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[8] The density decreases with radius as a zero order Bessel function. When ω_{p0}^2/ω^2 is just greater than 1 the enhanced emission originates close to the center of the column and its effect is "diluted" by the nonresonant plasma at larger radii. As ω_{p0}^2/ω^2 is increased the point of origin of the enhanced emission moves to a larger radius and the dilution is diminished.

[9] Even though the temperature enhancement is a consequence of metastable reactions, it surprisingly does not depend strongly on N_m or σ_{se}. The enhancement is determined not by $F(x)$ but by $F(x)/F'(x)$ for the suprathermal electrons [see Eq. (2)] and this ratio is not strongly dependent on the rate of production of fast electrons.

[10] Enhancement can also be expected as a result of coupling between longitudinal and transverse waves at density inhomogeneities. At the sharp boundary of a uniform, non-Maxwellian plasma, for example, a coupling exists which is apparently more efficient than scattering on the ions as has been discussed by F. L. Hinton, Phys. Fluids 10, 2408 (1967). This theory is not directly applicable to our experiment, however, and in any case it cannot explain the observed magnitude of the radiation temperature.

[11] The suprathermal electrons do, however, influence the time rate of change of $\bar{E}$. Electron heating due to metastable reactions has been studied previously, for example by Ingraham and Brown, Ref. 5; J. W. Poukey, J. B. Gerardo, and M. A. Gusinow, Phys. Rev. 179, 211 (1969).

COMPLETE CALCULATIONS OF THE ELECTRONIC ENERGIES OF SOLIDS*

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A method is described for the complete calculation of electronic energies in crystalline solids without approximating overlap, electron-repulsion, or exchange contributions. The practicality of the method is confirmed by preliminary results, which also indicate reasons for the considerable success of independent-electron methods.

Although much work has been done on the electronic states of crystalline solids, the overwhelming majority of the effort has been on independent-electron formulations. Recently there has been increasing interest in making more complete studies, and investigators such as Girifalco[1] have begun to examine the quantities which would enter all-electron calculations in the Wannier representation. The present communication sketches an approach which differs from those previously reported in that it seeks to use the lattice symmetry before attempting integral evaluations. This technique reduces the number of quantities needed in the theory, and substantially enhances their symmetry. The method we describe can be generalized to more complex systems, and can serve as a starting point for Hartree-Fock and electron correlation theories. We present here only an introductory illustration which exhibits the essence of our approach.

Consider a simple cubic lattice containing a proton fixed at each lattice point and an equal number of electrons. Let the Hamiltonian consist only of kinetic energy terms for the electrons and Coulombic interactions between all charges, and consider a wave function which is an antisymmetrized product of doubly-occupied Bloch sums.

Let $|\vec{k}\rangle$ denote a Bloch sum of the form

$$|\vec{k}\rangle = \sum\nolimits_j \exp(i\vec{R}\circ\vec{R}_j)\psi(\vec{r}-\vec{R}_j), \tag{1}$$

where $\vec{r}$ is a spatial point, $\vec{R}_j$ is a lattice point, and ψ is an atomic orbital. Except when explicitly indicated otherwise, summations are to be over all points of the lattice. For a lattice of N points and lattice spacing a, the total energy can be written in the form

$$E = 2N\left(\frac{a}{2\pi}\right)^3 \int d\vec{k}\frac{\langle\vec{k}|-\frac{1}{2}\nabla^2|\vec{k}\rangle}{\langle\vec{k}|\vec{k}\rangle} + 2N^2\left(\frac{a}{2\pi}\right)^6 \int \frac{d\vec{k}d\vec{k}'\,H(\vec{k},\vec{k}')}{\langle\vec{k}|\vec{k}\rangle\langle\vec{k}'|\vec{k}'\rangle}. \tag{2}$$

