Theory of the Knight shift in solids: Effect of electron-phonon interaction

G. S. Tripathi*
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

C. M. Misra and P. Tripathi
Department of Physics, Berhampur University, Berhampur 760007, Orissa, India

P. K. Misra
Department of Physics, Mesa State College, Grand Junction, Colorado 81502
and Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881
(Received 7 March 1988; revised manuscript received 6 July 1988)

We derive a theory of the Knight shift in the presence of a periodic potential and spin-orbit and electron-phonon interactions. We use a temperature Green's-function technique and solve the self-energy equations in the presence of a magnetic field. The spin, orbital, and spin-orbit contributions to the Knight shift are mainly affected by the electron-phonon interaction through the changes in the one-electron energies and wave functions. By considering both the electron-electron and electron-phonon interactions, we show that the Stoner factor is affected by about 13% in sodium. The theory presented in this work is general and, we believe, can be applied to metals, semiconductors, and intermetallic compounds with suitable modifications. In view of the present controversy in the role of the electron-phonon interaction on the magnetism of solids, our work is expected to pave the way for a better quantitative understanding of the subject.

I. INTRODUCTION

A first-principles analysis of the Knight shift (K) is an important tool to probe the electronic and magnetic properties of solids. The mechanisms that contribute to the Knight shift have been extensively discussed in earlier works.[1-8] The importance of these mechanisms has also been evaluated through various applications.[2,6,9-20] These mechanisms have contributed, in a very extensive way, to our understanding of both single-particle and many-particle effects both in the presence and absence of the magnetic field. However, there has not been any theory of the Knight shift, to date, which considers the effect of electron-phonon interactions from first principles.

Recently there has been considerable activity to assess the role of the electron-phonon interaction in the magnetism of solids.[21-30] However, there remains substantial disagreement among the findings of these investigations. It is well known that the Pauli paramagnetic susceptibility is exchange enhanced by the electron-electron interaction through the Stoner factor. Enz and Mathias[23] have proposed that this factor is affected by the electron-phonon coupling, and is responsible for the ferromagnetism of $ZrZn_2$. On the other hand, Fay and Appel[24] have proposed that the electron-phonon correction to the Stoner factor is of the order $(m/M)^{1/2}$, where m and M are the electron and atomic masses, respectively, and hence negligible. The idea that the Pauli susceptibility is not affected by electron-phonon interaction is also supported by Grimvall[25] and Pickett.[26] At the same time, Kim and co-workers[28-30] have emphasized the role of phonons in the ferromagnetism of solids. Thus the subject still remains controversial.

In view of the above remarks we have undertaken this work to probe in detail the effects of electron-phonon interaction on the Knight shift. This is a many-body problem and has been formulated as an extension of our earlier work,[6] which has considered the many-body and spin-orbit effects on the Knight shift.

We employ a temperature Green's-function technique to investigate this problem. The method has been successfully applied to derive first-principles theories of magnetic susceptibility,[31,32] indirect nuclear spin-spin interactions,[33] and chemical shift.[34] Furthermore, since the inertia of the ions is important, the interaction between the electrons which is mediated by phonons is not instantaneous but retarded. This makes the Green's functions a particularly useful vehicle for describing them.

The planning of the paper is as follows. In Sec. II we briefly review the general expression of K, obtained in our earlier work. In Sec. III we set up integral equations for the electron self-energy in the presence of electron-phonon interaction and the magnetic field. These equations are then solved to determine the modifications of the different contributions to the Knight shift by the electron-phonon interaction. We briefly summarize the work with a conclusion in Sec. IV. In Appendix A we discuss the mass renormalization due to the electron-phonon interaction, in the light of our theory; and in Appendix B we discuss the temperature dependence of the mass-enhancement factor.

II. GENERAL EXPRESSION OF THE KNIGHT SHIFT

The general expression of the Knight shift at the jth nuclear site for an interacting electron system is given by[6]

$$K_j^{\nu\mu}=(K_j^{\nu\mu})_s+(K_j^{\nu\mu})_o+(K_j^{\nu\mu})_{\rm so}\ , \tag{2.1}$$

where $(K_j^{\nu\mu})_s$, $(K_j^{\nu\mu})_o$, and $(K_j^{\nu\mu})_{\rm so}$ are the spin, orbital, and spin-orbit contributions to the Knight shift, and they are

$$(K_j^{\nu\mu})_s=-\tfrac{1}{2}\mu_B^2\sum_{n,\mathbf{k},\rho}X^{\nu}_{jn\rho,n\rho'}[g^{\mu}_{nn}(\mathbf{k})\sigma^{\mu}_{n\rho',n\rho}+(2/\mu_B)\tilde{\Sigma}^{1,\mu}_{n\rho',n\rho}]f'(E_{n\mathbf{k}})\ , \tag{2.2}$$

$$(K_j^{\nu\mu})_o=-(e^2/3mc^2)\sum_{n\mathbf{k}\rho}\left[\frac{1}{r_j}\right]_{n\rho,n\rho}\delta_{\nu\mu}f(E_{n\mathbf{k}})+(2\mu_B^2/m)\epsilon_{\alpha\beta\mu}\sum_{n,\mathbf{k},\rho}[(r_j^{\alpha}\pi^{\beta})_{n\rho,m\rho'}(L_j^{\nu}/r_j^3)_{m\rho',n\rho}$$
$$+(L_j^{\nu}/r_j^3)_{n\rho,m\rho'}(r_j^{\alpha}\pi^{\beta})_{m\rho',n\rho}]\frac{f(E_{n\mathbf{k}})}{E_{mn}}\ , \tag{2.3}$$

