16

States of lowest energy: dynamics

As for classical dynamics, in many applications the external potentials have a slow variation in space-time. The standard procedure is then to ignore the quantized Maxwell field and to proceed with an effective one-particle Hamiltonian. This is justified since the photons very rapidly adjust to the motion of the electron. To put it differently, if a classical trajectory of the electron is prescribed, then the photons are governed by a Hamiltonian of slow time-dependence and essentially remain in their momentarily lowest state of energy. We propose first to study slow time variation, which abstractly falls under the auspices of the time-adiabatic theorem. However, the real issue is how, from the slow variation in space, to extract, rather than assume, the slow variation in time. It seems appropriate to call such a situation *space*-adiabatic.

We will work for a start with time-dependent perturbation theory using the insights gained from the time-adiabatic theorem. It turns out that these methods lead us astray in the case of slowly varying external vector potentials. Thus we are forced to develop more powerful techniques. They come from the area of pseudo-differential operators. In fact this theory provides a much sharper picture of adiabatic decoupling and a systematic scheme for computing effective Hamiltonians. To avoid technical complications we restrict ourselves to matrix-valued symbols. Transcribing these results formally to the Pauli–Fierz Hamiltonian we will compute the effective Hamiltonian governing the motion of the electron in the band of lowest energy, including spin precession. The effective Hamiltonian can be analysed through semiclassical methods which eventually leads to the nonperturbative definition of the gyromagnetic ratio.

There are other properties of the Pauli–Fierz Hamiltonian which can be handled semiclassically. Most notably we may consider a physical situation, where classical currents are prescribed. Then the Pauli–Fierz operator reduces to a time-dependent operator on Fock space quadratic in the bosonic annihilation/creation operators. Such quasi-free theories can be studied in great detail. In particular,

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coherent states of the photon field evolve in time according to the classical inhomogeneous Maxwell equations. Under standard macroscopic conditions field fluctuations are small and the classical Maxwell theory can be used safely. For example, a city radio station with a power of 100 kW at a wavelength of 100 m emits 10^{30} photons per second, and at a distance of 100 km a flux of 10^{15} photons s^{-1} cm^{-2} is still observed. On the other hand, experimentally even the smallest field intensities can be controlled and quantum features are of importance, as for example in photon counting statistics. For the Maxwell field an amazingly wide span of scales can be probed, from the classical deterministic behavior down to single-photon randomness.

16.1 The time-adiabatic theorem

In the case where no external forces are present, the total momentum is conserved; compare with sections 13.5 and 15.2. Thus under slowly varying external potentials the total momentum can be expected to change slowly, and the appropriate starting point is the Pauli–Fierz Hamiltonian in the representation diagonal with respect to the total momentum, i.e.

$$H = \frac{1}{2m}\big(\sigma \cdot (p - P_{\mathrm{f}} - eA_{\varphi} - eA_{\mathrm{ex}}(\varepsilon x))\big)^2 + e\phi_{\mathrm{ex}}(\varepsilon x) + H_{\mathrm{f}}. \tag{16.1}$$

Here p refers to the total momentum and ε is a dimensionless parameter regulating the variation of the external potentials ϕ_{ex}, A_{ex}. Let us assume for the moment that a classical trajectory of the electron is given. Because of the slow variation of ϕ_{ex}, A_{ex} it has to be of the form $(q_{\varepsilon t}, p_{\varepsilon t})$, $0 \le t \le \varepsilon^{-1}\tau$ with $(\varepsilon q_{\varepsilon t}, p_{\varepsilon t})$ of order 1. Inserting in (16.1), the time-dependent Hamiltonian can be written as

$$\begin{aligned} H(\varepsilon t) = {} & \frac{1}{2m}\big(p_{\varepsilon t} - P_{\mathrm{f}} - eA_{\varphi} - eA_{\mathrm{ex}}(\varepsilon q_{\varepsilon t})\big)^2 - \frac{e}{2m}\sigma \cdot (B_{\varphi} + \varepsilon B_{\mathrm{ex}}(\varepsilon q_{\varepsilon t})) \\ & + e\phi_{\mathrm{ex}}(\varepsilon q_{\varepsilon t}), \end{aligned} \tag{16.2}$$

which governs the motion of photons and acts on $\mathcal{F}$. t is measured in atomic units. $B_{\varphi} = B_{\varphi}(0)$ is the quantized magnetic field. We have already studied the spectrum of $H(t)$ for fixed t. The term proportional to B_{ex} is of order ε and can be neglected. Provided $|p_t| < p_{\mathrm{c}}$, $H(t)$ has a two-fold degenerate ground state with energy

$$E(t) = E(p_t - eA_{\mathrm{ex}}(\varepsilon q_t)) + e\phi_{\mathrm{ex}}(\varepsilon q_t). \tag{16.3}$$

Physically it is expected that through radiation the photons approach very rapidly a state of lowest energy. Subsequently only very few photons escape, since the time variation is slow and $E(t)$ is separated by a gap from the continuous spectrum.

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The time-adiabatic theorem of quantum mechanics makes an abstraction of the particular situation and simply postulates the time-dependent Hamiltonian $H(t)$ as given and acting on the Hilbert space $\mathcal{H}$. The role of the ground state subspace is played by a physically distinguished, "relevant" subspace with corresponding instantaneous spectral projection $P(t)$ and energy $E(t)$, i.e. $H(t)P(t) = E(t)P(t)$. It is assumed that for every t the energy $E(t)$ is isolated by a finite gap from the rest of the spectrum of $H(t)$. The slow variation in time is introduced through $H(\varepsilon t)$ with $\varepsilon \ll 1$ as a dimensionless adiabaticity parameter and one is interested in the solution of the Schrödinger equation

$$\mathrm{i}\partial_t \psi(t) = H(\varepsilon t)\psi(t), \tag{16.4}$$

where the initial wave function $\psi(0)$ is assumed to lie already in the relevant subspace, $P(0)\psi(0) = \psi(0)$. t is chosen to be so long that $P(t)$ rotates by some finite amount, implying that

$$0 \leq t \leq \varepsilon^{-1}\tau, \quad \tau = \mathcal{O}(1). \tag{16.5}$$

Sometimes it is convenient to switch to the slow time scale

$$t' = \varepsilon t. \tag{16.6}$$

Then our problem becomes

$$\mathrm{i}\varepsilon\partial_{t'}\psi(t') = H(t')\psi(t'), \quad P(0)\psi(0) = \psi(0), \quad 0 \leq t' \leq \tau. \tag{16.7}$$

To stress the similarity with the space-adiabatic situation, however, we stick to the fast time scale of (16.4).

As one of the basic results it is established that the subspace $P(\varepsilon t)$ is adiabatically protected in the sense that

$$\|(1 - P(\varepsilon t))\psi(t)\| \leq c_0\varepsilon \quad \text{for} \quad 0 \leq t \leq \varepsilon^{-1}\tau \tag{16.8}$$

with some suitable constant c_0. Up to an error of order ε the solution to the Schrödinger equation (16.4) clings to the relevant subspace $P(\varepsilon t)\mathcal{H}$.

It is of interest briefly to recall the proof of (16.8), since some central elements will reappear later. We denote the unitary propagator for (16.4) by $U^\varepsilon(t, s)$. The idea is to define a "diagonal" propagator $U^\varepsilon_{\mathrm{dg}}(t, s)$ such that it preserves $P(t)$ exactly, i.e.

$$P(\varepsilon t)U^\varepsilon_{\mathrm{dg}}(t, s) = U^\varepsilon_{\mathrm{dg}}(t, s)P(\varepsilon s). \tag{16.9}$$

The unitary propagator $U^\varepsilon_{\mathrm{dg}}(t, s)$ is generated by the Hamiltonian $H_{\mathrm{dg}}(\varepsilon t)$. From (16.9) it follows that

$$[H_{\mathrm{dg}}(\varepsilon t), P(\varepsilon t)] = \mathrm{i}\varepsilon\dot{P}(\varepsilon t). \tag{16.10}$$

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We look for a solution which is ε-close to $H(\varepsilon t)$. Using the identities $P(t)\dot{P}(t)P(t) = 0$, $(1 - P(t))\dot{P}(t)(1 - P(t)) = 0$, we obtain

$$H_{\mathrm{dg}}(\varepsilon t) = H(\varepsilon t) + \mathrm{i}\varepsilon[\dot{P}(\varepsilon t), P(\varepsilon t)]. \tag{16.11}$$

To prove (16.8) one thus has to estimate the difference

$$U^{\varepsilon}(t, 0) - U^{\varepsilon}_{\mathrm{dg}}(t, 0) = -\varepsilon \int_0^t \mathrm{d}s U^{\varepsilon}(t, s)[\dot{P}(\varepsilon s), P(\varepsilon s)]U^{\varepsilon}_{\mathrm{dg}}(s, 0). \tag{16.12}$$

While $H(\varepsilon t) - H_{\mathrm{dg}}(\varepsilon t)$ is of order ε, this is not good enough, since errors might add up over the long times $\varepsilon^{-1}\tau$. To make progress we note that $P[\dot{P}, P]P = 0 = (1 - P)[\dot{P}, P](1 - P)$, whereas $P[\dot{P}, P](1 - P) \neq 0$. Thus to improve on (16.12) one has to exploit the time averaging, which is most easily achieved by writing $[\dot{P}, P]$ as a time derivative. Let us assume for a moment that the commutator equation

$$[H(t), X(t)] = [\dot{P}(t), P(t)] \tag{16.13}$$

has a bounded solution $X(t)$. Then, using again (16.11),

$$\begin{aligned}
&U^{\varepsilon}(\varepsilon^{-1}\tau, 0) - U^{\varepsilon}_{\mathrm{dg}}(\varepsilon^{-1}\tau, 0) \qquad (16.14)\\
&= -\varepsilon\int_0^{\varepsilon^{-1}\tau} \mathrm{d}s U^{\varepsilon}(\varepsilon^{-1}\tau, s)\big(H(\varepsilon s)X(\varepsilon s) - X(\varepsilon s)H_{\mathrm{dg}}(\varepsilon s)\big)U^{\varepsilon}_{\mathrm{dg}}(s, 0) + \mathcal{O}(\varepsilon)\\
&= \mathrm{i}\varepsilon\int_0^{\varepsilon^{-1}\tau} \mathrm{d}s\Big(\frac{\mathrm{d}}{\mathrm{d}s}U^{\varepsilon}(\varepsilon^{-1}\tau, s)X(\varepsilon s)U^{\varepsilon}_{\mathrm{dg}}(s, 0) - U^{\varepsilon}(\varepsilon^{-1}\tau, s)X(\varepsilon s)\frac{\mathrm{d}}{\mathrm{d}s}U^{\varepsilon}_{\mathrm{dg}}(s, 0)\Big)\\
&\quad + \mathcal{O}(\varepsilon)\\
&= \mathrm{i}\varepsilon\int_0^{\varepsilon^{-1}\tau} \mathrm{d}s\Big(\frac{\mathrm{d}}{\mathrm{d}s}\big(U^{\varepsilon}(\varepsilon^{-1}\tau, s)X(\varepsilon s)U^{\varepsilon}_{\mathrm{dg}}(s, 0)\big) - U^{\varepsilon}(\varepsilon^{-1}\tau, 0)\varepsilon\dot{X}(\varepsilon s)U^{\varepsilon}_{\mathrm{dg}}(s, 0)\Big)\\
&\quad + \mathcal{O}(\varepsilon),
\end{aligned}$$

which implies

$$\|U^{\varepsilon}(\varepsilon^{-1}\tau, 0) - U^{\varepsilon}_{\mathrm{dg}}(\varepsilon^{-1}\tau, 0)\| \leq c_0(1 + \tau)\varepsilon. \tag{16.15}$$

The adiabatic theorem (16.8) follows from

$$\begin{aligned}
\|(1 - P(\tau))U^{\varepsilon}(\varepsilon^{-1}\tau, 0)P(0)\psi\| &= \|(1 - P(\tau))U^{\varepsilon}_{\mathrm{dg}}(\varepsilon^{-1}\tau, 0)P(0)\psi\| + \mathcal{O}(\varepsilon)\\
&= \|(1 - P(\tau))P(\tau)U^{\varepsilon}_{\mathrm{dg}}(\varepsilon^{-1}\tau, 0)\psi\| + \mathcal{O}(\varepsilon)\\
&= \mathcal{O}(\varepsilon), \qquad (16.16)
\end{aligned}$$

where (16.9) has been used.

