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On the theory of the Larmor clock and time delay

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Abstract. Using the time-dependent scattering theory we prove that, in any spatial dimension and for arbitrary spin, the reading of the Larmor clock agrees with the global (Eisenbud–Wigner) time delay in the limit of an infinitesimal magnetic field. We show that convergence is also achieved at fixed energy (without oscillating terms) in the limit where the spatial switching on of the field occurs on a much larger scale than the de Broglie wavelength of the particle. Finally, we investigate the functioning of the spin clock beyond the linear response regime.

1. Introduction

In recent years, the concept of the tunnelling time of a quantum mechanical particle has been the subject of many studies, mainly motivated by the prospect of high speed devices based on tunnelling structures in semiconductors (see the review paper [1] and references therein). One of the proposals (the Larmor clock originally introduced in [2, 3]) is to measure the duration of a scattering event by means of the precession of a spin in a weak homogeneous magnetic field. Heuristically, a constant magnetic field applied to the region where the scattering takes place will set the spin into uniform rotation, and so the total precession angle will be proportional to the time elapsed during the collision process.

This picture has been substantiated in [4] by a detailled study of the motion of a one-dimensional wave packet through a potential barrier in the presence of a magnetic field. A freely moving wave packet first enters a region where a uniform magnetic field is applied, far away from the scattering centre. Then, it undergoes the scattering process in presence of the field, and finally the scattered waves leave the field region. By retaining in the phase of the wavefunction only the contributions that are linear in the field, the authors show that the reading of the clock agrees with the Eisenbud–Wigner time delay (see [5] and references therein, and [6], ch 7-2), i.e. the derivative of the phase shift with respect to energy (also called classic or asymptotic phase time).

In [7], the authors point out the intimate relation between the linear response of the scattering operator to an additional external perturbation and the sojourn (or dwell) time for a particle in some spatial region. With this relation they can easily establish that the (infinitesimal) rotation of the spin of a neutral particle is proportional to the sojourn time, so the difference between the precession angles relative to the interacting and free motion is proportional to the difference of the

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corresponding sojourn times. Since the latter quantity converges to the Eisenbud–Wigner time delay for large spatial regions [5, 6], it was found that the reading of the clock coincides with the classical phase time for infinitesimal fields. All the considerations in [7] are restricted to one dimension and rely on formulae for the stationary scattering states formalism.

The purpose of this work is twofold. To begin with we generalize in sections 2 and 3 the result of [7] to all space dimensions $d = 1,2,3$ and arbitrary spin s (for a neutral or charged particle). We feel that the connection between the linear response of the S-operator and the sojourn time can be exhibited more simply and with greater generality by using the methods of time-dependent scattering theory†. We find that in any dimension d the reading of the Larmor clock constituted by a (neutral or charged) particle with spin s in an infinitesimal field is always given by the Eisenbud–Wigner time delay, provided that one works with wave packets and extends the field region to the whole $\mathbb{R}^d$.

Then, in section 4, we again consider the problem from the viewpoint of time-independent scattering theory with spherically symmetric potentials. When the magnetic field is switched on abruptly in space (i.e. a step function), it was noted a long time ago that the convergence to the Eisenbud–Wigner time delay is not achieved at fixed energy because of the existence of oscillating terms. These oscillating terms, the physical origin of which is the interference of reflected waves at the boundaries of the magnetic field, have been the subject of several discussions in the literature (see for example [4, 9, 10]). In a good spin clock, the magnetic field should be responsible for the precession of the spin, but should not cause additional perturbative effects on the orbital degrees of freedom, which would interfere with those due to the scattering process under investigation. Our point here is that this can be achieved if the magnetic field is produced by a macroscopic device with the following properties: it extends to a region of much larger size than that of the (microscopic) range of the scattering potential and its spatial switching on occurs on a much larger scale than the de Broglie wavelength of the scattered particle. With such a model of the magnetic field (precisely defined in section 4) we prove the convergence to the Eisenbud–Wigner time delay at fixed energy when the field covers the whole space and its gradient becomes vanishingly small in the transition region.

So far, all the above results have been obtained in the framework of the linear response theory. In section 5 we address the problem of the functioning of the spin-clock, for a neutral particle, beyond the linear response regime for the case of a spherically symmetric potential. With the same model as in section 4 we show that, in the scattering operator, the magnetic field results asymptotically in a phase factor depending only on the energy and the spin component, but not on the angular momentum. Consequently, the magnetic field is transparent in the sense that it causes no deflection of the particle. Then we find in a weak, but not necessarily infinitesimal field, when there is no dispersion in energy, that the measure of the rotation angle of a spin-$\frac{1}{2}$ particle after the scattering process (relative to the free motion) still provides relevant information, which can be expressed in terms of finite energy differences of phase shifts. Only the linear term, which agrees with the energy derivative of the phase shifts found previously, has the legitimate interpretation of the time delay of the scattering process. Finally, when the incoming state has some non-negligible

† After submission of this work, the authors of [7] kindly informed us of their forthcoming paper [8] where the same generalization is considered.

dispersion in energy, one observes an attenuation of the outgoing spin vector, due to a spatial splitting, inside the magnetic field region, of the up and down parts of the incoming wave packet (relative to the field direction).

2. Response of a scattering system to a perturbation

We consider a quantum particle in d dimensions ($d = 1, 2, 3$), with kinetic energy $H_0 = -\hbar^2\Delta/2m$ (Δ is the Laplacian in $\mathbb{R}^d$), which is scattered by a potential $\nu(\boldsymbol{x}) + \lambda\omega(\boldsymbol{x})$, where $\lambda\omega(\boldsymbol{x})$ is a perturbation of $\nu(\boldsymbol{x})$; $\omega(\boldsymbol{x})$ is supposed to be bounded and with compact support, λ is a coupling constant in the range $|\lambda| \leqslant \lambda_0 < \infty$. We denote by $U_t = \exp(-\mathrm{i}H_0 t/\hbar)$ and $V_t(\lambda) = \exp(-\mathrm{i}H(\lambda)t/\hbar)$ the evolution groups generated by H_0 and $H(\lambda) = H_0 + \nu + \lambda\omega$. We assume that for each λ in the range $|\lambda| \leqslant \lambda_0$, $(H_0, H(\lambda))$ forms a complete scattering system [6] with wave operators

$$\Omega_\pm(\lambda) = \operatorname*{s-lim}_{t\to\infty} \Omega_{\pm,t}(\lambda) \qquad \Omega_{\pm,t}(\lambda) = V^\dagger_{\pm t}(\lambda)U_{\pm t} \tag{2.1}$$

such that Range $\Omega_+(\lambda) =$ Range $\Omega_-(\lambda)$. The scattering operator is defined by

$$S(\lambda) = \Omega^\dagger_+(\lambda)\Omega_-(\lambda) = \operatorname*{s-lim}_{t\to\infty} S_t(\lambda) \tag{2.2}$$

with

$$S_t(\lambda) = \Omega^\dagger_{+,t}(\lambda)\Omega_{-,t}(\lambda) = U^\dagger_t V_{2t}(\lambda)U_{-t}. \tag{2.3}$$

We would like to compute the linear response of the scattering operator to the perturbation $\lambda\omega$. For this we note that $S_t(\lambda)$ can be easily expanded around $\lambda = 0$, using the usual time-dependent perturbation (Dyson's) series at first order in λ (the series converge for a bounded ω)

$$S_t(\lambda) = \Omega^\dagger_{+,t}\left(1 - \frac{\mathrm{i}\lambda}{\hbar}\int_{-t}^{t} \mathrm{d}s\, V^\dagger_s\,\omega\, V_s\right)\Omega_{-,t} + \mathrm{O}(\lambda^2) \tag{2.4}$$

giving

$$\frac{\partial}{\partial\lambda}S_t(\lambda)\big|_{\lambda=0} = -\frac{\mathrm{i}}{\hbar}\Omega^\dagger_{+,t}\left(\int_{-t}^{t}\mathrm{d}s\, V^\dagger_s\omega V_s\right)\Omega_{-,t}. \tag{2.5}$$

In (2.4) and (2.5), the operators $V_t \equiv V_t(0)$, $\Omega_t \equiv \Omega_t(0)$ and $S_t \equiv S_t(0)$ refer to the unperturbed scattering system $(H_0, H = H_0 + \nu)$. Permuting the infinite time limit and the derivative with respect to λ we obtain formally from (2.1), (2.2) and (2.5) the linear response formula

$$\frac{\partial}{\partial\lambda}S(\lambda)\Big|_{\lambda=0} = \operatorname*{n-lim}_{t\to\infty}\frac{\partial}{\partial\lambda}S_t(\lambda)\Big|_{\lambda=0} = -\frac{\mathrm{i}}{\hbar}\Omega^\dagger_+\left(\int_{-\infty}^{\infty}\mathrm{d}s\, V^\dagger_s\omega V_s\right)\Omega_-. \tag{2.6}$$