$$(K_j^{\nu\mu})_{\rm so}=\sum_{n\mathbf{k}\rho}\Bigg[(i\mu_B^2/m)\epsilon_{\alpha\beta\mu}\Bigg[(-3X^{\nu}_{jn\rho,n\rho'}\pi^{\alpha}_{n\rho',m\rho''}\pi^{\beta}_{m\rho'',n\rho}+\pi^{\alpha}_{n\rho,n\rho}X^{\nu}_{jn\rho,m\rho'}\pi^{\beta}_{m\rho',n\rho}-\pi^{\alpha}_{n\rho,n\rho}\pi^{\beta}_{n\rho,m\rho'}X^{\nu}_{jm\rho',n\rho})\frac{1}{E_{mn}^2}$$
$$+(\pi^{\alpha}_{n\rho,m\rho'}\pi^{\beta}_{m\rho',q\rho''}X^{0\nu}_{jq\rho'',n\rho}+\pi^{\alpha}_{n\rho,m\rho'}X^{0\nu}_{jm\rho',q\rho''}\pi^{\beta}_{q\rho'',n\rho}+X^{0\nu}_{jn\rho,m\rho'}\pi^{\alpha}_{m\rho',q\rho''}\pi^{\beta}_{q\rho'',n\rho})\frac{1}{E_{mn}E_{qn}}\Bigg]$$
$$+\frac{1}{2}g_0\mu_B(X^{\nu}_{jn\rho,m\rho'}F^{\mu}_{m\rho',n\rho}+F^{\mu}_{n\rho,m\rho'}X^{\nu}_{jm\rho',n\rho})\frac{1}{E_{mn}}\Bigg]f(E_{n\mathbf{k}})\ . \tag{2.4}$$

In Eqs. (2.2)–(2.4), μ_B is the Bohr magneton, m is the mass of the electron except that when used as an index it represents the band index, q and n are other band indices, and the ρ's are the spin indices. $\epsilon_{\alpha\beta\mu}$ is an antisymmetric tensor of the third rank and we follow the Einstein summation convention. Repeated band and spin indices imply summation. π is the electronic momentum operator in the presence of spin-orbit and self-energy interactions represented by $\tilde{\Sigma}$. $f(E_{n\mathbf{k}})$ is the Fermi distribution function, $E_{mn}=E_m(\mathbf{k})-E_n(\mathbf{k})$, σ are the Pauli spin matrices, and $\mathbf{r}_j=\mathbf{r}-\mathbf{R}_j$, $\mathbf{R}_j$ being the position vector of the jth nucleus with respect to $\mathbf{r}$. g_{nn} is the intraband g matrix defined by

$$g^{\mu}_{nn}(\mathbf{k})\sigma^{\mu}_{n\rho,n\rho'}(\mathbf{k})=g_0\sigma^{\mu}_{n\rho,n\rho'}(\mathbf{k})+\frac{2i}{m}\epsilon_{\alpha\beta\mu}\sum_{m,\rho''}\frac{\pi^{\alpha}_{n\rho,m\rho''}\pi^{\beta}_{m\rho'',n\rho'}}{E_{mn}}\ , \tag{2.5}$$

where g_0 is the free-electron g-factor:

$$X_j^{\nu}=\left[\frac{8\pi}{3}\sigma^{\nu}\delta(\mathbf{r}_j)+\frac{3(\sigma\cdot\hat{\mathbf{r}}_j)\hat{\mathbf{r}}_j^{\nu}-\sigma^{\nu}}{r_j^3}\right]+2\epsilon_{\nu\mu\eta}\frac{\hat{\mathbf{r}}_j^{\mu}(\pi+\hbar\mathbf{k})^{\eta}}{\hbar r_j^2}$$
$$\equiv X_j^{0\nu}+X_j^{1\nu}\ . \tag{2.6}$$

Here, the first term is a sum of the contact and the dipolar parts of the hyperfine vertex and the last term represents the orbital hyperfine vertex:

$$F^{\mu}=\sigma^{\mu}+(2/g_0\mu_B)\tilde{\Sigma}^{1,\mu}\ , \tag{2.7}$$

where $\tilde{\Sigma}^{1,\mu}$ is defined through the following expression which is obtained by assuming the magnetic field and the nuclear-moment ($\mathbf{M}_j$) dependence of the electron self-energy:[6]

$$\tilde{\Sigma}(\mathbf{k},\mathbf{B},\mathbf{M}_j,E_n)=\tilde{\Sigma}^0(\mathbf{k},E_n)+B^{\mu}\tilde{\Sigma}_j^{1,\mu}(\mathbf{k},E_n)+M_j^{\nu}\tilde{\Sigma}_j^{1,\nu}(\mathbf{k},E_n)+B^{\mu}M_j^{\nu}\tilde{\Sigma}_j^{3,\mu\nu}(\mathbf{k},E_n)+\cdots\ . \tag{2.8}$$

The matrix elements occurring in Eqs. (2.2)–(2.4) are, in general, represented by

$$O^{\alpha}_{n\rho,m\rho'}(\mathbf{k})=\int u^*_{n\mathbf{k}\rho}(\mathbf{r})O^{\alpha}u_{m\mathbf{k}\rho'}(\mathbf{r})d^3r\ , \tag{2.9}$$

where $u_{\mathbf{k}}(r)$ is the periodic part of the Bloch function.

It may be noted that, although $(K_j^{\nu\mu})_{\rm so}$ represents the spin-orbit contribution, it does so only partly. The effect of spin-orbit interaction also enters in the spin contribution, $(K_j^{\nu\mu})_s$, through the effective g factor defined earlier. $(K_j^{\nu\mu})_s$ is, for all purposes, the dominant term; however, $(K_j^{\nu\mu})_{\rm so}$ is of the same order as $(K_j^{\nu\mu})_s$ in narrow-gap semiconductors with large g factors.[6] In some of the heavy metals and semimetals, too, $(K_j^{\nu\mu})_{\rm so}$ is expected to contribute significantly.

The self-energy term includes both the electron-electron and the electron-phonon interactions. Since the electron-electron interaction has been discussed in detail in our earlier work,[6] we skip this effect in this paper. It is included insofar as it contributes to the screening of the electron-phonon interaction.