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It remains to see whether the commutator equation (16.13) has a solution. Because of the spectral gap we may set

$$X = P\dot{P}(1-P)(H-E)^{-1} + (H-E)^{-1}(1-P)\dot{P}P \tag{16.17}$$

and verify (16.13) directly. In particular, $\|X(t)\| \leq g^{-1}\|\dot{P}(t)\|$, with g the width of the gap and $\|\dot{X}(t)\| \leq 3g^{-2}\|\dot{H}(t)\|\|\dot{P}(t)\|$.

While undoubtedly correct the estimate (16.8) does not specify the origin of the error. As we will explain below the order ε is not due to dispersion into all of $\mathcal{H}$. Rather the true solution $\psi(t)$ is slightly tilted out of the subspace $P(\varepsilon t)\mathcal{H}$. If this effect is properly taken into account, the error in (16.8) can be made smaller than any given power ε^n at the expense of adjusting the projection $P(t)$ to the slightly tilted projection $P^\varepsilon(t)$. The second missing aspect is more of a computational nature. Since $(1-P^\varepsilon(t))\mathcal{H}$ is in essence decoupled from the relevant subspace, one would like to have an, in our case time-dependent, effective Hamiltonian governing the solution in the subspace $P^\varepsilon(t)\mathcal{H}$, at least approximately. We will return to this point below.

16.2 The space-adiabatic limit

With these preparations done we return to the Pauli–Fierz model with the slowly varying electrostatic potential $V(\varepsilon x) = e\phi_{\mathrm{ex}}(\varepsilon x)$,

$$H = \frac{1}{2m}(p - P_{\mathrm{f}} - eA_\varphi)^2 + H_{\mathrm{f}} + V(\varepsilon x) = H_0 + V(\varepsilon x). \tag{16.18}$$

The case of a slowly varying vector potential will be discussed in section 16.6. Spin is omitted only for notational simplicity. H acts on $L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes \mathcal{F}$. For the wave functions it is convenient to use the momentum representation $\psi(k, \underline{k})$, also for the electron, with the shorthand $\underline{k} = (k_1, \lambda_1, \ldots, k_n, \lambda_n)$, n arbitrary, $\psi(k, \emptyset) = \psi(k) \otimes \Omega$. H_0 then has the direct integral decomposition

$$H_0 = \int^{\oplus} \mathrm{d}^3k\, H_0(k). \tag{16.19}$$

We assume a small photon mass and the validity of claim 15.4. Then, for every k, $|k| < p_{\mathrm{c}}$, $H_0(k)$ has a unique ground state ψ_{g}, $H_0(k)\psi_{\mathrm{g}}(k, \underline{k}) = E(k)\psi_{\mathrm{g}}(k, \underline{k})$. Since in the momentum representation $H_0(k)$ is a real operator, the phase of $\psi_{\mathrm{g}}(k)$ can be chosen such that the wave function is real. In particular, using $\langle \psi_{\mathrm{g}}(k), \psi_{\mathrm{g}}(k)\rangle_{\mathcal{F}} = 1$, this implies $\langle \psi_{\mathrm{g}}(k), \nabla_k \psi_{\mathrm{g}}(k)\rangle_{\mathcal{F}} = 0$. $E(k)$ is separated by a finite gap from the continuum edge $E_{\mathrm{c}}(k)$. Since our aim is to demonstrate the basic principle, we deliberately ignore the fact that the ground state band exists only up to p_{c} and continue as if $p_{\mathrm{c}} = \infty$. At the cost of a suitable restriction on

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the initial state, the assumption $p_c = \infty$ can be avoided. We refer to the Notes at the end of the chapter for further explanations.

The ground state band is the subspace of wave functions of the form $\widehat{f}(k)\psi_g(k, \underline{k})$, and the corresponding projection is denoted by P_g. $P_g\mathcal{H}$ is invariant under e^{-iH_0t}, $[H_0, P_g] = 0$, and

$$(e^{-iH_0t}\,\widehat{f}\psi_g)(k, \underline{k}) = \big(e^{-iE(k)t}\,\widehat{f}(k)\big)\psi_g(k, \underline{k}). \tag{16.20}$$

Thus wave functions in the ground state band propagate according to a free quantum evolution with the effective energy–momentum relation $E(k)$.

If the slowly varying potential is turned on, the subspace $P_g\mathcal{H}$ is no longer invariant. The in-band dynamics is modified and there are transitions to excited states. For times which are not too long their effect remains negligible and one expects that

$$(e^{-iHt}\,\widehat{f}\psi_g)(k, \underline{k}) = \big(e^{-iH_{\rm eff}t}\,\widehat{f}(k)\big)\psi_g(k, \underline{k}) + \mathcal{O}(\varepsilon), \quad 0 \le t \le \varepsilon^{-1}\tau, \tag{16.21}$$

where, as for the time-adiabatic theorem, the time scale is determined by the condition that the electron should feel the presence of the potential V. The effective one-particle Hamiltonian, $H_{\rm eff}$, is defined through the *Peierls substitution*

$$H_{\rm eff} = E(p) + V(\varepsilon x). \tag{16.22}$$

Coupling to the Maxwell field renormalizes the kinetic energy of the quantum particle. In particular, for small velocities we have

$$H_{\rm eff} = \frac{1}{2m_{\rm eff}}p^2 + V(\varepsilon x). \tag{16.23}$$

The mass is renormalized, but the coupling to the electrostatic potential is still given by the bare charge e.

Let us now argue with some care that the Peierls substitution gives the correct time evolution in the ground state band. The Hamiltonian is the one specified in (16.18) and the relevant subspace is the ground state band $P_g\mathcal{H}$. In particular, initially $P_g\psi(0) = \psi(0)$. By construction, $[H_0, P_g] = 0$ and one has to understand the transitions between $P_g\mathcal{H}$ and $(1 - P_g)\mathcal{H} = Q_g\mathcal{H}$ induced by $V(\varepsilon x)$. For this purpose we decompose into a diagonal and an off-diagonal piece as

$$\begin{aligned} &V = V_{\rm dg} + V_{\rm od}, \\ &V_{\rm dg} = P_gVP_g + Q_gVQ_g\,, \quad V_{\rm od} = P_gVQ_g + Q_gVP_g. \end{aligned} \tag{16.24}$$

It should be recalled that the time evolution must be controlled over the time span $\varepsilon^{-1}\tau$, $\tau = \mathcal{O}(1)$. Thus only terms of order ε^2 can be ignored safely.

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We consider first $P_{\mathrm{g}} V P_{\mathrm{g}}$, which in the ground state band acts as

$$(P_{\mathrm{g}} V P_{\mathrm{g}} \psi)(k, \underline{k}) = \int \mathrm{d}^3 k' \widehat{V}(k') \widehat{f}(k - \varepsilon k') \langle \psi_{\mathrm{g}}(k), \psi_{\mathrm{g}}(k - \varepsilon k') \rangle_{\mathcal{F}} \psi_{\mathrm{g}}(k, \underline{k}) \tag{16.25}$$

with $\widehat{f}(k) = \langle \psi_{\mathrm{g}}(k), \psi(k) \rangle_{\mathcal{F}}$. The Peierls substitution amounts to $V(\varepsilon P_{\mathrm{g}} x P_{\mathrm{g}})$, since

$$P_{\mathrm{g}} x P_{\mathrm{g}} \psi(k, \underline{k}) = \mathrm{i} \nabla_k \widehat{f}(k) \psi_{\mathrm{g}}(k, \underline{k}) + \mathrm{i} \widehat{f}(k) \langle \psi_{\mathrm{g}}(k), \nabla_k \psi_{\mathrm{g}}(k) \rangle_{\mathcal{F}} \psi_{\mathrm{g}}(k, \underline{k}) \tag{16.26}$$

with the second term vanishing by the argument given above. The difference is estimated as

$$\begin{aligned} &\big(P_{\mathrm{g}} V(\varepsilon x) P_{\mathrm{g}} - V(\varepsilon P_{\mathrm{g}} x P_{\mathrm{g}})\big) \psi(k, \underline{k}) \\ &\quad = \int \mathrm{d}^3 k' \widehat{V}(k') \widehat{f}(k - \varepsilon k') \big(\langle \psi_{\mathrm{g}}(k), \psi_{\mathrm{g}}(k - \varepsilon k') \rangle_{\mathcal{F}} - 1 \big) \psi_{\mathrm{g}}(k, \underline{k}). \end{aligned} \tag{16.27}$$

In the Taylor expansion, the first order vanishes, since $\langle \psi_{\mathrm{g}}(k), \nabla_k \psi_{\mathrm{g}}(k) \rangle_{\mathcal{F}} = 0$ as before, and the error is $\mathcal{O}(\varepsilon^2)$. Thus we are left with showing that V_{od} acts as a small perturbation only.

Since $H_0(k) = \frac{1}{2m}(k - P_{\mathrm{f}} - eA_\varphi)^2 + H_{\mathrm{f}}$, one has $\nabla_k H_0(k) = \frac{1}{m}(k - P_{\mathrm{f}} - eA_\varphi)$ and, with $P(k)$ denoting the projection onto $\psi_{\mathrm{g}}(k)$, then $P_{\mathrm{g}} = \int^{\oplus} \mathrm{d}^3 k P(k)$, $Q(k) = 1 - P(k)$, and $Q_{\mathrm{g}} = 1 - P_{\mathrm{g}}$. If clear from the context, the variable "$\underline{k}$" will be dropped. With these conventions

$$\begin{aligned} V(\varepsilon x) P_{\mathrm{g}} \psi(k) &= \int \mathrm{d}^3 k' \widehat{V}(k') P(k - \varepsilon k') \psi(k - \varepsilon k') \\ &= \int \mathrm{d}^3 k' \widehat{V}(k') P(k) \psi(k - \varepsilon k') \\ &\quad - \varepsilon \int \mathrm{d}^3 k' \widehat{V}(k') k' \cdot \nabla_k P(k) \psi(k - \varepsilon k') + \mathcal{O}(\varepsilon^2). \end{aligned} \tag{16.28}$$

By first-order perturbation theory

$$\nabla_k P(k) = -Q(k)(H_0(k) - E(k))^{-1} \nabla_k H_0(k) P(k) + \mathrm{h.c.}, \tag{16.29}$$

h.c. denoting the Hermitian conjugate. Therefore

$$Q_{\mathrm{g}} V(\varepsilon x) P_{\mathrm{g}} = -\mathrm{i}\varepsilon Q_{\mathrm{g}} \nabla P_{\mathrm{g}} \cdot F(\varepsilon x) + \mathcal{O}(\varepsilon^2) \tag{16.30}$$

with the shorthand $\nabla P_{\mathrm{g}} = \int^{\oplus} \mathrm{d}^3 k \nabla_k P(k)$ and the force $F(x) = -\nabla V(x)$.

