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A hybrid gauge transformation of the Hamiltonian for a coupled hydrogen atom–field system

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Abstract. A gauge transformation of the minimal-coupling Hamiltonian for a non-relativistic hydrogen atom is induced by a generating function that rescales the charges and their positions. The result is consistent with Maxwell's equations and the Lorentz force formula, and contains the *Power-Zienau-Woolley* Hamiltonian as a special case. The dipole approximation simplifies the Hamiltonian, giving a mixing of $\boldsymbol{p}\cdot\boldsymbol{A}$ and $\boldsymbol{q}\cdot\boldsymbol{E}$ interactions.

The Hamiltonian of a bound system incorporating the charges as a source of the quantised electromagnetic field has been referred to as the Power-Zienau-Woolley (PZW) Hamiltonian (Power and Zienau 1959, Woolley 1971). Here, the sources are the electric and magnetic polarisation vectors, and the coupling occurs via the displacement $\boldsymbol{D}$ and the magnetic flux density $\boldsymbol{B}$, rather than the potentials. The gauge can be arbitrary (Babiker and Loudon 1983), and this generalisation of the original dipole approximation theory to include all the higher-order multipoles, in closed form, is widely applied in quantum optics (Healy 1977a, b, Babiker *et al* 1973, 1974, Woolley 1975). The theory has been reviewed by Power and Thirunamachandran (1978).

The minimal-coupling Hamiltonian in arbitrary (a) gauge of a hydrogen atom interacting with an electromagnetic field is

$$H_{\min}^{(a)}=\frac{1}{2m}(\boldsymbol{p}+e\boldsymbol{A})^2+\tfrac{1}{2}\int \mathrm{d}^3\boldsymbol{r}(\varepsilon_0^{-1}\boldsymbol{\Pi}^2+\mu_0^{-1}\boldsymbol{B}^2). \tag{1}$$

The conjugate momenta are

$$\boldsymbol{p}=m\dot{\boldsymbol{q}}-e\boldsymbol{A}(\boldsymbol{q}) \tag{2}$$

$$\boldsymbol{\Pi}(r)=-\varepsilon_0\boldsymbol{E}(\boldsymbol{r}). \tag{3}$$

Here, $\boldsymbol{q}$ is the position of $-e$ with respect to $+e$. The mass of the electron is m, while the proton is assumed to be *massive*. The charge and current densities are respectively

$$\rho(\boldsymbol{r})=-e\delta(\boldsymbol{r}-\boldsymbol{q})+e\delta(\boldsymbol{r}) \tag{4}$$

$$\boldsymbol{J}(\boldsymbol{r})=-e\dot{\boldsymbol{q}}\delta(\boldsymbol{r}-\boldsymbol{q}). \tag{5}$$

The dynamical variables are q-numbers at the Hamiltonian level, obeying equal time commutators

$$[q_i,p_j]=\mathrm{i}\hbar\delta_{ij} \tag{6}$$

$$[A_i(r),\Pi_j(\boldsymbol{r}')]=\mathrm{i}\hbar\delta_{ij}\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{7}$$

A gauge transformation is equivalent to

$$\boldsymbol{A}\rightarrow\boldsymbol{A}-\nabla\chi(\boldsymbol{r})$$
$$\varphi\rightarrow\varphi+\dot{\chi}(\boldsymbol{r}).$$

We introduce a gauge density $\tilde{\chi}$ (Babiker and Loudon 1983) that is itself a functional of the potential $\boldsymbol{A}$ at some general position $\boldsymbol{r}'$:

$$\chi(\boldsymbol{r})=\int \mathrm{d}^3\boldsymbol{r}'\tilde{\chi}(\boldsymbol{r},\boldsymbol{r}',\{\boldsymbol{A}(\boldsymbol{r}')\}). \tag{8}$$

The gauge density function is written in a shorthand form as $\tilde{\chi}(\boldsymbol{r},\boldsymbol{r}')$. Note that $\tilde{\chi}$ depends on time only through $\boldsymbol{A}$. The momenta transform as

$$\boldsymbol{p}\rightarrow\boldsymbol{p}+e\nabla\chi(\boldsymbol{q}) \tag{9}$$
$$\boldsymbol{\Pi}(\boldsymbol{r})\rightarrow\boldsymbol{\Pi}(\boldsymbol{r})-\boldsymbol{G}(\boldsymbol{r}) \tag{10}$$

where the vector $\boldsymbol{G}(\boldsymbol{r})$ is defined as

$$\boldsymbol{G}(\boldsymbol{r})=\int \mathrm{d}^3\boldsymbol{r}'\left\{\frac{\partial\tilde{\chi}(\boldsymbol{r}',\boldsymbol{r})}{\partial\boldsymbol{A}(\boldsymbol{r})}\right\}\rho(\boldsymbol{r}'). \tag{11}$$