Using $S^\dagger\Omega^\dagger_+ = \Omega^\dagger_-$ one can also write (2.6) in the form

$$\mathrm{i}\hbar S^\dagger\frac{\partial}{\partial\lambda}S(\lambda)\Big|_{\lambda=0} \equiv T(\omega) \tag{2.7}$$

with

$$T(\omega) = \Omega_-^\dagger \left(\int_{-\infty}^{\infty} \mathrm{d}s\, V_s^\dagger \omega V_s \right) \Omega_- = \int_{-\infty}^{\infty} \mathrm{d}s\, U_s^\dagger \Omega_-^\dagger \omega \Omega_- U_s \tag{2.8}$$

where the last equality follows from the intertwining relations $V_t \Omega_\pm = \Omega_\pm U_t$. In appendix A we give conditions for the validity of formulae (2.6)–(2.8). They hold for sufficiently regular short-ranged potentials on a dense set of states $\mathcal{D}$ and the limit (2.6) has to be understood in the weak sense. If $\omega(\boldsymbol{x}) = \chi_R(\boldsymbol{x})$ is the characteristic function of the sphere of radius R, we see that

$$(\varphi, T(\chi_R)\varphi) = \int_{-\infty}^{\infty} \mathrm{d}s\, \| \chi_R V_s \psi \|^2 \qquad \psi = \Omega_- \varphi \qquad \varphi \in \mathcal{D} \tag{2.9}$$

is the sojourn time in the sphere of the particle scattered by the potential ν and with incoming state φ.

3. The Larmor clock

A neutral particle of spin s is scattered by the potential $\nu(\boldsymbol{x})$ and submitted to a static magnetic field $\boldsymbol{B}(\boldsymbol{x}) = (0, 0, B_z(\boldsymbol{x}))$ applied in the z-direction on the region where the scattering takes place. We write the magnetic energy $-\mu B_z(\boldsymbol{x})\Sigma_z$ (Σ_z is the z-component of the spin operator and μ the magnetic moment) in the form $\lambda\omega(\boldsymbol{x})\Sigma_z$ where $\omega(\boldsymbol{x})$ is a dimensionless local bounded function whose support determines the spatial region where the field is applied and λ is a measure of the field strength (λ has the dimension of a frequency). Specific forms of the cut-off function $\omega(\boldsymbol{x})$ will be discussed in the next section. The total Hamiltonian, still denoted by $H(\lambda)$, is $H(\lambda) = H_0 + \nu + \lambda\omega\Sigma_z$. The scattering system $(H_0, H(\lambda))$ has wave and scattering operators acting on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^{2s+1}$ still denoted by $\Omega_\pm(\lambda)$ and $S(\lambda)$.

Let $\phi = \varphi \otimes \chi$ be a normalized incoming state with orbital wavefunction $\varphi \in \mathcal{D}$, spin state χ and Σ a spin operator (Σ may be, for example, a combination $\Sigma_\pm = \Sigma_x \pm \mathrm{i}\Sigma_y$). The average value of Σ after the scattering process, denoted by $\langle\Sigma\rangle^{\mathrm{out}}(\lambda)$, is given by

$$\langle\Sigma\rangle^{\mathrm{out}}(\lambda) = (S(\lambda)\phi, \Sigma S(\lambda)\phi). \tag{3.1}$$

The response of $\langle\Sigma\rangle^{\mathrm{out}}(\lambda)$ to an infinitesimal field can be computed from (2.7) and (2.8) with ω replaced by $\omega\Sigma_z$. Using the fact that $S \equiv S(0)$ commute with the spin operators and $T^\dagger(\omega\Sigma_z) = T(\omega\Sigma_z)$, we find

$$\begin{aligned} \frac{\partial}{\partial\lambda}\langle\Sigma\rangle^{\mathrm{out}}(\lambda)\big|_{\lambda=0} &= \left(\frac{\partial S}{\partial\lambda}(\lambda)\big|_{\lambda=0}\phi, \Sigma S\phi\right) + \left(S\phi, \Sigma\frac{\partial S}{\partial\lambda}(\lambda)\big|_{\lambda=0}\phi\right) \\ &= \frac{\mathrm{i}}{\hbar}\,(\phi, [T(\omega\Sigma_z), \Sigma]\phi) \\ &= \frac{\mathrm{i}}{\hbar}\,(\chi, [\Sigma_z, \Sigma]\chi)(\varphi, T(\omega)\varphi) \end{aligned} \tag{3.2}$$

where $[\Sigma_z, \Sigma]$ denotes the commutator between Σ_z and Σ. If, for instance, we set $\Sigma = \Sigma_\pm$ and $\omega = \chi_R$ in (3.2), we deduce that up to the first order in λ

$$\langle\Sigma_\pm\rangle^{\mathrm{out}}(\lambda) = (1 \pm \mathrm{i}\lambda(\varphi, T(\chi_R)\varphi))\langle\Sigma_\pm\rangle^{\mathrm{in}} + \mathrm{O}(\lambda^2) \tag{3.3}$$

which means that during the scattering process, the spin vector $\langle\Sigma\rangle^{\text{in}} = (\langle\Sigma_x\rangle^{\text{in}}, \langle\Sigma_y\rangle^{\text{in}})$ has accomplished an infinitesimal rotation of angle

$$\alpha_\varphi(\chi_R, \lambda) = \lambda(\varphi, T(\chi_R)\varphi) + \mathrm{O}(\lambda^3) \tag{3.4}$$

given by the product of the Larmor frequency of the field with the sojourn time of the particle in the region $|x| \leqslant R$ where the field is applied. If we subtract from $\alpha_\varphi(\chi_R, \lambda)$ the angle which would occur if the potential ν is set equal to zero and then take the limit of an infinitly extended space region, we obtain

$$\begin{aligned}\lim_{R\to\infty} \frac{\partial}{\partial\lambda} \left(\alpha_\varphi(\chi_R, \lambda) - \alpha_{0\varphi}(\chi_R, \lambda)\right)\Big|_{\lambda=0} &= \lim_{R\to\infty} \left((\varphi, T(\chi_R)\varphi) - (\varphi, T_0(\chi_R)\varphi)\right) \\ &= (\varphi, \tau\varphi).\end{aligned} \tag{3.5}$$

In (3.5), the quantities with an index 0 refer to the system $(H_0, H_0 + \chi_R\Sigma_z)$ without scattering potential ν and τ is the Eisenbud–Wigner time delay operator with energy shell components [6, ch 7-2]

$$\tau_E = -\mathrm{i}\hbar S_E^\dagger \frac{\partial S_E}{\partial E} \tag{3.6}$$

where S_E is the scattering operator of the system (H_0, H) at fixed energy E (i.e. a unitary operator acting on $L^2(\sigma^{d-1})$, the square integrable functions of the surface σ^{d-1} of the unit sphere in $\mathbb{R}^d$). More generally, for any spin observable Σ, one obtains from (3.2) and (3.5)

$$\lim_{R\to\infty} \frac{\partial}{\partial\lambda} \left(\langle\Sigma\rangle^{\text{out}}(\lambda) - \langle\Sigma\rangle_0^{\text{out}}(\lambda)\right)\big|_{\lambda=0} = \frac{\mathrm{i}}{\hbar}(\chi, [\Sigma_z, \Sigma]\chi)(\varphi, \tau\varphi). \tag{3.7}$$

The existence of the infinite space limit, (3.5) and (3.7) for suitable wave packets φ, has been established in a number of works (e.g. [11, 12] for spherically symmetric potentials and [13] for potentials which are not necessarly rotation invariant; in the context of one-dimensional tunnelling, see [4, 14] and also [7] where the corresponding linear response relation (2.6) can be found). Notice that the existence of the limit (3.5) does not require the choice $\omega(\boldsymbol{x}) = \chi_R(\boldsymbol{x})$ (corresponding to an abrupt spatial switching on of the magnetic field), but also holds for sequences $\omega(\boldsymbol{x}) = \omega_R(\boldsymbol{x})$ of smooth spherically symmetric cut-off functions, corresponding to a smooth switching on of the field, such that $\lim_{R\to\infty}\omega_R(\boldsymbol{x}) = 1$ (e.g. [13, 15, 16]). In any case there is a large class of potentials ν and cut-off functions ω_R for which the limit (3.5) holds. We therefore see that the linear response to a magnetic field of a scattered neutral particle in d dimensions with arbitrary spin s gives the Eisenbud–Wigner time delay in the sense of formulae (3.5) and (3.7). These formulae involve three limiting procedures: the infinite time limit (2.2), the linearization with respect to the field strength and the extension of the field action to the whole space $\mathbb{R}^d$. The infinite time limit is required as usual to have a complete scattering event. The need for the existence of the last limit is justified by the request that the spin clock should provide intrinsic information on the scattering process, independent of the size of the region and the manner in which the field is applied. This limit cannot be permuted with the two first ones. If the field is taken to be constant on $\mathbb{R}^d$ at first (i.e. $\omega(\boldsymbol{x}) = 1$ in

$H(\lambda)$), it is clear that the spin decouples from the orbital degrees of freedom and is not affected by the scattering process.