The approximate time evolution is generated by

$$H_{\mathrm{dg}} = H_0 + V_{\mathrm{dg}}, \quad U_{\mathrm{dg}}(t) = \mathrm{e}^{-\mathrm{i} H_{\mathrm{dg}} t}, \tag{16.31}$$

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and our goal is to compare it with the full time evolution $\mathrm{e}^{-\mathrm{i}Ht} = U(t)$ over times of order ε^{-1}, i.e. to estimate the difference

$$U(\varepsilon^{-1}t) - U_{\mathrm{dg}}(\varepsilon^{-1}t) = -\mathrm{i}\int_0^{t/\varepsilon} \mathrm{d}s\, U(\varepsilon^{-1}t - s) V_{\mathrm{od}} U_{\mathrm{dg}}(s) \tag{16.32}$$

with $t = \mathcal{O}(1)$.

At this point we have arrived at a structure very similar to the time-adiabatic difference (16.14). $V_{\mathrm{od}} = \mathcal{O}(\varepsilon)$ and time averaging must be used. As before, the trick is to write V_{od} as a time derivate, i.e. as a commutator with H_0, up to unavoidable errors of order ε^2. We set

$$B(k) = -Q(k)(H_0(k) - E(k))^{-2}\nabla_k H_0(k) P(k). \tag{16.33}$$

Then

$$Q(k)\nabla_k P(k) = -[H_0(k), B(k)]. \tag{16.34}$$

With the shorthand $B = \int^{\oplus} \mathrm{d}^3k\, B(k)$ one has

$$Q_{\mathrm{g}}\nabla P_{\mathrm{g}} \cdot F = [H_0, B]\cdot F = [H_0, B\cdot F] - B\cdot[H_0, F] = [H_0, B\cdot F] + \mathcal{O}(\varepsilon), \tag{16.35}$$

since $[H_0, F] = \frac{1}{m}(p - P_{\mathrm{f}} - eA_\varphi)\cdot[p, F] +$ h.c. and $[p, F] = -\mathrm{i}\varepsilon\nabla_x F(\varepsilon x)$. It remains to substitute H_{dg} for H_0. One has $[V_{\mathrm{dg}}, B] = Q_{\mathrm{g}}[V, B]P_{\mathrm{g}}$. Since $B = \int^{\oplus} \mathrm{d}^3k\, B(k)$ and $V = V(\mathrm{i}\varepsilon\nabla_k)$, the commutator is of order ε, hence

$$Q_{\mathrm{g}}\nabla P_{\mathrm{g}} \cdot F = [H_{\mathrm{dg}}, B\cdot F] + \mathcal{O}(\varepsilon). \tag{16.36}$$

On inserting in (16.32), we get

$$\begin{aligned}
U(\varepsilon^{-1}t) - U_{\mathrm{dg}}(\varepsilon^{-1}t) &= -\varepsilon\int_0^{t/\varepsilon} \mathrm{d}s\, U(\varepsilon^{-1}t - s)[H_{\mathrm{dg}}, B\cdot F + F\cdot B^*]U_{\mathrm{dg}}(s) \\
&\quad + \mathcal{O}(\varepsilon) \\
&= -\varepsilon\int_0^{t/\varepsilon} \mathrm{d}s\, U(\varepsilon^{-1}t - s)U_{\mathrm{dg}}(s)U_{\mathrm{dg}}(-s)[H_{\mathrm{dg}}, B\cdot F + F\cdot B^*]U_{\mathrm{dg}}(s) + \mathcal{O}(\varepsilon) \\
&= \mathrm{i}\varepsilon\int_0^{t/\varepsilon} \mathrm{d}s\, U(\varepsilon^{-1}t - s)U_{\mathrm{dg}}(s)\frac{\mathrm{d}}{\mathrm{d}s}(B\cdot F + F\cdot B^*)(s) + \mathcal{O}(\varepsilon) \\
&= \mathrm{i}\varepsilon(B\cdot F + F\cdot B^*)U_{\mathrm{dg}}(\varepsilon^{-1}t) - \mathrm{i}\varepsilon U(\varepsilon^{-1}t)(B\cdot F + F\cdot B^*) \\
&\quad - \mathrm{i}\varepsilon\int_0^{t/\varepsilon} \mathrm{d}s\Big(\frac{\mathrm{d}}{\mathrm{d}s}U(\varepsilon^{-1}t - s)U_{\mathrm{dg}}(s)\Big)(B\cdot F + F\cdot B^*)(s) + \mathcal{O}(\varepsilon) \\
&= \mathcal{O}(\varepsilon),
\end{aligned} \tag{16.37}$$

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since $\frac{\mathrm{d}}{\mathrm{d}s}U(-s)U_{\mathrm{dg}}(s) = \mathrm{i}U(-s)V_{\mathrm{od}}U_{\mathrm{dg}}(s) = \mathcal{O}(\varepsilon)$ by (16.30). As in the time-adiabatic setting the leakage out of the ground state subspace $P_{\mathrm{g}}\mathcal{H}$ is $\mathcal{O}(\varepsilon)$ for times of order ε^{-1}. In addition we have identified the effective Hamiltonian (16.22) which approximately governs the time evolution inside $P_{\mathrm{g}}\mathcal{H}$.

16.3 Matrix-valued symbols

If in (16.18) a slowly varying vector potential is added through minimal coupling, then even on a formal level the argument of the previous section breaks down. The reason is that the ground state subspace $P_{\mathrm{g}}\mathcal{H}$ is no longer even approximately invariant under the time evolution. There is another subspace to take its role, but it has to be computed rather than guessed. We immediately consider the general case (16.1) and switch to the macroscopic space scale through the substitution x for εx. Then the Hamiltonian under study is

$$H = \frac{1}{2m}\big(-\mathrm{i}\varepsilon\nabla_x - P_{\mathrm{f}} - eA_\varphi - eA_{\mathrm{ex}}(x)\big)^2 - \frac{e}{2m}\sigma\cdot(B_\varphi + \varepsilon B_{\mathrm{ex}}(x)) + e\phi_{\mathrm{ex}}(x) + H_{\mathrm{f}}. \tag{16.38}$$

As before, $-\mathrm{i}\nabla_x$ refers to the total momentum, $A_\varphi = A_\varphi(0)$, $B_\varphi = B_\varphi(0)$.

The first step is to mold (16.38) into the canonical space-adiabatic form. For this purpose we have to distinguish between the classical phase space variable (q, p) and the corresponding operators, which exclusively for the purpose of sections 16.3–16.5 are denoted by $\widehat{q} = x$, $\widehat{p} = -\mathrm{i}\varepsilon\nabla_x$. To the Hamiltonian (16.38) in the obvious way we associate the operator-valued function (= symbol)

$$\begin{aligned} H(q,p) &= H_0(q,p) + \varepsilon H_1(q,p),\\ H_0(q,p) &= \frac{1}{2m}\big(p - P_{\mathrm{f}} - eA_\varphi - eA_{\mathrm{ex}}(q)\big)^2 - \frac{e}{2m}\sigma\cdot B_\varphi + e\phi_{\mathrm{ex}}(q) + H_{\mathrm{f}},\\ H_1(q,p) &= -\frac{e}{2m}\sigma\cdot B_{\mathrm{ex}}(q). \end{aligned} \tag{16.39}$$

For fixed (q, p), $H(q, p)$ acts as an operator on $\mathbb{C}^2\otimes\mathcal{F}$, $\mathbb{C}^2$ standing for the spin degrees of freedom. H_0 is called the leading symbol and H_1 the subleading symbol for H because of the extra prefactor of ε in the first line of (16.39). To a symbol one associates an operator through the Weyl quantization, which can be thought of as a specific prescription for ordering x and $-\mathrm{i}\varepsilon\nabla_x$. To be general, let $A(q, p)$ be an operator-valued function with Fourier transform $\widetilde{A}(\eta, \xi)$,

$$A(q,p) = (2\pi)^{-3}\int \mathrm{d}^3\eta\mathrm{d}^3\xi\,\widetilde{A}(\eta,\xi)\mathrm{e}^{\mathrm{i}(\eta\cdot q+\xi\cdot p)}. \tag{16.40}$$

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The Weyl quantization of A is then simply

$$\mathcal{W}_\varepsilon(A) = (2\pi)^{-3} \int \mathrm{d}^3\eta \mathrm{d}^3\xi \, \widetilde{A}(\eta, \xi) \mathrm{e}^{\mathrm{i}(\eta\cdot\widehat{q}+\xi\cdot\widehat{p})}. \tag{16.41}$$

$A(q, p)$ is an operator-valued function and $\mathcal{W}_\varepsilon(A)$ is an operator on the large Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2 \otimes \mathcal{F}$. We will also use the notation

$$\mathcal{W}_\varepsilon(A) = A(\widehat{q}, \widehat{p}) = \widehat{A} \tag{16.42}$$

as a shorthand. Using the inverse Fourier transform in (16.40), $\mathcal{W}_\varepsilon(A)$ can be written in the form of an integral operator as

$$\mathcal{W}_\varepsilon(A)\psi(x) = (2\pi)^{-3} \int \mathrm{d}^3\xi \mathrm{d}^3 y A(\tfrac{1}{2}(x+y), \varepsilon\xi) \mathrm{e}^{\mathrm{i}\xi\cdot(x-y)} \psi(y). \tag{16.43}$$

Here A acts on $\psi(x)$ which is a $\mathbb{C}^2 \otimes \mathcal{F}$-valued wave function, $\psi \in L^2(\mathbb{R}^3, \mathbb{C}^2 \otimes \mathcal{F}) = L^2(\mathbb{R}^3) \otimes (\mathbb{C}^2 \otimes \mathcal{F}) = \mathcal{H}$, and $\mathcal{W}_\varepsilon(A)$ is an operator acting on $\mathcal{H}$. Note that $f(\widehat{q}) = f(x)$, $f(\widehat{p}) = f(-\mathrm{i}\varepsilon\nabla_x)$ as operators. Also $\mathcal{W}_\varepsilon(A)$ being Hermitian is equivalent to $A(q, p) = A(q, p)^*$ for all (q, p). For the Weyl quantization of $H(q, p)$ from (16.39) one obtains simply

$$H(\widehat{q}, \widehat{p}) = H, \tag{16.44}$$

as it should be. Thus the adiabatic evolution problem associated with (16.38) can be written as

$$\mathrm{i}\varepsilon \frac{\partial}{\partial t}\psi(x, t) = H(x, -\mathrm{i}\varepsilon\nabla_x)\psi(x, t) \tag{16.45}$$

with the Weyl rule for the ordering of operators. Consistent with the macroscopic space scale we switched also to macroscopic times through the substitution of t for εt. Equation (16.45) looks like a standard Schrödinger equation, apart from the fact that $\psi(x, t)$ takes values in $\mathbb{C}^2 \otimes \mathcal{F}$ and $H(q, p)$ acts as an operator on $\mathbb{C}^2 \otimes \mathcal{F}$.

