

The Effect of a Magnetic Field on Electrons in a Periodic Potential

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A theorem due to Wannier for treating the motion of electrons in a perturbed periodic field is generalized to include the effect of a slowly varying magnetic field. It is shown that the problem reduces to that of solving an effective Schrödinger equation, which is known as soon as we have solved the problem without perturbing fields.

I. INTRODUCTION

RECENTLY Slater¹ has revived interest in a theorem due to Wannier² which enables one to study the behavior of electrons in a perturbed periodic potential. This theorem may be stated as follows: Say the energy for the unperturbed periodic potential as a function of the quasi-momentum \mathbf{p}' is known, and is given by $E_0(\mathbf{p}')$. Let the perturbing potential be $e\varphi(\mathbf{r})$, where $\varphi(\mathbf{r})$ is a function which does not change appreciably over one lattice spacing (for example, the potential of an applied electric field). Then the allowed energies E of the perturbed problem are given approximately by solving the equation

$$\{E_0(-i\hbar\nabla) + e\varphi(\mathbf{r})\}\psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad (1)$$

The operator $E_0(-i\hbar\nabla)$ is the same function of $-i\hbar\partial/\partial x$, $-i\hbar\partial/\partial y$, $-i\hbar\partial/\partial z$ as it was of p_x' , p_y' , p_z' .

The question now arises as to what modifications of (1) are necessary when an external magnetic field is also imposed. This problem has been studied and to some degree solved by Peierls,³ in connection with his investigation of the diamagnetism of strongly bound electrons in metals. Our results will be a simplification and generalization of those of Peierls.

The simplest modification of (1) consistent with the requirements of gauge invariance⁴ would be obtained by replacing $-i\hbar\nabla$ by $-i\hbar\nabla - (e/c)\mathbf{A}$, where \mathbf{A} is the vector potential of the magnetic field. It is by no means clear that these are the only terms which arise, for one could add to the resulting hamiltonian any terms which depend on the magnetic field only, and which would therefore be automatically gauge invariant. It is the purpose of this paper to show that in fact no such extra terms occur, and, therefore, that the energy levels in the presence of a magnetic field are approximately given by

$$\{E_0[-ie\nabla - (e/c)\mathbf{A}] + e\varphi\}\psi = E\psi. \quad (2)$$

II. EFFECT OF A SLOWLY VARYING MAGNETIC FIELD

Let the hamiltonian of the electron in the unperturbed periodic lattice be given by $\mathcal{H}_0 = \mathbf{p}^2/2m + V(\mathbf{r})$,

¹ J. C. Slater, Phys. Rev. **76**, 1592 (1949).

² G. H. Wannier, Phys. Rev. **52**, 191 (1937).

³ R. Peierls, Z. Physik **80**, 763 (1933).

⁴ The requirements of gauge invariance for velocity dependent operators have been investigated by R. G. Sachs and N. Austern, Phys. Rev. **81**, 705 (1951).

$V(\mathbf{r})$ being the periodic potential. We will assume that we can solve this unperturbed problem; that is, we can obtain the energy as a function of the quasi-momentum \mathbf{p}' . Let this energy be $E_0(\mathbf{p}')$, and let the corresponding normalized Bloch function be $\psi_{\mathbf{p}'}(\mathbf{r})$, i.e.,

$$\mathcal{H}_0\psi_{\mathbf{p}'}(\mathbf{r}) = E_0(\mathbf{p}')\psi_{\mathbf{p}'}(\mathbf{r}).$$

Now let us construct the Wannier localized atomic functions $a(\mathbf{r} - \mathbf{Q}_k)$,⁵ where \mathbf{Q}_k is the vector to the k th lattice point. These functions are defined as

$$a(\mathbf{r} - \mathbf{Q}_k) = \frac{1}{\sqrt{N}} \sum_{\mathbf{p}'} \exp\left\{-\frac{i\mathbf{p}' \cdot \mathbf{Q}_k}{\hbar}\right\} \psi_{\mathbf{p}'}(\mathbf{r}) \quad (3)$$

where the summation on \mathbf{p}' is extended over all N levels of the band in question, N being the number of atoms in the lattice. One may easily show¹ that these functions are orthonormal,

$$(a(\mathbf{r} - \mathbf{Q}_k), a(\mathbf{r} - \mathbf{Q}_l)) = \delta_{kl}. \quad (4)$$