The $\vec{k}$ integrations are over the occupied part of the first Brillouin zone, and $H(\vec{k},\vec{k}')$ stands for the two-electron matrix element

$$H(\vec{k},\vec{k}')=\langle\vec{k}\vec{k}'|r_{12}{}^{-1}-\frac{1}{N}\sum_{\mu}|\vec{r}_1-\vec{R}_\mu|^{-1}-\frac{1}{N}\sum_{\nu}|\vec{r}_2-\vec{R}_\nu|^{-1}+\frac{1}{N^2}\sum_{\substack{\mu\nu\\ \mu\neq\nu}}R_{\mu\nu}{}^{-1}|\vec{k}\vec{k}'\rangle-\tfrac{1}{2}\langle\vec{k}\vec{k}'|r_{12}{}^{-1}|\vec{k}'\vec{k}\rangle. \tag{3}$$

Here $\vec{r}_1$ and $\vec{r}_2$ refer to spatial coordinates of the two electrons, $\vec{r}_{12}=\vec{r}_2-\vec{r}_1$, and $\vec{R}_{\mu\nu}=\vec{R}_\nu-\vec{R}_\mu$. Equation (3) is exact except for terms of order less than N. All quantities are in atomic units (1 bohr = 0.5292 Å, 1 hartree = 27.21 eV).

We now introduce the Bloch sums, obtaining for $\langle\vec{k}|\vec{k}\rangle$

$$\langle\vec{k}|\vec{k}\rangle=\sum_{i,l}\exp(i\vec{k}\cdot\vec{R}_{il})\langle\psi_i|\psi_l\rangle, \tag{4}$$

where ψ_i stands for $\psi(\vec{r}-\vec{R}_i)$. Equation (4) can be simplified by recognizing that $\langle\psi_i|\psi_l\rangle$ has Fourier integral representation

$$\langle\psi_i|\psi_l\rangle=\frac{1}{(2\pi)^3}\int d\vec{p}\,|\overline{\psi}(\vec{p})|^2\exp(i\vec{p}\cdot\vec{R}_{il}), \tag{5}$$

where $\overline{\psi}$ is the Fourier transform of ψ. We now insert Eq. (5) into Eq. (4), performing the summations with the aid of the lattice orthogonality relation

$$\sum\nolimits_l\exp(i\vec{p}\cdot\vec{R}_{il})=(2\pi/a)^3\sum\nolimits_\mu\delta(\vec{p}-\vec{p}_\mu), \tag{6}$$

where the $\vec{p}_\mu$ are points in the reciprocal lattice (in this problem simple cubic, of cell dimension $2\pi/a$). The result is

$$\langle\vec{k}|\vec{k}\rangle=(N/a^3)\sum\nolimits_\mu|\overline{\psi}(\vec{p}_\mu-\vec{k})|^2. \tag{7}$$

A parallel discussion for the kinetic energy integral yields

$$T(\vec{k})=\frac{\langle\vec{k}|-\frac{1}{2}\nabla^2|\vec{k}\rangle}{\langle\vec{k}|\vec{k}\rangle}=\frac{N}{2a^3\langle\vec{k}|\vec{k}\rangle}\sum_\mu(\vec{p}_\mu-\vec{k})^2|\overline{\psi}(\vec{p}_\mu-\vec{k})|^2. \tag{8}$$

As a preliminary to a complete discussion of $H(\vec{k},\vec{k}')$, we examine the "Coulomb" term

$$\langle\vec{k}\vec{k}'|r_{12}{}^{-1}|\vec{k}\vec{k}'\rangle=\sum_{i,j,l,m}\exp(i\vec{k}\cdot\vec{R}_{il}+i\vec{k}'\cdot\vec{R}_{jm})\langle\psi_i\psi_j|r_{12}{}^{-1}|\psi_l\psi_m\rangle. \tag{9}$$

The two-electron four-center integrals on the right-hand side of Eq. (9) may also be expressed by Fourier integral representations, as is done in one of the standard methods for evaluating such integrals.[2] The necessary formula is

$$\langle\psi_i\psi_j|r_{12}{}^{-1}|\psi_l\psi_m\rangle=\frac{1}{2\pi^2}\int\frac{d\vec{q}}{q^2}\overline{\psi}_{il}(\vec{q})\overline{\psi}_{jm}(-\vec{q})\exp(i\vec{q}\cdot\vec{R}_{ij}), \tag{10}$$