III. SELF-ENERGY EQUATIONS

The expressions [Eqs. (2.2)–(2.4)] are not in computable form, because of the presence of the self-energy terms. In order that the different contributions to K are expressed in physically meaningful forms, we have to set

up integral equations for the self-energy. Viewed as a field theoretical problem it might appear that one has little hope of handling this fermion-boson coupling in an accurate manner. However, it may be possible to treat this problem exactly, following Migdal's approach.[35] He showed that in normal metals one can calculate the one-electron self-energy to an accuracy of $(m/M)^{1/2}$, where M is the ionic mass, by what amounts to second-order self-consistent perturbation theory. This remarkable result does not depend on the strength of the electron-phonon coupling, but rather depends on the existence of a small parameter $(m/M)^{1/2}$ in the problem. Thus, in the presence of the electron-phonon interaction, one can write[36]

$$\Sigma(\mathbf{k},J_l)=-\frac{1}{\beta}\sum_{\mathbf{k}',J_{l'}}|M_{\mathbf{k}\mathbf{k}'}|^2D(\mathbf{k}-\mathbf{k}',J_l-J_{l'})G(\mathbf{k}',J_{l'})\ , \tag{3.1}$$

where $M_{kk'}$ is the electron-phonon coupling function, D is the phonon propagator, G is the exact one-electron propagator, and

$$J_l=\frac{(2l+1)i\pi}{\beta}+\mu;\quad l=0,\pm1,\ \pm2,\ \cdots\ , \tag{3.2}$$

in which μ is the chemical potential and $\beta=(k_BT)^{-1}$. We consider the field dependence of the electron self-energy and write

$$\tilde{\Sigma}(\mathbf{k},\mathbf{B},\mathbf{M}_j,J_l)=-\frac{1}{\beta}\sum_{\mathbf{k}',J_{l'}}|M_{\mathbf{k}\mathbf{k}'}|^2D(\mathbf{k}-\mathbf{k}',J_l-J_{l'})\tilde{G}(\mathbf{k}',\mathbf{B},\mathbf{M}_j,J_{l'})\ , \tag{3.3}$$

where $\tilde{G}(\mathbf{k}',\mathbf{B},\mathbf{M}_j,J_{l'})$ is defined[6] as

$$\begin{aligned}\tilde{G}(\mathbf{k}',\mathbf{B},\mathbf{M}_j,J_{l'})=&G_0(\mathbf{k}',J_{l'})-\frac{i\hbar^2}{m^2}h_{\alpha\beta}G_0(\mathbf{k}',J_{l'})\pi^\alpha G_0(\mathbf{k}',J_{l'})\pi^\beta G_0(\mathbf{k}',J_{l'})\\&+\tfrac{1}{2}g_0\mu_BB^\mu G_0(\mathbf{k}',J_{l'})F^\mu G_0(\mathbf{k}',J_{l'})+O(\mathbf{M}_j)+\text{higher-order terms}\ .\end{aligned} \tag{3.4}$$

In Eq. (3.4) $O(\mathbf{M}_j)$ includes terms which are functions of $\mathbf{M}_j$, and $h_{\alpha\beta}=\epsilon_{\alpha\beta\mu}h^\mu$, $h^\mu=eB^\mu/2\hbar c$; and G_0 is the electron propagator in the absence of the magnetic field and $\mathbf{M}_j$, and is diagonal in the periodic part of the Bloch function. Using Eqs. (2.8) and (3.4) in Eq. (3.1), and comparing the coefficients of B^μ we have

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}(\mathbf{k},J_l)=&-\frac{1}{\beta}\sum_{\mathbf{k}',J_{l'}}|M_{\mathbf{k}\mathbf{k}'}|^2D(\mathbf{k}-\mathbf{k}',J_l-J_{l'})\\&\times\left[-\frac{ie\hbar}{2m^2c}\epsilon_{\alpha\beta\mu}G_0(\mathbf{k}',J_{l'})\pi^\alpha G_0(\mathbf{k}',J_{l'})\pi^\beta G_0(\mathbf{k}',J_{l'})+\tfrac{1}{2}g_0\mu_BG_0(\mathbf{k}',J_{l'})\sigma^\mu G_0(\mathbf{k}',J_{l'})\right.\\&\left.+G_0(\mathbf{k}',J_{l'})\tilde{\Sigma}^{1,\mu}(\mathbf{k}',J_{l'})G_0(\mathbf{k}',J_{l'})\right]\ .\end{aligned} \tag{3.5}$$

Equation (3.5) can be rewritten with the introduction of the band and spin indices as

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k},E_{n\mathbf{k}})=&-\frac{1}{\beta}\sum_{\mathbf{k}',J_{l'}}|M_{n\mathbf{k},n\mathbf{k}'}|^2D(\mathbf{k}-\mathbf{k}',E_{n\mathbf{k}}-J_{l'})\\&\times\left[-\frac{ie\hbar}{2m^2c}\epsilon_{\alpha\beta\mu}G_0\pi^\alpha G_0\pi^\beta G_0+\tfrac{1}{2}g_0\mu_BG_0\sigma^\mu G_0+G_0\tilde{\Sigma}^{1,\mu}G_0\right]_{n\mathbf{k}'\rho,n\mathbf{k}'\rho'}\ .\end{aligned} \tag{3.6}$$

