1 System description

1.1 Coordinates and quantities

Consider a dumbbell-like system consisting of two equal masses at a distance l from one another, and let m be the total mass. The system can be freely translated and rotated throughout space, so let x, y, z be the position of the centre off mass, and θ_r, φ_r be the polar and azimuthal angle respectively of the axis connecting the two masses. Notate these coordinates compactly as the vector

$$\vec{\mathbf{r}} = \begin{pmatrix} x \\ y \\ z \\ \vartheta_r \\ \varphi_r \end{pmatrix}.$$

Fix the angles such that a polar angle of $\varphi_r = m_0$ implies a dumbbell parallell to the z-axis and so that an azimuthal angle of $\vartheta_r = 0$ implies that the dumbbell axis lies in the xz-plane.

Now, consider also each of the masses of the dumbbell to carry spin, intrinsic angular momentum, of size $\frac{1}{2}$ each. The state of the spin components must be described quantum mechanically, so let $|s, m'\rangle$ denote the state of the system with *total* spin magnitude squared $s(s+1)\hbar^2$ and *total* spin measured along the z-axis $\hbar m'$. An external field $\vec{\mathbf{B}}$ is present, which we can describe by its magnitude B and its angular direction ϑ_B, φ_B in analogue with the angles defined above.

1.2 The Hamiltonian

The time evolution of such a system is governed in both classical and quantum mechanics by its Hamiltonian. Since spin is the epitome of a phenomena demanding a quantum mechanical interpretation we have no choice but to model the whole system quantum mechanically.The Hamiltonian which will be assumed for the system here is:

$$\mathcal{H} = \sum_{i=1}^{5} \frac{\vec{\mathbf{p}_\mathbf{i}}^2}{2m_i} + \frac{4J}{\hbar} S_z^{(1)} S_z^{(2)} - \gamma \vec{\mathbf{B}} \cdot \vec{\mathbf{S}}. \tag{1}$$

The first sum is over the five degrees of translational and rotational coordinates in $\vec{\mathbf{r}}$. The momentum and angular momentum operators are taken to be $p_i = i\hbar\partial_i$ with ∂_i as the derivative with respect to the corresponding coordinate. Note that it is not a priori clear that the effective masses m_i for all degrees of freedom are the same, but we can until later note that at least the first three are equal to m.

For the potential energy the spin-spin interaction is taken to be of Ising form, which is the first term after the sum, while the interaction between spin and magnetic field is considered in the final term. The parameters J and γ are the strengths of both of these interactions, while the operators $\vec{\mathbf{S}}$ and $S_z^{(n)}$ are respectively the one related to the total spin of the system and the spin in the z-direction of one of the system components.

1.3 Effective mass

To clearly see the values of the effective masses paired with the rotational momenta a quick derivation of the kinetic part of the Hamiltonian is in order. The kinetic energy related to rotation is of the form

$$K_{rot} = \frac{m}{2}\left(\frac{l}{2}\right)^2 \left(\dot{\vartheta}_r^2 + \dot{\varphi}_r^2\right),$$

which is the same as the relevant terms of the Lagrangian. The quantum mechanical momenta correspond to the momenta received from differentiating the classical Lagrangian, and as of such we have in the classical picture that

$$p_4 = \frac{\partial K}{\partial \dot{\vartheta}_r} = \frac{ml^2}{4}\dot{\vartheta}_r$$
$$p_5 = \frac{\partial K}{\partial \dot{\varphi}_r} = \frac{ml^2}{4}\dot{\varphi}_r$$

.

Performing the Legendre transform from the Lagrangian to the Hamiltonian yields:

$$\mathcal{H}_{rot} = p_4\dot{\vartheta}_r + p_5\dot{\varphi}_r - K = \frac{p_4^2 + p_5^2}{2}\frac{4}{ml^2}.$$

It is then clear that the effective masses to be used in equation 1 are:

$$m_i = \begin{cases} m & i = 1,2,3 \\ \frac{ml^2}{4} & i = 4,5 \end{cases}.$$

1.4 Rotation matrices

The potential energy operators will be of great use in some matrix form, so let the spin state be described as a coordinate vector in the basis $(|0,0\rangle, |1,-1\rangle, |1,0\rangle, |1,1\rangle)$. In the special case where the axis of the dumbbell (henceforth "Ising axis") and the magnetic field $\vec{\mathbf{B}}$ is parallell to the z-axis, it is clear that the operators take the form:

$$\vec{\mathbf{B}} \cdot \vec{\mathbf{S}} = B\hbar \begin{pmatrix} 0 & & & \\ & -1 & & \\ & & 0 & \\ & & & 1 \end{pmatrix} \tag{2}$$

$$S_z^{(1)} S_z^{(2)} = \frac{\hbar^2}{4} \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}. \tag{3}$$