We used the standard notation (ψ_1, ψ_2) for the scalar product of the functions ψ_1 and ψ_2 ,

$$(\psi_1, \psi_2) = \iiint dx dy dz (\psi_1^* \psi_2).$$

Further they have the property that they are localized² about the point \mathbf{Q}_k : they drop off rapidly as we move away from \mathbf{Q}_k . It is these properties that make them so useful in discussing the perturbed periodic lattice. In the presence of a perturbing electric and magnetic field the hamiltonian \mathcal{H} takes the form

$$\mathcal{H} = (\mathbf{p} - e\mathbf{A}/c)^2/2m + V(\mathbf{r}) + e\varphi(\mathbf{r}),$$

\mathbf{A} being the vector potential of the perturbing magnetic field. We want to solve the Schrödinger equation

$$\mathcal{H}\psi = i\hbar\partial\psi/\partial t.$$

For the case of no magnetic field Slater (see reference 1) shows that it is convenient to expand ψ in terms of the Wannier functions, that is to put

$$\psi = \sum_m \Psi(\mathbf{Q}_m) a(\mathbf{r} - \mathbf{Q}_m) \quad (5)$$

$\Psi(\mathbf{Q}_m)$ being coefficients to be determined. Here the

⁵ We shall follow most of the notation of Slater, see reference 1, Appendix I.

summation is extended over all the points in the lattice. Such an expansion is always possible as long as we assume that the electric and magnetic fields are weak enough so that we may neglect contributions from different bands. According to well known calculations of Zener⁶ this is usually an excellent approximation, and we shall assume it throughout this paper. A little consideration shows, however, that the expansion (5) is no longer quite suitable when a magnetic field is present. This is because of the perturbing term of the form $\mathbf{A} \cdot \mathbf{p}$ in \mathcal{H} . This term contains a derivative operator, and the method used by Slater is only directly applicable to perturbing terms which are functions of the coordinates alone. By suitably modifying the expansion (5), we shall be able to use most of the apparatus of Slater's proof. Let us replace (5) by

$$\psi = \sum_m \Psi(\mathbf{Q}_m) \exp\{ (ie/\hbar c) G_m \} a(\mathbf{r} - \mathbf{Q}_m), \quad (6)$$

where

$$G_m \equiv \int_{\mathbf{Q}_m}^{\mathbf{r}} \mathbf{A}(\xi) d\xi,$$

the integral being taken along the straight line path joining \mathbf{Q}_m to \mathbf{r} . The exponential term has the effect of approximately removing the troublesome $\mathbf{A} \cdot \mathbf{p}$ term. One may write G_m in another form, which is convenient for calculation:

$$G_m = \int_0^1 d\lambda (\mathbf{r} - \mathbf{Q}_m) \cdot \mathbf{A}(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)). \quad (7)$$

Equation (7) is obtained simply by parametrizing the line integral in the original definition of G_m .

We must now calculate $\mathcal{H}\psi$. Using the notation

$$\Psi(\mathbf{Q}_m) = \Psi_m, \quad a(\mathbf{r} - \mathbf{Q}_m) = a_m,$$

we have

$$\begin{aligned} \mathcal{H}\psi &= \mathcal{H} \sum_m \Psi_m \exp\{ (ie/\hbar c) G_m \} a_m \\ &= \sum_m \Psi_m [(\mathbf{p} - e\mathbf{A}/c)^2/2m + V + e\varphi] \exp\{ (ie/\hbar c) G_m \} a_m \\ &= \sum_m \Psi_m \exp\{ (ie/\hbar c) G_m \} \\ &\quad \times \left(\frac{[\mathbf{p} - (e/c)(\mathbf{A} - \nabla G_m)]^2}{2m} + V + e\varphi \right) a_m. \end{aligned}$$

It is a straightforward matter to compute ∇G_m (see Appendix I). One obtains

$$\nabla G_m = \mathbf{A}(\mathbf{r}) + \int_0^1 \lambda d\lambda (\mathbf{r} - \mathbf{Q}_m) \times \mathbf{H}(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)).$$

$\mathbf{H}(\xi)$ is the magnetic field at the point ξ , $\mathbf{H}(\xi) = \nabla_\xi \times \mathbf{A}(\xi)$.