$H_0(q, p)$ has a subspace of lowest energy with the corresponding projection denoted by $P(q, p)$. Deliberately ignoring $p_c < \infty$, from section 15.3 we know already that $\mathrm{tr}[P(q, p)] = 2$ and

$$H_0(q, p)P(q, p) = E(q, p)P(q, p) \tag{16.46}$$

with the eigenvalue

$$E(q, p) = E(p - eA_{\mathrm{ex}}(q)) + e\phi_{\mathrm{ex}}(q). \tag{16.47}$$

One would expect that the Peierls substitution $E(\widehat{q}, \widehat{p})$ somehow plays the role of the effective one-particle Hamiltonian. Note that this would leave spin precession

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still hidden and, in fact, it will appear as the ε-order correction to the Peierls substitution $E(\widehat{q}, \widehat{p})$.

At this stage, as for the time-adiabatic theorem, it is convenient to abstract from the specific origin of the space-adiabatic evolution (16.45). Thereby the general structure of space-adiabatic problems becomes visible with the bonus of wide applicability. For simplicity $\mathbb{C}^2 \otimes \mathcal{F}$ is replaced by $\mathbb{C}^n$ with n arbitrary. In fact, a finite-dimensional internal Hilbert space is not essential and only allows us to remain in familiar territory. We record that the Hamiltonian $H(q, p) = H_0(q, p) + \varepsilon H_1(q, p)$ is a matrix-valued function, assumed to be smooth in q, p. There is a relevant subspace of physical interest with energy band $E(q, p)$ of constant multiplicity ℓ. This means that $H_0(q, p)$ has the eigenprojection $P(q, p)$, $[H_0(q, p), P(q, p)] = 0$, with $\mathrm{tr}[P(q, p)] = \ell$, $1 \leq \ell < n$, such that

$$H_0(q, p)P(q, p) = E(q, p)P(q, p). \tag{16.48}$$

Most importantly, H_0 is assumed to have a spectral gap in the sense that

$$|E(q, p) - E_j(q, p)| \geq g > 0 \tag{16.49}$$

for all (q, p) and all other eigenvalues $E_j(q, p)$ of $H_0(q, p)$. As before, the space-adiabatic evolution is governed by

$$\mathrm{i}\varepsilon \frac{\partial}{\partial t}\psi(x, t) = H(\widehat{q}, \widehat{p})\psi(x, t) \tag{16.50}$$

with $\psi(x, t)$ an n-spinor, i.e. the Hilbert space for the Schrödinger equation (16.50) is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^n = \mathcal{H}$. Note that, if in (16.50) $H(\widehat{q}, \widehat{p})$ is replaced by $H(t)$, then (16.50) turns into its time-adiabatic cousin (16.7) where the role of the relevant projection $P(q, p)$ is taken over by $P(t)$.

The analysis of (16.50) will be carried out in such a way as to make use only of (16.48) and (16.49) with no further assumptions at all on the spectrum of $H_0(q, p)$ in the subspace orthogonal to $P(q, p)\mathbb{C}^n$. For this reason we are confident that the final result will apply also to the Pauli–Fierz Hamiltonian.

With the more general perspective gained, one can understand why the case $A_{\mathrm{ex}} = 0$ can be handled by more elementary means. In that case $H_0(q, p) = \frac{1}{2m}(p - P_{\mathrm{f}} - eA_\varphi)^2 + e\phi_{\mathrm{ex}}(q)$. Thus $P(q, p)$ depends only on p and $P(\widehat{q}, \widehat{p}) = P_{\mathrm{g}}$, the projection onto the ground state subspace. This suggests that also in the general case $P(\widehat{q}, \widehat{p})\mathcal{H}$ is the adiabatically decoupled subspace. Unfortunately $P(\widehat{q}, \widehat{p})^2 \neq P(\widehat{q}, \widehat{p})$, in general, although $P(q, p)^2 = P(q, p)$. On the other hand, as will be shown, $P(\widehat{q}, \widehat{p})(1 - P(\widehat{q}, \widehat{p})) = \mathcal{O}(\varepsilon)$. Since $P(\widehat{q}, \widehat{p})$ is Hermitian, its spectrum is of order ε concentrated near 0 and 1. Thus, at the expense of an error of order ε, we can associate to $P(\widehat{q}, \widehat{p})$ a true projection operator $\widetilde{P}(\widehat{q}, \widehat{p})$, and $\widetilde{P}(\widehat{q}, \widehat{p})\mathcal{H}$ is the adiabatically protected subspace in lowest-order approximation.

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From the example of $P(\widehat{q}, \widehat{p})$ just discussed, it is clear that for a study of the Schrödinger equation (16.50) in the limit of small ε one has to understand the relationship between the multiplication of symbols and the multiplication of their Weyl quantization, which is taken up next. Let A, B be two matrix-valued functions. One defines their Moyal product $A\#B$ implicitly through the condition

$$\mathcal{W}_\varepsilon(A)\mathcal{W}_\varepsilon(B) = \mathcal{W}_\varepsilon(A\#B). \tag{16.51}$$

The Moyal product is best grasped in the case where the symbols are given as formal power series,

$$A(q, p) = \sum_{j\geq 0} \varepsilon^j A_j(q, p), \quad B(q, p) = \sum_{j\geq 0} \varepsilon^j B_j(q, p), \tag{16.52}$$

where the expansion coefficients A_j, B_j do not depend on ε. The equality is understood as $|A - \sum_{j\geq 0}^{n-1} \varepsilon^j A_j| \leq c_n \varepsilon^n$ with constants c_n possibly growing so fast in n that the partial sums in (16.52) do not converge. Then $A\#B$ also has a formal power series, which is written as

$$A\#B = \sum_{j\geq 0} \varepsilon^j (A\#B)_j. \tag{16.53}$$

Equating power by power in (16.51) one finds

$$(A\#B)_j(q, p) = \sum_{|\alpha|+|\beta|+l+m=j} (2i)^{-(|\alpha|+|\beta|)} \frac{(-1)^{|\beta|}}{|\alpha|!|\beta|!} \partial_q^\alpha \partial_p^\beta A_l(q, p) \partial_p^\alpha \partial_q^\beta B_m(q, p), \tag{16.54}$$

where it is understood that $j, l, m \in \mathbb{N}$ and α, β are multi-indices, $\alpha, \beta \in \mathbb{N}^3$. To lowest order

$$(A\#B)_0 = A_0 B_0, \quad (A\#B)_1 = A_0 B_1 + A_1 B_0 - \frac{\mathrm{i}}{2}\{A_0, B_0\}. \tag{16.55}$$

We introduced here the Poisson bracket $\{\cdot, \cdot\}$ for matrix-valued functions. It is defined by

$$\{A, B\} = \nabla_p A \cdot \nabla_q B - \nabla_q A \cdot \nabla_p B, \tag{16.56}$$

the dot referring to the scalar product of the two gradients. Thus even if the formal power series for A, B consists only of the leading term, $A = A_0$, $B = B_0$, as is the case for $P(q, p)$, their Moyal product is a formal power series starting with

$$A\#B = AB - \varepsilon \frac{\mathrm{i}}{2}\{A, B\} + \mathcal{O}(\varepsilon^2) \tag{16.57}$$

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and, by definition, the lowest-order product becomes

$$\mathcal{W}_\varepsilon(A)\mathcal{W}_\varepsilon(B) = \mathcal{W}_\varepsilon(AB - \varepsilon\frac{\mathrm{i}}{2}\{A, B\}) + \mathcal{O}(\varepsilon^2). \tag{16.58}$$

Note that in (16.56) the order of matrices must be respected. In general, it is *not* true that $\{A, A\} = 0$, or $\{A, B\} = -\{B, A\}$, as one is used to from the standard calculus of Poisson brackets.

In the sequel, very roughly the idea is to use (16.51) as a link between functions of operators, like the time-evolved position operator $\widehat{q}(t) = \mathrm{e}^{\mathrm{i}Ht/\varepsilon}\widehat{q}\mathrm{e}^{-\mathrm{i}Ht/\varepsilon}$, and matrix-valued symbols. In particular, one can regard the matrix-valued function $P(q, p)$ as the lowest-order symbol for the true Hilbert space projection onto the adiabatically decoupled relevant subspace.

16.4 Adiabatic decoupling, effective Hamiltonians

As noticed already, in general $P(\widehat{q}, \widehat{p})$ is not a projection, due to errors of order ε. This suggests to successively correct $P(q, p)$ with the goal in Weyl quantization to get a projection up to precision ε^n, n arbitrary, a situation denoted by the symbol $\mathcal{O}(\varepsilon^\infty)$. We make the ansatz

$$\pi(q, p) = \sum_{j\geq 0} \varepsilon^j \pi_j(q, p), \quad \pi_0(q, p) = P(q, p) \tag{16.59}$$

and recall that in general

$$H(q, p) = \sum_{j\geq 0} \varepsilon^j H_j(q, p), \tag{16.60}$$

where in our specific application $H_j = 0$ for $j \geq 2$. The Weyl quantization for π should be a projection and commute with $H(\widehat{q}, \widehat{p})$ up to errors $\mathcal{O}(\varepsilon^\infty)$. π has then to satisfy the conditions

$$\pi^* = \pi, \quad \pi\#\pi = \pi, \quad \pi\#H = H\#\pi. \tag{16.61}$$

Through an iterative procedure it can be shown that the symbol π is in fact uniquely determined by (16.61). By construction $\mathcal{W}_\varepsilon(\pi)^2 = \mathcal{W}_\varepsilon(\pi) + \mathcal{O}(\varepsilon^\infty)$ and there is a projection operator Π on $\mathcal{H}$ naturally associated to $\mathcal{W}_\varepsilon(\pi)$. If we assume the initial wave function ψ to lie in $\Pi\mathcal{H}$, $\Pi\psi = \psi$, then for the true solution $\psi(t) = \mathrm{e}^{-\mathrm{i}Ht/\varepsilon}\psi$ one has

$$(1 - \Pi)\psi(t) = \mathcal{O}(\varepsilon^\infty). \tag{16.62}$$

For this reason $\Pi\mathcal{H}$ is called an almost invariant subspace, associated to the relevant projection $P(q, q)$. On the adiabatic scale transitions out of $\Pi\mathcal{H}$ are

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exponentially suppressed as $\mathrm{e}^{-(1/\varepsilon)}$ and the dynamics on $\Pi\mathcal{H}$ is governed by the diagonal Hamiltonian $H_{\mathrm{dg}} = \Pi\widehat{H}\Pi$.

Equation (16.62) solves the adiabatic problem only in principle. To have a workable scheme it is required to have a basis in $\Pi\mathcal{H}$ which is in some sense naturally adapted to the slow degrees of freedom and in which H_{dg} can be computed perturbatively. Of course, the hope is that low-order perturbation will suffice. For this purpose we pick a fixed (q, p)-independent basis $|\chi_\alpha\rangle$, $\alpha = 1, \ldots, n$, in $\mathbb{C}^n$ and define the ℓ-dimensional *reference projection*

$$\pi_{\mathrm{r}} = \sum_{\alpha=1}^{\ell} |\chi_\alpha\rangle\langle\chi_\alpha|. \tag{16.63}$$

Since $|\chi_\alpha\rangle$ does not depend on (q, p), $1 \otimes \pi_{\mathrm{r}} = \widehat{\pi}_{\mathrm{r}} = \mathcal{W}_\varepsilon(\pi_{\mathrm{r}})$ is a projection and its range defines the *reference Hilbert space* $L^2(\mathbb{R}^3) \otimes \pi_{\mathrm{r}}\mathbb{C}^n = \mathcal{H}_{\mathrm{r}}$ as a subspace of $\mathcal{H}$. Of course, at this stage the reference subspace is fairly arbitrary and a convenient choice must be made in concrete applications. The projection $P(q, p)$ is spanned by the eigenvectors $\psi_\alpha(q, p)$, $\alpha = 1, \ldots, \ell$, of $H_0(q, p)$, $\langle\psi_\alpha(q, p), \psi_\beta(q, p)\rangle_{\mathbb{C}^n} = \delta_{\alpha\beta}$. The unitary map from $P(q, p)\mathbb{C}^n$ to the reference subspace is then

$$u_0(q, p) = \sum_{\alpha=1}^{\ell} |\chi_\alpha\rangle\langle\psi_\alpha(q, p)|. \tag{16.64}$$

If u_0 were completed to a unitary operator $\widetilde{u}_0$ on $\mathbb{C}^n$, then for every q, p the $n \times n$ matrix $\widetilde{u}_0 H_0 \widetilde{u}_0^*$ is block diagonal, with block sizes ℓ and $n - \ell$, and has in the $\ell \times \ell$ left upper block only the diagonal entries $E(q, p)$.