We have considered, for simplicity, the case of a neutral particle. If the particle has a charge q, the formulae (3.2)–(3.5) remain the same. Indeed, the total Hamiltonian for a charged particle has the form

$$H(\lambda) = H_0 + \lambda\omega\Sigma_z + \frac{q}{2m}(\boldsymbol{P}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{P}) + \frac{q^2}{2m}|\boldsymbol{A}|^2 \tag{3.8}$$

where $\boldsymbol{P}$ is the momentum and $\boldsymbol{A}(\boldsymbol{x})$ is the potential vector ($\boldsymbol{B} = \boldsymbol{\nabla}\wedge\boldsymbol{A}$). Thus $\lambda\omega$ has to be replaced in the linear response formula (2.6) by the part of the interaction which is linear in the field strength, i.e. by $\lambda\omega\Sigma_z + (q/2m)(\boldsymbol{P}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{P})$, but the contribution to (3.2) of this additional term vanishes since it commutes with the spin operators.

It is worth emphasizing that in (3.1) and the subsequent discussion, we have considered the average outgoing spin without the specification of any scattering direction. In particular, since Σ_z is a constant of the motion, it commutes with $S(\lambda)$ and thus $\langle\Sigma_z\rangle^{\mathrm{out}}(\lambda) = \langle\Sigma_z\rangle^{\mathrm{in}}$.

Let P_Ω be the projection on some solid angle Ω in momentum space. Then, one can also consider the average spin when the outgoing particle is found in Ω (in one dimension, the spin associated with the transmitted or reflected waves separately) i.e.

$$\langle\Sigma P_\Omega\rangle^{\mathrm{out}}(\lambda) = (S(\lambda)\phi, \Sigma P_\Omega S(\lambda)\phi). \tag{3.9}$$

Since P_Ω does not commute with the scattering operator, a change of the z-component of the spin is found when the particle is detected in Ω. Working out the linear response term in this case, we obtain

$$\langle\Sigma_z P_\Omega\rangle^{\mathrm{out}}(\lambda) = \langle\Sigma_z\rangle^{\mathrm{in}}(\varphi, S^\dagger P_\Omega S\varphi) + \frac{2\lambda}{\hbar}\langle\Sigma_z^2\rangle^{\mathrm{in}}\mathrm{Im}(\varphi, S^\dagger P_\Omega S T(\omega)\varphi) + \mathrm{O}(\lambda^2). \tag{3.10}$$

In the context of one-dimensional scattering, this observation led Büttiker [17] to associate transmission and reflection times with this change in the z-component of the spin. The definition and possible interpretation of these times are also discussed in [18]. In the present paper, we shall only be interested in the total outgoing spin (3.1) and its relation to the global (Eisenbud–Wigner) time delay.

4. The Larmor clock on the energy shell: the smooth switching on of the magnetic field

In the preceding section, we have seen that in order to observe a non-trivial effect of the scattering on the spin motion it is necessary for the particle to enter and leave the field region, however weak the field is and however large the region is. In principle, the dynamics of the particle should depend on the nature of the transition region for the field. It is a non-trivial result in the theory of the Eisenbud–Wigner time delay that, when dealing with wave packets and ultimately extending the field to the whole space, the limit (3.5) is in fact independent of the details of this transition region (see references quoted after (3.7)).

The situation is, however, very different when one works in the formalism of stationary scattering theory at fixed energy E (without averaging the energy of the packet). Let $\omega(r)$ be a spherically symmetric spatial cut-off function, and let $S_E(\lambda)$ denote the scattering operator at fixed energy E for the system $(H_0, H(\lambda))$ described in section 2 ($S_E(\lambda)$ acts on $L^2(\sigma^{d-1})$). In the rest of this section we shall mainly be concerned with the three-dimensional scattering problem with a rotation invariant potential $\nu(r)$. Then, $S_E(\lambda)$ is diagonal in the basis $|l, m\rangle$ of eigenvectors of the orbital momentum, with matrix elements

$$\langle \ell, m|S_E(\lambda)|\ell, m\rangle = S_E^\ell(\lambda) = \mathrm{e}^{2\mathrm{i}\delta_E^\ell(\lambda)} \tag{4.1}$$

expressed in terms of the phase shifts $\delta_E^\ell(\lambda)$ in the usual way.

The response equivalent to (2.6) in the stationary formalism follows from the observation that the perturbed and unperturberd phase shifts $\delta_E^\ell(\lambda)$ and $\delta_E^\ell \equiv \delta_E^\ell(0)$ are related by [19, ch X, section 17]

$$\sin(\delta_E^\ell(\lambda) - \delta_E^\ell) = -\frac{2m\lambda}{\hbar^2 k}\int_0^\infty \mathrm{d}r\, u_E^\ell(r,\lambda)\omega(r)u_E^\ell(r) \qquad \hbar k = \sqrt{2mE} \tag{4.2}$$

where $u_E^\ell(r,\lambda)$ is the regular solution of the radial Schrödinger equation

$$\left(\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + E - \nu(r) - \lambda\omega(r) - \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)u_E^\ell(r,\lambda) = 0 \tag{4.3}$$

with asymptotic form

$$u_E^\ell(r,\lambda) = \sin\left(kr - \frac{\ell\pi}{2} + \delta_E^\ell(\lambda)\right) + \mathrm{O}(r^{-1}) \tag{4.4}$$

as $r \to \infty$ and $u_E^\ell(r)$ is the corresponding solution of (4.3) with $\lambda = 0$. Differentiating (4.2) with respect to λ at $\lambda = 0$ gives

$$\begin{aligned} \mathrm{i}\hbar S_E^{\ell\,*} \frac{\partial}{\partial\lambda}S_E^\ell(\lambda)\Big|_{\lambda=0} &= -2\hbar\frac{\partial}{\partial\lambda}\delta_E^\ell(\lambda)\Big|_{\lambda=0} \\ &= \frac{4m}{\hbar k}\int_0^\infty \mathrm{d}r\,\omega(r)(u_E^\ell(r))^2 \equiv T_E^\ell(\omega) \end{aligned} \tag{4.5}$$

which are the energy shell and orbital momentum components of the operator (2.7). In particular, if $\omega(r) = \chi_R(r)$ (the characteristic function of the sphere of radius R), one recovers the well known expression of the sojourn time at fixed energy [5, 10]

$$T_E^\ell(\chi_R) = \frac{4m}{\hbar k}\int_0^R \mathrm{d}r\,(u_E^\ell(r))^2. \tag{4.6}$$

If the Hamiltonian of section 3 is considered (with spin included), the corresponding energy shell scattering operator $S_E(\lambda)$ is diagonal in the basis of eigenvectors of Σ_z and is simply obtained replacing ω in (4.2) and (4.3) by $\Sigma_z\omega$. In particular, the stationary representation of (3.2) is

$$\frac{\partial}{\partial\lambda}\langle\Sigma\rangle_{E,\ell}^{\mathrm{out}}(\lambda)\Big|_{\lambda=0} = \frac{\mathrm{i}}{\hbar}(\chi, [\Sigma_z, \Sigma]\chi)T_E^\ell(\chi_R). \tag{4.7}$$

The asymptotic behaviour of $T_E^\ell(\chi_R)$ for large R has been studied in several papers (e.g. [10] in the context of sojourn times and [2, 3] in connection with the spin clock) and is given by

$$T_E^\ell(\chi_R) = \frac{2mR}{\hbar k} + 2\hbar\frac{\partial \delta_E^\ell}{\partial E} - \frac{\hbar}{2E}\sin(2kR - \ell\pi + 2\,\delta_E^\ell) + \mathrm{o}(1). \tag{4.8}$$

An important point here is the occurrence of oscillating terms with R as $R \to \infty$. Because of these, the difference

$$T_E^\ell(\chi_R) - T_{0E}^{\,\ell}(\chi_R) = 2\hbar\frac{\partial \delta_E^\ell}{\partial E} - \frac{\hbar}{2E}[\sin(2kR-\ell\pi+2\,\delta_E^\ell) - \sin(2kR-\ell\pi)] + \mathrm{o}(1) \tag{4.9}$$

between the full sojourn time $T_E^\ell(\chi_R)$ and the free sojourn time $T_{0E}^{\,\ell}(\chi_R)$ (obtained by setting $\delta_E^\ell = 0$ in (4.8)) does not converge at fixed energy as $R \to \infty$ (the oscillating terms do not compensate). This is not in contradiction with the existence of the limit (3.5) for wave packets; when (4.8) is averaged over a smooth energy distribution, the oscillating contribution vanishes by the Riemann–Lebesgue lemma. As a consequence the limit (3.5) is not uniform with respect to the choice of the incoming packet; the better the energy definition of the incoming beam, the wider the field region must be. In fact the oscillating terms in (4.8) have a clear physical origin which is discussed in [9] (three-dimensional scattering) and [4] (one-dimensional problem). They result from interferences due to reflected waves at the sharp frontiers of the magnetic field (described as a step potential). These interference terms remain at the linear order in the field. It has been argued that these terms are 'spurious' in the sense that they do not pertain only to the scattering process by the potential ν under investigation, but originate in the boundaries of the magnetic field; thus they have to be disregarded in one way or another.

