彭桓武选集

SELECTED WORKS OF PENG HUAN-WU

中国学术出版社
CHINA ACADEMIC PUBLISHERS

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中国科学院理论物理研究所
北京应用物理和计算数学研究所 编

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序

很久以来，和彭桓武教授一起工作过的同事和他的学生都希望有一个机会将他历年的工作汇集成书，这个愿望终于实现了．随着时代的转移和国家的需要，彭桓武教授不断地开辟新的研究方向，带出了一批又一批的学生。我国的理论物理工作者为国民经济和国防建设作出的贡献、在科学发展上的成就无不与彭桓武教授的努力密切相关．他早年在英国从事固体理论、介子物理和量子场论的研究，１９４８年回国以后，转向核物理和核工程，领导了我国反应堆和核武器的理论设计工作．最近十年来为了加强我国固体和统计物理，原子和分子物理，加速器等新原理，他作了大量的组织和研究工作。

彭桓武教授对待科学工作十分严肃认真，他的物理思想深入问题的本质，数学技巧非常熟练，研究的对象具体实在．无论是基础研究还是应用研究，在当时的历史背景下，他的著作都是走在最前列的创造性的工作，并解决了实践中提出的大量实际问题。

这本书收集了彭桓武教授部分公开发表的论文．从这些论文中，读者可以领略彭桓武教授的工作风格，学习他将深刻的理论观点应用来解决具体问题的本领。

我们衷心祝愿彭桓武教授健康长寿，为发展我国的科学事业作出更大的贡献。

周光召

１９８５年１０月

PREFACE

This collection of Professor Peng Huan-wu represents his finished works over the years. Its publication has fulfilled the long-cherished wishes of his colleagues and his students. To catch up with changes of times and to meet the need of the state Professor Peng took great pains in his sustained efforts in exploring new fields and bringing up young physicists. The Chinese theoretical physicists owed much to Professor Peng in their contributions to national economy, building up national defense as well as in their achievements in scientific developments, for they are closely related to the labors of professor Peng Huan-wu.

In his early years Professor Peng engaged in the studies of solid state theory, meson physics and quantum field theory in Britain. After his return to China in 1948, he shifted his attention to nuclear physics and nuclear engineering. The theoretical designs of China's nuclear reactors and nuclear weapons were completed under his leadership. In the last decade, he has made strong endeavors to stimulate and promote new theories in the areas of solid state and statistical physics, atomic and molecular physics, and accelerators.

Professor Peng is deeply conscientious towards scientific work. His physical thoughts reach the very core of problems. He is thoroughly proficient in the techniques of mathematics. His research targets are tangible and definite. Whether in basic research or applied research his papers always stood in the forefront among the creative works at their given time and have solved a good many practical problems.

Included in this book are a portion of Peng's published papers. From these papers readers will get some idea of Professor Peng's working style and learn from him the skill of tackling actual problems in their deep theoretical perspectives.

Finally, we give professor Peng Huan-wu our best wishes for his health as well as his research work.

K.C. Chou

October, 1985

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Perturbation theory for the self-consistent field

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The perturbation theory has been applied to the Fock-Dirac system of equations. To obtain the perturbed Fock functions, it is necessary to solve a system of linear algebraic equations. To obtain the perturbation energy of the ith order, the perturbed Fock functions up to the $(i-1)$th order are needed.

In treating n-electron problems by quantum mechanics, it is necessary to adopt approximate methods; the most accurate of these involving the use of one-electron functions is, at present, the method of the self-consistent field. When the Hamiltonian contains some terms small compared with the rest—a state of affairs that often occurs—it is convenient to regard these small terms as 'perturbations'. In what follows we shall investigate the effect of these perturbations on the wave functions and the energy of an n-electron problem to the approximation of the self-consistent field.