where $\overline{\psi}_{il}(\vec{q})$ is the Fourier transform of $\psi_i{}^*\psi_l$ in a coordinate system centered at lattice point i. Inserting Eq. (10) into Eq. (9) and appropriately grouping terms, we obtain

$$\langle\vec{k}\vec{k}'|r_{12}{}^{-1}|\vec{k}\vec{k}'\rangle=\frac{1}{2\pi^2}\int\frac{d\vec{q}}{q^2}\Big[\sum_l\overline{\psi}_{il}(\vec{q})\exp(i\vec{k}\cdot\vec{R}_{il})\Big]\Big[\sum_m\overline{\psi}_{jm}(-\vec{q})\exp(i\vec{k}'\cdot\vec{R}_{jm})\Big]\Big[\sum_{i,j}\exp(-i\vec{q}\cdot\vec{R}_{ij})\Big]. \tag{11}$$

The first two summations in Eq. (11) are, because of their short-range nature and the crystal symmetry, actually independent of i and j, and that is why they have been removed from within the i and j summations. The sums over i and j can therefore be evaluated according to Eq. (6), leading to

$$\langle\vec{k}\vec{k}'|r_{12}{}^{-1}|\vec{k}\vec{k}'\rangle=\frac{N}{2\pi^2}\left(\frac{2\pi}{a}\right)^3\sum_\mu\frac{1}{q_\mu{}^2}\Big[\sum_l\overline{\psi}_{il}(\vec{q}_\mu)\exp(i\vec{k}\cdot\vec{R}_{il})\Big]\Big[\sum_m\overline{\psi}_{jm}(-\vec{q}_\mu)\exp(i\vec{k}'\cdot\vec{R}_{jm})\Big]. \tag{12}$$

The form of $\overline{\psi}_{il}(\vec{q})$ insures that the μ summation in Eq. (12) converges. However, there is a singularity at $\vec{q}_\mu=0$ which can be shown to cancel exactly against corresponding contributions from other terms of $H(\vec{k},\vec{k}')$, so that we may simply omit $\vec{q}_\mu=0$ from the sum. The cancellation indicates the absence of a net long-range contribution from an electrically neutral crystal.

The l and m summations of Eq. (12) can be further manipulated in a manner parallel to that used for

$\langle\overleftrightarrow{\mathrm{k}}|\overleftrightarrow{\mathrm{k}}\rangle$. The result is

$$\textstyle\sum_l \bar{\psi}_{il}(\vec{\mathrm{q}}_\mu)\exp(i\vec{\mathrm{k}}\cdot\vec{\mathrm{R}}_{il}) = (1/a^3)\sum_\nu \bar{\psi}^*(\vec{\mathrm{p}}_\nu-\vec{\mathrm{q}}_\mu-\vec{\mathrm{k}})\bar{\psi}(\vec{\mathrm{p}}_\nu-\vec{\mathrm{k}}). \tag{13}$$

The "Coulomb" term thus contributes to $H(\overleftrightarrow{\mathrm{k}},\overleftrightarrow{\mathrm{k}}')$ proportionally to

$$J(\vec{\mathrm{k}},\vec{\mathrm{k}}') = \frac{4\pi}{a^3}\sum_{\substack{\mu\\ \vec{\mathrm{q}}\neq 0}}\frac{1}{q_\mu{}^2}\sum_\nu \bar{\psi}^*(\vec{\mathrm{p}}_\nu-\vec{\mathrm{q}}_\mu-\vec{\mathrm{k}})\bar{\psi}(\vec{\mathrm{p}}_\nu-\vec{\mathrm{k}})\sum_\lambda \bar{\psi}^*(\vec{\mathrm{p}}_\lambda+\vec{\mathrm{q}}_\mu-\vec{\mathrm{k}}')\bar{\psi}(\vec{\mathrm{p}}_\lambda-\vec{\mathrm{k}}'). \tag{14}$$