The second matrix follows from the well known representation of a two-component spin-$\frac{1}{2}$ system as singlet and triplet states: Let $|m_1, m_2\rangle_1$ be the state with spin-z number m_1 for the first component and m_2 for the second component. Then

$$\begin{aligned} |0,0\rangle &= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1 - \left|-\frac{1}{2},\frac{1}{2}\right\rangle_1\right] \\ |1,-1\rangle &= \left|-\frac{1}{2},-\frac{1}{2}\right\rangle_1 \\ |1,0\rangle &= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1 + \left|-\frac{1}{2},\frac{1}{2}\right\rangle_1\right] \\ |1,1\rangle &= \left|\frac{1}{2},\frac{1}{2}\right\rangle_1. \end{aligned}$$

Both matrices above assume that the basis is aligned with $\vec{\mathbf{B}}$ and the Ising axis respectively. Therefore we must find some rotation operator that can describe our state given in the z-axis basis in a basis aligned with $\vec{\mathbf{B}}$ or the Ising axis.

Consider therefore first a rotation of the *state* vectors, which can then easily be inverted to receive the forward transformation also necessary for the transformation of operator matrices. The inversion process is but a complex conjugation since the operator in question is unitary. It can be shown that the rotation about three Euler angles α, β, δ of a state is given by the matrix with elements as:

$$\mathcal{U}_{m'm''} = \langle s, m'| e^{\frac{-iS_z\alpha}{\hbar}} e^{\frac{-iS_y\beta}{\hbar}} e^{\frac{-iS_z\delta}{\hbar}} |s, m''\rangle.$$

Here s, m', m'' are spin quantum numbers of the system, which in the more general case can be replaced by angular momentum quantum numbers. The rotations α, β and δ are done about the $z-$, $y-$ and then $z-$ body axes of the system in turn. Since the spin states considered here are symmetric about their body z-axes the final rotation δ is superfluous and thus will be discarded. Identifying the angles $\alpha = \varphi$ and $\beta = \vartheta$ for rotation to some spherical coordinates it can further be shown that the exponential operators amount to:

$$\mathcal{U} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{e^{-i\varphi}}{2}(1+\cos(\vartheta)) & \frac{e^{-i\varphi}}{\sqrt{2}}\sin(\vartheta) & \frac{e^{-i\varphi}}{2}(1-\cos(\vartheta)) \\ 0 & -\frac{1}{\sqrt{2}}\sin(\vartheta) & \cos(\vartheta) & \frac{1}{\sqrt{2}}\sin(\vartheta) \\ 0 & \frac{e^{i\varphi}}{2}(1-\cos(\vartheta)) & -\frac{e^{i\varphi}}{\sqrt{2}}\sin(\vartheta) & \frac{e^{i\varphi}}{2}(1+\cos(\vartheta)) \end{pmatrix}.$$

An operator matrix A transforms under rotation as $A_{rot} = \mathcal{U}A\mathcal{U}^\dagger$, so the operator of equation 2 which is expressed in terms of a basis rotated by angles ϑ_B and φ_B can be written in the z-axis basis as:

$$\vec{\mathbf{B}} \cdot \vec{\mathbf{S}} = B\hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\cos(\vartheta_B) & \frac{e^{-i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) & 0 \\ 0 & \frac{e^{i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) & 0 & \frac{e^{-i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) \\ 0 & 0 & \frac{e^{i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) & \cos(\vartheta_B) \end{pmatrix}. \tag{4}$$

Analogously the matrix of equation 3 is expressed in a basis rotated through angles ϑ_r and φ_r, so in the z-axis basis it can be written:

$$S_z^{(1)} S_z^{(2)} = \frac{\hbar^2}{4} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & \cos^2(\vartheta_r) & -\frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & e^{-2i\varphi_r}\sin^2(\vartheta_r) \\ 0 & -\frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & -\cos(2\vartheta_r) & \frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) \\ 0 & e^{2i\varphi_r}\sin^2(\vartheta_r) & \frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & \cos^2(\vartheta_r) \end{pmatrix}. \tag{5}$$

In equation 4 and 5 it is readily visible that the spin singlet state $|0,0\rangle$ is unaffected by the external magnetic field, as could be concluded even without the explicit Hamiltonian. As a result the total Hamiltonian for the singlet state is but the sum of two terms dependent on different sets of variables. This is to say that separation of variables can be used to solve the eigenstate problem, so the qualities presently at interest are lost. For this reason henceforth only the non-singlet (so called triplet) states are considered, and matrices will often be reduced to the relevant three-dimensional subspace for simplicity's sake.