Using the completeness property of $u_{n\mathbf{k}\rho}$ and replacing the phonon propagator D by the bare-phonon propagator D_0, where

$$D_0=\frac{2\hbar\omega_{k-k'}}{(E_{n\mathbf{k}}-J_{l'})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}\ , \tag{3.7}$$

we can write Eq. (3.6) as

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k},E_n)=&-\frac{1}{\beta}\sum_{\mathbf{k}',J_{l'}}|M_{n\mathbf{k},n\mathbf{k}'}|^2\frac{2\hbar\omega_{k-k'}}{(E_{n\mathbf{k}}-J_{l'})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}\\&\times\left[-\frac{ie\hbar}{2m^2c}\epsilon_{\alpha\beta\mu}\frac{\pi^\alpha_{n\rho,m\rho''}(\mathbf{k}')\pi^\beta_{m\rho'',n\rho'}(\mathbf{k}')}{(J_{l'}-E_{n\mathbf{k}'})^2(J_{l'}-E_{m\mathbf{k}'})}+\frac{1}{2}g_0\mu_B[\sigma^\mu_{n\rho,n\rho'}(\mathbf{k}')+\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k}')]\frac{1}{(J_{l'}-E_{n\mathbf{k}'})^2}\right],\end{aligned} \tag{3.8}$$

where, as before, repeated indices imply summation. The frequency summation can be carried out using the Luttinger-Ward indentity[37]

$$\frac{1}{\beta}\sum_{J_{l'}}\frac{1}{(J_{l'}-E_n)^m}=-\frac{1}{2\pi i}\oint_\Gamma\frac{1}{(J'-E_n)^m}f(J')dJ' \ , \tag{3.9}$$

where the contour Γ encircles the imaginary axis in an anticlockwise direction. Using Eq. (3.9) in Eq. (3.8), and neglecting the terms proportional to f, which are not expected to be important for the intraband matrix element, we obtain

$$\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k},E_{n\mathbf{k}})\simeq-\sum_{\mathbf{k}'}\frac{|M_{n\mathbf{k},n\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}}{(E_{n\mathbf{k}}-E_{n\mathbf{k}'})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}[\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k}')+\tfrac{1}{2}\mu_B g^\mu_{nn}(\mathbf{k}')\sigma^\mu_{n\rho,n\rho'}(\mathbf{k}')]f'(E_{n\mathbf{k}'}) \ . \tag{3.10}$$

Following an average-interaction ansatz, in which case the self-energy is independent of $\mathbf{k}$, we obtain

$$\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k},E_n)\simeq[\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\mathbf{k},E_n)+\tfrac{1}{2}\mu_B g^\mu_{nn}(\mathbf{k})\sigma^\mu_{n\rho,n\rho'}(\mathbf{k})]\beta_n(\mathbf{k}) \ , \tag{3.11}$$

where

$$\beta_n(\mathbf{k})=-\sum_{\mathbf{k}'}\frac{2\hbar\omega_{\mathbf{k}-\mathbf{k}'}|M_{n\mathbf{k},n\mathbf{k}'}|^2}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}f'(E_{n\mathbf{k}'}) \ . \tag{3.12}$$

The apparent singularity in Eq. (3.12) is due to the fact that in evaluating frequency summations, we have considered only the real part of the energy. The imaginary part is proportional to the lifetime, which is not of interest here.

The solution of Eq. (3.11) becomes

$$\tilde{\Sigma}^{1,\mu}_{n\rho,m\rho'}(\mathbf{k},E_n)=\tfrac{1}{2}\mu_B\frac{\beta_n(\mathbf{k})}{1-\beta_n(\mathbf{k})}g^\mu_{nn}(\mathbf{k})\sigma^\mu_{n\rho,m\rho'}(\mathbf{k}) \ , \tag{3.13}$$

Following a similar but more tedious method we can obtain

$$\tilde{\Sigma}^{1,\mu}_{n\rho,m\rho'}=\tfrac{1}{2}\mu_B\frac{\beta_{nm}(\mathbf{k})}{1-\beta_{nm}(\mathbf{k})}g^\mu_{nm}(\mathbf{k})\sigma^\mu_{n\rho,m\rho'}(\mathbf{k}) \ , \tag{3.14}$$

where

$$\beta_{nm}(\mathbf{k})=-\sum_{\mathbf{k}'}\frac{|M_{n\mathbf{k},m\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}}{E_{nm}(\mathbf{k}')}\left[\frac{f(E_{n\mathbf{k}'})}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}-\frac{f(E_{m\mathbf{k}'})}{(E_{m\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}\right] \tag{3.15}$$

and the interband g matrix is defined as

$$g^\mu_{nm}\sigma^\mu_{n\rho,m\rho'}(\mathbf{k})=g_0\sigma^\mu_{n\rho,m\rho'}(\mathbf{k})+\frac{i\mu_B}{m}\epsilon_{\alpha\beta\mu}\sum_{\substack{q,\rho''\\ q\neq m}}\frac{\pi^\alpha_{n\rho,q\rho''}\pi^\beta_{q\rho'',m\rho'}}{E_{qm}} \ . \tag{3.16}$$

In the limit of m going to n, β_{nm} reduces to β_n and $\tilde{\Sigma}_{n\rho,m\rho'}$ goes to $\tilde{\Sigma}_{n\rho,n\rho'}$. We shall now use these results to obtain tractable expressions for $(K_j^{\nu\mu})_s$ and $(K_j^{\nu\mu})_{so}$, since $(K_j^{\nu\mu})_o$ does not have explicit dependence on $\tilde{\Sigma}$. Substituting Eq. (3.13) into Eq. (2.2) we obtain

$$(K_j^{\nu\mu})_s=-\tfrac{1}{2}\mu_B^2\sum_{n,\mathbf{k},\rho}\frac{1}{1-\beta_n(\mathbf{k})}X^\nu_{jn\rho,n\rho'}g^\mu_{nn}(\mathbf{k})\sigma^\mu_{n\rho',n\rho}f'(E_{n\mathbf{k}}) \ . \tag{3.17}$$