The wave equations for the self-consistent field are the following due to Fock (1930) and Dirac (1930):

$$(K+G-W_\gamma)\,\phi_\gamma = 0, \quad (\gamma = 1, 2, \ldots, n). \tag{1}$$

They form a system of n simultaneous equations. The operator K denotes the one-electron Hamiltonian in the ideal case of vanishing interaction among the electrons, while G, defined by

$$G\phi_\gamma = \sum_{\lambda=1}^{n} \{(\phi_\lambda \,.\, \mathscr{G}\phi_\lambda)\,\phi_\gamma - (\phi_\lambda \,.\, \mathscr{G}\phi_\gamma)\,\phi_\lambda\}, \tag{2}$$

represents the ordinary and the exchange potentials due to the interactions of the electrons. The expression $(\phi_\lambda \,.\, \mathscr{G}\phi_\gamma)$ stands for

$$\sum_{s'} \int d\mathbf{r}'\, \phi_\lambda^*(\mathbf{r}'s')\, \mathscr{G}(\mathbf{r}s, \mathbf{r}'s')\, \phi_\gamma(\mathbf{r}'s'), \tag{3}$$

with $\mathscr{G}(\mathbf{r}s, \mathbf{r}'s')$ denoting the interaction between the electron at $\mathbf{r}$ with spin co-ordinate s and that at $\mathbf{r}'$ with spin co-ordinate s'. The interaction

$\mathscr{G}$ must be a self-adjoint operator and must be symmetric in the two electrons, i.e.

$$\mathscr{G}^\dagger = \mathscr{G}, \quad \mathscr{G}(\mathbf{r}s, \mathbf{r}'s') = \mathscr{G}(\mathbf{r}'s', \mathbf{r}s). \tag{4}$$

In most applications $\mathscr{G}$ is simply the Coulomb interaction $e^2/|\mathbf{r}-\mathbf{r}'|$.

The energy parameters W_γ which occur in (1) do not give the total energy E of the electrons directly. Since the interaction energy of electron pairs must be counted only once, E is given by

$$E = \sum_{\gamma=1}^{n} (\phi_\gamma . (K + \tfrac{1}{2}G)\,\phi_\gamma) = \sum_{\gamma=1}^{n} \{W_\gamma - \tfrac{1}{2}(\phi_\gamma . G\phi_\gamma)\}. \tag{5}$$

The main difficulty in solving (1) is due to the non-linear character of these equations, as may be seen from (2). We consider only the case when K and $\mathscr{G}$ can be expanded into series of descending terms

$$K = K^{(0)} + K^{(1)} + K^{(2)} + \ldots, \quad \mathscr{G} = \mathscr{G}^{(0)} + \mathscr{G}^{(1)} + \mathscr{G}^{(2)} + \ldots. \tag{6}$$

The system (1) can then be split into systems of various orders according to the usual practice of the perturbation method. As the perturbation equations are always linear, the solution of (1) is thereby greatly simplified.

1. Perturbation equations

Let us suppose that the Fock-Dirac system of equations for $K^{(0)}$ and $\mathscr{G}^{(0)}$ has been solved. In order to have a complete set of orthogonal, normalized functions at our disposal so that all other functions may be expressed as linear combinations of these, we introduce the following eigenvalue problem:

$$(K^{(0)} + G^{(0)} - W_\beta^{(0)})\,\phi_\beta^{(0)} = 0, \tag{7}$$

where the linear operator $G^{(0)}$ is defined, with the help of the known functions $\phi_1^{(0)}, \phi_2^{(0)}, \ldots, \phi_n^{(0)}$, by

$$G^{(0)}\phi = \sum_{\lambda=1}^{n} \{(\phi_\lambda^{(0)} . \mathscr{G}^{(0)}\phi_\lambda^{(0)})\,\phi - (\phi_\lambda^{(0)} . \mathscr{G}^{(0)}\phi)\,\phi_\lambda^{(0)}\}, \tag{8}$$

and is, by (4), self-adjoint. It follows from the definition that the complete set $\{\phi_\beta^{(0)}\}$ of orthonormal functions includes the functions $\phi_\beta^{(0)}, \phi_2^{(0)}, \ldots, \phi_n^{(0)}$.

