l)\psi_{n'\mathbf{k}'\rho'}(\mathbf{r}') \ . \tag{A4}$$

Using the transformation properties of the Bloch function and the Green's function

$$G(\mathbf{r},\mathbf{r}',\mathbf{I},\zeta_l)=G(\mathbf{r}+\mathbf{R},\mathbf{r}'+\mathbf{R},\mathbf{I},\zeta_l) \ , \tag{A5}$$

where $\mathbf{R}$ is the crystal translation vector, Eq. (A4) can be written as

$$T_1=\int d\mathbf{r}\, d\mathbf{r}'\psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})\left[\zeta_l-\frac{p^2}{2m}-V(\mathbf{r})-\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}-\frac{\hbar^2}{8m^2c^2}\nabla^2V\right.$$
$$\left.-\mu_0\mu_{0N}\sum_{j,\alpha} g_{I_j}I_j^\alpha X^\alpha(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}\right]G(\mathbf{r},\mathbf{r}',\mathbf{I},\zeta_l)\psi_{n'\mathbf{k}'\rho'}(\mathbf{r}') \ . \tag{A6}$$

Equation (A6) can further be written through the use of the completeness property of the Bloch function [Eq. (A1)] as

$$T_1=\sum_{n'',\mathbf{k}'',\rho''}\left[\zeta_l-\frac{p^2}{2m}-V(\mathbf{r})-\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}-\frac{\hbar^2}{8m^2c^2}\nabla^2V\right.$$
$$\left.-\mu_0\mu_{0N}\sum_{j,\alpha} g_{I_j}I_j^\alpha X^\alpha(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}\right]_{n\mathbf{k}\rho,n''\mathbf{k}''\rho''} G(\mathbf{r}'',\mathbf{r}',\mathbf{I},\zeta_l)_{n''\mathbf{k}''\rho'',n'\mathbf{k}'\rho'} \ , \tag{A7}$$

where

$$\left[\zeta_l-\frac{p^2}{2m}-V(\mathbf{r})-\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}-\frac{\hbar^2}{8m^2c^2}\nabla^2V-\mu_0\mu_{0N}\sum_{j\alpha} g_{I_j}I_j^\alpha X^\alpha(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}\right]_{n\mathbf{k}\rho,n''\mathbf{k}''\rho''}$$
$$=\int d\mathbf{r}\psi^\dagger_{n\mathbf{k}\rho}(\mathbf{r})\left[\zeta_l-\frac{p^2}{2m}-V(\mathbf{r})-\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}-\frac{\hbar^2}{8m^2c^2}V^2V\right.$$
$$\left.-\mu_0\mu_{0N}\sum_{j,\alpha} g_{I_j}I_j^\alpha X^\alpha(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}\right]\psi_{n''\mathbf{k}''\rho''}(\mathbf{r}) \tag{A8}$$

and

$$G(\mathbf{r}'',\mathbf{r}',\mathbf{I},\zeta_l)_{n''\mathbf{k}''\rho'',n'\mathbf{k}'\rho'}=\int d\mathbf{r}'\, d\mathbf{r}''\psi_{n''\mathbf{k}''\rho''}(\mathbf{r}'')G(\mathbf{r}'',\mathbf{r}',\mathbf{I},\zeta_l)\psi_{n'\mathbf{k}'\rho'}(\mathbf{r}') \ . \tag{A9}$$

Similarly, T_2 can be written as

$$T_2=\sum_{n'',k'',\rho''}[\Sigma(\mathbf{r},\mathbf{r}'',\mathbf{I},\zeta_l)]_{n\mathbf{k}\rho,n''\mathbf{k}''\rho''}G(\mathbf{r}''',\mathbf{r}',\mathbf{I},\zeta_l)_{n''\mathbf{k}''\rho'',n'\mathbf{k}'\rho'}\ , \tag{A10}$$

where

$$[\Sigma(\mathbf{r},\mathbf{r}'',\mathbf{I},\zeta_l)]_{n\mathbf{k}\rho,n''\mathbf{k}''\rho''}=\int d\mathbf{r}\,d\mathbf{r}''\psi^{\dagger}_{n\mathbf{k}\rho}(\mathbf{r})\Sigma(\mathbf{r},\mathbf{r}'',\mathbf{I},\zeta_l)\psi_{n''\mathbf{k}''\rho''}(\mathbf{r}'')\ . \tag{A11}$$