Thus, by considering the magnetic field dependence of the self-energy, we have seen that $(K_j^{\nu\mu})_s$ is modified by a factor of $[1-\beta_n(\mathbf{k})]^{-1}$. In order to understand the physical meaning of this modification, let us write Eq. (3.13) as

$$\beta_n(\mathbf{k})=-\sum_{\mathbf{k}'}u_{nn}(\mathbf{k},\mathbf{k}')f'(E_{n\mathbf{k}'}) \ , \tag{3.18}$$

where $u_{nn}(\mathbf{k},\mathbf{k}')$ is an effective electron-electron interaction mediated by phonon and is given by

$$u_{nn}(\mathbf{k},\mathbf{k}')=\frac{2\hbar\omega_{\mathbf{k}-\mathbf{k}'}|M_{n\mathbf{k},n\mathbf{k}'}|^2}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2} \tag{3.19}$$

The interaction given by Eq. (3.19) can be either attractive or repulsive. If the states $\mathbf{k}$ and $\mathbf{k}'$ are separated by an energy larger than $\hbar\omega_{\mathbf{k}-\mathbf{k}'}$, the effect is repulsive, but if the energy difference is smaller than this, attraction is present. It may be noted, in passing, that an attractive interaction of this type led to the explanation of low-temperature superconductivity through the formation of Cooper pairs. Since the present work does not envisage such a pairing we confine ourselves to the discussion of electron-phonon interaction effects in the normal state.

Thus far, we have not considered the effect of mass renormalization on the spin contribution to the Knight shift. In order to do this let us rewrite Eq. (3.17) as

$$(K_j^{\nu\mu})_s = -\tfrac{1}{2}\mu_B^2 \sum_{n,\mathbf{k},\rho} \frac{1}{1-\beta_n(\mathbf{k})} X^{\nu}_{jn\rho,n\rho'} g^{\mu}_{nn}(\mathbf{k}) \sigma^{\mu}_{n\rho',n\rho} f'(\bar{E}_{n\mathbf{k}}) \ , \tag{3.20}$$

where $\bar{E}_{n\mathbf{k}}$ is the modified one-electron energy in the presence of electron-phonon interaction. Equation (3.20) can be further simplified as

$$(K_j^{\nu\mu})_s = -\tfrac{1}{2}\mu_B^2 \sum_{n,\mathbf{k},\rho} \frac{1}{1-\beta_n(\mathbf{k})} X^{\nu}_{jn\rho,n\rho'} g^{\mu}_{nn}(\mathbf{k}) \sigma^{\mu}_{n\rho,'n\rho} \frac{\partial f(\bar{E}_{n\mathbf{k}})}{\partial \mathbf{k}} (\nabla_{\mathbf{k}} \bar{E}_{n\mathbf{k}})^{-1} \ . \tag{3.21}$$

In Appendix A we have shown that

$$(\nabla_{\mathbf{k}} \bar{E}_{n\mathbf{k}})^{-1} = (\nabla_{\mathbf{k}} E_{n\mathbf{k}})^{-1} [1+\gamma_n(\mathbf{k})] \tag{3.22}$$

and

$$\beta_n(\mathbf{k}) = -\gamma_n(\mathbf{k}) \ , \tag{3.23}$$

where $\gamma_n(\mathbf{k})$ is the mass-renormalization function. Substituting Eqs. (3.22) and (3.23) into Eq. (3.21) we obtain

$$(K_j^{\nu\mu})_s = -\tfrac{1}{2}\mu_B^2 \sum_{n,\mathbf{k},\rho} X^{\nu}_{jn\rho,n\rho'} g^{\mu}_{nn}(\mathbf{k}) \sigma^{\mu}_{n\rho',n\rho} f'(E_{n\mathbf{k}}) \ . \tag{3.24}$$

Thus we have seen that the modifications caused by the magnetic field dependence of the self-energy are canceled by the mass-renormalization effects. In other words, $(K_j^{\nu\mu})_s$ is modified only through the changes in the one-particle energies and wave functions, in the presence of electron-phonon interaction.

Let us now consider the combined effects of both the electron-electron and electron-phonon interactions and see how the electron-phonon interaction modifies the Stoner factor. $(K_j^{\nu\mu})_s$, in the presence of electron-electron interaction only, is given by[6]

$$(K_j^{\nu\mu})_s = -\tfrac{1}{2}\mu_B^2 \sum_{n,\mathbf{k},\rho} \frac{1}{1-\alpha_n(\mathbf{k})} X^{\nu}_{jn\rho,n\rho'} g^{\mu}_{nn}(\mathbf{k}) \sigma^{\mu}_{n\rho',n\rho} f'(E_{n\mathbf{k}}) \ , \tag{3.25}$$

where $[1-\alpha_n(\mathbf{k})]^{-1}$ is the Stoner factor:

$$\alpha_n(\mathbf{k}) = -\sum_{m,\mathbf{k}'} \bar{v}_{nm}(\mathbf{k},\mathbf{k}') f'(E_{m\mathbf{k}'}) \tag{3.26}$$

and $\bar{v}$ is the strength of an average exchange interaction. It is now easy to see that by considering both the electron-electron and electron-phonon interaction effects in the self-energy equations, we would finally obtain

$$(K_j^{\nu\mu})_s = -\tfrac{1}{2}\mu_B^2 \sum_{n,\mathbf{k},\rho} \frac{1}{[1+\gamma_n(\mathbf{k})-\alpha_n(\mathbf{k})]} X^{\nu}_{jn\rho,n\rho'} g^{\mu}_{nn}(\mathbf{k}) \sigma^{\mu}_{n\rho',n\rho} f'(\bar{E}_{n\mathbf{k}}) \ . \tag{3.27}$$

Following a procedure as we have done in obtaining Eq. (3.24), $(K_j^{\nu\mu})_s$ would be modified:

$$(K_j^{\nu\mu})_s = \frac{(\bar{K}_j^{\nu\mu})_s(0)}{[1-\bar{\alpha}|(1+\bar{\gamma})]} \ , \tag{3.28}$$

where $(\bar{K}_j^{\nu\mu})_s(0)$ is the Knight shift in the absence of the electron-electron and electron-phonon interactions, and the overbars above the quantities denote average values. Thus the Stoner factor $[1-\bar{\alpha}]^{-1}$ changes to $[1-\bar{\alpha}\,|\,(1+\bar{\gamma})]^{-1}$ in the presence of the electron-phonon interaction. Let us now estimate the effect in a free-electron-like system, sodium. The mass enhancement parameter $\bar{\gamma}$ in sodium is about 0.26 and $\bar{\alpha}$ is about 0.4 (Ref. 38). With these data, it is easy to see that the Stoner factor is affected roughly by 13%. In general, the mass enhancement parameter $\bar{\gamma}$ varies by about 20–40 % in simple metals.[38] Thus $\bar{\alpha}$ would be correspondingly reduced by about 20–30 % in these systems. However, it would not be possible here to predict as to what would be the status for more complicated systems. The effect might be important.