As in the case of the projection $P(q, p)$, $\mathcal{W}_\varepsilon(u_0)$ is in general not unitary with an error of order ε. Thus we iteratively correct so as to obtain a proper unitary operator from $\Pi\mathcal{H}$ to the reference subspace $\mathcal{H}_{\mathrm{r}}$. The ansatz is

$$u(q, p) = \sum_{j\geq 0} \varepsilon^j u_j(q, p), \tag{16.65}$$

with u_0 as in (16.64). Unitarity and transformation of π to π_{r} translates into

$$u^{*}\#u = 1, \quad u\#u^{*} = 1, \quad u\#\pi\#u^{*} = \pi_{\mathrm{r}}. \tag{16.66}$$

One can show that such a symbol u exists. Since u_0 is already not unique, neither is u. As with $\pi(q, p)$, one associates with u a unitary operator $U : \Pi\mathcal{H} \to \mathcal{H}_{\mathrm{r}}$. On $\mathcal{H}_{\mathrm{r}}$ the motion is governed by $U\Pi\widehat{H}\Pi U^*$ and it agrees with the true solution up to $\mathcal{O}(\varepsilon^\infty)$. $U\Pi\widehat{H}\Pi U^*$ has a symbol determined through

$$h = u\#H\#u^{*}. \tag{16.67}$$

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We call h the *effective Hamiltonian*, associated to the almost invariant subspace $\Pi\mathcal{H}$. The crux of the construction is that h can be represented by a formal power series,

$$h = \sum_{j\geq 0} \varepsilon^j h_j \tag{16.68}$$

and the effective Hamiltonian is successively approximated through the Weyl quantization

$$\mathcal{W}_\varepsilon(h) = \mathcal{W}_\varepsilon(\pi_{\rm r} h_0 \pi_{\rm r}) + \varepsilon \mathcal{W}_\varepsilon(\pi_{\rm r} h_1 \pi_{\rm r}) + \cdots . \tag{16.69}$$

Let us work out the two lowest orders. Clearly

$$\pi_{\rm r} h_0 \pi_{\rm r} = \pi_{\rm r} u_0^* H_0 u_0 \pi_{\rm r} = E(q, p)\pi_{\rm r}. \tag{16.70}$$

Its Weyl quantization is $E(\widehat{q}, \widehat{p})\pi_{\rm r}$ which is the anticipated Peierls substitution. In spinor space $E(q, p)\pi_{\rm r}$ is diagonal, see (16.63), and there is no internal motion at this order yet. For h_1 it is easier to rewrite (16.67) as $H\#u = u\#h$ and therefore $(H_0 + \varepsilon H_1)\#(u_0 + \varepsilon u_1) = (u_0 + \varepsilon u_1)\#(h_0 + \varepsilon h_1)$. Using (16.57) one thus obtains

$$h_1 = \Big(u_1 H_0 + u_0 H_1 - h_0 u_1 - \frac{\rm i}{2}\{u_0, H_0\} + \frac{\rm i}{2}\{h_0, u_0\}\Big) u_0^*. \tag{16.71}$$

Projecting onto $\pi_{\rm r}$, the terms $H_0 u_1$ and $u_1 h_0$ cancel and h_1 simplifies to

$$\pi_{\rm r} h_1 \pi_{\rm r} = \pi_{\rm r}\Big(u_0 H_1 u_0^* - \frac{\rm i}{2}\{u_0, H_0\} u_0^* + \frac{\rm i}{2}\{E, u_0\} u_0^*\Big)\pi_{\rm r}. \tag{16.72}$$

u_0 is inserted from Eq. (16.64). In the basis of the reference Hilbert space one then obtains to first order

$$\langle \chi_\alpha, (h_0 + \varepsilon h_1)\chi_\beta\rangle_{\mathbb{C}^n} = E\delta_{\alpha\beta} + \varepsilon\langle \psi_\alpha, H_1 \psi_\beta\rangle_{\mathbb{C}^n} - \varepsilon\frac{\rm i}{2}\langle \psi_\alpha, \{H_0 + E, \psi_\beta\}\rangle_{\mathbb{C}^n} + \mathcal{O}(\varepsilon^2), \tag{16.73}$$

where $\alpha, \beta = 1, \ldots, \ell$, and where the Poisson bracket is understood as

$$\{H_0, \psi_\alpha\} = \nabla_p H_0 \cdot \nabla_q \psi_\alpha - \nabla_q H_0 \cdot \nabla_p \psi_\alpha \tag{16.74}$$

with H_0 acting on ψ_α as a matrix. The Weyl quantization of $h_0 + \varepsilon h_1$ is the effective Hamiltonian in $L^2(\mathbb{R}^3) \otimes \mathbb{C}^\ell$ to that order.

In principle, our scheme can be pushed up to arbitrary order. Formulas for h_2 are available, but they are already so involved that h_3 is out of reach. Physically the dominant effects are in h_0, h_1, and to some extent in h_2. Further terms will add only a minute correction. Of course, the adiabatic decoupling relies on the gap

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assumption (16.49). In the case where the energy bands of $H_0(q, p)$ cross, or almost cross, transition between bands become possible and the qualitative picture developed so far breaks down. Away from crossings the description through the effective Hamiltonian is still accurate, but close to nearly avoided crossings new techniques come into play.

The formula (16.73) looks unfamiliar. To get acquainted, a simple but instructive way is to return to the time-adiabatic setting of section 16.1, where $H(t)$ is a time-dependent $n \times n$ matrix and the relevant subspace has a constant multiplicity ℓ. It is spanned by the instantaneous eigenvectors $\varphi_\alpha(t)$, $H(t)\varphi_\alpha(t) = E(t)\varphi_\alpha(t)$, $\alpha = 1, \dots, \ell$, and the projection onto the relevant subspace is given by $P(t) = \sum_{\alpha=1}^{\ell} |\varphi_\alpha(t)\rangle\langle\varphi_\alpha(t)|$. As before, one needs a reference subspace of dimension ℓ with time-*independent* basis $|\chi_\alpha\rangle$, $\alpha = 1, \dots, \ell$. We do not spell out the details of the computation, but state the final result. Including order ε, the unitary $U^\varepsilon(t)^*$ from the reference space $\mathbb{C}^\ell$ into $\mathbb{C}^n = \mathcal{H}_\mathrm{f}$ is given by

$$U^\varepsilon(t)^* = \sum_{\alpha=1}^{\ell} (|\varphi_\alpha(t)\rangle + |\mathrm{i}\varepsilon(H(t) - E(t))^{-1}(1 - P(t))\dot{\varphi}_\alpha(t)\rangle)\langle\chi_\alpha| + \mathcal{O}(\varepsilon^2). \tag{16.75}$$

$U^\varepsilon(t)^*$ should be thought of as a kinematical component. It says, for each t, how the adiabatically protected subspace lies in $\mathbb{C}^n$. To order 1 the subspace is just $P(t)\mathbb{C}^n$ and (16.75) provides the first-order correction. The dynamical piece provides the information of how the solution vector rotates inside the almost invariant subspace. It is governed by the effective Hamiltonian acting in $\mathbb{C}^\ell$, which to order ε^2 has the form

$$\begin{aligned} h_{\alpha\beta}(t) = {} & \delta_{\alpha\beta}E(t) - \mathrm{i}\varepsilon\langle\varphi_\alpha(t), \dot{\varphi}_\beta(t)\rangle_{\mathbb{C}^n} \\ & + \frac{1}{2}\varepsilon^2\langle\dot{\varphi}_\alpha(t), (H(t) - E(t))^{-1}(1 - P(t))\dot{\varphi}_\beta(t)\rangle_{\mathbb{C}^n} + \mathcal{O}(\varepsilon^3), \end{aligned} \tag{16.76}$$

$\alpha, \beta = 1, \dots, \ell$. The second term of $h(t)$ is the Berry phase. The approximate solution to (16.7) is obtained by first solving the time-dependent Schrödinger equation with $h_\mathrm{eff}(t)$ in the reference subspace $\mathbb{C}^\ell$ and then mapping into $\mathcal{H}$ through the unitary (16.75). Thereby the error in (16.8) is improved to order ε^2. In addition we know how the vector $\psi(t)$ rotates inside the relevant subspace. With some effort the precision could be improved to $\mathcal{O}(\varepsilon^3)$. Abstractly, an error $\mathcal{O}(\varepsilon^\infty)$ is guaranteed.

Matrix-valued symbols are a very powerful tool in the analysis of the space-adiabatic limit. But, in the end, one would like to have a result on the Schrödinger equation (16.45). This is always possible because the two frames of description

are linked through Weyl quantization. To order ε the result is

$$\mathrm{e}^{-\mathrm{i}H(\widehat{q},\widehat{p})t/\varepsilon}\psi = u_0(\widehat{q},\widehat{p})^*\mathrm{e}^{-\mathrm{i}(h_0(\widehat{q},\widehat{p})+\varepsilon h_1(\widehat{q},\widehat{p}))t/\varepsilon}u_0(\widehat{q},\widehat{p})\psi + (1+|t|)\mathcal{O}(\varepsilon) \tag{16.77}$$

provided the initial wave function lies in the relevant subspace, i.e. $\pi_0(\widehat{q},\widehat{p})\psi = \psi$. On the right, one has the effective dynamics in the reference subspace $L^2(\mathbb{R}^3)\otimes\mathbb{C}^\ell$ as generated by $\mathcal{W}_\varepsilon(h_0+\varepsilon h_1)$. Then $\mathcal{W}_\varepsilon(u_0)$ which, up to error ε, is unitary turns the effective evolution into the physical Hilbert space $L^2(\mathbb{R}^3)\otimes\mathbb{C}^n$. The error $(1+|t|)\mathcal{O}(\varepsilon)$ comes from the correction of π_0 to $\pi_0+\varepsilon\pi_1$, of u_0 to $u_0+\varepsilon u_1$, and from the correction of $h_0+\varepsilon h_1$ to $h_0+\varepsilon h_1+\varepsilon^2 h_2$. Equation (16.77) agrees with our findings for the particular case studied in section 16.2. There $h_0(q,p)=E(p)+V(q)$ and $h_1(p)=-\mathrm{i}\langle\psi_\mathrm{g}(p),\nabla_p\psi_\mathrm{g}(p)\rangle_\mathcal{F}=0$ by our choice of the phase for $\psi_\mathrm{g}(p)$. Once the spin is included, h_1 no longer vanishes, see section 16.6.