⁶ C. Zener, Proc. Roy. Soc. (London) A145, 523 (1934).

Thus

$$\begin{aligned} \mathcal{H}\psi &= \sum_m \Psi_m \exp\{ (ie/\hbar c) G_m \} \\ &\quad \times \left[\frac{\left[\mathbf{p} + (e/c) \int_0^1 d\lambda \lambda (\mathbf{r} - \mathbf{Q}_m) \times \mathbf{H} \right]^2}{2m} + V + e\varphi \right] a_m. \end{aligned}$$

We may now invoke (following Slater) the localization of the a_m . This allows us to put $\mathbf{r} \cong \mathbf{Q}_m$ in the operator on a_m , as long as the electric and magnetic fields are not too rapidly varying.⁷ When we do this we obtain very simply

$$\begin{aligned} \mathcal{H}\psi &= \sum_m \Psi_m \exp\{ (ie/\hbar c) G_m \} [p^2/2m + V + e\varphi(\mathbf{Q}_m)] a_m, \\ \text{or,} \quad \mathcal{H}\psi &= \sum_m \Psi_m \exp\{ (ie/\hbar c) G_m \} [\mathcal{H}_0 + e\varphi(\mathbf{Q}_m)] a_m. \quad (8) \end{aligned}$$

To complete the evaluation of the right-hand side of (8) we must have $\mathcal{H}_0 a_m$. This is easily accomplished as follows: Using (3),

$$\begin{aligned} \mathcal{H}_0 a_m &= N^{-1} \sum_{p'} \mathcal{H}_0 \exp\{ -i\mathbf{p}' \cdot \mathbf{Q}_m/\hbar \} \psi_{p'} \\ &= N^{-1} \sum_{p'} E_0(\mathbf{p}') \exp\{ -i\mathbf{p}' \cdot \mathbf{Q}_m/\hbar \} \psi_{p'}. \end{aligned}$$

Expressing $\psi_{p'}$ in terms of the a_m we have

$$\psi_{p'} = N^{-1} \sum_l \exp\{ i\mathbf{p}' \cdot \mathbf{Q}_l/\hbar \} a_l,$$

so that we have finally

$$\mathcal{H}_0 a_m = N^{-1} \sum_l \sum_{p'} E_0(\mathbf{p}') \exp\{ i\mathbf{p}' \cdot (\mathbf{Q}_l - \mathbf{Q}_m)/\hbar \} a_l. \quad (9)$$

Now as is well known $E_0(\mathbf{p}')$ is a periodic function of \mathbf{p}' , having the periodicity of the reciprocal lattice. Thus we may expand

$$E_0(\mathbf{p}') = \sum_s B_s \exp\{ -i\mathbf{p}' \cdot \mathbf{Q}_s/\hbar \}. \quad (10)$$

Using (10) in (9) we obtain

$$\begin{aligned} \mathcal{H}_0 a_m &= N^{-1} \sum_l \sum_s \sum_{p'} B_s \exp\{ i\mathbf{p}' \cdot (\mathbf{Q}_l - \mathbf{Q}_s - \mathbf{Q}_m)/\hbar \} a_l \\ &= \sum_{l,s} B_s \delta_{l,m+s} a_l \end{aligned}$$

or

$$\mathcal{H}_0 a_m = \sum_s B_s a_{m+s}. \quad (11)$$

Substitution of (11) into (8) then yields

$$\mathcal{H}\psi = \sum_m \Psi_m \exp\{ (ie/\hbar c) G_m \} [\sum_s B_s a_{m+s} + e\varphi(\mathbf{Q}_m) a_m].$$