I can now expand the ϕ_γ's of (1) in the set $\{\phi_\beta^{(0)}\}$ and write

$$\phi_\gamma = \sum_\beta \phi_\beta^{(0)} \mathscr{U}_{\beta\gamma}. \tag{9}$$

Denoting, for brevity, the constants $(\phi_\alpha^{(0)}.K\phi_\beta^{(0)})$, $(\phi_\alpha^{(0)}.(\phi_\mu^{(0)}.\mathscr{G}\phi_\nu^{(0)})\phi_\beta^{(0)})$ by $K_{\alpha\beta}$, $\mathscr{G}_{\alpha\mu\nu\beta}$, we obtain, from (1), (2) and (9), the system of algebraic equations

$$\sum_\beta \left\{K_{\alpha\beta}+\sum_{\lambda=1}^{n}\sum_{\mu\nu}\mathscr{U}^*_{\mu\lambda}(\mathscr{G}_{\alpha\mu\nu\beta}-\mathscr{G}_{\alpha\mu\beta\nu})\mathscr{U}_{\nu\lambda}-W_\gamma\delta_{\alpha\beta}\right\}\mathscr{U}_{\beta\gamma}=0. \tag{10}$$

By expanding $\mathscr{U}_{\beta\gamma}$ and W_γ in accordance with the perturbation,

$$\left.\begin{aligned}\mathscr{U}_{\beta\gamma}&=\delta_{\beta\gamma}+\mathscr{U}^{(1)}_{\beta\gamma}+\mathscr{U}^{(2)}_{\beta\gamma}+\ldots,\\ W_\gamma&=W^{(0)}_\gamma+W^{(1)}_\gamma+W^{(2)}_\gamma+\ldots,\end{aligned}\right\} \tag{11}$$

(10) splits into systems of various orders,† viz.

$$-W^{(0)}_\gamma\delta_{\alpha\gamma}+K^{(0)}_{\alpha\gamma}+\sum_{\lambda=1}^{n}(\mathscr{G}^{(0)}_{\alpha\lambda\lambda\gamma}-\mathscr{G}^{(0)}_{\alpha\lambda\gamma\lambda})=0, \tag{10·0}$$

$$\begin{aligned}&-W^{(1)}_\gamma\delta_{\alpha\gamma}+K^{(1)}_{\alpha\gamma}+\sum_{\lambda=1}^{n}(\mathscr{G}^{(0)}_{\alpha\lambda\lambda\gamma}-\mathscr{G}^{(0)}_{\alpha\lambda\gamma\lambda})\\&\quad+\sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(0)}_{\alpha\mu\nu\gamma}-\mathscr{G}^{(0)}_{\alpha\mu\gamma\nu})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda}+\delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\\&\quad+\sum_\beta\left\{K^{(0)}_{\alpha\beta}+\sum_{\lambda=1}^{n}(\mathscr{G}^{(0)}_{\alpha\lambda\lambda\beta}-\mathscr{G}^{(0)}_{\alpha\lambda\beta\lambda})-W^{(0)}_\gamma\delta_{\alpha\beta}\right\}\mathscr{U}^{(1)}_{\beta\gamma}=0,\end{aligned} \tag{10·1}$$

$$\begin{aligned}&-W^{(2)}_\gamma\delta_{\alpha\gamma}+K^{(2)}_{\alpha\gamma}+\sum_{\lambda=1}^{n}(\mathscr{G}^{(0)}_{\alpha\lambda\lambda\gamma}-\mathscr{G}^{(0)}_{\alpha\lambda\gamma\lambda})\\&\quad+\sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(1)}_{\alpha\mu\nu\gamma}-\mathscr{G}^{(1)}_{\alpha\mu\gamma\nu})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda}+\delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\\&\quad+\sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(0)}_{\alpha\mu\nu\gamma}-\mathscr{G}^{(0)}_{\alpha\mu\gamma\nu})(\mathscr{U}^{(2)*}_{\mu\lambda}\delta_{\nu\lambda}+\delta_{\mu\lambda}\mathscr{U}^{(2)}_{\nu\lambda}+\mathscr{U}^{(1)*}_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\\&\quad+\sum_\beta\left\{-W^{(1)}_\lambda\delta_{\alpha\beta}+K^{(1)}_{\alpha\beta}+\sum_{\lambda=1}^{n}(\mathscr{G}^{(1)}_{\alpha\lambda\lambda\beta}-\mathscr{G}^{(1)}_{\alpha\lambda\beta\lambda})\right.\\&\quad\left.+\sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(0)}_{\alpha\mu\nu\beta}-\mathscr{G}^{(0)}_{\alpha\mu\beta\nu})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda}+\delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\right\}\mathscr{U}^{(1)}_{\beta\gamma}\\&\quad+\sum_\beta\left\{K^{(0)}_{\alpha\beta}+\sum_{\lambda=1}^{n}(\mathscr{G}^{(0)}_{\alpha\lambda\lambda\beta}-\mathscr{G}^{(0)}_{\alpha\lambda\beta\lambda})-W^{(0)}_\gamma\delta_{\alpha\beta}\right\}\mathscr{U}^{(2)}_{\beta\lambda}=0,\end{aligned} \tag{10·2}$$

etc.