At last all parts of the potential energy are expressed in a single basis, such that the potential part of the Hamiltonian takes the form:

$$\mathcal{H}_f = \gamma B\hbar \begin{pmatrix} \xi\cos^2(\vartheta_r) + \cos(\vartheta_B) & -\frac{e^{-i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) - \xi\frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & \xi e^{-2i\varphi_r}\sin^2(\vartheta_r) \\ -\frac{e^{i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) - \xi\frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & -\xi\cos(2\vartheta_r) & -\frac{e^{-i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) + \xi\frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) \\ \xi e^{2i\varphi_r}\sin^2(\vartheta_r) & -\frac{e^{i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) + \xi\frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & \xi\cos^2(\vartheta_r) - \cos(\vartheta_B) \end{pmatrix}. \tag{6}$$

Here $\xi = \frac{J}{\gamma B}$ is a proportionality factor between the spin-spin and spin-field interactions which will simplify calculations. This together with the kinetic part of the Hamiltonian $\mathcal{H}_s$ will determine the time evolution of the system:

$$\mathcal{H}_s = \sum_{n=1}^{5} \frac{p_i^2}{2m_i}. \tag{7}$$

2 The Born-Oppenheimer approximation

2.1 Derivation

Solving for the eigenstates of such a Hamiltonian as described above is a mighty task. Note in particular that the contribution from potential energy to the Hamiltonian, equation 6, is heavily dependent on the position and rotation of the dumbbell through all parameters ϑ_r, ϑ_B, φ_r, φ_B and B. This couples all degrees of freedom for the system, which complicates the problem greatly.

An approximation is therefore in order. If the position and rotation, henceforth the "slow" parameters, is more or less static in comparison with the spin degrees of freedom, henceforth "fast parameters", the so-called Born-Oppenheimer approximation is applicable. A version of the adiabatic approximation, it assumes that a "fast" subsystem, described by the fast parameters, can be described by eigenstates to a Hamiltonian parametrised by the slow parameters. A fast system in such an eigenstate can be considered to remain in the same eigenstate as the associated "fast" Hamiltonian slowly changes, changing but its eigenvalue as the slow parameters evolve. So far this is what is known as the adiabatic approximation.

The Born-Oppenheimer approximation involves the extension of this to also consider how the "slow" system evolves, in practice finding an effective Hamiltonian to the slow system as well. The full system is then considered to be described by the product of a wave function to the slow system Ψ_s and some eigenstate to the fast Hamiltonian $|n\rangle$, i.e.:

$$|\Psi_{full}\rangle = \Psi_s |n\rangle .$$

The aforementioned fast and slow Hamiltonians are for the system in consideration the previously found $\mathcal{H}_f$ and $\mathcal{H}_s$ respectively. The full solution to the fast system is assumed to be found, i.e.:

$$\mathcal{H}_f \left|n\right\rangle = E_n \left|n\right\rangle .$$

The Schrödinger equation then implies, since $\frac{\partial}{\partial t}\left|n\right\rangle = 0$:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}(\Psi_s \left|n\right\rangle) &= (\mathcal{H}_f + \mathcal{H}_s)\Psi_s \left|n\right\rangle \\ i\hbar\frac{\partial \Psi_s}{\partial t} &= \left\langle n\right| (\mathcal{H}_f + \mathcal{H}_s) \left|n\right\rangle \Psi_s = (\left\langle n\right| \mathcal{H}_s \left|n\right\rangle + E_n)\Psi_s. \end{aligned}$$

This can be interpreted as an effective Hamiltonian $\mathcal{H}_{eff} = \left\langle n\right| \mathcal{H}_s \left|n\right\rangle + E_n$ governing the slow wave function. The inner product term can be further manipulated as follows:

$$\left\langle n\right| \mathcal{H}_s \left|n\right\rangle \Psi_s = \sum_{i=1}^{5} \left[\left\langle n\right| \frac{p_i^2}{2m_i} \left|n\right\rangle \Psi_s + \left\langle n\right| \frac{p_i}{m_i} \left|n\right\rangle p\Psi_s + p_i^2 \Psi \right].$$