If we replace $m+s$ by m' in the first term in the square bracket, we obtain (on dropping the prime)

$$\begin{aligned} \mathcal{H}\psi &= \sum_m a_m [\sum_s B_s \Psi(\mathbf{Q}_m - \mathbf{Q}_s) \exp\{ (ie/\hbar c) G_{m-s} \} \\ &\quad + e\varphi(\mathbf{Q}_m) \Psi(\mathbf{Q}_m) \exp\{ (ie/\hbar c) G_m \}]. \quad (12) \end{aligned}$$

Equation (12) may be put in a more elegant form if we make use of the well-known operator identity

$$\Psi(\mathbf{Q}_m - \mathbf{Q}_s) = \exp\{ -\mathbf{Q}_s \cdot \nabla_m \} \Psi(\mathbf{Q}_m)$$

⁷ Unfortunately it seems rather difficult within this formalism to make an estimate of the error involved here, and therefore it is impossible to say exactly what the conditions are under which the theorem to be proved is valid. This is so even without the presence of the magnetic field.

where ∇_m is the gradient operation with respect to the position vector \mathbf{Q}_m . Using this, (12) takes the form

$$\mathcal{H}\psi = \sum_m a_m \left[\sum_s B_s \exp\left\{ \frac{ie}{\hbar c} G_{m-s} \right\} \exp\left\{ -\mathbf{Q}_s \cdot \nabla_m \right\} + e\varphi(\mathbf{Q}_m) \exp\left\{ \frac{ie}{\hbar c} G_m \right\} \right] \Psi(\mathbf{Q}_m).$$

Now this equation may further be simplified by using once again the localization of the a_m . This tells us that in G_{m-s} , and in G_m we can put $\mathbf{r} \cong \mathbf{Q}_m$. We have

$$\begin{aligned} G_m(\mathbf{r} = \mathbf{Q}_m) &= 0 \\ G_{m-s}(\mathbf{r} = \mathbf{Q}_m) &= \int_0^1 d\lambda \mathbf{Q}_s \cdot \mathbf{A}(\mathbf{Q}_m - (1-\lambda)\mathbf{Q}_s) \\ &= \int_0^1 d\lambda \mathbf{Q}_s \cdot \mathbf{A}(\mathbf{Q}_m - \lambda\mathbf{Q}_s). \end{aligned}$$

Substituting, we obtain

$$\begin{aligned} \mathcal{H}\psi &= \sum_m a_m \left[\sum_s B_s \exp\left\{ \frac{ie}{\hbar c} \right. \right. \\ &\quad \times \int_0^1 d\lambda \mathbf{Q}_s \cdot \mathbf{A}(\mathbf{Q}_m - \lambda\mathbf{Q}_s) \left. \left. \right\} \exp\left\{ -\mathbf{Q}_s \cdot \nabla_m \right\} \right. \\ &\quad \left. + e\varphi(\mathbf{Q}_m) \right] \Psi(\mathbf{Q}_m). \end{aligned}$$

We now make use of the operator identity (for a proof, see Appendix II)

$$\begin{aligned} \exp\left\{ \frac{ie}{\hbar c} \int_0^1 d\lambda \mathbf{Q}_s \cdot \mathbf{A}(\mathbf{Q}_m - \lambda\mathbf{Q}_s) \right\} \exp\left\{ -\mathbf{Q}_s \cdot \nabla_m \right\} \\ = \exp\left\{ -\mathbf{Q}_s \cdot \left[\nabla_m - \frac{ie}{\hbar c} \mathbf{A}(\mathbf{Q}_m) \right] \right\} \\ = \exp\left\{ -i\mathbf{Q}_s \cdot \left[\mathbf{p}_m - (e/c)\mathbf{A}_m \right] / \hbar \right\}, \end{aligned}$$

where $\mathbf{p}_m \equiv -i\hbar\nabla_m$. Thus

$$\mathcal{H}\psi = \sum_m a_m \left[\sum_s B_s \exp\left\{ -i\mathbf{Q}_s \cdot \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right] / \hbar \right\} + e\varphi(\mathbf{Q}_m) \right] \Psi(\mathbf{Q}_m). \quad (13)$$