The zero-order system (10·0) is but a repetition, in algebraic form, of either the unperturbed Fock-Dirac system or the unperturbed eigenvalue

† The restriction ($\gamma = 1, 2, \ldots, n$) has been purposely omitted in (9)–(14) as (1) can be extended into an eigenvalue problem similar to (7) as soon as $\phi_1, \phi_2, \ldots, \phi_n$ are determined.

problem (7) according to whether the index γ is restricted to vary from 1 to n or not. With the help of the equation obtained by putting the index γ of (10·0) equal to β, the last bracket of (10·1) and (10·2) becomes simply

$$\{(W_\beta^{(0)} - W_\gamma^{(0)})\,\delta_{\alpha\beta}\} = \{(W_\alpha^{(0)} - W_\gamma^{(0)})\,\delta_{\alpha\beta}\}, \tag{12}$$

and vanishes identically when we take $\alpha = \gamma$. Because of the appearance of $\mathscr{U}_{\nu\lambda}^{(1)}$ and $\mathscr{U}_{\nu\lambda}^{(2)}$ elsewhere in (10·1) and (10·2), the perturbation energy parameters $W_\gamma^{(1)}$ and $W_\gamma^{(2)}$ cannot be calculated before $\mathscr{U}_{\nu\lambda}^{(1)}$ and $\mathscr{U}_{\nu\lambda}^{(2)}$ are obtained. To obtain $\mathscr{U}_{\nu\lambda}^{(1)}$, for example, I take the index α of (10·1) different from γ. Remembering (12), I have, for the equations for $\mathscr{U}_{\alpha\gamma}^{(1)}$ $(\alpha \neq \gamma)$,

$$(W_\alpha^{(0)} - W_\gamma^{(0)})\,\mathscr{U}_{\alpha\gamma}^{(1)} + \sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}_{\alpha\mu\nu\gamma}^{(0)} - \mathscr{G}_{\alpha\mu\gamma\nu}^{(0)})\,(\mathscr{U}_{\mu\lambda}^{(1)*}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}_{\nu\lambda}^{(1)}) = -\left\{K_{\alpha\gamma}^{(1)} + \sum_{\lambda=1}^{n}(\mathscr{G}_{\alpha\lambda\lambda\gamma}^{(1)} - \mathscr{G}_{\alpha\lambda\gamma\lambda}^{(1)})\right\}. \tag{13·1}$$

Successively the equations for $\mathscr{U}_{\alpha\lambda}^{(i)}$ $(i = 1, 2, \ldots; \alpha \neq \gamma)$ are all of the form

$$(W_\alpha^{(0)} - W_\gamma^{(0)})\,\mathscr{U}_{\alpha\gamma}^{(i)} + \sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}_{\alpha\mu\nu\gamma}^{(0)} - \mathscr{G}_{\alpha\mu\gamma\nu}^{(0)})\,(\mathscr{U}_{\mu\lambda}^{(i)*}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}_{\nu\lambda}^{(i)}) = \text{known quantities.} \tag{13·i}$$

These equations, being algebraic and linear, are in principle solvable. The elements $\mathscr{U}_{\gamma\gamma}^{(1)}$, $\mathscr{U}_{\gamma\gamma}^{(2)}$, etc. are, as usual, not determined by these equations but, owing to the normalization of the ϕ_γ's of (1) and the $\phi_\beta^{(0)}$'s of (7), they are given by

$$\mathscr{U}_{\gamma\gamma}^{(1)*} + \mathscr{U}_{\gamma\gamma}^{(1)} = 0, \quad \mathscr{U}_{\gamma\gamma}^{(2)*} + \mathscr{U}_{\gamma\gamma}^{(2)} = -\sum_\beta \mathscr{U}_{\beta\gamma}^{(1)*}\mathscr{U}_{\beta\gamma}^{(1)}, \text{ etc.} \tag{14}$$