Here it is to be understood that the momentum operators in $\mathcal{H}_s$ act on *both* the spin ket and and the slow wave fucntion. An operator to the left of a ket and wave function product will however be understood to act on the ket only, if no clarifying parentheses are written out explicitly. Since all p_i are hermitian operators and can thus be acted on bras to the left without conjugation the most troublesome term can also be written as:

$$\begin{aligned} \left\langle n\right| p_i^2 \left|n\right\rangle &= \left\langle p_i n | p_i n\right\rangle \\ &= \left\langle p_i n | n\right\rangle \left\langle n | p_i n\right\rangle + \left\langle p_i n\right| (\mathbb{1} - \left|n\right\rangle \left\langle n\right|) \left|p_i n\right\rangle \\ &= \left\langle n | p_i n\right\rangle^2 + \left\langle p_i n\right| (\mathbb{1} - \left|n\right\rangle \left\langle n\right|) \left|p_i n\right\rangle . \end{aligned}$$

An identity relation was used in the second step, where $\mathbb{1}$ is the identity operator. Inserting the derivative form of the momentum operator as seen in section 1.2 and rearranging terms with some convenient notation we arrive to the Hamiltonian providing the interesting properties sought after.

$$\mathcal{H}_{eff} = \sum_{i=5}^{5} \frac{(p_i - A_i)^2}{2m_i} + \Phi + E_n \tag{8}$$

$$A_i = i\hbar \left\langle n | \partial_i n\right\rangle \tag{9}$$

$$\Phi = \sum_{i=1}^{5} \frac{\hbar^2}{2m_i} \left\langle \partial_i n\right| (\mathbb{1} - \left|n\right\rangle \left\langle n\right|) \left|\partial_i n\right\rangle . \tag{10}$$

2.2 Interpretation

[Något om magnetfältskopplingen, monopolerna, $\vec{\mathbf{A}} = \sum_{i=1}^{5} A_i$, $\vec{\mathbf{p}} = \sum_{i=1}^{5} p_i$. En första blick på att det är här den fina fysiken händer]

2.3 Dynamics

Having found an effective Hamiltonian to the slow system the application of this Hamiltonian to the dynamics of the system remains to be performed. One could proceed with the quantum mechanical methods applied so far, solving for eigenstates to $\mathcal{H}_{eff}$. This however requires finding the dependence of the eigenstates to $\mathcal{H}_f$ on the slow parameters, which may not be achievable analytically. Instead the slow system can be considered to be effectively lying in the classical domain, and the Hamiltonian derived by quantum mechanical means will be utilized in the role of the Hamiltonian for classical mechanics.

Hamilton's canonical equations indicate the time evolution of $\vec{\mathbf{r}}$:

$$\begin{aligned} \frac{\partial \vec{\mathbf{r}}}{\partial t} &= \frac{\partial \mathcal{H}_{eff}}{\partial \vec{\mathbf{p}}} = \frac{\vec{\mathbf{p}} - \vec{\mathbf{A}}}{m} \\ \frac{\partial \vec{\mathbf{p}}}{\partial t} &= -\frac{\partial \mathcal{H}_{eff}}{\partial \vec{\mathbf{r}}} = \left(\frac{\partial \vec{\mathbf{A}}}{\partial \vec{\mathbf{r}}}\right)^T \frac{\vec{\mathbf{p}} - \vec{\mathbf{A}}}{m} - \frac{\partial \Phi}{\partial \vec{\mathbf{r}}} - \frac{\partial E_n}{\partial \vec{\mathbf{r}}} = \left(\frac{\partial \vec{\mathbf{A}}}{\partial \vec{\mathbf{r}}}\right)^T \frac{\partial \vec{\mathbf{r}}}{\partial t} - \frac{\partial \Phi}{\partial \vec{\mathbf{r}}} - \frac{\partial E_n}{\partial \vec{\mathbf{r}}}. \end{aligned}$$