The χ-gauge-transformed Hamiltonian is

$$H_\chi^{(a)}=\frac{1}{2m}(\boldsymbol{p}+e\boldsymbol{A}-e\nabla\chi)^2+\tfrac{1}{2}\int \mathrm{d}^3\boldsymbol{r}[\varepsilon_0^{-1}(\boldsymbol{\Pi}+\boldsymbol{G})^2+\mu_0^{-1}\boldsymbol{B}^2]. \tag{12}$$

It must be remembered that apparently identical operators have different significance in $H_{\min}^{(a)}$ compared with $H_\chi^{(a)}$.

Consider a gauge transformation induced by

$$\boldsymbol{G}(\boldsymbol{r},\boldsymbol{q})=-e\alpha\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda\boldsymbol{q}\delta(\boldsymbol{r}-\lambda\boldsymbol{q}) \tag{13}$$

where α, β_1 and β_2 are arbitrary, dimensionless scalars. If $\alpha=\beta_2=1$ and $\beta_1=0$ then $\boldsymbol{G}$ reduces to the multipolar polarisation $\boldsymbol{P}_\mathrm{M}$, and $H_\chi^{(a)}$ becomes the PZW Hamiltonian (Babiker and Loudon 1983). From (11) the gauge generated by (13) is

$$\chi(\boldsymbol{r})=\alpha\int \mathrm{d}^3\boldsymbol{r}'\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda A_j(\boldsymbol{r}')r_j\delta(\boldsymbol{r}'-\lambda\boldsymbol{r}). \tag{14}$$

The ith component of $\nabla\chi$ is

$$\nabla_{i\chi}=\alpha\beta_2A_i(\beta_2\boldsymbol{r})-\alpha\beta_1A_i(\beta_1\boldsymbol{r})$$
$$+\alpha\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda\int \mathrm{d}^3\boldsymbol{r}'\left\{A_i(\boldsymbol{r}')\lambda\boldsymbol{r}\cdot\boldsymbol{\nabla}'\delta(\boldsymbol{r}'-\lambda\boldsymbol{r})+\sum_j A_j(\boldsymbol{r}')r_j\nabla_i\delta(\boldsymbol{r}'-\lambda\boldsymbol{r})\right\} \tag{15}$$

where use has been made of the identity

$$\alpha\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda\{1-\lambda\boldsymbol{r}\cdot\boldsymbol{\nabla}'\}\delta(\boldsymbol{r}'-\lambda\boldsymbol{r})=\alpha\beta_2\delta(\boldsymbol{r}'-\beta_2\boldsymbol{r})-\alpha\beta_1\delta(\boldsymbol{r}'-\beta_1\boldsymbol{r}). \tag{16}$$

Since, by definition,

$$\delta(\boldsymbol{r}'-\lambda\boldsymbol{r})=\delta(r_1'-\lambda r_1)\delta(r_2'-\lambda r_2)\delta(r_3'-\lambda r_3)$$

where r_1, r_2 and r_3 are the Cartesian components of $\boldsymbol{r}$, we can write

$$\int_{\beta_1}^{\beta_2} \mathrm{d}\lambda\, \lambda r_j \nabla'_i \delta(\boldsymbol{r}'-\lambda\boldsymbol{r}) = -\int_{\beta_1}^{\beta_2} \mathrm{d}\lambda\, r_j \nabla_i \delta(\boldsymbol{r}'-\lambda\boldsymbol{r}). \tag{17}$$

Substituting (17) into (16) gives

$$\nabla_{i\chi} = \alpha\beta_2 A_i(\beta_2\boldsymbol{r}) - \alpha\beta_1 A_i(\beta_2\boldsymbol{r}) + \alpha \int_{\beta_1}^{\beta_2} \mathrm{d}\lambda \int \mathrm{d}^3\boldsymbol{r}'\lambda \left\{ A_i(\boldsymbol{r}')\boldsymbol{r}\cdot\boldsymbol{\nabla}' - \sum_j A_j(\boldsymbol{r}') r_j \nabla'_i \right\} \delta(\boldsymbol{r}'-\lambda\boldsymbol{r}).$$