2. Perturbation energy

The algebraic expression for the total energy of the electrons, obtained by substituting (9) into (5), is

$$E = \sum_{\gamma=1}^{n} W_\gamma - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}\sum_{\alpha\beta\mu\nu}\mathscr{U}_{\alpha\gamma}^{*}\mathscr{U}_{\mu\lambda}^{*}(\mathscr{G}_{\alpha\mu\nu\beta} - \mathscr{G}_{\alpha\mu\beta\nu})\,\mathscr{U}_{\nu\lambda}\mathscr{U}_{\beta\gamma}. \tag{15}$$

This, being expanded according to the perturbation into series of the form (11), yields

$$E^{(0)} = \sum_{\gamma=1}^{n} W_\gamma^{(0)} - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}(\mathscr{G}_{\gamma\lambda\lambda\gamma}^{(0)} - \mathscr{G}_{\gamma\lambda\gamma\lambda}^{(0)}), \tag{15·0}$$

$$E^{(1)} = \sum_{\gamma=1}^{n} W_\gamma^{(1)} - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}(\mathscr{G}^{(1)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(1)}_{\gamma\lambda\gamma\lambda}) - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}\sum_{\alpha\beta\mu\nu}(\mathscr{G}^{(0)}_{\alpha\mu\nu\beta} - \mathscr{G}^{(0)}_{\alpha\mu\beta\nu}) \times \{(\mathscr{U}^{(1)*}_{\alpha\gamma}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\mathscr{U}^{(1)}_{\beta\gamma})\delta_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\alpha\gamma}\delta_{\beta\gamma}(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\}, \quad (15\cdot1)$$

$$E^{(2)} = \sum_{\gamma=1}^{n} W_\gamma^{(2)} - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}(\mathscr{G}^{(2)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(2)}_{\gamma\lambda\gamma\lambda}) - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}\sum_{\alpha\beta\mu\nu}(\mathscr{G}^{(1)}_{\alpha\mu\nu\beta} - \mathscr{G}^{(1)}_{\alpha\mu\beta\nu}) \times \{(\mathscr{U}^{(1)*}_{\alpha\gamma}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\mathscr{U}^{(1)}_{\beta\gamma})\delta_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\alpha\gamma}\delta_{\beta\gamma}(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\} - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}\sum_{\alpha\beta\mu\nu}(\mathscr{G}^{(0)}_{\alpha\mu\nu\beta} - \mathscr{G}^{(0)}_{\alpha\mu\beta\nu}) \times \{(\mathscr{U}^{(2)*}_{\alpha\gamma}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\mathscr{U}^{(2)}_{\beta\gamma} + \mathscr{U}^{(1)*}_{\alpha\gamma}\mathscr{U}^{(1)}_{\beta\gamma})\delta_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\alpha\gamma}\delta_{\beta\gamma}(\mathscr{U}^{(2)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(2)}_{\nu\lambda} + \mathscr{U}^{(1)*}_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda}) + (\mathscr{U}^{(1)*}_{\alpha\gamma}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\mathscr{U}^{(1)}_{\beta\gamma})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda})\}, \quad (15\cdot2)$$

etc. If I had applied the ordinary perturbation method to the original Schrödinger equation for the assembly of electrons and then introduced the one-electron approximation, I should have obtained some expressions for calculating the perturbation energy of the first and the second order from the Fock functions of zero-order and the first order. Hence the explicit appearance of $\mathscr{U}^{(1)}_{\beta\gamma}$ in (15·1) and $\mathscr{U}^{(2)}_{\beta\gamma}$ in (15·2) must be only apparent. I can get rid of them by substituting (10·1) and (10·2) for $W^{(1)}_\gamma$ and $W^{(2)}_\gamma$ and then cancelling terms, as will be shown immediately.