The attraction and exchange terms of $H(\overleftrightarrow{\mathrm{k}},\overleftrightarrow{\mathrm{k}}')$ may be treated by methods similar to those used above. The results are that their noncanceling contributions are, respectively,

$$V(\vec{\mathrm{k}}) = \frac{4\pi}{a^3}\sum_{\substack{\mu\\ q_\mu\neq 0}}\frac{1}{q_\mu{}^2}\sum_\nu \bar{\psi}^*(\vec{\mathrm{p}}_\nu-\vec{\mathrm{q}}_\mu-\vec{\mathrm{k}})\bar{\psi}(\vec{\mathrm{p}}_\nu-\vec{\mathrm{k}}), \tag{15}$$

$$X(\overleftrightarrow{\mathrm{k}},\overleftrightarrow{\mathrm{k}}') = \frac{4\pi}{a^3}\sum_\mu \frac{1}{|\vec{\mathrm{q}}_\mu+\vec{\mathrm{k}}-\vec{\mathrm{k}}'|^2}\sum_\nu \bar{\psi}^*(\vec{\mathrm{p}}_\nu-\vec{\mathrm{q}}_\mu-\vec{\mathrm{k}})\bar{\psi}(\vec{\mathrm{p}}_\nu-\vec{\mathrm{k}}')\sum_\lambda \bar{\psi}^*(\vec{\mathrm{p}}_\lambda+\vec{\mathrm{q}}_\mu-\vec{\mathrm{k}}')\bar{\psi}(\vec{\mathrm{p}}_\lambda-\vec{\mathrm{k}}). \tag{16}$$

The remaining term of $H(\overleftrightarrow{\mathrm{k}},\overleftrightarrow{\mathrm{k}}')$, containing $R_{\mu\nu}{}^{-1}$, warrants additional discussion. The Fourier integral representation of $R_{\mu\nu}{}^{-1}$ is

$$R_{\mu\nu}{}^{-1} = \frac{1}{2\pi^2}\int\frac{d\vec{\mathrm{q}}}{q^2}\exp[-i\vec{\mathrm{q}}\cdot(\vec{\mathrm{R}}_\nu-\vec{\mathrm{R}}_\mu)], \tag{17}$$

and its summation over μ and ν leads with the aid of Eq. (6) to

$$\begin{aligned}\sum_{\substack{\mu\nu\\ \mu\neq\nu}} R_{\mu\nu}{}^{-1} &= \frac{N}{2\pi^2}\int\frac{d\vec{\mathrm{q}}}{q^2}\sum_{\substack{\nu\\ \nu\neq\mu}}\exp[-i\vec{\mathrm{q}}\cdot(\vec{\mathrm{R}}_\nu-\vec{\mathrm{R}}_\mu)] = \frac{N}{2\pi^2}\int\frac{d\vec{\mathrm{q}}}{q^2}\Big\{\sum_\nu\exp[-i\vec{\mathrm{q}}\cdot(\vec{\mathrm{R}}_\nu-\vec{\mathrm{R}}_\mu)]-1\Big\}\\ &= \frac{N}{2\pi^2}\left[\left(\frac{2\pi}{a}\right)^3\sum_\mu\frac{1}{q_\mu{}^2}-\int\frac{d\vec{\mathrm{q}}}{q^2}\right].\end{aligned} \tag{18}$$

The term for $\vec{\mathrm{q}}_\mu=0$ completes the long-range cancellation and is therefore to be omitted, while the remainder of the right-hand side of Eq. (18), though consisting of a divergent sum and a divergent integral, converges as a whole to a definite limit.

The cancellation and limiting process encountered in Eq. (18) is by no means inherently quantum mechanical, as it would also occur in a parallel treatment of classical lattice sums for Madelung energies. In fact, a good check of the mathematical procedures described herein is provided by the study of classical Madelung sums. Such sums exhibit cancellations of opposing apparently singular terms at $\vec{\mathrm{q}}_\mu=0$ and contain limits such as that of Eq. (18). We have accordingly made an investigation of Madelung sums, determining the limit of Eq. (18) to have the value $-8.913\,633(2\pi/a)$ for a simple cubic lattice and verifying that proper values are obtained for various Madelung constants.[3]