At the risk of repeating the obvious: expectations of physical observables have the form $\langle\psi_t, A\psi_t\rangle$. Thus if ψ_t is unitarily transformed so must be the observable A. When using the effective Hamiltonian of (16.67) one has to properly transform the observables of physical interest. To lowest order x and $-\mathrm{i}\nabla_x$ transform into themselves. But, in general, to first order there will be corrections. Also, the basis $\psi_\alpha(q,p), \alpha=1,\ldots,\ell$, of the relevant subspace must be selected judiciously such that in the $|\chi_\alpha\rangle$-basis observables of interest have a simple representation. We will come back to this point in the context of the Pauli–Fierz operator; see section 16.6 below. The Weyl quantization of the effective Hamiltonian (16.67) still carries the small parameter ε which suggests using semiclassical methods, a subject to be taken up in the following section. For general $E(q,p)$, the semiclassical regime is limited by the Ehrenfest time which in our units is of order $\log\varepsilon^{-1}$. We stress that the adiabatic limit has no such restrictions, as can be seen from (16.77): if one had included the term h_2, the approximation with the given precision would be valid for macroscopic times of order ε^{-1}.

16.5 Semiclassical limit

According to Eq. (16.73) the effective Hamiltonian has the form

$$H = H(\widehat{q},\widehat{p}) = E(\widehat{q},\widehat{p})\mathbb{1} + \varepsilon H_\mathrm{sp}(\widehat{q},\widehat{p}) \tag{16.78}$$

acting on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^\ell$, where for clarity $\mathbb{1}$ denotes the $\ell\times\ell$ unit matrix. The last two terms in (16.73) have been renamed as H_sp anticipating that they are responsible for the precession of the ℓ-spinor.

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The semiclassical limit can be guessed most directly by considering the Heisenberg evolution of the semiclassical observable $\widehat{a} = a(\widehat{q}, \widehat{p})$ as

$$\widehat{a}(t) = \mathrm{e}^{\mathrm{i}Ht/\varepsilon}\widehat{a}\mathrm{e}^{-\mathrm{i}Ht/\varepsilon}. \tag{16.79}$$

$\widehat{a}(t)$ has a semiclassical representation through $a(q, p, t) = \sum_{j\geq 0}\varepsilon^j a_j(q, p, t)$. From the equations of motion

$$\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\widehat{a}(t) = \mathrm{i}[H, \widehat{a}(t)], \tag{16.80}$$

using $[E\mathbb{1}, a_j(t)] = 0$, one finds to lowest order

$$\frac{\mathrm{d}}{\mathrm{d}t}a_0(t) = \{E, a_0(t)\} + \mathrm{i}[H_{\mathrm{sp}}, a_0(t)] + \mathcal{O}(\varepsilon) \tag{16.81}$$

with initial conditions $a_0(0) = a$.

Ignoring the error $\mathcal{O}(\varepsilon)$, the solution to (16.81) is easily constructed. First one defines the classical flow Φ_t on phase space through

$$\dot{q}_t = \nabla_p E(q_t, p_t), \quad \dot{p}_t = -\nabla_q E(q_t, p_t). \tag{16.82}$$

Secondly, given the initial condition (q, p) with corresponding trajectory (q_t, p_t) one obtains the time-dependent spin Hamiltonian $H_{\mathrm{sp}}(t) = H_{\mathrm{sp}}(q_t, p_t)$. It determines the spinor evolution as

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\chi(t) = H_{\mathrm{sp}}(t)\chi(t), \quad \chi(t) \in \mathbb{C}^\ell. \tag{16.83}$$

The unitary propagator for (16.83) from s to t is denoted by $U(t, s|q, p)$, recalling that it depends on the trajectory through its initial conditions. Then

$$a_0(q, p, t) = U(t, 0|q, p)^* a(\Phi_t(q, p))U(t, 0|q, p), \tag{16.84}$$

as can be verified by inserting in (16.81).

In the semiclassical limit there is no back-reaction of the spin on the orbit. Such an effect could be seen in corrections to the semiclassical limit and in the next-order correction, h_2, to the effective Hamiltonian.

The predictions of the semiclassical limit move more sharply into focus through considering the dual Schrödinger picture. One picks a possibly ε-dependent initial wave function such that for expectations of semiclassical observables the limit

$$\lim_{\varepsilon\to 0}\langle\psi^\varepsilon, a(\widehat{q}, \widehat{p})\psi^\varepsilon\rangle = \int \mathrm{tr}[\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p)a(q, p)] \tag{16.85}$$

holds, examples being listed below. Here tr is over $\mathbb{C}^\ell$. $\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p)$ is a matrix-valued classical probability measure on phase space, $\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p) \geq 0$ as a matrix

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and $\int \mathrm{tr}[\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p)] = 1$. Then at later times, from (16.82) and (16.84),

$$\begin{aligned}\lim_{\varepsilon\to 0}\langle \mathrm{e}^{-\mathrm{i}Ht/\varepsilon}\psi^\varepsilon, \widehat{a}\mathrm{e}^{-\mathrm{i}Ht/\varepsilon}\psi^\varepsilon\rangle &= \lim_{\varepsilon\to 0}\langle \psi^\varepsilon, \widehat{a}(t)\psi^\varepsilon\rangle \\ &= \int \mathrm{tr}[\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p)U(t,0|q,p)^* a(\Phi_t(q,p))U(t,0|q,p)] \\ &= \int \mathrm{tr}[U(t,0|q,p)\rho_{\mathrm{cl}}\circ\Phi_{-t}(\mathrm{d}^3q\mathrm{d}^3p)U(t,0|q,p)^* a(q,p)]. \quad (16.86)\end{aligned}$$

The classical part of the measure is transported through the classical flow, while the spinor part evolves through the spin Hamiltonian $H_{\mathrm{sp}}(q_t, p_t)$. In this sense the quantum expectation on the left of (16.86) is approximated by the classical average on the right, keeping in mind that the internal spinor motion remains of full quantum nature.

We list a few conventional choices, where the position variable refers to the macroscopic scale. In *wave packet dynamics* one assumes a sharp concentration as $\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p) = |\chi\rangle\langle\chi|\delta(q-q_0)\delta(p-p_0)\mathrm{d}^3q\mathrm{d}^3p$. Then at later times the wave packet is concentrated at (q_t, p_t) and the spin χ_t precesses according to (16.83). A particular choice would be an initially Gaussian wave packet, which depends on ε such that $\langle x\rangle_\varepsilon = q_0$, $\langle -\mathrm{i}\varepsilon\nabla_x\rangle = p_0$, $\langle (x-q_0)^2\rangle_\varepsilon \to 0$, and $\langle(-\mathrm{i}\varepsilon\nabla_x - p_0)^2\rangle_\varepsilon \to 0$ as $\varepsilon\to 0$. Note that to achieve the concentration in momentum the position is necessarily broadly distributed on the atomic scale. A *WKB wave function* is of the form $\psi^\varepsilon(x) = \chi(x)\mathrm{e}^{\mathrm{i}S(x)/\varepsilon}$. In the limit $\varepsilon\to 0$ it defines the initial distribution $\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p) = |\chi(q)\rangle\langle\chi(q)|\delta(p-\nabla S(q))\mathrm{d}^3q\mathrm{d}^3p$. As a measure on the six-dimensional phase space it is concentrated on a three-dimensional hypersurface, a property which is retained by the flow Φ_t. Since this surface may in general fold up in the course of time, it cannot be represented as the graph of a function. For fixed q there could be several values of p. The wave function $U^\varepsilon(t)\psi^\varepsilon$ has the standard WKB form only locally in phase space. A further choice is a *microscopic wave packet* which in our units reads as $\psi^\varepsilon(x) = \chi\varepsilon^{-3/2}\psi(x/\varepsilon)$ with some given wave function ψ on the microscopic scale. Then $\rho_{\mathrm{cl}}(\mathrm{d}^3q\mathrm{d}^3p) = |\chi\rangle\langle\chi|\delta(q)|\widehat{\psi}(p)|^2\mathrm{d}^3q\mathrm{d}^3p$. The wave packet is spatially localized, necessarily with a spread in momentum. ρ_{cl} is concentrated on the three-dimensional surface $\{(q,p)|q=0\}$ in phase space. Thus at a later time it will be of WKB form locally.

If we look back at our starting point, an electron subject to slowly varying external potentials governed by the Hamiltonian (16.1), it may appear that we have lost sight of our goal. To improve, we summarize our main findings on a qualitative level. First, slow variation is satisfied for all laboratory fields including those employed in the big accelerator machines. The translational degrees of freedom of the electron are thus governed in an excellent approximation by an effective Hamiltonian obtained from the Peierls substitution, $H_{\mathrm{eff}} = E(\widehat{p} - eA_{\mathrm{ex}}(\widehat{q})) + e\phi_{\mathrm{ex}}(\widehat{q})$.

In particular for small velocities, relying on the results from chapter 15,

$$H_{\text{eff}} = \frac{1}{2m_{\text{eff}}}(\widehat{p} - eA_{\text{ex}}(\widehat{q}))^2 + e\phi_{\text{ex}}(\widehat{q}). \tag{16.87}$$

To understand the spin precession, one has to compute the first-order correction h_1 to the effective Hamiltonian, which is the topic of the section to follow.

16.6 Spin precession and the gyromagnetic ratio

The time of pleasant harvest has come. The Hamiltonian is (16.38) with principal symbol

$$H_0(q, p) = H(p - eA_{\text{ex}}(q)) + e\phi_{\text{ex}}(q); \tag{16.88}$$

compare with (16.39). $H(p)$ acts on $\mathbb{C}^2 \otimes \mathcal{F}$ and is defined in (15.68), where for notational convenience we use $H(p)$ instead of H_p. From section 15.3 we know that $H(p)$ has a two-fold degenerate ground state with energy $E(p)$ and projector $P(p)$, $\operatorname{tr}[P(p)] = 2$ provided $|p| \leq p_{\text{c}}$ ($\cong m$). Therefore $P(q, p) = P(p - eA_{\text{ex}}(q))$ as a projection operator on $\mathbb{C}^2 \otimes \mathcal{F}$ defines the relevant subspace for $H_0(q, p)$ with corresponding eigenvalue $E(q, p) = E(p - eA_{\text{ex}}(q)) + e\phi_{\text{ex}}(q)$. To lowest order the symbol of the effective Hamiltonian is then

$$h_0(q, p) = E(q, p)\mathbb{1} = \big(E(p - eA_{\text{ex}}(q)) + e\phi_{\text{ex}}(q)\big)\mathbb{1}, \tag{16.89}$$

with $\mathbb{1}$ the 2×2 unit matrix, and the orbital motion is approximately governed by

$$h_0(\widehat{q}, \widehat{p}) = \big(E(-\mathrm{i}\varepsilon\nabla_x - eA_{\text{ex}}(x)) + e\phi_{\text{ex}}(x)\big)\mathbb{1}. \tag{16.90}$$