However, using (10) we see that the summation over s is easily performed:

$$\begin{aligned} \sum_s B_s \exp\left\{ -i\mathbf{Q}_s \cdot \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right] / \hbar \right\} \\ = E_0 \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right], \quad (14) \end{aligned}$$

where $E_0 \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right]$ is the same function⁸ of $\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m)$ as $E_0(\mathbf{p}')$ is of \mathbf{p}' . Using (14), we may rewrite (13) as

$$\mathcal{H}\psi = \sum_m a_m \left\{ E_0 \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right] + e\varphi(\mathbf{Q}_m) \right\} \Psi(\mathbf{Q}_m). \quad (15)$$

⁸ Since $\mathbf{A}(\mathbf{Q}_m)$ does not commute with \mathbf{p}_m , there may be some ambiguity in the ordering of the factors in $E_0 \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right]$. In such cases the order is uniquely determined by returning to the expansion (14).

The Schrödinger equation reads

$$\begin{aligned} \mathcal{H}\psi &= i\hbar \partial\psi / \partial t \\ &= i\hbar \sum_m a_m \exp\left\{ \frac{ie}{\hbar c} G_m \right\} \dot{\Psi}(\mathbf{Q}_m) \\ &\quad - (e/c) \sum_m \dot{G}_m a_m \Psi(\mathbf{Q}_m) \cong i\hbar \sum_m a_m \dot{\Psi}(\mathbf{Q}_m), \end{aligned}$$

on using once again the localization of the a_m . Using (15), we obtain

$$\begin{aligned} \sum_m a_m \left\{ E_0 \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right] + e\varphi(\mathbf{Q}_m) \right\} \Psi(\mathbf{Q}_m) \\ = i\hbar \sum_m a_m \dot{\Psi}(\mathbf{Q}_m). \end{aligned}$$

Finally, taking the scalar product of both sides with a_i , and using the orthonormality of the a_k , we obtain

$$\left\{ E_0 \left[\mathbf{p}_m - (e/c)\mathbf{A}(\mathbf{Q}_m) \right] + e\varphi(\mathbf{Q}_m) \right\} \dot{\Psi}(\mathbf{Q}_m) = i\hbar \dot{\Psi}(\mathbf{Q}_m), \quad (2')$$

The eigenvalue problem associated with Eq. (2') is identical (apart from notation) with Eq. (2), so that we have proven that for fields which vary slowly enough approximate eigenvalues of the energy may be obtained by solving (2).

III. THE MOTION OF WAVE PACKETS

Following Slater¹ we can also investigate the motion of wave packets of electrons in the perturbed lattice. If we construct our wave packets from the solutions of (2), then we know (Ehrenfest's theorem) that the center of gravity of such a wave packet moves according to the classical canonical equations. In our case this hamiltonian is

$$\mathcal{H} = E_0 \left[\mathbf{p} - (e/c)\mathbf{A} \right] + e\varphi.$$

The equations of motion are therefore

$$dx/dt = v_x = \partial\mathcal{H} / \partial p_x, \text{ etc.},$$

and

$$dp_x/dt = -\partial\mathcal{H} / \partial x, \text{ etc.}$$

Let us use the notation

$$\mathbf{P} = \mathbf{p} - (e/c)\mathbf{A}.$$

Then

$$v_x = \partial\mathcal{H} / \partial p_x = \partial E_0(\mathbf{P}) / \partial p_x = \partial E_0(\mathbf{P}) / \partial P_x,$$

or

$$\mathbf{v} = \nabla_{\mathbf{P}} E_0(\mathbf{P}). \quad (16)$$

The other canonical equation gives

$$\begin{aligned} \frac{dp_x}{dt} &= -\frac{\partial}{\partial x} \left[E_0(\mathbf{P}) + e\varphi \right] \\ &= -e \frac{\partial \varphi}{\partial x} - \left(\frac{\partial E_0}{\partial P_x} \frac{\partial P_x}{\partial x} + \frac{\partial E_0}{\partial P_y} \frac{\partial P_y}{\partial x} + \frac{\partial E_0}{\partial P_z} \frac{\partial P_z}{\partial x} \right) \\ &= -e \frac{\partial \varphi}{\partial x} + \frac{e}{c} \left(v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_y}{\partial x} + v_z \frac{\partial A_z}{\partial x} \right). \end{aligned}$$