Consolidating the results obtainable by a complete treatment along the lines of the foregoing discussion, we find

$$\frac{H(\overleftrightarrow{\mathrm{k}},\overleftrightarrow{\mathrm{k}}')}{\langle\overleftrightarrow{\mathrm{k}}|\overleftrightarrow{\mathrm{k}}\rangle\langle\overleftrightarrow{\mathrm{k}}'|\overleftrightarrow{\mathrm{k}}\rangle} = \frac{1}{N}\left[\frac{-8.913\,633}{\pi a}-V(\vec{\mathrm{k}})-V(\vec{\mathrm{k}}')+J(\vec{\mathrm{k}},\vec{\mathrm{k}}')-\tfrac{1}{2}X(\vec{\mathrm{k}},\vec{\mathrm{k}}')\right]. \tag{19}$$

To gain confidence that the above-described methods are practical, we undertook the evaluation of some sums of each of the types that occur when ψ is taken to be a 1s orbital of screening parameter ζ. We first looked at the overlap and kinetic-energy summations. When programmed straightforwardly, these were found to take, for a given $\vec{\mathrm{k}}$, about 20 msec each (five-significant-figure results on Univac 1108 equipment). The potential-energy summations were found more cumbersome, requiring 20 sec for an electron-nuclear sum or 30 sec for an electron-repulsion sum. These evaluation times reflect no savings resulting from manipulations to more advantageous analytical forms. There are a number of possible ways of improving the computational efficiency, and we hope to incorporate them into a fuller report on this work.

Although the summations we evaluated for this preliminary strudy are for a relatively unrealistic simple cubic hydrogen-atom lattice, the re-

Table I. Kinetic energies $T(\vec{k})$, in hartrees. Values are for the indicated magnitudes of $\vec{k}$ in units $2\pi/a$ in the symmetry directions Δ (=$u00$), Σ (=$uu0$), and Λ (=uuu).

k	Δ	Σ	Λ	Δ	Σ	Λ
	ζ = 1.0, a = 1.5			ζ = 1.0, a = 2.0		
0.00	0.0006	0.0006	0.0006	0.0032	0.0032	0.0032
0.10	0.0890	0.0890	0.0890	0.0541	0.0541	0.0541
0.20	0.3570	0.3568	0.3568	0.2106	0.2103	0.2102
0.30	0.8277	0.8234	0.8224	0.4941	0.4900	0.4890
0.40	1.6043	1.5690	1.5597	0.9645	0.9485	0.9424
0.45	2.0965	2.1002	2.0819	1.2394	1.2718	1.2631
0.50	2.3544	2.7564	2.7390	1.3726	1.6585	1.6585
	ζ = 1.4, a = 1.5			ζ = 1.4 a = 2.0		
0.00	0.0081	0.0081	0.0081	0.0357	0.0357	0.0357
0.10	0.0993	0.0993	0.0993	0.0933	0.0933	0.0933
0.20	0.3810	0.3804	0.3802	0.2754	0.2746	0.2743
0.30	0.8943	0.8865	0.8844	0.6166	0.6110	0.6092
0.40	1.7440	1.7187	1.7078	1.1495	1.1611	1.1575
0.45	2.2313	2.3029	2.2888	1.4120	1.5263	1.5295
0.50	2.4635	2.9963	3.0012	1.5251	1.9314	1.9623

sults nevertheless contain some information of physical interest. In Table I we give values of $T(\vec{k})$, for $\vec{k}$ vectors in the three symmetry directions Δ, Σ, and Λ (in the notation of Bouckaert, Smoluchowski, and Wigner[4]), and for two values each of ζ and a. Particularly at low screening and short lattice spacing, we see that T is very nearly spherical almost all the way out to $k=\frac{1}{2}$ (in units $2\pi/a$). In a more realistic body-centered or face-centered lattice, T would be expected to deviate less from spherical symmetry than in the present calculation, and besides, the Fermi surface would not be as close to the zone boundary. Although T is quite spherical, Table I indicates that the localization of the 1s functions causes T to deviate substantially from the free-electron value $\frac{1}{2}k^2$.