From (4), I derive

$$\mathscr{G}^{(i)*}_{\beta\nu\mu\alpha} = \mathscr{G}^{(i)}_{\alpha\mu\nu\beta} = \mathscr{G}^{(i)}_{\mu\alpha\beta\nu}, \quad (i = 0, 1, 2, \ldots). \quad (16)$$

This may be used to simplify the last term of (15·1). I then have for $E^{(1)}$,

$$E^{(1)} = \sum_{\gamma=1}^{n} W_\gamma^{(1)} - \frac{1}{2}\sum_{\lambda,\gamma=1}^{n}(\mathscr{G}^{(1)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(1)}_{\gamma\lambda\gamma\lambda}) - \sum_{\gamma,\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(0)}_{\gamma\mu\nu\gamma} - \mathscr{G}^{(0)}_{\gamma\mu\gamma\nu})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda}). \quad (15\cdot1a)$$

To obtain $W^{(1)}_\gamma$ from (10·1), take $\alpha = \gamma$. The last line of (10·1) then drops out by (12). Hence for $W^{(1)}_\gamma$,

$$W^{(1)}_\gamma = K^{(1)}_{\gamma\gamma} + \sum_{\lambda=1}^{n}(\mathscr{G}^{(1)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(1)}_{\gamma\lambda\gamma\lambda}) + \sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(0)}_{\gamma\mu\nu\gamma} - \mathscr{G}^{(0)}_{\gamma\mu\gamma\nu})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\mu}). \quad (17)$$

Substituting (17) into (15·1a) and cancelling terms, I obtain for the perturbation energy of the first order,

$$E^{(1)} = \sum_{\gamma=1}^{n} K^{(1)}_{\gamma\gamma} + \frac{1}{2}\sum_{\gamma,\lambda=1}^{n} (\mathscr{G}^{(1)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(1)}_{\gamma\lambda\gamma\lambda}), \tag{18·1}$$

which is indeed free from $\mathscr{U}^{(1)}_{\beta\gamma}$. A similar combination of (10·2) and (15·2) yields for the perturbation energy of the second order,

$$\begin{aligned} E^{(2)} = {} & \sum_{\gamma=1}^{n} K^{(2)}_{\gamma\gamma} + \frac{1}{2}\sum_{\gamma,\lambda=1}^{n} (\mathscr{G}^{(2)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(2)}_{\gamma\lambda\gamma\lambda}) \\ & + \sum_{\gamma=1}^{n}\sum_{\beta}\Big\{K^{(1)}_{\gamma\beta} + \sum_{\lambda=1}^{n}\sum_{\mu\nu}(\mathscr{G}^{(0)}_{\gamma\mu\nu\beta} - \mathscr{G}^{(0)}_{\gamma\mu\beta\nu})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda}) \\ & \qquad + \sum_{\lambda=1}^{n}(\mathscr{G}^{(1)}_{\gamma\lambda\lambda\beta} - \mathscr{G}^{(1)}_{\gamma\lambda\beta\lambda}) - W^{(1)}_{\gamma}\delta_{\gamma\beta}\Big\}\mathscr{U}^{(1)}_{\beta\gamma} \\ & - \frac{1}{2}\sum_{\gamma,\lambda=1}^{n}\sum_{\alpha\beta\mu\nu}(\mathscr{G}^{(0)}_{\alpha\mu\nu\beta} - \mathscr{G}^{(0)}_{\alpha\mu\beta\nu})(\mathscr{U}^{(1)*}_{\alpha\gamma}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\mathscr{U}^{(1)}_{\beta\gamma})(\mathscr{U}^{(1)*}_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\mathscr{U}^{(1)}_{\nu\lambda}). \end{aligned} \tag{18·2}$$

Since the above expression is necessarily real, I can replace the right-hand side by its real part. The real part of the coefficient of $W^{(1)}_{\gamma}$ vanishes by (14) and the real part of the terms containing $\mathscr{G}^{(0)}$ cancel by (18). Hence I get finally for $E^{(2)}$,

$$\begin{aligned} E^{(2)} = {} & \sum_{\gamma=1}^{n} K^{(2)}_{\gamma\gamma} + \frac{1}{2}\sum_{\gamma,\lambda=1}^{n} (\mathscr{G}^{(2)}_{\gamma\lambda\lambda\gamma} - \mathscr{G}^{(2)}_{\gamma\lambda\gamma\lambda}) \\ & + \text{real part of } \sum_{\gamma=1}^{n}\sum_{\beta}\Big\{K^{(1)}_{\gamma\beta} + \sum_{\lambda=1}^{n}(\mathscr{G}^{(1)}_{\gamma\lambda\lambda\beta} - \mathscr{G}^{(1)}_{\gamma\lambda\beta\lambda})\Big\}\mathscr{U}^{(1)}_{\beta\gamma}. \end{aligned} \tag{18·3}$$