As regards $(K_j^{\nu\mu})_0$, since it does not explicitly depend on the self-energy term, it is modified only through the changes in the energy eigenvalues and eigenfunctions.

In order to discuss the effect of electron-phonon interaction on $(K_j^{\nu\mu})_{so}$, we write using Eqs. (2.7) and (3.14):

$$F^{\mu}_{n\rho,m\rho'} = A^{\mu}_{nm} \sigma^{\mu}_{n\rho' m\rho'} \ , \tag{3.29}$$

where

$$A^{\mu}_{nm} = 1 + \frac{\beta_{nm}(\mathbf{k})}{1-\beta_{nm}(\mathbf{k})} g^{\mu}_{nm} \ . \tag{3.30}$$

Assuming $\beta_{nm} = \beta_{mn}$ we can write

$$A^{\mu}_{mn} = 1 + \frac{\beta_{nm}(\mathbf{k})}{1-\beta_{nm}(\mathbf{k})} g^{\mu}_{mn} \tag{3.31}$$

and

$$F_{m\rho',n\rho} = A^{\mu}_{mn} \sigma^{\mu}_{m\rho',n\rho} \ . \tag{3.32}$$

Substituting Eqs. (3.28) and (3.31) into Eq. (2.4) we have

$$(K_j^{\nu\mu})_{\rm so}=\sum_{n,\mathbf{k},\rho}\left[\frac{i\mu_B^2}{m}\epsilon_{\alpha\beta\mu}\left\{(-3X^{\nu}_{jn\rho,n\rho'}\pi^{\alpha}_{n\rho',m\rho''}\pi^{\beta}_{m\rho'',n\rho}+\pi^{\alpha}_{n\rho,n\rho'}X^{\nu}_{jn\rho,m\rho'}\pi^{\beta}_{m\rho',n\rho}-\pi^{\alpha}_{n\rho,n\rho}\pi^{\beta}_{n\rho,m\rho'}X^{\nu}_{jm\rho',n\rho})\frac{1}{E_{mn}^2}\right.\right.$$
$$\left.\left.+(\pi^{\alpha}_{n\rho,m\rho'}\pi^{\beta}_{m\rho',q\rho''}X^{0\nu}_{jq\rho'',n\rho}+\pi^{\alpha}_{n\rho,m\rho'}X^{0\nu}_{jm\rho',q\rho''}\pi^{\beta}_{q\rho'',n\rho}+X^{0\nu}_{jn\rho,m\rho'}\pi^{\alpha}_{m\rho',q\rho''}\pi^{\beta}_{q\rho'',n\rho})\frac{1}{E_{qn}E_{mn}}\right\}\right.$$
$$\left.+\tfrac{1}{2}g_0\mu_B\frac{A^{\mu}_{mn}X^{\nu}_{jn\rho,m\rho'}\sigma^{\mu}_{m\rho',n\rho}+A^{\mu}_{nm}\sigma^{\mu}_{n\rho,m\rho'}X^{\nu}_{jm\rho',n\rho}}{E_{mn}}\right]f(E_{n\mathbf{k}})\ . \tag{3.33}$$

In Eq. (3.33) only the last term depends on the interband electron-phonon parameter β_{nm}. However, this term is normally small and is not expected to contribute significantly to $(K_j^{\nu\mu})_{\rm so}$. Thus $(K_j^{\nu\mu})_{\rm so}$ is also mainly modified through only the energy eigenvalues and eigenfunctions.

IV. SUMMARY AND CONCLUSIONS

In this paper we have made a detailed investigation of the electron-phonon interaction effects on the Knight shift. The contributions to $K_j^{\nu\mu}$ as we have found out, are mainly modified through the changes in energies and wave functions. However, by considering the combined effects of electron-electron and electron-phonon interactions on the Knight shift, we have shown that the Stoner factor appearing in the spin contribution to the Knight shift is affected, in the free-electronlike system sodium, by about 13%. However, the theory is general and can be applied to different types of systems, such as metals, semiconductors, etc. Indeed, the electron-phonon interaction makes a substantial contribution to the variation of the energy gap in narrow-gap semiconductors, and is partly responsible for the temperature dependence of the Knight shift in these systems.[20]

In conclusion, the theory presented in this paper is the first of its kind to investigate in detail the electron-phonon interaction effects on the Knight shift. In view of the controversy still existing in the assessment of the electron-phonon interaction on the magnetism of solids, the theory, we believe would pave the way for a better quantitative understanding of the effect.

ACKNOWLEDGMENTS

Financial support is acknowledged by one of the authors (G.S.T.) from National Science Foundation Grant No. DMR-8504259 and the Ministry of Human Resource Development, Department of Education, Government of India and by another author (P.T.) from the Council of Scientific and Industrial Research (India).