As we have already emphasized, the particle has to enter and leave the field region and the physical effects of the transition region (if there are some) have to be taken into account in the theory of the Larmor clock; in principle, they cannot be observationally disentangled from those due to the scattering potential ν alone. To our knowledge, the existing literature has only discussed the abrupt switching on of the field (step function) and the resulting oscillating terms in (4.8). This switching on, which idealizes a situation where the field strength changes on a much smaller scale than the de Broglie wavelength of the particle, is admittedly not very realistic if the field is supposed to be produced by a macroscopic device. In this case it is more legitimate to assume that in the transition region the field variation occurs on distances much larger than the de Broglie wavelength of the particle. We model this situation with a cut-off function $\omega_R(r)$ such that

$$\omega_R(r) = \begin{cases} 1 & r \leqslant R \\ g\left(\dfrac{r-R}{\rho}\right) & r > R \end{cases} \tag{4.10}$$

where $g(r)$ is a twice continuously differentiable function with compact support, $0 \leqslant g(r) \leqslant 1$ and $g(0) = 1$. Clearly $\mathrm{d}\omega_R(r)/\mathrm{d}r = \mathrm{O}(\rho^{-1})$ for $r > R$, so ρ^{-1} is a measure of the size of the field gradient in the transition region. We have the following result.

Proposition 1. Assume that the potential $\nu(r)$ fulfils the condition

$$\int_r^\infty \mathrm{d}s\, s|\nu(s)| = N(r) < \infty \qquad 0 \leqslant r < \infty. \tag{4.11}$$

Then, for any fixed ℓ and $E > 0$, we have

$$-2\hbar \frac{\partial}{\partial\lambda}\delta_E^\ell(\lambda)\bigg|_{\lambda=0} = T_E^\ell(\omega_R) = \frac{2m}{\hbar k}\int_0^\infty \mathrm{d}r\, \omega_R(r)$$
$$+ 2\hbar\frac{\mathrm{d}\delta_E^\ell}{\mathrm{d}E} + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}) + \mathrm{O}(N(R)). \tag{4.12}$$

Proof. Since $u_E^\ell(r)$ verifies (4.3) (with $\lambda = 0$), one has the identity

$$(u_E^\ell(r))^2 = \frac{\mathrm{d}}{\mathrm{d}r} h_E^\ell(r) \tag{4.13}$$

with

$$h_E^\ell(r) = \frac{\hbar^2}{2m}\left(\frac{\partial u_E^\ell}{\partial r}\frac{\partial u_E^\ell}{\partial E} - u_E^\ell \frac{\partial^2 u_E^\ell}{\partial r \partial E}\right)(r). \tag{4.14}$$

It is shown in appendix B that under the condition (4.11), $h_E^\ell(r)$ has asymptotic behaviour as $r \to \infty$

$$h_E^\ell(r) = \frac{r}{2} + \frac{\hbar^2 k}{2m}\frac{\mathrm{d}\delta_E^\ell}{\mathrm{d}E} - \frac{1}{4k}\sin(2kr - \ell\pi + 2\delta_E^\ell) + \mathrm{O}(r^{-1}) + \mathrm{O}(N(r)). \tag{4.15}$$

Since $h_E^\ell(0) = 0$ ($u_E^\ell(r)$ is the regular solution of (4.3)) and $\omega_R(r)$ is constant for $r \leqslant R$, an integration by parts of (4.5) gives

$$\begin{aligned} T_E^\ell(\omega_R) &= -\frac{4m}{\hbar k}\int_R^\infty \mathrm{d}r\, g'\left(\frac{r-R}{\rho}\right) h_E^\ell(r) \\ &= -\frac{4m}{\hbar k}\int_0^\infty \mathrm{d}r\, g'(r) h_E^\ell(\rho r + R) \end{aligned} \tag{4.16}$$

where $g'(r) = \mathrm{d}g(r)/\mathrm{d}r$. For R large enough we can insert in (4.16) the asymptotic behaviour (4.15). After an integration by parts of the linear term in r and using $g(0) = 1$, we obtain

$$T_E^\ell(\omega_R) = \frac{2mR}{\hbar k} + \frac{2m\rho}{\hbar k}\int_0^\infty \mathrm{d}r\, g(r) + 2\hbar\frac{\mathrm{d}\delta_E^\ell}{\mathrm{d}E}$$
$$+ \frac{\hbar}{2E}\int_0^\infty \mathrm{d}r\, g'(r)\sin(2k\rho r + 2kR - \ell\pi + 2\delta_E^\ell)$$
$$+ \frac{\hbar}{2E}\int_0^\infty \mathrm{d}r\, g'(r)\left(\mathrm{O}\left(\frac{1}{\rho r + R}\right) + \mathrm{O}(N(\rho r + R)\right). \tag{4.17}$$

Since $(\rho r + R)^{-1} < R^{-1}$, the last term is $\mathrm{O}(1/R) + \mathrm{O}(N(R))$ for all ρ. Moreover, after an integration by parts, we find that the fourth term in (4.17) is less than

$$\left(\frac{1}{k\rho}\right)\frac{\hbar}{4E}\left(|g''(0)| + \int_0^\infty \mathrm{d}r\, |g''(r)|\right) = \mathrm{O}(\rho^{-1}) \tag{4.18}$$

uniformly with respect to R. Finally, the sum of the two first terms of (4.17) equals $(2m/\hbar k)\int_0^\infty \mathrm{d}r\,\omega_R(r)$ and this proves (4.12).

We now see that

$$\lim_{\substack{R\to\infty\\ \rho\to\infty}} (T_E^\ell(\omega_R) - T_{0E}^{\ \ell}(\omega_R)) = 2\hbar\,\frac{\mathrm{d}\delta_E^\ell}{\mathrm{d}E} \tag{4.19}$$

for each E and ℓ fixed. Because of the smooth transition region (in the sense $k\rho \gg 1$), there are no more reflections at the boundaries of the field and we obtain the expected limit (3.6).

The common divergent term (the first term of (4.12)) is a purely classical quantity. It can be written as $\int_{-\infty}^{\infty} \mathrm{d}s\,\omega_R(s/v)$, i.e. the time needed by a classical particle of velocity $v = \hbar k/m$ to cross the field region along its diameter, weighted by the function ω_R.

It is worth noting that if $\omega_R(r)$ is assumed to be infinitely differentiable (i.e. $g(r)$ is infinitely differentiable with vanishing derivatives at $r = 0$), then the correction due to the transition region (the fourth term of (4.17)) vanishes faster than any power of the field gradient ρ^{-1}. On the other hand, if one lets $\rho \to 0$, ω_R approaches the step function χ_R and one recovers from (4.17) the result (4.8) with oscillating terms.

The present analysis can be extended to potentials ν which are not necessarily rotation invariant. For this one can follow the method of [20], replacing the characteristic function of the sphere by our ω_R (4.10). Then, one obtains the result of the main theorem of [20] as $R \to \infty$, $\rho \to \infty$ without using the somewhat artificial spatial averaging procedure introduced there.

5. The spin scattering beyond the linear response

In this section, we consider the scattering of a neutral particle in a weak (but not necessarily infinitesimal) field. To do this, we first study the scattering, at fixed energy $E > \lambda$ and angular momentum ℓ, by the potential $\nu + \lambda\omega_R$ where ω_R is as in (4.10). We shall show that in the limit $R \to \infty$, $\rho \to \infty$, the matrix elements $S_E^\ell(\lambda)$ factorize into a product of two terms, one due to the crossing of the region where $\lambda\omega_R$ acts and the other one due to the scattering by the potential ν at energy $E - \lambda$. Equivalently, the effects of the potentials ν and $\lambda\omega_R$ become additive in the phase shifts $\delta_E^\ell(\lambda)$.

Proposition 2. Let $\omega_R(r)$ be defined as in (4.10). Assume that there exist $a > 0$ such that $\int_0^a \mathrm{d}r\,r|\nu(r)| < \infty$ and for $r > a$, $\nu(r)$ is twice continuously differentiable and $\nu(r)$, $\nu'(r)$, $\nu''(r)$ are $\mathrm{O}(r^{-\eta})$, $\eta > 2$. Then, for any fixed ℓ, $E > 0$ and $\lambda < E$, we have

$$\delta_E^\ell(\lambda) = \int_0^\infty \mathrm{d}r\,(\kappa(r) - k) + \delta_{E-\lambda}^\ell + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}) \tag{5.1}$$

where $\hbar\kappa(r) = \sqrt{2m(E - \lambda\omega_R(r))}$ and δ_E^ℓ are the phase shifts of the scattering system $(H_0, H_0 + \nu)$.