From Eqs. (A3), (A7), and (A10) we can write the equation of motion of the Green's function in the Bloch representation as

$$[\zeta_l-H(\mathbf{k},\mathbf{k}',\zeta_l)]G(\mathbf{k},\mathbf{k}',\zeta_l)=\delta_{\mathbf{k}\mathbf{k}'}\ . \tag{A12}$$

APPENDIX B

In configuration space, the exchange self-energy is nonlocal and is expressed as

$$\Sigma(\mathbf{r},\mathbf{r}',\zeta_l)=-\frac{1}{\beta}\sum_{\zeta_{l'}}v_{\text{eff}}(\mathbf{r}-\mathbf{r}')G(\mathbf{r},\mathbf{r}',\zeta_l-\zeta_{l'})\ , \tag{B1}$$

where a simple static screening approximation is made in obtaining $v_{\text{eff}}(\mathbf{r},\mathbf{r}')$ from $v(\mathbf{r},\mathbf{r}')$. In this approximation the self-energy is independent of ζ_l and one has

$$\Sigma(\mathbf{r},\mathbf{r}')=-\frac{1}{\beta}\sum_{\zeta_l}v_{\text{eff}}(\mathbf{r},\mathbf{r}')G(\mathbf{r},\mathbf{r}',\zeta_l)\ . \tag{B2}$$

Assuming $v_{\text{eff}}(\mathbf{r},\mathbf{r}')$ to be independent of nuclear spin, Eq. (B2) can be written as

$$\Sigma(\mathbf{r},\mathbf{r}',\mathbf{I})=-\frac{1}{\beta}\sum_{\zeta_l}v_{\text{eff}}(\mathbf{r},\mathbf{r}')G(\mathbf{r},\mathbf{r}',\mathbf{I},\zeta_l)\ . \tag{B3}$$

Σ and G can be expanded in terms of the Bloch states as

$$\Sigma(\mathbf{r},\mathbf{r}',I)=\sum_{\substack{n,n',\mathbf{k},\mathbf{k}'\\ \rho,\rho'}}\Sigma_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(\mathbf{k},\mathbf{k}',\mathbf{I})\psi_{n\mathbf{k}\rho}(\mathbf{r})\psi^{\dagger}_{n'\mathbf{k}'\rho'}(\mathbf{r}') \tag{B4}$$

and

$$G(\mathbf{r},\mathbf{r}',\mathbf{I})=\sum_{\substack{n,n',\mathbf{k},\mathbf{k}'\\ \rho,\rho'}}G_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(\mathbf{k},\mathbf{k}',\mathbf{I})\psi_{n\mathbf{k}\rho}(\mathbf{r})\psi^{\dagger}_{n'\mathbf{k}'\rho'}(\mathbf{r}')\ . \tag{B5}$$

Substituting Eqs. (B4) and (B5) in Eq. (B3), we obtain

$$\sum_{\substack{n,n',\mathbf{k},\mathbf{k}'\\ \rho,\rho'}}\Sigma_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(\mathbf{k},\mathbf{k}',\mathbf{I})\psi_{n\mathbf{k}\rho}(\mathbf{r})\psi^{\dagger}_{n'\mathbf{k}'\psi'}(\mathbf{r}')=-\frac{1}{\beta}\sum_{\zeta_l}\sum_{\substack{p,q,\mathbf{k},\mathbf{k}'\\ \bar\rho,\bar\rho'}}v_{\text{eff}}(\mathbf{r},\mathbf{r}')G_{p\bar\rho,q\bar\rho'}(\mathbf{k},\mathbf{k}',I)\psi_{p\mathbf{k}\bar\rho}(\mathbf{r})\psi^{\dagger}_{q\mathbf{k}'\bar\rho'}(\mathbf{r}')\ . \tag{B6}$$