The spin precession requires more attention. First of all one has to specify a basis in $P(p)\mathbb{C}^2 \otimes \mathcal{F}$. The singled-out choice is the eigenvectors of the total angular momentum component parallel to p, which we denote by $\psi_{\text{g}\pm}(p, \underline{k})$, $\langle \psi_{\text{g}-}(p), \psi_{\text{g}+}(p) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} = 0$. To define them properly, we follow section 13.5 and introduce the total angular momentum

$$J = \frac{1}{2}\sigma + J_{\text{f}} + S_{\text{f}}, \tag{16.91}$$

see (13.96), (13.97). If R is a rotation by angle θ relative to the axis of rotation $\widehat{n}$ through the origin, then

$$\mathrm{e}^{\mathrm{i}\theta\widehat{n}\cdot J} e_\lambda(k) a(k, \lambda) \mathrm{e}^{-\mathrm{i}\theta\widehat{n}\cdot J} = R e_\lambda(R^{-1}k) a(R^{-1}k, \lambda) \tag{16.92}$$

and therefore

$$\mathrm{e}^{\mathrm{i}\theta\widehat{n}\cdot J} A_\varphi \mathrm{e}^{-\mathrm{i}\theta\widehat{n}\cdot J} = RA_\varphi, \quad \mathrm{e}^{\mathrm{i}\theta\widehat{n}\cdot J} B_\varphi \mathrm{e}^{-\mathrm{i}\theta\widehat{n}\cdot J} = RB_\varphi, \quad \mathrm{e}^{\mathrm{i}\theta\widehat{n}\cdot J} \sigma \mathrm{e}^{-\mathrm{i}\theta\widehat{n}\cdot J} = R\sigma. \tag{16.93}$$

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If $\widehat{n}$ is parallel to p, $\widehat{n} = p/|p|$, these relations imply that the component of J along p is conserved,

$$[H(p),\, p \cdot J] = 0. \tag{16.94}$$

$|p|^{-1} p \cdot J$ has the eigenvalues $\pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$. For $e = 0$, $|p|^{-1} p \cdot J$ has eigenvalues $\pm\frac{1}{2}$ in the ground state subspace of $H(p)$. By continuity, for $e \neq 0$, the eigenvalue equations $H(p)\psi_{\mathrm{g}\pm}(p) = E(p)\psi_{\mathrm{g}\pm}(p)$, $|p|^{-1} p \cdot J \psi_{\mathrm{g}\pm}(p) = \pm\frac{1}{2}\psi_{\mathrm{g}\pm}(p)$ uniquely determine the basis vectors $\psi_{\mathrm{g}\pm}(p)$, up to phase factors $\mathrm{e}^{-\mathrm{i}\theta_{\pm}(p)}$. We interpret these states as having spin pointing parallel, eigenvalue $\frac{1}{2}$, and antiparallel, eigenvalue $-\frac{1}{2}$, to p. On the other hand, except for $p = 0$, one has $[H(p),\, p' \cdot J] \neq 0$ unless $|p|^{-1} p = \pm |p'|^{-1} p'$.

The effective spin Hamiltonian in the $p \cdot J$-basis is derived with the help of (16.73), recalling the subprincipal symbol $H_1(q, p)$ from (16.39). Setting $\psi_{\mathrm{g}\pm}(q, p) = \psi_{\mathrm{g}\pm}(p - eA_{\mathrm{ex}}(q))$ one obtains

$$\begin{aligned}\langle \alpha | H_{\mathrm{sp}}(q, p) | \beta \rangle = &- \frac{e}{2m} B_{\mathrm{ex}}(q) \cdot \langle \psi_{\mathrm{g}\alpha}(q, p), \sigma \psi_{\mathrm{g}\beta}(q, p) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} \\ &- \frac{\mathrm{i}}{2} \langle \psi_{\mathrm{g}\alpha}(q, p), \{H_0(q, p) + E(q, p), \psi_{\mathrm{g}\beta}(q, p)\} \rangle_{\mathbb{C}^2 \otimes \mathcal{F}},\end{aligned} \tag{16.95}$$

$\alpha, \beta = \pm$. Working out the Poisson bracket yields

$$\begin{aligned}\langle \alpha | H_{\mathrm{sp}}(q, p) | \beta \rangle = &- B_{\mathrm{ex}}(q) \cdot \Big(\frac{e}{2m} \langle \psi_{\mathrm{g}\alpha}(\tilde{p}), \sigma \psi_{\mathrm{g}\beta}(\tilde{p}) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} \\ &- \frac{\mathrm{i}}{2} e \langle \nabla_p \psi_{\mathrm{g}\alpha}(\tilde{p}), \times (H(\tilde{p}) - E(\tilde{p})) \nabla_p \psi_{\mathrm{g}\beta}(\tilde{p}) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} \Big) \\ &+ e\big(- \nabla_q \phi_{\mathrm{ex}}(q) + v \times B_{\mathrm{ex}}(q) \big) \cdot \langle \psi_{\mathrm{g}\alpha}(\tilde{p}), \mathrm{i} \nabla_p \psi_{\mathrm{g}\beta}(\tilde{p}) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}}\end{aligned} \tag{16.96}$$

with the velocity $v = \nabla_p E(\tilde{p})$ and $\tilde{p} = p - eA_{\mathrm{ex}}(q)$. The spin Hamiltonian has a simple interpretation: through the coupling to the field the electron acquires the effective magnetic moment

$$\begin{aligned}\langle \alpha | M_{\mathrm{m}}(\tilde{p}) | \beta \rangle = &\frac{e}{2m} \langle \psi_{\mathrm{g}\alpha}(\tilde{p}), \sigma \psi_{\mathrm{g}\beta}(\tilde{p}) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} \\ &- \frac{\mathrm{i}}{2} e \langle \nabla_p \psi_{\mathrm{g}\alpha}(\tilde{p}), \times (H(\tilde{p}) - E(\tilde{p})) \nabla_p \psi_{\mathrm{g}\beta}(\tilde{p}) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}}\end{aligned} \tag{16.97}$$

and the effective electric moment

$$\langle \alpha | M_{\mathrm{e}}(\tilde{p}) | \beta \rangle = -e \langle \psi_{\mathrm{g}\alpha}(\tilde{p}), \mathrm{i} \nabla_p \psi_{\mathrm{g}\beta}(\tilde{p}) \rangle_{\mathbb{C}^2 \otimes \mathcal{F}}. \tag{16.98}$$

They are operators on spin space depending on the kinetic momentum $\tilde{p}$. The spin Hamiltonian then reads

$$H_{\mathrm{sp}} = -B_{\mathrm{ex}} \cdot M_{\mathrm{m}} - F_{\mathrm{L}} \cdot M_{\mathrm{e}} \tag{16.99}$$

with the Lorentz force $F_{\mathrm{L}} = -\nabla_q \phi_{\mathrm{ex}}(q) + v \times B_{\mathrm{ex}}(q)$. Note that on top of the obvious magnetic splitting, the effective moments are determined through geometric phases.

The semiclassical analysis of (16.90) together with (16.96) was discussed in the previous section. Of particular interest is the case of a small uniform magnetic field B, i.e. $\phi_{\mathrm{ex}} = 0$, $A_{\mathrm{ex}}(q) = \frac{1}{2} B \times q$. For small velocities the orbital motion is then governed by

$$m_{\mathrm{eff}} \frac{\mathrm{d}}{\mathrm{d}t} v_t = e v_t \times B; \tag{16.100}$$

see (15.23) for the definition of the effective mass, which yields the cyclotron frequency

$$\omega_{\mathrm{c}} = e|B|/m_{\mathrm{eff}}. \tag{16.101}$$

Since $\tilde{p} = 0$, we may pick arbitrarily the J_3-basis with eigenvectors $\psi_{\mathrm{g}\pm} = \psi_{\mathrm{g}\pm}(0)$ determined through $H(0)\psi_{\mathrm{g}\pm} = E(0)\psi_{\mathrm{g}\pm}$, $J_3 \psi_{\mathrm{g}\pm} = \pm\frac{1}{2}\psi_{\mathrm{g}\pm}$. Using first-order perturbation theory for $\nabla_p \psi_{\mathrm{g}\pm}(0)$, the spin Hamiltonian simplifies to

$$\begin{aligned}\langle \alpha | H_{\mathrm{sp}} | \beta \rangle = & -\frac{e}{2m} B \cdot \langle \psi_{\mathrm{g}\alpha}, \sigma \psi_{\mathrm{g}\beta} \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} \\ & + \frac{\mathrm{i}}{2} e B \cdot \langle \psi_{\mathrm{g}\alpha}, \frac{1}{m}(P_{\mathrm{f}} + eA_\varphi) \times \frac{1}{H(0) - E(0)} \frac{1}{m}(P_{\mathrm{f}} + eA_\varphi) \psi_{\mathrm{g}\beta} \rangle_{\mathbb{C}^2 \otimes \mathcal{F}}.\end{aligned} \tag{16.102}$$

$H(0)$ is rotation invariant; see the discussion leading to (16.94). Therefore H_{sp} is necessarily of the form

$$H_{\mathrm{sp}} = -\frac{e}{2m} \frac{\widetilde{g}}{2} B \cdot \sigma, \tag{16.103}$$

which yields $\widetilde{g}$ as

$$\begin{aligned}\frac{1}{2}\widetilde{g} = & \langle \psi_{\mathrm{g}+}, \sigma_3 \psi_{\mathrm{g}+} \rangle_{\mathbb{C}^2 \otimes \mathcal{F}} \\ & - \frac{2}{m} \mathrm{Im} \langle \psi_{\mathrm{g}+}, (P_{\mathrm{f}} + eA_\varphi)_2 \frac{1}{H(0) - E(0)} (P_{\mathrm{f}} + eA_\varphi)_1 \psi_{\mathrm{g}+} \rangle_{\mathbb{C}^2 \otimes \mathcal{F}}.\end{aligned} \tag{16.104}$$

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Note that $H_{\rm sp}$ does not depend on the choice of the phase $\mathrm{e}^{-\mathrm{i}\theta_+(p)}$ for $\psi_{\mathrm{g}+}(p)$. In our approximation, the spin motion is governed by

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma(t) = -\frac{e}{2m}\widetilde{g}B \times \sigma(t), \tag{16.105}$$

from which the frequency of spin precession

$$\omega_{\rm s} = e|B|\widetilde{g}/2m \tag{16.106}$$

follows.

The conventional definition of the gyromagnetic factor is

$$g = 2\omega_{\rm s}/\omega_{\rm c}. \tag{16.107}$$

Comparing (16.100) and (16.105) yields

$$g = \frac{m_{\rm eff}}{m}\widetilde{g}. \tag{16.108}$$

We stress that Eq. (16.108) is nonperturbative in the sense that it is valid for any coupling strength e. In the derivation it is assumed that the external magnetic field is weak, an assumption which certainly holds, since experimentally the radius of gyration is of the order of meters. Equation (16.108) is the g-factor at $p = 0$. At $p \neq 0$, since the Pauli–Fierz model is nonrelativistic, there is a p-dependent g-factor with components parallel and transverse to p.