Proof. Throughout all the proof we set $R > a$. Given ℓ, $\lambda < E$ and $\varepsilon > 0$, there exist R sufficiently large such that (we recall that $0 \leqslant \omega_R(r) \leqslant 1$)

$$\gamma(r) \equiv \nu(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + \lambda\omega_R(r) \leqslant E - \varepsilon \qquad r \geqslant R. \tag{5.2}$$

If $r \geqslant R$, we write the solution of (4.3) in the form (dropping now the indices ℓ, E)

$$u(r) = C_+(r)f_+(r) + C_-(r)f_-(r) \tag{5.3}$$

$$u'(r) = \mathrm{i}\,k(r)\left(C_+(r)f_+(r) - C_-(r)f_-(r)\right) \tag{5.4}$$

where $u'(r) = \mathrm{d}u(r)/\mathrm{d}r$,

$$\hbar k(r) = \sqrt{2m(E-\gamma(r))} \geqslant \sqrt{2m\varepsilon} > 0 \tag{5.5}$$

and $f_\pm(r)$ has the WKB form

$$f_\pm(r) = \frac{1}{\sqrt{k(r)}}\exp\left(\pm\mathrm{i}\int_R^r \mathrm{d}s\,k(s)\right). \tag{5.6}$$

It is not difficult to check that $u(r)$ verifies (4.3) if and only if the functions $C_\pm(r)$ obey the first-order differential system

$$C'_\pm(r) = C_\mp(r)\frac{k'(r)}{2k(r)}\exp\left(\mp 2\mathrm{i}\int_R^r \mathrm{d}s\,k(s)\right) \tag{5.7}$$

with initial conditions determined by the continuity of $u(r)$ and $u'(r)$ at $r = R$

$$C_\pm(R) = \tfrac{1}{2}\left((k(R))^{1/2}u(R) \mp \mathrm{i}\,(k(R))^{-1/2}u'(R)\right). \tag{5.8}$$

For $r \leqslant R$, we have $\lambda\omega_R(r) = \lambda$, thus $u(r) = u^\ell_{E-\lambda}(r)$ is the regular stationary solution of the radial equation with potential $\nu(r)$ and energy $E - \lambda$. Hence it has the asymptotic behaviour

$$u(R) = u^\ell_{E-\lambda}(R) = A\sin(\kappa R - \ell\pi/2 + \delta^\ell_{E-\lambda}) + \mathrm{O}(R^{-1}) \tag{5.9}$$

$$u'(R) = \left(u^\ell_{E-\lambda}\right)'(R) = A\kappa\cos(\kappa R - \ell\pi/2 + \delta^\ell_{E-\lambda}) + \mathrm{O}(R^{-1}) \tag{5.10}$$

where $\hbar\kappa = \sqrt{2m(E-\lambda)}$ and A is a constant to be determined later. We observe that, according to (5.2) and (5.5), one has

$$k(r) = \kappa(r) + \mathrm{O}(r^{-2}) \qquad r \geqslant R \tag{5.11}$$

with $\kappa(R) = \kappa$ and $\kappa(r) = k$ for r sufficiently large (since $\omega_R(r)$ has compact support). Combining (5.9), (5.10) and (5.11) in (5.8) gives

$$C_\pm(R) = \pm A\frac{\sqrt{\kappa}}{2\mathrm{i}}\exp\left(\pm\mathrm{i}\,(\kappa R - \ell\frac{\pi}{2} + \delta^\ell_{E-\lambda})\right) + \mathrm{O}(R^{-1}). \tag{5.12}$$

Furthermore, it is shown in appendix C that for $r \geqslant R$

$$C_\pm(r) = C_\pm(R) + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}). \tag{5.13}$$

This implies that for $r \geqslant R$

$$u(r) = C_+(R)f_+(r) + C_-(R)f_-(r) + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}) \tag{5.14}$$

is, in fact, given by the usual WKB approximation provided that R is sufficiently large and that the field gradient is sufficiently small in the transition region. In view of (5.6) and (5.11), $f_\pm(r)$ have the asymptotic behaviour

$$f_\pm(r) = \frac{1}{\sqrt{k}} \exp\left(\pm \mathrm{i}\,(kr - kR + \int_R^\infty \mathrm{d}s\,(\kappa(s) - k)\right) + \mathrm{O}(R^{-1}). \tag{5.15}$$

Thus, for $r \geqslant R$, r sufficiently large, (5.12), (5.15) and (5.14) lead to

$$u(r) = A\sqrt{\frac{\kappa}{k}}\,\sin\left(kr - \ell\frac{\pi}{2} + (\kappa - k)R + \int_R^\infty \mathrm{d}s\,(\kappa(s) - k) + \delta^\ell_{E-\lambda}\right) + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}). \tag{5.16}$$

The comparison of (5.16) with (4.4) shows that $A = \sqrt{k/\kappa}$. Moreover, since $S^\ell_E(\lambda)$ is continuous in λ, we choose the determination of $\delta^\ell_E(\lambda)$ which is continuous in λ with $\delta^\ell_E(\lambda = 0) \equiv \delta^\ell_E$ and conclude from (5.16) that (5.1) is true.

We see that the phase shifts have a well defined asymptotic behaviour (5.1) without oscillations. This has to be contrasted with the case $\omega_R(r) = \chi_R(r)$ (abrupt switching on) which produces the phase shifts

$$\delta^\ell_E(\lambda) = -kR + \arctan\left(\frac{k}{\kappa}\tan\left(\kappa R - \ell\frac{\pi}{2} + \delta^\ell_{E-\lambda}\right)\right) + \mathrm{O}(R^{-1}). \tag{5.17}$$

If one calculates $2\hbar\,\partial\delta^\ell_E(\lambda)/\partial\lambda\big|_{\lambda=0}$ from (5.1) and (5.17) respectively, one recovers (4.12) and (4.8).

Expression (5.1) has the following interpretation: the Eisenbud–Wigner time delay associated with the scattering of the particle by the potential $\nu + \lambda\omega_R$, i.e. $\tau^\ell_E(\lambda) = 2\hbar\partial\delta^\ell_E(\lambda)/\partial E$, is equal to the sum of two contributions

$$\tau^\ell_E(\lambda) = \tau^{\mathrm{cl}}_E(\lambda) + \tau^\ell_{E-\lambda} \tag{5.18}$$

where

$$\tau^{\mathrm{cl}}_E(\lambda) = \int_0^\infty \mathrm{d}r\left(\sqrt{\frac{2m}{E - \lambda\omega_R(r)}} - \sqrt{\frac{2m}{E}}\right) \tag{5.19}$$

and $\tau^\ell_{E-\lambda}$ is the time delay due to the potential ν alone at energy $E - \lambda$. It is not hard to check that as $R \to \infty$, $\tau^{\mathrm{cl}}_E(\lambda)$ is the asymptotic form of the time delay corresponding to the scattering of a classical particle by the potential $\lambda\omega_R(r)$.

Expression (5.1) may also be compared with the standard WKB phase shifts [21]. The difference is that here the semiclassical treatement only applies to the transition region for $\lambda\omega_R$ (because of its weak gradient), whereas the full quantum mechanical scattering by the potential ν is taken into account.

The main consequence of the result (5.1) is that, in the limit $R \to \infty$ and $\rho \to \infty$, the potential $\lambda\omega_R$ has no effects on the scattering by ν, except for the energy shift $E - \lambda$ and the additional classical time delay (5.19). This is because the first factor in (5.1) is an overall phase depending only on the energy and thus commuting with the momentum operator. More specifically, if $F_E(\hat{p})$ is any function of the momentum p on the energy shell (i.e. depending only on the angles $\hat{p} = p/|p|$ of p with $|p| = (2mE/\hbar^2)^{1/2}$ fixed), the matrix elements of the asymptotic operator

$$\lim_{\substack{R\to\infty\\ \rho\to\infty}} \langle \ell, m|S_E^\dagger(\lambda)F_E(\hat{p})S_E(\lambda)|\ell', m'\rangle = \lim_{\substack{R\to\infty\\ \rho\to\infty}} S_E^{\ell\,*}(\lambda)S_E^{\ell'}(\lambda)\langle \ell, m|F_E(\hat{p})|\ell', m'\rangle$$
$$= \mathrm{e}^{2\mathrm{i}(\delta_{E-\lambda}^{\ell'} - \delta_{E-\lambda}^{\ell})}\langle \ell, m|F_E(\hat{p})|\ell', m'\rangle \tag{5.20}$$

converge to those due to the potential ν alone. In particular, if $\nu = 0$, there is no scattering at all and the cross section vanishes.