If the effective electron-electron interaction is spin independent, then $\rho=\bar\rho$, $\rho'=\bar\rho'$, and we have

$$\Sigma_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(\mathbf{k},\mathbf{k}',\mathbf{I})=-\frac{1}{\beta}\sum_{\zeta_l}\sum_{p,q,\mathbf{k}'',\mathbf{k}'''}\langle nn'\,|\,v_{\text{eff}}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\,|\,pq\,\rangle_{\rho\rho'}G_{p\rho,q\rho'}(\mathbf{k}'',\mathbf{k}''',\mathbf{I})\ , \tag{B7}$$

where

$$\langle nn'\,|\,v_{\text{eff}}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\,|\,pq\,\rangle_{\rho\rho'}=\int d\mathbf{r}\,d\mathbf{r}'\psi^{\dagger}_{n\mathbf{k}\rho}(\mathbf{r})\psi_{n'k'\rho'}(\mathbf{r}')v_{\text{eff}}(\mathbf{r},\mathbf{r}')\psi_{p\mathbf{k}''\rho}(\mathbf{r})\psi^{\dagger}_{q\mathbf{k}'''\rho'}(\mathbf{r}')\ . \tag{B8}$$

We make the approximation

$$\langle nn'\,|\,v_{\text{eff}}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\,|\,pq\,\rangle\cong v_{nn'}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\delta_{np}\delta_{n'q}\ . \tag{B9}$$

Using Eq. (B9) in Eq. (B7), we obtain

$$\Sigma_{n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(\mathbf{k},\mathbf{k}',\mathbf{I})=-\frac{1}{\beta}\sum_{\zeta_l}\sum_{\mathbf{k}'',\mathbf{k}'''}v_{nn'}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')G_{n\rho,n'\rho'}(\mathbf{k}'',\mathbf{k}''',\mathbf{I})\ . \tag{B10}$$

Substituting the expression of G from Eq. (2.16) in Eq. (B10), using (2.8) and (3.14), and comparing the coefficients of $I^{\beta}_{j'}$, we obtain

$$\Sigma^{l,\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}'\rho'}(\mathbf{k},\mathbf{k}')=-\sum_{\mathbf{k}'',\mathbf{k}'''}v_{nn'}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')(P^{\beta}_{j'n\mathbf{k}''\rho,n'\mathbf{k}'''\rho'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}+\Sigma^{1,\beta}_{j'n\mathbf{k}''\rho,n'\mathbf{k}'''\rho'})\frac{f(E_{n\mathbf{k}''})-f(E_{n'\mathbf{k}'''})}{E_{n\mathbf{k}''}-E_{n'\mathbf{k}'''}}\ . \tag{B11}$$

We make an average exchange-enhancement ansatz, which is equivalent to the assumption that $\Sigma^{1,\beta}$ is independent of $\mathbf{k}$, to obtain

$$\Sigma^{l,\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}'\rho'}=\frac{\alpha_{nn'}(\mathbf{k},\mathbf{k}')}{1-\alpha_{nn'}(\mathbf{k},\mathbf{k}')}P^{\beta}_{j'n\mathbf{k}\rho,n'\mathbf{k}'\rho'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{j'}}\ , \tag{B12}$$

where

$$\alpha_{nn'}(\mathbf{k},\mathbf{k}')=-\sum_{\mathbf{k}'',\mathbf{k}'''}\bar{v}_{nn}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\frac{f(E_{n\mathbf{k}''})-f(E_{n'\mathbf{k}'''})}{E_{n\mathbf{k}''}-E_{n'\mathbf{k}'''}}\ . \tag{B13}$$