Therefore

$$\nabla\chi = \alpha\beta_2 \boldsymbol{A}(\beta_2\boldsymbol{r}) - \alpha\beta_1 \boldsymbol{A}(\beta_1\boldsymbol{r}) - \frac{1}{e}\int \mathrm{d}^3\boldsymbol{r}' \boldsymbol{\Theta}(\boldsymbol{r}', \boldsymbol{r}) \times \boldsymbol{B}(\boldsymbol{r}') \tag{18}$$

where the vector $\boldsymbol{\Theta}$ is defined by the equation

$$\boldsymbol{\Theta}(\boldsymbol{r}', \boldsymbol{r}) = -\alpha e \int_{\beta_1}^{\beta_2} \mathrm{d}\lambda\, \lambda \boldsymbol{r} \delta(\boldsymbol{r}'-\boldsymbol{r}). \tag{19}$$

Finally, a substitution of (18) and (13) into (12) gives the transformed Hamiltonian

$$H_\chi^{(a)} = \frac{1}{2m}\left(\boldsymbol{p} + e\boldsymbol{A}(\boldsymbol{r}) - \alpha e\beta_2 \boldsymbol{A}(\beta_2\boldsymbol{r}) + \alpha e \beta_1 \boldsymbol{A}(\beta_1\boldsymbol{r}) + \int \mathrm{d}^3\boldsymbol{r}'\boldsymbol{\Theta}(\boldsymbol{r}', \boldsymbol{r})\times\boldsymbol{B}(\boldsymbol{r}')\right)^2 + \tfrac{1}{2}\int \mathrm{d}^3\boldsymbol{r}[\varepsilon_0^{-1}(\boldsymbol{\Pi}+\boldsymbol{G})^2 + \mu_0^{-1}\boldsymbol{B}^2] \tag{20}$$

with conjugate momenta

$$\boldsymbol{p} = m\dot{\boldsymbol{q}} - e\boldsymbol{A}(\boldsymbol{q}) + e\alpha\beta_2\boldsymbol{A}(\beta_2\boldsymbol{q}) - e\alpha\beta_1\boldsymbol{A}(\beta_1\boldsymbol{q}) - \int \mathrm{d}^3\boldsymbol{r}'\boldsymbol{\Theta}(\boldsymbol{r}', \boldsymbol{r})\times\boldsymbol{B}(\boldsymbol{r}') \tag{21}$$

$$\boldsymbol{\Pi}(\boldsymbol{r}) = -\varepsilon_0 \boldsymbol{E}(\boldsymbol{r}) - e\alpha\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda\, \boldsymbol{q}\delta(\boldsymbol{r}-\boldsymbol{q}). \tag{22}$$

If the transformation is canonical then the gauge and transformed momenta obey the relationship (Babiker and Loudon 1983)

$$[\Pi_i(\boldsymbol{r}), \nabla_j\chi(\boldsymbol{q})] = -\left[\left\{\frac{\partial\tilde{\chi}(\boldsymbol{q}, \boldsymbol{r})}{\partial A_i(\boldsymbol{r})}\right\}, p_j\right]. \tag{23}$$

It is not difficult to verify (23) for a gauge generated by (13).

We will now look at the nature of $\boldsymbol{\Pi}$. From standard vector analysis

$$\boldsymbol{\nabla}\cdot\boldsymbol{G}(\boldsymbol{r}) = -e\alpha\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda\, \boldsymbol{q}\cdot\boldsymbol{\nabla}\delta(\boldsymbol{r}-\lambda\boldsymbol{q}).$$

Using the representation of the δ function

$$\delta(\boldsymbol{r}-\lambda\boldsymbol{q}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{+\infty}\mathrm{d}^3\boldsymbol{k}\exp\{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\lambda\boldsymbol{q})\}$$

we find that

$$\boldsymbol{\nabla}\cdot\boldsymbol{G}(\boldsymbol{r}) = -\frac{e\alpha}{(2\pi)^3}\int_{\beta_1}^{\beta_2}\mathrm{d}\lambda\int_{-\infty}^{+\infty}\mathrm{d}^3\boldsymbol{k}\,\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{k}\exp\{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\lambda\boldsymbol{q})\}.$$

Integrating with respect to λ and reverting back to δ notation gives

$$\nabla \cdot \boldsymbol{G}(\boldsymbol{r}) = \alpha e\delta(\boldsymbol{r} - \beta_2\boldsymbol{q}) - \alpha e\delta(\boldsymbol{r} - \beta_1\boldsymbol{q}). \tag{24}$$

The vector $\boldsymbol{G}$ can be thought of as an 'effective polarisation', leading to a transformed charge density

$$\rho'(\boldsymbol{r}) = -e\delta(\boldsymbol{r} - \beta_2\boldsymbol{q}) + e\delta(\boldsymbol{r} - \beta_1\boldsymbol{q}). \tag{25}$$