We now consider the scattering of a neutral particle of spin s. For each E and ℓ, $S_E^\ell(\lambda)$ is now a $(2s+1)\times(2s+1)$ matrix, diagonal in the basis of eigenvectors of Σ_z, with elements $S_E^\ell(m_s\lambda)$, $-s \leqslant m_s \leqslant s$ obtained by replacing λ by $m_s\lambda$ in (5.1). For a spin-$\frac{1}{2}$, we find according to (5.1)

$$\langle\Sigma_\pm\rangle_{E,\ell}^{\mathrm{out}}(\lambda) = \mathrm{e}^{\pm\mathrm{i}\alpha_E^\ell(\omega_R,\lambda)}\langle\Sigma_\pm\rangle^{\mathrm{in}} \tag{5.21}$$

with

$$\alpha_E^\ell(\omega_R,\lambda) = \alpha_{0\,E}(\omega_R,\lambda) + 2(\delta_{E+\hbar\lambda/2}^\ell - \delta_{E-\hbar\lambda/2}^\ell) + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}) \tag{5.22}$$

$$\alpha_{0\,E}(\omega_R,\lambda) = 2\int_0^\infty \mathrm{d}r\,(\kappa_-(r) - \kappa_+(r)) \tag{5.23}$$

$$\hbar\kappa_\pm(r) = \sqrt{2m\,(E \mp (\hbar\lambda/2)\omega_R(r))}. \tag{5.24}$$

When there is no dispersion in energy, the spin vector $\langle\Sigma\rangle^{\mathrm{in}} = (\langle\Sigma_x\rangle^{\mathrm{in}}, \langle\Sigma_y\rangle^{\mathrm{in}})$ undergoes a rotation in the (x,y) plane of angle $\alpha_E^\ell(\omega_R,\lambda)$ which is the sum of two terms. The first of these two terms, $\alpha_{0\,E}(\omega_R,\lambda)$, diverges as $R\to\infty$ and is the rotation angle of the outgoing spin vector in the magnetic field when the scattering potential ν is set equal to zero. Therefore, the difference

$$\alpha_E^\ell(\omega_R,\lambda) - \alpha_{0\,E}(\omega_R,\lambda) = 2\lambda\hbar\,\frac{\delta_{E+\hbar\lambda/2}^\ell - \delta_{E-\hbar\lambda/2}^\ell}{\lambda\hbar} + \mathrm{O}(R^{-1}) + \mathrm{O}(\rho^{-1}) \tag{5.25}$$

has a well defined limit as $R\to\infty$ and $\rho\to\infty$ which is the generalization of (4.19) for a spin-$\frac{1}{2}$ at fixed energy E and ℓ, for a cut-off function given by (4.10). At the first order in λ, one recovers the Eisenbud–Wigner time-delay and higher order terms in λ give access to the higher order derivatives of the phase shifts δ_E^ℓ with respect to the energy.

However, if the incoming state φ has some dispersion in energy (but with no contributions below $\lambda\hbar/2$), (5.21) has to be replaced by

$$\langle\Sigma_\pm\rangle_\ell^{\mathrm{out}}(\lambda) = \langle\Sigma_\pm\rangle^{\mathrm{in}}\int \mathrm{d}E\,|\varphi_\ell(E)|^2\mathrm{e}^{\pm\mathrm{i}\alpha_E^\ell(\omega_R,\lambda)}. \tag{5.26}$$

Since $\alpha^{\ell}_{E}(\omega_{R},\lambda)$ varies rapidly for large R, $\langle\Sigma_{\pm}\rangle^{\text{out}}_{\ell}(\lambda)$ is now subjected to an attenuation (for instance, an integration by parts of (5.26) gives $|\langle\Sigma_{\pm}\rangle^{\text{out}}_{\ell}(\lambda)| = O(R^{-1})$ as $R \to \infty$). This attenuation is due to fact that in the field region, the spin up and down parts of the wave packet (relative to the field direction) have different effective momenta $\hbar\kappa_{\pm}(r)$ (see (5.24)) and thus propagate at different speeds. This produces a spatial splitting of the incoming wave packet which is the reason for the attenuation. This effect has been discussed in the context of neutron beam experiments [22]. It is easy to check using (5.26) that this attenuation is negligible if $\sqrt{mE^{-3}}\lambda\Delta R << 1$ where Δ is the energy width of the wave packet which peaks at about E.

All the results of sections 4 and 5 can be easily specialized to the one-dimensional scattering problem. We define the cut-off function as in (4.10) with $r = |x|$, $x \in \mathbb{R}$. If the potential is invariant under the reflection $x \to -x$, the scattering operator at fixed energy is diagonal in the representation of even and odd functions of the momentum $\hbar k$. Then, $\ell = 0, 1$, where 0 corresponds to the odd functions and 1 to the even ones. The phase shifts $\delta^{0}_{E}(\lambda)$ and $\delta^{1}_{E}(\lambda)$ are connected with the transmission and reflection coefficients by

$$e^{2i\delta^{0}_{E}(\lambda)} = \mathcal{T}_{E}(\lambda) - \mathcal{R}_{E}(\lambda) \qquad e^{2i\delta^{1}_{E}(\lambda)} = \mathcal{T}_{E}(\lambda) + \mathcal{R}_{E}(\lambda) \tag{5.27}$$

and the results of propositions 1 and 2 are the same for $\delta^{0}_{E}(\lambda)$ and $\delta^{1}_{E}(\lambda)$.

In one dimension, it is possible to apply the WKB method of proposition 2 to a potential ν which is not necessarily invariant under space reflection (but still keeping the same form (4.10) of ω_{R}). Working now in the two-valued energy representation specified by E and $k/|k|$, the S-operator of the scattering system $(H_0, H_0 + \nu)$, on the energy shell, is given by the following 2×2 unitary matrix

$$S_{E} = \begin{pmatrix} \mathcal{T}_{E} & \mathcal{R}'_{E} \\ \mathcal{R}_{E} & \mathcal{T}_{E} \end{pmatrix}. \tag{5.28}$$

In (5.28) $\mathcal{T}_{E}$ and $\mathcal{R}_{E}$ are the transmission and reflection coefficients for a particle with energy E coming from the left and $\mathcal{R}'_{E}$ is the reflection coefficient for the particle coming from the right. The equivalent of proposition 2 is now that $S_{E}(\lambda)$, $\lambda < E$, is asymptotic to $\mathcal{T}_{0E}(\lambda)\, S_{E-\lambda}$ as $R \to \infty$ and $\rho \to \infty$, where $\mathcal{T}_{0E}(\lambda) = \exp\left(2i\int_0^\infty dr\,(\kappa(r) - k)\right)$ is the transmission coefficient for the scattering system without the potential ν. Notice that $|\mathcal{T}_{0E}(\lambda)| = 1$, i.e. the potential $\lambda\omega_{R}$ causes no reflections. Since $\mathcal{T}_{0E}(\lambda)$ is a pure phase factor, we find that, at fixed energy E and for a spin-$\frac{1}{2}$, the length of the difference of the spin vector in the (x, y) plane

$$\begin{aligned} &\left|\langle\Sigma\rangle^{\text{out}}_{E}(\lambda) - \langle\Sigma\rangle^{\text{out}}_{0E}(\lambda)\right| \\ &\quad = 2\lambda\hbar|\langle\Sigma\rangle^{\text{in}}|\left|\left\langle S^{\dagger}_{E-\lambda\hbar/2}\left(\frac{S_{E+\lambda\hbar/2} - S_{E-\lambda\hbar/2}}{\lambda\hbar}\right)\right\rangle_{E}\right| + O(1) \end{aligned} \tag{5.29}$$

again has a well defined limit as $R \to \infty$ and $\rho \to \infty$.

6. Concluding remarks

The scattering of a quantum mechanical particle by a (non-random) potential (here $\nu + \lambda\omega$) is a fully coherent process; all interactions, wherever they take place, contribute coherently to the wavefunction. By a rigorous quantum mechanical treatment of the full process (field and potential), we have shown that the spin clock agrees with the (classic) Eisenbud–Wigner time delay, at fixed energy as well as for wave packets, under the following conditions:

(i) one considers the average value of the total outgoing spin (i.e. summing up the contributions of all scattering directions);

(ii) the magnetic field is switched on smoothly in space in a spherically symmetric region;

(iii) one retains the linear response term in the field strength;

(iv) the field region is eventually extended to the whole space.

Under the same conditions (i), (ii) and (iv), we have also investigated the functioning of the spin clock beyond the linear response regime. At fixed energy relevant information can be obtained on finite-energy differences of phase shifts. When there is some dispersion in energy, the outgoing spin magnitude is attenuated because of a (Stern–Gerlach) splitting of the spin component waves inside the field region. This confirms the view that the apparent pure spin rotation occurring in the linear response should be interpreted as a coherent interference between the spin component waves in the field region, rather than as a classical Larmor precession (see [22] for a discussion of this point).

Conditions (i) and (iv) may also be dropped by performing a spin measurement in a definite outgoing direction and/or considering cases where the magnetic field acts only locally on some region of microscopic size.