From this we can construct the equation of motion

for P_x :

$$\begin{aligned} \frac{dP_x}{dt} &= \frac{d\dot{p}_x}{dt} - \frac{e}{c} \frac{dA_x}{dt} \\ &= \frac{d\dot{p}_x}{dt} - \frac{e}{c} \left(\frac{\partial A_x}{\partial t} + \frac{\partial A_x}{\partial x} v_x + \frac{\partial A_x}{\partial y} v_y + \frac{\partial A_x}{\partial z} v_z \right) \\ &= e \left[-\frac{\partial \varphi}{\partial x} - \frac{1}{c} \frac{\partial A_x}{\partial t} + \frac{1}{c} \left(v_y \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \right. \right. \\ &\quad \left. \left. - v_z \left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) \right) \right]. \end{aligned}$$

Using the defining equations for the electric and magnetic fields

$$\begin{aligned} \mathbf{E} &= -\nabla\varphi - (1/c)\partial\mathbf{A}/\partial t \\ \mathbf{H} &= \nabla \times \mathbf{A}, \end{aligned}$$

we obtain

$$dP_x/dt = e[E_x + (1/c)(\mathbf{v} \times \mathbf{H})_x]$$

of finally,

$$d\mathbf{P}/dt = e[\mathbf{E} + (1/c)(\mathbf{v} \times \mathbf{H})]. \quad (17)$$

Equations (16) and (17) are actually well known,⁹ though the derivations previously given differ considerably from the one presented here.

In conclusion I should like to express my warmest thanks to Professor R. G. Sachs and to Professor J. Powell for many stimulating and helpful discussions.

APPENDIX I

We must construct the gradient of G_m .

$$\begin{aligned} \nabla G_m &= \int_0^1 d\lambda \nabla [(\mathbf{r} - \mathbf{Q}_m) \cdot \mathbf{A}(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m))] \\ &= \int_0^1 d\lambda [(\mathbf{r} - \mathbf{Q}_m) \times (\nabla \times \mathbf{A}) + \mathbf{A} \times (\nabla \times (\mathbf{r} - \mathbf{Q}_m)) \\ &\quad + (\mathbf{A} \cdot \nabla)(\mathbf{r} - \mathbf{Q}_m) + ((\mathbf{r} - \mathbf{Q}_m) \cdot \nabla)\mathbf{A}], \end{aligned}$$

by a well-known expansion in vector analysis. Using

$$\begin{aligned} \nabla \times \mathbf{A}[\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)] &= \lambda \mathbf{H}[\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)] \\ \nabla \times \mathbf{r} &= 0, \quad (\mathbf{A} \cdot \nabla)\mathbf{r} = \mathbf{A}, \end{aligned}$$

we get

$$\nabla G_m = \int_0^1 d\lambda [\lambda(\mathbf{r} - \mathbf{Q}_m) \times \mathbf{H} + \mathbf{A} + ((\mathbf{r} - \mathbf{Q}_m) \cdot \nabla)\mathbf{A}].$$

⁹ A. H. Wilson, *Theory of Metals* (Cambridge University Press, London, 1935), p. 61 ff., and W. Shockley, *Electrons and Holes in Semi-Conductors* (D. Van Nostrand Company, Inc., New York, 1950), p. 424 ff. The form in which we have given these equations is that of Shockley, who makes extensive application of them in the theory of semiconductors. A discussion of the range of validity of these equations is also to be found in Shockley's book.