The above derivation of (18·3) is quite general. Similar expressions for the perturbation energy of higher orders can all be obtained in the same way. In evaluating the energy to the third order, for example, it is necessary to solve the equations (10·2) for $\mathscr{U}^{(2)}_{\beta\gamma}$, which, however, does not present any new feature as the perturbation equations of higher orders are all of the same form as that of the equations of the first order.

3. Separation of the spin

In treating $2n$-electron problems with zero resultant spin by the method of the self-consistent field, the $2n$ one-electron functions may be taken as the products of n functions $\psi_1, \psi_2, \ldots, \psi_n$ of the spatial co-ordinates r with the two spin eigenfunctions $\delta_{-1}(s)$, $\delta_{+1}(s)$. The spin eigenfunctions $\delta_{\sigma}(s)$ assume the value zero when s differs from σ and the value unity when s

equals σ. In all the scalar products (cf. (3)) of the preceding sections, the summation over the spin co-ordinates can then be performed independently according to the normalization

$$\sum_s \delta_\sigma(s)\,\delta_{\sigma'}(s) = \delta_{\sigma\sigma'}. \tag{19}$$

The important consequence of this is that all electrons contribute to the ordinary potential but only electrons with parallel spins contribute to the exchange potential. The spin eigenfunctions may be factorized and hence removed from (1). For the details of this reduction, we refer to Brillouin's book (1934).

The reduced Fock-Dirac system of equations in the case of zero resultant spin consists of n simultaneous equations in the n ψ-functions of r. These may be obtained formally from (1) by changing ϕ into ψ provided that a factor 2 is added to the first (the ordinary potential) term on the right of (2). This means that the perturbation equations for the ψ-functions of the $2n$-electron problem may be obtained from the corresponding equations of § 1 by adding a factor 2 to the first term of every bracket containing the difference of two $\mathscr{G}$'s. The constants $K_{\alpha\beta}$, $\mathscr{G}_{\alpha\mu\nu\beta}$ now stand for $(\psi_\alpha^{(0)}.K\psi_\beta^{(0)})$, $(\psi_\alpha^{(0)}.(\psi_\mu^{(0)}.\mathscr{G}\psi_\nu^{(0)})\,\psi_\beta^{(0)})$, involving volume integrations of the spatial co-ordinates only.

To obtain the expressions for the perturbation energy for the $2n$-electron problem from those of § 2, we need to add the factor 2 in the above way and then double the whole expressions on the right-hand sides.

The above perturbation theory has been applied to the calculation of the elastic constants and the thermal frequencies of metallic crystals which will be treated in separate papers.

I wish to acknowledge my indebtedness to Professor M. Born and Dr K. Fuchs for much valuable advice.

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Crystal theory of metals: calculation of the elastic constants

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The approximate equations of motion for the electrons in a cyclic lattice of a metal are set up with the help of the self-consistent field. The displacements of the ions are then considered as perturbations of the motion of the electrons. The change of the boundary is compensated by a co-ordinate transformation. The change of the potential energy of the lattice due to a homogeneous deformation is calculated by the perturbation method. The calculated values of the elastic constants are found to be in satisfactory agreement with the observed values.

Introduction

The character of metallic binding has been revealed by the calculations of Wigner & Seitz (1933, 1934). But little progress has since been made in developing a crystal theory of metals comparable with the classical crystal theory of ionic lattices of Born (1923), apart from the calculation of the elastic properties (Fröhlich 1937; Fuchs 1936*a*; Bardeen 1938).

Recently one of us (Fuchs 1940) suggested that the method of the operator calculus is suitable for further progress in this direction. In this paper we wish to attempt such a development, and the general method of treatment

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