The behavior of typical potential-energy contributions is indicated in Table II, which reports electron-nuclear contributions $V(\vec{k})$ for $\zeta=1$, $a=2$. We note that $V(\vec{k})$ is also quite spherical, but the most striking aspect of Table II is the small magnitude of its entries. This is best understood if we recognize that the cancellation of opposing potential-energy contributions, leading to the term in Eq. (19) containing $-8.913\,633$, would have no remainder represented by V, J, or X if the electron density were completely uniform.[5] In other words, $-8.913\,633/\pi a$ represents the exact potential energy of a lattice of positive ions in a uniform negative charge distribution. The terms V, J, X describe corrections due to the fact that the electron density is not completely uniform, and therefore may be thought of as localization energies. The essential message of Table II is that not only is the localization contribution of the electron-nuclear attraction spherical, but it is also small relative to the total potential energy and to the kinetic energy. What is true of V will be even more true of J and X, as J and X describe interactions between charges

Table II. Electron-nuclear energy contributions $V(\vec{k})$ in hartrees, for $\zeta=1$, $a=2$. Values are for the indicated magnitudes of $\vec{k}$ in units $2\pi/a$ in the symmetry directions Δ (=$u00$), Σ (=$uu0$), and Λ (=uuu).

k	Δ	Σ	Λ
0.00	0.0241	0.0241	0.0241
0.10	0.0296	0.0296	0.0296
0.20	0.0509	0.0504	0.0503
0.30	0.1063	0.1015	0.1003
0.40	0.2344	0.2122	0.2065
0.45	0.3188	0.2995	0.2906
0.50	0.3576	0.4050	0.3965

both of which are mainly delocalized. This result points up a key reason for the success of independent-electron models for solids, namely that the variable part of the electron-interaction energy is a very small part of the total interaction energy.

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NUCLEAR ACOUSTIC RESONANCE IN ALUMINUM VIA COUPLING TO THE MAGNETIC DIPOLE MOMENT

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We have observed a new interaction mechanism between a sound wave and the nuclear spin system in a single crystal of aluminum. The coupling is via the oscillating magnetic field induced by the sound wave in the presence of a large applied magnetic field and the magnetic moment of the nucleus. The experimental results agree with the theoretical predictions based on this mechanism.

The acoustic excitation of nuclear-spin resonance in metals has been reported unambiguously in tantalum.[1] We have recently observed the nuclear acoustic resonance in single crystals of niobium.[2] The interaction mechanism for both tantalum and niobium is the coupling between the oscillating electric field gradient created by the sound wave and the electric quadrupole moment of the nucleus. This is indicated by the observation of the $\Delta m=2$ transition as well as the $\Delta m=1$ transition. We report in this Letter the observation of the acoustic excitation of the $\Delta m=1$ nuclear spin transition in a single crystal of aluminum[3] (at 300 and 77°K) and we present evidence that the coupling mechanism is the interaction between the oscillating magnetic field induced by the sound wave in the presence of a large applied magnetic field and the magnetic moment of the nucleus.

According to the mechanism of Alpher and Rubin[4] the sound wave forces a mechanical motion of the charged particles in a conducting medium. In the presence of an applied magnetic field these charges are deflected and a transverse current is set up, which generates an electromagnetic field propagating in a metal at the velocity of the sound wave. The induced fields modify slightly the velocity[5] of the sound wave as well as the attenuation. Both effects are proportional to the square of the applied magnetic field and have been observed in aluminum.[6, 7]

On the basis of this mechanism, we have calculated the acoustic attenuation coefficient for the absorption of energy by the nuclear spin system. The attenuation coefficient, α_n, is defined as $\frac{1}{2}P_n/P_0$, where P_0 is the incident acoustic power per unit area and is equal to $\frac{1}{2}\rho v_s{}^3\epsilon^2$, where ρ is the density of the metal, v_s the velocity of the sound wave appropriate to shear or longitudinal wave propagation, and ϵ the peak value of the strain.[8] P_n is the power per unit volume absorbed by the nuclear spin system and is given by

$$P_n=\frac{N(h\nu)^2}{(2I+1)kT}\sum_m W_{mm'}, \tag{1}$$

where N is the number of nuclear spins per unit volume, ν is the frequency of the sound wave, and $W_{mm'}$ the transition probability per unit time from the spin state m to the state m'. For magnetic dipole coupling, $W_{mm'}$ is well known[9] and is proportional to the square of the oscillating magnetic field component perpendicular to the applied