APPENDIX A

Here we discuss the mass renormalization due to the electron-phonon interaction. The total one-electron energy in the presence of this interaction is

$$\bar{E}_{n\mathbf{k}}=E_{n\mathbf{k}}+\Sigma^0(\mathbf{k},E_{n\mathbf{k}})\ , \tag{A1}$$

where

$$\Sigma^0(\mathbf{k},E_{n\mathbf{k}})=-\frac{1}{\beta}\sum_{\mathbf{k}',J_{l'}}\frac{|M_{n\mathbf{k},n\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}}{(J_{l'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}G(\mathbf{k}',J_{l'})\ . \tag{A2}$$

Performing the frequency summation using Eq. (3.9), we obtain after neglecting the first-order correction

$$\bar{E}_{n\mathbf{k}}=E_{n\mathbf{k}}-\sum_{\mathbf{k}'}\frac{|M_{n\mathbf{k},n\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}f(E_{n\mathbf{k}'})}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}\ . \tag{A3}$$

Since we are interested in the electronic states near the Fermi surface we can write

$$\nabla_{\mathbf{k}}\bar{E}_{n\mathbf{k}}\simeq\nabla_{\mathbf{k}}E_{n\mathbf{k}}-\sum_{\mathbf{k}'}\frac{|M_{n\mathbf{k},n\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}\nabla_{k'}f(E_{n\mathbf{k}'})}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}$$
$$=\nabla_{\mathbf{k}}E_{n\mathbf{k}}-\sum_{\mathbf{k}'}\frac{|M_{n\mathbf{k},n\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}\nabla_{\mathbf{k}'}E_{n\mathbf{k}'}}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}f'(E_{n\mathbf{k}'})\ . \tag{A4}$$

If we make a further approximation, i.e., by replacing $\nabla_{\mathbf{k}'}E_{n\mathbf{k}'}$ by $\nabla_{\mathbf{k}}E_{n\mathbf{k}}$, we can obtain

$$\nabla_{\mathbf{k}}\bar{E}_{n\mathbf{k}}=\nabla_{\mathbf{k}}E_{n\mathbf{k}}[1-\gamma(\mathbf{k})]\ , \tag{A5}$$

where

$$\gamma(\mathbf{k})=\sum_{\mathbf{k}'}\frac{|M_{n\mathbf{k},n\mathbf{k}'}|^2 2\hbar\omega_{\mathbf{k}-\mathbf{k}'}}{(E_{n\mathbf{k}'}-E_{n\mathbf{k}})^2-(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2}f'(E_{n\mathbf{k}'})=-\beta(\mathbf{k})\ . \tag{A6}$$

Since the density of states is proportional to $|\nabla_k\bar{E}|^{-1}$, we have to the first order of $\gamma(k)$

$$G(\bar{E}_{n\mathbf{k}})=G(E_{n\mathbf{k}})[1+\gamma(\mathbf{k})]\ , \tag{A7}$$

where $G(\bar{E}_{n\mathbf{k}})$ is the renormalized density of states and $G(E_{n\mathbf{k}})$ is the density of states in the absence of electron-phonon interaction. Now we shall further simplify $\gamma(\mathbf{k})$. Since the electron-phonon interaction is short range we can consider $|M_{n\mathbf{k},n\mathbf{k}'}|^2$ as a constant $|M|^2$. Again, since in the low-temperature limit, $\hbar\omega_{\mathbf{k}-\mathbf{k}'}$ is greater than $|E_{n\mathbf{k}'}-E_{n\mathbf{k}}|$, we replace the phonon frequency by an average frequency; say the Debye frequency ω_D. In this limit, the value of $\gamma(\mathbf{k})$averaged over the Fermi surface is given by

$$\bar{\gamma}=\frac{|M|^2G(E_F)}{\hbar}\omega_D \tag{A8}$$

which is a positive quantity. Here $G(E_F)$ is the density of states at the Fermi surface. Thus, the density of states is enhanced by a factor of $(1+\bar{\gamma})$. The increase in the density of states implies a change in the effective mass by the same factor:

$$m_{e-p}=m(1+\bar{\gamma}) , \tag{A9}$$

where m_{e-p} is the renormalized mass due to the electron-phonon interaction.

APPENDIX B

In this appendix we consider the temperature dependence of $\beta_n(\mathbf{k})$ through the Fermi function $f_T(E_{\mathbf{k}}-\mu)$. We assume the electron-phonon matrix element and the phonon frequency to be constants. Dropping the band index and using cylindrical coordinates, Eq. (3.12) can be written

$$\beta(\mathbf{k})=-\frac{|M|^2\hbar\omega_D}{8\pi^2}\int_{-k_{l'}}^{+k_{l'}}dk'_z\int_0^{k'^2_\rho}dk'^2_\rho\phi(E_{\mathbf{k}'},E_{\mathbf{k}},\hbar\omega_D)f'_T(E_{\mathbf{k}'}-\mu) , \tag{B1}$$

where

$$\phi(E_{\mathbf{k}'},E_{\mathbf{k}},\hbar\omega_D)=\frac{1}{(E_{\mathbf{k}'}-E_{\mathbf{k}})^2-(\hbar\omega_D)^2};\quad k'^2_\rho=k'^2_x+k'^2_y , \tag{B2}$$

and μ is the chemical potential. For simplicity we consider a system of free electrons. In this case $k_l'=\sqrt{2m\mu/\hbar^2}$, and $\beta(\mathbf{k})$ becomes

$$\beta(\mathbf{k})=-\frac{\hbar\omega_D|M|^2}{2\pi^2}\left[\frac{2m}{\hbar 2}\right]^{3/2}\mu^{1/2}\int dE_{\mathbf{k}'}\phi(E_{\mathbf{k}'},E_{\mathbf{k}},\hbar\omega_D)f'_T(E_{\mathbf{k}'}-\mu) . \tag{B3}$$

Integrating by parts and noting that the surface integral vanishes for a periodic integrand, we have

$$\beta(\mathbf{k})=\frac{\hbar\omega_D|M|^2}{2\pi^2}\left[\frac{2m}{\hbar^2}\right]^{3/2}\mu^{1/2}\int_0^{\mu}dE_{\mathbf{k}'},\phi'(\mathbf{E}_{\mathbf{k}'},E_{\mathbf{k}},\hbar\omega_D)f_T(E_{\mathbf{k}'}-\mu) . \tag{B4}$$