It is certainly of interest to investigate what information can be obtained on tunnelling processes from a partial spin measurement (for instance, in one dimension, the spin associated with transmitted or reflected waves separately; see the comment at the end of section 3). This aspect was not discussed in this paper but we shall return to this point in further work in relation to the concept of 'angular time delay' (see for instance [23]).

If the magnetic field has a strictly local action in some region there will be, in principle, quantum mechanical interferences due to the non-vanishing gradients at the finite distance boundaries of this region. To what extent they can be disentangled from the scattering waves due to the potential ν has to be examined in each case.

The sojourn time also has a local character. As emphasized in [24] it is an idealized quantity obtained by a continuous observation in the limit of weak disturbance of the system by the measurement procedure. In fact, the linear response of the scattering system to an applied field, as described in section 2, precisely provides such a measurement. We understand then that the sojourn time also unavoidedly embodies the physical consequences of the spatial switching on of the field specified by a choice of the cut-off function ω.

Many studies have been devoted to local tunnelling times (see for instance [1, 25] and references cited therein) but, in our opinion (and this is also a conclusion in [1]), the Eisenbud–Wigner phase shift is the only concept of time delay intrinsically attached to the potential ν: it has to be a non-local quantity by the very nature of quantum mechanics (a wave packet cannot have compact support for all times).

A final remark is in order. To our knowledge, in the present work as well as in almost all the existing literature, the cut-off function ω is always chosen to be spherically symmetric (or reflection invariant in one dimension). The only exceptions are the one-dimensional case [14] and the treatment of the trace $\mathrm{Tr}\,\tau_E$ of the time delay operator [26]. A spherically symmetric cut-off has the advantage that it leads to the expected result (the usual Eisenbud–Wigner phase shift) and facilitates the analysis (for instance a simple application of the WKB method of proposition 2 is only possible with the radial ordinary differential equation). We think that the reason for this choice is, in fact, more fundamental: if more general cut-off functions are allowed the convergence (3.5) is no larger guaranteed [27].

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Appendix A

In this appendix, we establish the formula (2.6) for a class of spherically symmetric potentials. We have from (2.3)

$$\frac{\partial}{\partial\lambda}S_t(\lambda) = -\frac{\mathrm{i}}{\hbar}\Omega^\dagger_{+,t}(\lambda)A_t(\lambda)\Omega_{-,t}(\lambda) \tag{A.1}$$

with

$$A_t(\lambda) = \int_{-t}^{t} \mathrm{d}s\, V_s^\dagger(\lambda)\omega V_s(\lambda) \tag{A.2}$$

$$\| A_t(\lambda) \| \leqslant 2t \, \|\omega\| \, . \tag{A.3}$$

One proceeds with the following steps:

(i) the strong limits (2.1) hold on $L^2(\mathbb{R}^3)$ uniformly with respect to λ ($|\lambda| \leqslant \lambda_0$);

(ii) there exists a dense set $\mathcal{D} \subset L^2(\mathbb{R}^3)$ such that $\operatorname{s-lim}_{t\to\infty} A_t(\lambda)\Omega_-(\lambda)\varphi = A(\lambda)\Omega_-(\lambda)\varphi$, uniformly with respect to λ, on the set $\Omega_-(\lambda)\varphi$, $\varphi \in \mathcal{D}$, where $A(\lambda) = A_\infty(\lambda)$ is given by the integral (A.2) with infinite integration range;

(iii) $\operatorname{s-lim}_{t\to\infty} A_t(\lambda)\Omega_{-,t}(\lambda)\varphi = A(\lambda)\Omega_-(\lambda)\varphi$, $\varphi \in \mathcal{D}$, uniformly with respect to λ.

The assertions (i) and (iii) imply that, for $\psi \in L^2(\mathbb{R}^3)$ and $\varphi \in \mathcal{D}$, the sequence of derivatives

$$\begin{aligned} \lim_{t\to\infty} \frac{\partial}{\partial\lambda}(\psi, S_t(\lambda)\varphi) &= -\frac{\mathrm{i}}{\hbar}\lim_{t\to\infty}(\Omega_{+,t}(\lambda)\psi, A_t(\lambda)\Omega_{-,t}(\lambda)\varphi) \\ &= -\frac{\mathrm{i}}{\hbar}(\psi, \Omega_+^\dagger(\lambda)A(\lambda)\Omega_-(\lambda)\varphi) \end{aligned} \tag{A.4}$$

converge uniformly with respect to λ. This justifies the exchange of the infinite time limit with the λ derivative and gives (2.6) when λ is set equal to zero in (A.4). Point (i) follows from the standard Cook estimate

$$\begin{aligned} \| (\Omega_\pm(\lambda) - V_t^\dagger(\lambda)U_t)\varphi \| &\leqslant \left| \int_t^{\pm\infty} \mathrm{d}s \; \| (\nu + \lambda\omega)U_t\varphi \| \right| \\ &\leqslant \left| \int_t^{\pm\infty} \mathrm{d}s \; \| \nu\, U_t\varphi \| \right| + \lambda_0 \left| \int_t^{\pm\infty} \mathrm{d}s \; \| \omega\, U_t\varphi \| \right| \end{aligned} \tag{A.5}$$

which is obviously uniform with respect to λ, $|\lambda| \leqslant \lambda_0$. To establish (ii), we show that $(A_{t_2}(\lambda) - A_{t_1}(\lambda))\Omega_-(\lambda)\varphi$, $t_2 > t_1$, $\varphi \in \mathcal{D}$, form a strong Cauchy sequence uniform in λ. We omit the variable λ from now on, remembering that the total potential is $\nu + \lambda\omega$. We use the inequalities

$$\begin{aligned} \| (A_{t_2} - A_{t_1})\Omega_-\varphi \| &= \left\| \int_{t_1}^{t_2} \mathrm{d}s \frac{\mathrm{d}}{\mathrm{d}s} A_s \Omega_-\varphi \right\| \\ &\leqslant \int_{-t_2}^{-t_1} \mathrm{d}s \ \| \omega V_s \Omega_-\varphi \| + \int_{t_1}^{t_2} \mathrm{d}s \ \| \omega V_s \Omega_-\varphi \| \\ &\leqslant \int_{-t_2}^{-t_1} \mathrm{d}s \ \| \omega U_s \varphi \| + \| \omega \| \int_{-t_2}^{-t_1} \mathrm{d}s \ \| (V_s \Omega_- - U_s)\varphi \| \\ &\quad + \int_{t_1}^{t_2} \mathrm{d}s \ \| \omega U_s S\varphi \| + \| \omega \| \int_{t_1}^{t_2} \mathrm{d}s \ \| (V_s\Omega_- - U_s S)\varphi \| . \end{aligned} \tag{A.6}$$

We note that the integrability of the functions occurring in (A.6) is precisely the condition under which the existence of the time delay is proven in [12], i.e. it holds if $\mathcal{D} = \{\varphi \in L^2(\mathbb{R}^3); \hat{\varphi}(\boldsymbol{k}) = \int \mathrm{d}^3x \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \varphi(\boldsymbol{x})$ is three times continuously differentiable with compact support and no support in a neigbourhood of $\boldsymbol{k} = 0\}$, ν is spherically symmetric and $\nu(r) = \mathrm{O}(r^{-5/2-\varepsilon})$ (we recall that ω has compact support). The analysis of [12] relies on the Cook estimate (A.5) and on the finitness of the moments

$$\int \mathrm{d}r \, r^\gamma |\nu(r) + \lambda\omega(r)| \leqslant \int \mathrm{d}r \, r^\gamma |\nu(r)| + \lambda_0 \int \mathrm{d}r \, r^\gamma |\omega(r)| \qquad 0 \leqslant \gamma \leqslant \tfrac{3}{2} + \varepsilon. \tag{A.7}$$

Both estimates (A.5) and (A.7) are uniform with respect to λ, and this completes the proof of (ii). For (iii), we have with (A.3)

$$\begin{aligned} \| (A_t\Omega_{-,t} - A\Omega_-)\varphi \| &\leqslant \| (A_t - A)\Omega_-\varphi \| + \| A_t \| \| (\Omega_{-,t} - \Omega_-)\varphi \| \\ &\leqslant \| (A_t - A)\Omega_-\varphi \| + 2 \| \omega \| \, t \, \| (\Omega_{-,t} - \Omega_-)\varphi \| . \end{aligned} \tag{A.8}$$

The first term in the right-hand side of (A.8) tends to zero uniformly with respect to λ by (ii). So does the second term since by the Cook estimate $\| (\Omega_{-,t} - \Omega_-)\varphi \| = \mathrm{O}(t^{-1-\varepsilon})$, $\varphi \in \mathcal{D}$, uniformly with respect to λ (see [12]). This completes the proof of (2.6) for $\varphi \in \mathcal{D}$ and for spherically symmetric potentials ν decreasing at infinity more rapidly than $r^{-5/2}$. The proof could be extended to non-spherically symmetric potentials by the methods of [13].