Under our standard assumptions, g depends analytically on the coupling strength e and it is of interest to obtain the order e^2 correction to $g = 2$ at $e = 0$. For this purpose it is convenient to switch to the dimensionless units of section 19.3. The effective mass is defined through (15.23). Compared to (15.36) there is an extra contribution from the fluctuating magnetic field and one obtains

$$\begin{aligned}\frac{m_{\rm eff}}{m} = 1 &+ \frac{2}{3}e^2\int \mathrm{d}^3k|\widehat{\varphi}(k/\lambda_{\rm c})|^2\Big[k^2\Big(1+\frac{1}{2}|k|\Big)\Big]^{-1}\\ &+ \frac{1}{6}e^2\int \mathrm{d}^3k|\widehat{\varphi}(k/\lambda_{\rm c})|^2\Big[\Big(1+\frac{1}{2}|k|\Big)^3\Big]^{-1} + \mathcal{O}(e^4).\end{aligned} \tag{16.109}$$

Next we have to determine $\widetilde{g}$, which is the sum $\widetilde{g}_1 + \widetilde{g}_2$. $H(0)$ is written as $H(0) = H_0 + eH_1 + \frac{1}{2}e^2H_2$. At $e = 0$, $\psi_{\mathrm{g}+} = \chi_+ \otimes \Omega$, $\sigma_3\chi_+ = \chi_+$, and $\widetilde{g}_1 = 2$, $\widetilde{g}_2 = 0$. Expanding $\psi_{\mathrm{g}+}$ to first order in e as $\psi_{\mathrm{g}+} = \chi_+ \otimes \Omega + (e/2)H_0^{-1}\sigma \cdot B_\varphi\chi_+ \otimes \Omega + \mathcal{O}(e^2)$, we insert in (16.104). For $\widetilde{g}_1$ there is a contribution from the normalization of $\psi_{\mathrm{g}+}$ and one contribution involving $(e^2/4)\langle\chi_+ \otimes \Omega, \sigma \cdot B_\varphi H_0^{-1}\sigma_3 H_0^{-1}\sigma \cdot$

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$B_\varphi \chi_+ \otimes \Omega\rangle_{\mathbb{C}^2 \otimes \mathcal{F}}$. The net result is

$$\frac{1}{2}\widetilde{g}_1 = 1 - \frac{1}{4}e^2 \int \mathrm{d}^3k |\widehat{\varphi}(k/\lambda_c)|^2 \Big[|k|\Big(1 + \frac{1}{2}|k|\Big)^2\Big]^{-1} - \frac{1}{12}e^2 \int \mathrm{d}^3k |\widehat{\varphi}(k/\lambda_c)|^2 \Big[|k|\Big(1 + \frac{1}{2}|k|\Big)^2\Big]^{-1} + \mathcal{O}(e^4). \quad (16.110)$$

For $\widetilde{g}_2$ only one of the two ground states is expanded to order e. Hence one has a contribution proportional to $\langle \chi_+ \otimes \Omega,\ (A_{\varphi 2} H_0^{-1} P_{\mathrm{f}1} H_0^{-1} \sigma \cdot B_\varphi - \sigma \cdot B_\varphi H_0^{-1} P_{\mathrm{f}2} H_0^{-1} A_{\varphi 1}) \chi_+ \otimes \Omega\rangle_{\mathbb{C}^2 \otimes \mathcal{F}}$. The net result is

$$\frac{1}{2}\widetilde{g}_2 = -\frac{1}{3}e^2 \int \mathrm{d}^3k |\widehat{\varphi}(k/\lambda_c)|^2 \Big[|k|\Big(1 + \frac{1}{2}|k|\Big)^2\Big]^{-1}. \quad (16.111)$$

Adding up (16.109), (16.110), and (16.111), the g-factor to order e^2 is given by

$$g = 2\Big(1 + \frac{2}{3}e^2 \int \mathrm{d}^3k |\widehat{\varphi}(k/\lambda_c)|^2 \Big[k^2\Big(1 + \frac{1}{2}|k|\Big)^3\Big]^{-1}\Big) + \mathcal{O}(e^4). \quad (16.112)$$

In Heaviside–Lorentz units $e^2 = 4\pi\alpha$. We also set the sharp cutoff $\widehat{\varphi}(k) = (2\pi)^{-3/2}$ for $|k| \leq \Lambda$, $\widehat{\varphi}(k) = 0$ for $|k| > \Lambda$. Then

$$g = 2\Big(1 + \frac{8}{3}\Big(\frac{\alpha}{2\pi}\Big)\big(1 - (1 + (\Lambda/2\lambda_c))^{-2}\big) + \mathcal{O}(\alpha^2)\Big). \quad (16.113)$$

Clearly $g > 2$, as observed experimentally. It is remarkable that g stays bounded in the limit $\Lambda \to \infty$ and

$$g_\infty = 2\Big(1 + \frac{8}{3}\Big(\frac{\alpha}{2\pi}\Big)\Big) + \mathcal{O}(\alpha^2), \quad (16.114)$$

which is to be compared with $2\big(1 + (\alpha/2\pi)\big) + \mathcal{O}(\alpha^2)$ from fully relativistic QED. Evidently the nonrelativistic Pauli–Fierz model overestimates the contribution from large wave numbers by a factor 8/3. The result (16.114) is satisfactory, since it nourishes the hope that the Pauli–Fierz model makes reasonable predictions even when the ultraviolet cutoff Λ is removed.

Notes and references

Section 16.1

In the old quantum theory classical adiabatic invariants were associated with good quantum numbers (Ehrenfest 1916). Thus the time-adiabatic theorem was an

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important consistency check of the Heisenberg–Schrödinger quantum mechanics (Born 1926; Born and Fock 1928). Kato (1958) proves the adiabatic theorem under the condition that the relevant subspace has finite dimension and is separated by a spectral gap. In fact, the theorem holds in much greater generality than explained in the text. Only a corridor separating the relevant energy band from the rest is needed. The spectrum inside the band can be arbitrary. The error in (16.8) may be improved to any order at the expense of a slight tilt of the subspace $P(\varepsilon t)\mathcal{H}$, as first recognized by Lenard (1959) and further refined by Garrido (1965), Berry (1990), Joye *et al.* (1991), Nenciu (1993), and Joye and Pfister (1994). We refer also to the interesting collection of articles by Shapere and Wilczek (1989). Sjöstrand (1993) discusses the higher-order corrections from the point of view of pseudodifferential operators; compare with section 16.4 and Panati *et al.* (2003a). If $H(t)$ depends analytically on t, the error becomes $\mathrm{e}^{-1/\varepsilon}$, which complements the Landau–Zener formula for almost crossing of eigenvalues (Joye and Pfister 1993). If there is no gap, but a smooth t-dependence as before, the adiabatic theorem still holds (Avron and Elgart 1999; Bornemann 1998; Teufel 2001). The error depends on the context. It can be as small as in (16.8), but in general it will be larger.

Section 16.2

Our discussion of the space-adiabatic limit ignores technical details on purpose. They are supplied in Teufel and Spohn (2002), Spohn and Teufel (2001), and Teufel (2003). Most importantly, since $p_{\mathrm{c}} < \infty$, one needs a local version of the result explained in the text in the following sense. In the limit $\varepsilon \to 0$ the initial state defines a classical probability measure $\rho_{\mathrm{cl}}(\mathrm{d}^3q\,\mathrm{d}^3p)$ on phase space $\mathbb{R}^6$; compare with section 16.5. ρ_{cl} is transported by the classical flow Φ_t with Hamiltonian (16.22) as $\rho_{\mathrm{cl}} \circ \Phi_{-t}$. If ρ_{cl} is supported in $\mathbb{R}^3 \times \{p\,|\,|p| < p_{\mathrm{c}}\}$, then there is a first time t_{hit} at which the support of $\rho_{\mathrm{cl}} \circ \Phi_{-t}$ hits the boundary $\mathbb{R}^3 \times \{p\,|\,|p| = p_{\mathrm{c}}\}$. The approximation through an effective Hamiltonian is valid for times $0 \leq t < \varepsilon^{-1} t_{\mathrm{hit}}$.

Section 16.3

Weyl quantization, the Moyal product, and matrix-valued symbols are discussed in Robert (1987, 1998), Dimassi and Sjöstrand (1999), Martinez (2002), and Panati *et al.* (2003a). The Moyal product is introduced in Moyal (1949).

Section 16.4

The methods explained in this section have a rich history with motivations ranging from singular partial differential equations and Fourier integral operators to the motion of electrons in solids subject to a small magnetic field. Blount (1962a, b, c)

develops a similar scheme for computing effective Hamiltonians and applies it to Bloch electrons and to the Dirac equation. In particular, he computes the second-order symbol h_2. In the solid state physics literature his work is a standard reference, but his method is hardly applied to concrete problems. We refer to the discussion in Panati *et al.* (2003b) for an example in the case of magnetic Bloch bands. Starting from coupled wave equations Littlejohn and Flynn (1991) and Littlejohn and Weigert (1993) develop the technique of unitary operators close to the identity on the level of symbols in the case where the principal symbol is a nondegenerate matrix. They apply their scheme to Born–Oppenheimer-type problems, where $H_0(q, p) = p^2 \mathbb{1} + V(q)$ with $V(q)$ an $n \times n$ matrix. On an abstract level the Born–Oppenheimer approximation is similar to the Pauli–Fierz model with a slowly varying external electrostatic potential only. The role of the invariant subspace is emphasized by Nenciu (1993). The formal power series for the projector $\pi(q, p)$ is constructed by Brummelhuis and Nourrigat (1999) for the Dirac equation, by Martinez and Sordoni (2002) for Born–Oppenheimer-type Hamiltonians and in the general matrix-valued case by Nenciu and Sordoni (2001). Our discussion is based on Panati *et al.* (2003a). The lecture notes by Teufel (2003) give detailed coverage with many examples, including the case of Bloch electrons (Panati *et al.* 2003b). There also a more complete listing of the literature can be found.

Section 16.5

There is a vast literature on semiclassical methods, both on the theoretical physics and on the mathematical side; to mention only a few representatives: Maslov and Fedoriuk (1981), Gutzwiller (1990), and Robert (1987, 1998). These works are mostly concerned with the scalar case. An alternative technique is to employ matrix-valued Wigner functions (Gérard *et al.* 1997; Spohn 2000b). In this approach the adiabatic and semiclassical limits are fused, which is conceptually misleading. Also higher-order corrections are not accessible. An important example is the Dirac equation which has matrix dimension $n = 4$ and degeneracy $\ell = 2$ of, for example, the electron subspace. The adiabatic limit yields the BMT equation of chapter 10, as discussed in Panati *et al.* (2003a). Blount (1962c) computes the next-order correction. It seems to be of interest in accelerator physics (Heinemann and Barber 1999), despite its fairly complicated structure. Yajima (1992) studies the derivation of the BMT equation using WKB methods, which are rather difficult to handle because of the necessity to switch coordinate systems on the Lagrangian manifold.

The classical limit of the free Maxwell field with classical sources is regarded as sort of obvious. An instructive discussion is Thirring (1958) and Sakurai (1986). Photon counting statistics is covered by Carmichael (1999).

Section 16.6

The gyromagnetic ratio of the electron is the most famous and precise prediction of QED with the current value $g_{\text{theor}}/2 = 1.001\,159\,652\,459\,(135)$ as based on an eight-loop computation, see Kinoshita and Sapirstein (1984) for a review. This result compares extraordinarily well with the experimental value $g_{\text{exp}}/2 = 1.001\,159\,652\,193\,(4)$ of van Dyck, Schwinberg and Dehmelt (1986) based on measurements on a single electron in a Penning trap, see also Brown and Gabrielse (1986), and Dehmelt (1990). The nonrelativistic theory yields $g_{\text{non}}/2 = 1.0031$, with no cutoffs. The nonperturbative formula (16.108) seems to be novel and is described in Panati *et al.* (2002b). A rough approximation is provided by Welton (1948). Grotch and Kazes (1977) discuss the g-factor for the Pauli–Fierz model and obtain the second-order result (16.113) through computing energy shifts; compare with section 19.3.5. Surprisingly, they do not stress the obvious point: the g-factor is not too far off the truth even in the limit $\Lambda \to \infty$. After all, the mistrust in QED up to the early 1940s was based mainly on the results being cutoff-dependent and diverging as $\Lambda \to \infty$; see Schweber (1994).

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