Using the relation[39]

$$\int dE\,R(E)f_T(E-\mu)=\int_0^{\mu}R(E)dE+\frac{\pi^2}{6}(k_BT)^2\frac{dR(E)}{dE}\bigg|_{E=\mu} \tag{B5}$$

we have, from Eq. (B4),

$$\beta(\mathbf{k})=\hbar\omega_D|M|^2G(\mu)\left[\left[\frac{1}{(\mu-E_k)^2-(\hbar\omega_D)^2}-\frac{1}{E_k^2-(\hbar\omega_D)^2}\right]-\frac{\pi^2}{2}(K_BT)^2\frac{1}{(\mu-E_k)^2-(\hbar\omega_D)^2}\left[1-\frac{4(\mu-E_k)^2}{(\mu-E_k)^2-(\hbar\omega_D)^2}\right]\right] , \tag{B6}$$

where

$$G(\mu)=\frac{1}{2\pi^2}\left[\frac{2m}{\hbar^2}\right]^{3/2}\mu^{1/2} \tag{B7}$$

and is the density of states. In real systems, however, the energy and the electron-phonon matrix element will also have temperature dependence, which should also be considered for an actual calculation.

*On leave from the Department of Physics, Berhampur University, Berhampur 760 007, Orissa, India (address for correspondence).

[1]C. H. Townes, C. Herring, and W. D. Knight, Phys. Rev. 77, 852 (1950).

[2]S. D. Mahanti, L. Tterilikkis, and T. P. Das, in *Magnetic Resonance*, edited by C. K. Coogan *et al.* (Plenum, New York, 1970), p. 90.

[3]H. J. Zeiger and G. W. Pratt, *Magnetic Interactions in Solids* (Oxford, London, 1973).

[4]A. R. B. deCastro and R. T. Schumacher, Phys. Rev. B 7, 105 (1973).

[5]G. S. Tripathi, L. K. Das, P. K. Misra, and S. D. Mahanti, Solid State Commun. **38** 1207 (1981).

[6]G. S. Tripathi, L. K. Das, P. K. Misra, and S. D. Mahanti, Phys. Rev. B **25**, 3091 (1982).

[7]G. S. Tripathi, J. Phys. C **18**, L1157 (1985).

[8]G. S. Tripathi, B. Mishra, and P. K. Misra, J. Magn. Magn.

Mater. **67**, 271 (1987).
[9]P. Jena, S. D. Mahanti, and T. P. Das, Phys. Rev. Lett. **20**, 544 (1968).
[10]P. Jena, T. P. Das, and S. D. Mahanti, Phys. Rev. B **1**, 432 (1970); **2**, 2264 (1970).
[11]P. Jena, T. P. Das, G. D. Gaspari, and S. D. Mahanti, Phys. Rev. B **1**, 1160 (1970).
[12]M. M. Pant and B. Y. Tong, Phys. Lett. **36A**, 133 (1971).
[13]J. P. Perdew and J. W. Wilkins, Phys. Rev. B **1**, 2461 (1973).
[14]E. Zaremba and D. Zobin, Phys. Rev. Lett. **44**, 175 (1980).
[15]M. Manninen and P. Jena, J. Phys. F **10**, 1567 (1980).
[16]M. Nusair, L. Wilk, and S. H. Vosko, J. Phys. F **11**, 1683 (1981).
[17]L. Wilk, M. Nusair, and S. H. Vosko, Can J. Phys. **59**, 585 (1981).
[18]B. Mishra, L. K. Das, T. Sahu, G. S. Tripathi, and P. K. Misra, Phys. Lett. **106A**, 81 (1984).
[19]B. Mishra, T. Sahu, G. S. Tripathi, and P. K. Misra, Phys. Lett. **114A**, 272 (1986).
[20]S. Misra, G. S. Tripathi, and P. K. Misra, Phys. Lett. **110A**, 461 (1985); J. Phys. C **20**, 277 (1987).
[21]C. Herring, in *Magnetism,* edited by G. T. Rado and H. Suhl (Academic, New York, 1966), Vol. 4, p. 290.
[22]S. K. Joshi and A. K. Rajagopal, *in Solid State Physics,* edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1968), Vol. 22, p. 159.
[23]C. P. Enz and B. T. Mathias, Z. Phys. B **33**, 129 (1979).
[24]D. Fay and J. Appel, Phys. Rev. B **20**, 3705 (1979).
[25]G. Grimvall, *The Electron-Phonon Interaction in Metals* (North-Holland, Amsterdam, 1981), p. 140.
[26]W. E. Pickett, Phys. Rev. B **26**, 1186 (1982).
[27]V. M. Zvrev and V. P. Silin, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 178 (1987) [JETP Lett. **45**, 220 (1987)].
[28]D. J. Kim, Phys. Rev. B **17**, 468 (1978).
[29]D. J. Kim, Phys. Rev. B **25**, 6919 (1982).
[30]D. J. Kim and C. Tanaka, Phys. Rev. B **37**, 3948 (1988).
[31]S. K. Misra, P. K. Misra, and S. D. Mahanti, Solid State Commun. **39**, 58 (1981); Phys. Rev. B **26**, 1903 (1982).
[32]G. S. Tripathi, Phys. Lett. **115A**, 169 (1986); Phys. Rev. B **35**, 5247 (1987).
[33]G. S. Tripathi, Phys. Rev. B **31**, 5143 (1985).
[34]G. S. Tripathi, C. M. Misra, and P. K. Misra, J. Phys. C **18**, L935 (1985).
[35]A. B. Migdal, Zh. Eksp. Teor. Fiz. **34**, 1438 (1958) [Sov. Phys.–JETP **7**, 996 (1958)].
[36]J. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964), p. 198.
[37]J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
[38]C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1976).
[39]J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, 1973).