Appendix B

We give here a proof of (4.15) in section 4. Using the method of the variation of constants it is not difficult to show that the solution of (4.3) with asymptotic behaviour (4.4) obeys the Volterra-type integral equation (see [28] for the method)

$$u^\ell(k,r) = u_0^\ell(k,r) + u_1^\ell(k,r) \qquad \hbar k = \sqrt{2mE} \tag{B.1}$$

with

$$u_0^\ell(k,r) = \cos\delta^\ell(k) j_\ell(kr) + \sin\delta^\ell(k) n_\ell(kr) \tag{B.2}$$

$$u_1^\ell(k,r) = \frac{2m}{\hbar^2 k}\int_r^\infty \mathrm{d}s\, G_k^\ell(r,s)\nu(s)u^\ell(k,s) \tag{B.3}$$

$$G_k^\ell(r,s) = n_\ell(ks)j_\ell(kr) - n_\ell(kr)j_\ell(ks) \tag{B.4}$$

where $j_\ell(x)$ and $n_\ell(x)$ are the usual Riccati–Bessel and Riccati–Newmann functions with asymptotic behaviour

$$\begin{aligned} j_\ell(x) &= \sin(x - \ell\pi/2) + \mathrm{O}(1/x) \\ n_\ell(x) &= \cos(x - \ell\pi/2) + \mathrm{O}(1/x). \end{aligned} \tag{B.5}$$

Inserting (B.1) into (4.14) gives (dropping the indices E and ℓ)

$$h(k,r) = \sum_{\alpha,\beta=0}^{1} \frac{1}{2k} \overbrace{\left(\frac{\partial u_\alpha}{\partial r}\frac{\partial u_\beta}{\partial k} - u_\alpha \frac{\partial^2 u_\beta}{\partial r \partial k}\right)(k,r)}^{A_{\alpha,\beta}(k,r)}. \tag{B.6}$$

We first derive the asymptotic behaviour of $A_{0,0}(k,r)$, noting that, under the condition (4.11), the phase shifts $\delta^\ell(k)$ are continuously differentiable for $k \neq 0$ (see [28]). One obtains, setting $x = kr$,

$$\begin{aligned} A_{0,0}(k,r) &= \cos^2\delta(k)\left(k\frac{\mathrm{d}\delta(k)}{\mathrm{d}k}(n'j - nj')(x) + x(j''j - j'^2)(x) + j'(x)j(x)\right) \\ &\quad + \sin^2\delta(k)\left(k\frac{\mathrm{d}\delta(k)}{\mathrm{d}k}(n'j - nj')(x) + x(n''n - n'^2)(x) + n'(x)n(x)\right) \\ &\quad + \sin\delta(k)\cos\delta(k)(x(j''n - j'n')(x) \\ &\quad + (n''j - n'j')(x) + (j'n + n'j)(x)). \end{aligned} \tag{B.7}$$

Using the following properties of the spherical Bessel functions

$$\begin{aligned} & j''(x) = -j(x) + \mathrm{O}(x^{-2}) \qquad n''(x) = -n(x) + \mathrm{O}(x^{-2}) \\ & j'(x) = n(x) + \mathrm{O}(x^{-2}) \qquad n'(x) = -j(x) + \mathrm{O}(x^{-2}) \\ & n^2(x) + j^2(x) = 1 + \mathrm{O}(x^{-2}) \end{aligned} \tag{B.8}$$

(B.7) becomes

$$\begin{aligned} \frac{1}{2k}A_{0,0}(k,r) &= \frac{1}{2}\frac{\mathrm{d}\delta(k)}{\mathrm{d}k} + \frac{r}{2} - \frac{1}{4k}(j(kr)\cos\delta(k) + n(kr)\sin\delta(k))(n(kr)\cos\delta(k) \\ &\quad - j(x)\sin\delta(k)) + \mathrm{O}(r^{-1}) \\ &= \frac{1}{2}\frac{\hbar^2 k}{2m}\frac{\mathrm{d}\delta_E^\ell}{\mathrm{d}E} \\ &\quad + \frac{r}{2} - \frac{1}{4k}\sin(2kr - \ell\pi + 2\delta_E^\ell) + \mathrm{O}(r^{-1}) \end{aligned} \tag{B.9}$$

where the last equality follows from (B.5). This is the expected asymptotic behaviour of $h_E^\ell(r)$. To complete the proof of (4.15) it remains to show that under the conditions (4.11) the three last terms in the sum (B.5) do not contribute as $r \to \infty$. As a consequence of the fact that the spherical Bessel functions are uniformly bounded away from the origin, we have for $k \neq 0$ and $r \geqslant 1$

$$u_0^\ell(k,r), \frac{\mathrm{d}u_0^\ell}{\mathrm{d}r}(k,r) = \mathrm{O}(1) \qquad \frac{\mathrm{d}u_0^\ell}{\mathrm{d}k}(k,r), \frac{\mathrm{d}^2 u_0^\ell}{\mathrm{d}r\mathrm{d}k}(k,r) = \mathrm{O}(r) \tag{B.10}$$

and also, solving the integral equation (B.1)–(B.4) by iteration,

$$u^\ell(k,r) = \mathrm{O}(1) \qquad \frac{\mathrm{d}u^\ell}{\mathrm{d}k}(k,r) = \mathrm{O}(r). \tag{B.11}$$

Then one deduces from (B.3) that

$$u_1^\ell(k,r), \frac{\mathrm{d}u_1^\ell}{\mathrm{d}r}(k,r) = \mathrm{O}\left(\int_r^\infty \mathrm{d}s\, |\nu(s)|\right) \tag{B.12}$$

$$\frac{\mathrm{d}u_1^\ell}{\mathrm{d}k}(k,r), \frac{\mathrm{d}^2 u_1}{\mathrm{d}r\mathrm{d}k}(k,r) = \mathrm{O}\left(\int_r^\infty \mathrm{d}s\, s|\nu(s)|\right). \tag{B.13}$$

(B.12) and (B.13) imply that all the terms $A_{\alpha,\beta}(k,r)$, $(\alpha,\beta) \neq (0,0)$ are $\mathrm{O}(N(r))$.

Appendix C

We indicate here a proof of (5.13). For this we write (5.7) as an integral equation

$$C_\pm(r) = C_\pm(R) + \Delta_\pm(r) \tag{C.1}$$

where

$$\Delta_\pm(r) = \frac{1}{2}\int_R^r \mathrm{d}s\, \frac{k'(s)}{k(s)} C_\mp(s) \mathrm{e}^{\mp 2\mathrm{i}\int_R^s \mathrm{d}s'\, k(s')}. \tag{C.2}$$

An integration by parts of (C.2) gives

$$\Delta_\pm(r) = \mp\frac{1}{4\mathrm{i}}\frac{k'(s)}{k^2(s)} C_\mp(s)\mathrm{e}^{\mp 2\mathrm{i}\int_R^s \mathrm{d}s'\, k(s')}\bigg|_R^r - \frac{1}{4}\int_R^r \mathrm{d}s\, \left(\frac{k'(s)}{k^2(s)} C_\mp(s)\right)' \mathrm{e}^{\mp 2\mathrm{i}\int_R^s \mathrm{d}s'\, k(s')}. \tag{C.3}$$

We know that the regular solution $u(r)$ of (4.3) and its derivative $u'(r)$ are bounded (see for instance appendix B); the definitions (5.3) and (5.4) imply that the same is true for $C_+(r)$ and $C_-(r)$. Then, using (5.5), it is a simple matter to check that for $s \geqslant R$

$$\left|\frac{k'(s)}{k^2(s)} C_\mp(s)\right| \leqslant M_1\, |\gamma'(s)| \tag{C.4}$$

$$\left|\left(\frac{k'(s)}{k^2(s)} C_\mp(s)\right)'\right| \leqslant M_2\, (\gamma'(s))^2 + M_3\, |\gamma''(s)|. \tag{C.5}$$

To obtain (C.5) we have taken into account that, by (5.7), $C'_{\pm}(s)$ has the same bound as (C.4). Introducing (C.4) and (C.5) into (C.3) gives, after integrating $(\gamma'(s))^2$ by parts,

$$|\Delta_{\pm}(r)| \leqslant M_4 \sup_{s\geqslant R} |\gamma'(s)| + M_5 \int_R^\infty \mathrm{d}s\, |\gamma''(s)|. \tag{C.6}$$

In view of (4.10) and with the conditions assumed for the potential ν, one has the estimates

$$\sup_{s\geqslant R} |\gamma'(s)| \leqslant \rho^{-1} \sup_{s\geqslant 0} |g'(s)| + \mathrm{O}(R^{-\eta}) + \mathrm{O}(R^{-3}) \tag{C.7}$$

$$\int_R^\infty \mathrm{d}s\, |\gamma''(s)| \leqslant \rho^{-1} \int_0^\infty \mathrm{d}s\, |g''(s)| + \mathrm{O}(R^{-\eta+1}) + \mathrm{O}(R^{-3}) \tag{C.8}$$

implying that (5.13) holds when $\eta \geqslant 2$.

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