However, integrating by parts gives

$$\begin{aligned} \int_0^1 A(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)) d\lambda &= \lambda A(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)) \Big|_0^1 \\ &\quad - \int_0^1 d\lambda \cdot \lambda \cdot \frac{d}{d\lambda} A(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)) \\ &= A(\mathbf{r}) - \int_0^1 d\lambda ((\mathbf{r} - \mathbf{Q}_m) \cdot \nabla) A. \end{aligned}$$

Inserting this in our original expression we obtain

$$\nabla G_m = A(\mathbf{r}) + \int_0^1 d\lambda \cdot \lambda \cdot (\mathbf{r} - \mathbf{Q}_m) \times \mathbf{H}(\mathbf{Q}_m + \lambda(\mathbf{r} - \mathbf{Q}_m)),$$

which is the required result.

APPENDIX II

We wish to establish the identity¹⁰

$$\begin{aligned} \exp\{-\mathbf{Q} \cdot (\nabla - (ie/\hbar c)\mathbf{A})\} \\ = \exp\left\{ (ie/\hbar c) \int_0^1 d\lambda \mathbf{Q} \cdot \mathbf{A}(\mathbf{r} - \lambda \mathbf{Q}) \right\} \exp\{-\mathbf{Q} \cdot \nabla\}. \end{aligned}$$

To do this, let us define an operator $F(\eta)$ as follows:

$$F(\eta) = \exp\left\{ (ie/\hbar c) \int_0^\eta d\lambda \mathbf{Q} \cdot \mathbf{A}(\mathbf{r} - \lambda \mathbf{Q}) \right\} \exp\{-\eta \mathbf{Q} \cdot \nabla\}.$$

Then

$$\begin{aligned} dF/d\eta &= \exp\left\{ (ie/\hbar c) \int_0^\eta d\lambda \mathbf{Q} \cdot \mathbf{A}(\mathbf{r} - \lambda \mathbf{Q}) \right\} \\ &\quad \times [(ie/\hbar c)\mathbf{Q} \cdot \mathbf{A}(\mathbf{r} - \lambda \mathbf{Q})] \exp\{-\eta \mathbf{Q} \cdot \nabla\} \\ &\quad + \exp\left\{ (ie/\hbar c) \int_0^\eta \mathbf{Q} \cdot \mathbf{A}(\mathbf{r} - \lambda \mathbf{Q}) d\lambda \right\} \\ &\quad \times \exp\{-\eta \mathbf{Q} \cdot \nabla\} (-\mathbf{Q} \cdot \nabla). \end{aligned}$$

But

$$\begin{aligned} (ie/\hbar c)\mathbf{Q} \cdot \mathbf{A}(\mathbf{r} - \eta \mathbf{Q}) \exp\{\eta \mathbf{Q} \cdot \nabla\} \\ = \exp\{-\eta \mathbf{Q} \cdot \nabla\} (ie/\hbar c)\mathbf{Q} \cdot \mathbf{A}(\mathbf{r}), \end{aligned}$$

since $\exp\{-\eta \mathbf{Q} \cdot \nabla\}$ is just the displacement operator for the displacement $-\eta \mathbf{Q}$. Therefore, we obtain

$$\begin{aligned} dF/d\eta &= F(\eta)[- \mathbf{Q} \cdot \nabla + (ie/\hbar c)\mathbf{Q} \cdot \mathbf{A}(\mathbf{r})] \\ &= F(\eta)[- \mathbf{Q} \cdot (\nabla - (ie/\hbar c)\mathbf{A})]. \end{aligned}$$

This is a differential equation for $F(\eta)$, and may be integrated at once, giving

$$F(\eta) = \exp\{-\eta \mathbf{Q} \cdot (\nabla - (ie/\hbar c)\mathbf{A})\}$$

(the constant of integration being fixed by the condition $F(0) = 1$, which follows from the original definition of F). If we set $\eta = 1$ in this expression we obtain the identity in question.

¹⁰ This identity is given in a slightly different form, and with an entirely different proof in R. G. Sachs, *Phys. Rev.* **74**, 433 (1948), Sec. IV.