Thus, the gauge transformation has the effect of rescaling the charges to $-\alpha e$ and $+\alpha e$, and moving them to the positions $\beta_2\boldsymbol{q}$ and $\beta_1\boldsymbol{q}$ respectively. We can also define two charge systems

$$\rho_1(\boldsymbol{r}) = -e\delta(\boldsymbol{r} - \beta_1\boldsymbol{q}) + e\delta(\boldsymbol{r}) \tag{26}$$

$$\rho_2(\boldsymbol{r}) = -e\delta(\boldsymbol{r} - \beta_2\boldsymbol{q}) + e\delta(\boldsymbol{r}) \tag{27}$$

with the result

$$\nabla \cdot \boldsymbol{G}(\boldsymbol{r}) = \alpha(\rho_1 - \rho_2). \tag{28}$$

By Maxwell's equation

$$\varepsilon_0 \nabla \cdot \boldsymbol{E} = \rho \tag{29}$$

we obtain the interesting equation

$$\nabla \cdot \boldsymbol{\Pi} = -\rho \left\{ 1 - \frac{\alpha(\rho_2 - \rho_1)}{\rho} \right\} \tag{30}$$

where ρ is the actual charge density, defined in (4). In particular, in the PZW Hamiltonian $\nabla \cdot \boldsymbol{\Pi} = 0$ and $\boldsymbol{\Pi}$ is identified as the displacement $\boldsymbol{D}$. On the other hand, if $\alpha = 0$ then $\boldsymbol{\Pi}$ reverts back to the field $\boldsymbol{E}$, indicating a return to the minimal-coupling regime.

The transformed Hamiltonian exhibits a particularly interesting form when the dipole approximation is made. Here $\beta_1 = 0$, $\beta_2 = 1$ and

$$\boldsymbol{G}(\boldsymbol{r}, \boldsymbol{q}) = -\alpha e\boldsymbol{q}\delta(\boldsymbol{r}) = \alpha\boldsymbol{P}_{\mathrm{D}}(\boldsymbol{r}) \tag{31}$$

where $\boldsymbol{P}_{\mathrm{D}}(\boldsymbol{r})$ is the dipole approximation polarisation. The transformed Hamiltonian is

$$H_X^{(\alpha)} = \frac{1}{2m}\{\boldsymbol{p} + (1-\alpha)e\boldsymbol{A}\}^2 + \tfrac{1}{2}\int \mathrm{d}^3\boldsymbol{r}\{\varepsilon_0(\boldsymbol{\Pi} + \alpha\boldsymbol{P}_{\mathrm{D}})^2 + \mu_0\boldsymbol{B}^2\} \tag{32}$$

with conjugate momenta

$$\boldsymbol{p} = m\dot{\boldsymbol{q}} - (1-\alpha)e\boldsymbol{A} \tag{33}$$

$$\boldsymbol{\Pi} = -\varepsilon_0\boldsymbol{E} - \alpha\boldsymbol{P}_{\mathrm{D}}. \tag{34}$$

The dipole approximation dictates that $\boldsymbol{A}$ and $\boldsymbol{\Pi}$ in equations (32)–(34) are measured at the coordinate origin, that is at the position of $+e$. In a Coulomb gauge, (32) gives an interaction Hamiltonian in terms of transverse vectors

$$H_{\mathrm{I}}^{(c)} = \frac{e}{m}(1-\alpha)\boldsymbol{p}\cdot\boldsymbol{A}_\perp + \frac{e^2}{2m}(1-\alpha)^2\boldsymbol{A}_\perp^2 + \alpha e\boldsymbol{q}\cdot\boldsymbol{E}_\perp + \frac{\alpha^2}{2\varepsilon_0}\int \mathrm{d}^3\boldsymbol{r}\boldsymbol{P}_{\mathrm{D}_\perp}^2 \tag{35}$$

indicating a mix of $\boldsymbol{p}\cdot\boldsymbol{A}_\perp$ and $\boldsymbol{q}\cdot\boldsymbol{E}_\perp$ interactions. The interaction Hamiltonian of (35) leads to gauge-invariant photon transition processes; however, the multiplier α can be so chosen to eliminate the counter-rotating terms of a harmonic oscillator, or two-state atom, coupled to a field (Baxter *et al* 1989). The oscillator case has also been considered in a somewhat similar fashion by Drummond (1987), who diagonalised the minimal-coupling Hamiltonian by means of a double transformation of the annihilation and creation operators.

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