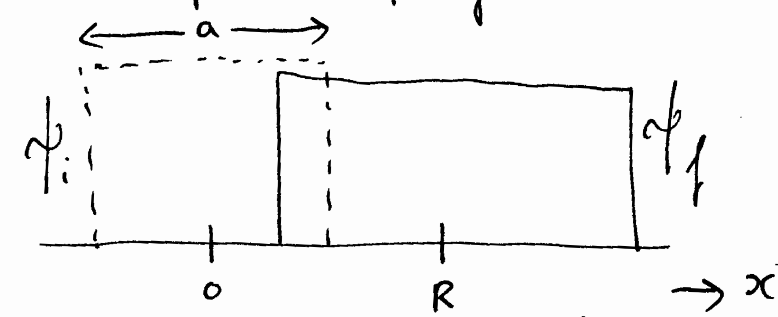
1)

Absorption, Oscillator Strength and Transition Moments

The absorption spectrum of an atom or molecule is described in terms of the oscillator strength (Atkins pp. 327 ff.) Since paper 59 deals with oscillations a connection can be forged between ECE theory and absorption theory. On page 328 Atkins gives a simple example of a charge-transfer transition



The initial state is modelled with a rectangular wavefunction centred at $x = 0$ and width a. The final state is modelled with a function of the same shape and size centred at $x = R$. The transition dipole moment is calculated as follows. Each wavefunction is normalized to unity and the integral $\int \phi_f \, x \, \phi_i \, d\tau$ is calculated, with $\phi_i = N$ for $-\frac{1}{2}a \leq x \leq \frac{1}{2}a$ and $\phi_i = 0$ elsewhere. Then:

$$\int \phi_i^2 \, d\tau = N^2 \int_{-\frac{1}{2}a}^{\frac{1}{2}a} dx = N^2 a = 1 \quad -(1)$$

Therefore:

$$N = 1 / \sqrt{a} \quad -(2)$$

This is the normalization factor. There is a similar result for ϕ_f. For the transition moment there is a contribution to the integral only where ϕ_i and ϕ_f are both

2) non-zero. Otherwise $\phi_f x \phi_i$ is zero. Therefore if $R > a$, $\mu_{fi} = 0$. If $R \leq a$:

$$\mu_{fi} = -e\int \phi_f x \phi_i \, d\tau = -e\int_{R-\frac{1}{2}a}^{\frac{1}{2}a} N x N \, dx = -eR(1 - R/a) \quad -(3)$$

The intensity of the transition is proportional to μ_{fi}^2.
The transition dipole moment is equivalent to a charge

$$q = -e(1 - R/a) \quad -(4)$$

shifting between the centres of the two distributions. This is what happens when the resonance Coulomb law applies to a molecule, or atom. In H for example oscillations of the electron occur at resonance.

In the example given by Atkins the overlap integral for the pair of states is 0 for $R > a$ and is:

$$S = 1 - \frac{R}{a} \quad \text{for } R < a \quad -(5)$$

The transition moment arises from the motion of a charge $-eS$ ~~through~~ the distance R.

Einstein Coefficient of Absorption

This is given by Atkins in Appendices 13 and 17:

$$B_{fi} = \frac{1}{6}\epsilon_0 \hbar^2 |\mu_{fi}|^2 \quad -(6)$$

So absorption may occur from the resonant Coulomb law. The absorbance is ~~then~~:

$$A = \frac{\hbar \omega_{fi}}{c} L B \quad -(7)$$

where L is Avogadro's constant and ω_{fi} the transition frequency. The oscillator strength of a transition is:

$$f = \frac{4 m_e c \epsilon_0}{L e^2} A \quad -(8)$$

where m_e is the mass of the electron.

For a one dimensional harmonic oscillator $f = 1/3$, and for an electron oscillating harmonically in ~~three~~ dimensions $f = 1$. Therefore the resonant Coulomb law should be used to calculate the transition dipole moment and oscillator strengths of transitions induced by spin - connection in atoms, molecules and materials. The Schrödinger equation is obtained from the ECE Lemma:

$$\Box q_\mu^a = R q_\mu^a \quad -(9)$$

in the slow motion or weak field limit:

$$\Box \rightarrow -\nabla^2 \quad -(10)$$

so

$$\nabla^2 q_\mu^a = kT q_\mu^a \quad -(11)$$

4) Eq. (11) has the same form as:

$$\hat{H}\psi = E\psi \quad -(12)$$

For a free electron:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 \quad -(13)$$

so:

$$\nabla^2\psi = -\frac{2mE}{\hbar^2}\psi \quad -(14)$$

This equation can be compared with the ECE Lemma in the slow motion limit:

$$\nabla^2\psi = -R\psi \quad -(15)$$

so:

$$\boxed{R = \frac{2mE}{\hbar^2}} \quad -(16)$$

is the scalar curvature of the free electron in the Schrödinger equation, $\boxed{R := \partial\omega / \partial Z.}$

Conclusion

Absorption and the Schrödinger eqn. are spacetime properties.