APPENDIX C

If we ignore the dipolar and orbital hyperfine interactions, the electron-electron interaction, and the interband terms, we have from Eq. (3.26)

$$A^{\alpha\beta}_{jj'}=\left[\frac{8\pi}{3}\right]^2\mu_0^2\mu_{0N}^2 g_{I_j}g_{I_{j'}}\sum_{\substack{\rho,\rho'\\ \mathbf{k},\mathbf{k}'}}\{[\sigma^\alpha\delta(\mathbf{r})]_{n\mathbf{k}\rho,n\mathbf{k}'\rho'}[\sigma^\beta\delta(\mathbf{r})]_{n\mathbf{k}'\rho',n\mathbf{k}\rho}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}$$
$$+[\sigma^\beta\delta(\mathbf{r})]_{n\mathbf{k}\rho,n\mathbf{k}'\rho'}[\sigma^\alpha\delta(\mathbf{r})]_{n\mathbf{k}'\rho',n\mathbf{k}\rho}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}\}\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}\ . \tag{C1}$$

In the absence of spin-orbit interaction, Eq. (C1) can be written as

$$A^{\alpha\beta}_{jj'}=\left[\frac{8\pi}{3}\right]^2\mu_0^2\mu_{0N}^2 g_{I_j}g_{I_{j'}}$$
$$\times\sum_{\mathbf{k},\mathbf{k}'}\{[\langle\psi_{n\mathbf{k}\uparrow}|\sigma^\alpha\delta(\mathbf{r})|\psi_{n\mathbf{k}'\uparrow}\rangle\langle\psi_{n\mathbf{k}'\uparrow}|\sigma^\beta\delta(\mathbf{r})|\psi_{n\mathbf{k}\uparrow}\rangle+\langle\psi_{n\mathbf{k}\uparrow}|\sigma^\alpha\delta(\mathbf{r})|\psi_{n\mathbf{k}'\downarrow}\rangle\langle\psi_{n\mathbf{k}'\downarrow}|\sigma^\beta\delta(\mathbf{r})|\psi_{n\mathbf{k}\uparrow}\rangle]e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}$$
$$+[\langle\psi_{n\mathbf{k}\uparrow}|\sigma^\beta\delta(\mathbf{r})|\psi_{n\mathbf{k}'\uparrow}\rangle\langle\psi_{n\mathbf{k}'\uparrow}|\sigma^\alpha\delta(\mathbf{r})|\psi_{n\mathbf{k}\uparrow}\rangle+\langle\psi_{n\mathbf{k}\uparrow}|\sigma^\beta\delta(\mathbf{r})|\psi_{n\mathbf{k}'\downarrow}\rangle\langle\psi_{n\mathbf{k}'\downarrow}|\sigma^\alpha\delta(\mathbf{r})|\psi_{n\mathbf{k}\uparrow}\rangle]$$
$$\times e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}}+\text{c.c.}\}\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}\ , \tag{C2}$$

where $\uparrow=\binom{1}{0}$ and $\downarrow=\binom{0}{1}$.

In this case, the coupling constant is isotropic and we have, using Eq. (2.5),

$$A^{zz}_{jj'}=A^{xx}_{jj'}=A^{yy}_{jj'}=4\left[\frac{8\pi}{3}\right]^2\mu_0^2\mu_{0N}^2 g_{I_j}g_{I_{j'}}\sum_{\mathbf{k},\mathbf{k}'}|U_{n\mathbf{k}}(0)|^2|U_{n\mathbf{k}'}(0)|^2\cos[(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}]\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}$$
$$=\frac{64\pi^2}{2}\hbar^4\gamma_e^2\gamma_j\gamma'_j\sum_{\mathbf{k},\mathbf{k}'}|U_{n\mathbf{k}}(0)|^2|U_{n\mathbf{k}'}(0)|^2\cos[(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{jj'}]\frac{f(E_{n\mathbf{k}})}{E_{n\mathbf{k}}-E_{n\mathbf{k}'}}\ , \tag{C3}$$

where γ_e, γ_j, and $\gamma_{j'}$ are the gyromagnetic ratios for the electron, jth and (j')th nuclei. Equation (C3) is the Ruderman-Kittel result.[33]

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