Note in particular that the first of these equations imply that the canonical momentum $\vec{\mathbf{p}}$ is *not* $m\frac{\partial \vec{\mathbf{r}}}{\partial t}$. The effective force acting on the system can be found, utilizing that the synthetic vector potential does not depend explicitly on time, i.e. that $\frac{\partial \vec{\mathbf{A}}}{\partial t} = 0$:

$$m\frac{\partial^2 \vec{\mathbf{r}}}{\partial t^2} = \frac{\partial \vec{\mathbf{p}}}{\partial t} - \frac{\partial \vec{\mathbf{A}}}{\partial t} = \left(\frac{\partial \vec{\mathbf{A}}}{\partial \vec{\mathbf{r}}}\right)^T \frac{\partial \vec{\mathbf{r}}}{\partial t} - \left(\frac{\partial \vec{\mathbf{r}}}{\partial t} \cdot \vec{\boldsymbol{\nabla}}\right)\vec{\mathbf{A}} - \frac{\partial \Phi}{\partial \vec{\mathbf{r}}} - \frac{\partial E_n}{\partial \vec{\mathbf{r}}}. \tag{11}$$

The Jacobian matrix can be treated elementwise, as well as the second term:

$$\frac{1}{i\hbar}\left(\frac{\partial \vec{\mathbf{A}}}{\partial \vec{\mathbf{r}}}\right)_{ji} = \partial_i \langle n|\partial_j n\rangle = \langle \partial_i n|\partial_j n\rangle + \langle n|\partial_i \partial_j n\rangle$$

$$\frac{1}{i\hbar}\left(\left(\frac{\partial \vec{\mathbf{r}}}{\partial t} \cdot \vec{\boldsymbol{\nabla}}\right)\vec{\mathbf{A}}\right)_i = \sum_{j=1}^{5} \frac{\partial r_j}{\partial t}\partial_j \langle n|\partial_i n\rangle = \sum_{j=1}^{5} \frac{\partial r_j}{\partial t}(\langle \partial_j n|\partial_i n\rangle + \langle n|\partial_j \partial_i n\rangle).$$

Insertion into equation 11 then yields a higher dimensional analogue to [the usual case] for the forces due to the synthetic magnetic field:

$$\begin{aligned}\frac{1}{i\hbar}\left[\left(\frac{\partial \vec{\mathbf{A}}}{\partial \vec{\mathbf{r}}}\right)^T \frac{\partial \vec{\mathbf{r}}}{\partial t} - \left(\frac{\partial \vec{\mathbf{r}}}{\partial t} \cdot \vec{\boldsymbol{\nabla}}\right)\vec{\mathbf{A}}\right]_i &= \frac{1}{i\hbar}F_i^A = \sum_{j=1}^{5} \frac{\partial r_j}{\partial t}[\langle \partial_i n|\partial_j n\rangle - \langle \partial_j n|\partial_i n\rangle] \\ &= \sum_{j=1}^{5}\sum_{l} \frac{\partial r_j}{\partial t}[\langle \partial_i n|l\rangle \langle l|\partial_j n\rangle - \langle \partial_j n|l\rangle \langle l|\partial_i n\rangle] \\ &= \sum_{j=1}^{5}\sum_{l\neq n} \frac{\partial r_j}{\partial t}[\langle \partial_i n|l\rangle \langle l|\partial_j n\rangle - \langle \partial_j n|l\rangle \langle l|\partial_i n\rangle].\end{aligned}$$

Here $|l\rangle$ simply denotes an eigenstate to $\mathcal{H}_f$ of some index l, and the sum over l is over all available states. The exclusion of $n = l$-terms follows as $\langle \partial_i n|n\rangle$ is pure imaginary, which can be seen from differentiating $\langle n|n\rangle$. This rearrangement is highly desirable, for it now so happens that this allows us to take derivatives of the Hamiltonian instead of the rather tricky differentiation of the eigenkets. Differentiating the Schrödinger equation and acting on it with some other eigenbra yields:

$$\begin{aligned}\mathcal{H}_f |n\rangle &= E_n |n\rangle \\ \partial\mathcal{H}_f |n\rangle + H_f |\partial n\rangle &= E_n |\partial n\rangle \\ \langle l| \partial\mathcal{H}_f |n\rangle &= \langle l|\partial n\rangle (E_n - E_l).\end{aligned}$$

Rearranging, a very useful relation emerges:

$$\langle l|\partial n\rangle = \frac{\langle l| \partial\mathcal{H}_f |n\rangle}{E_n - E_l}. \tag{12}$$

This we can insert into above:

$$\frac{1}{i\hbar}F_i^A = \sum_{j=1}^{5}\sum_{l\neq n} \frac{\frac{\partial r_j}{\partial t}}{(E_n - E_l)^2}[\langle n| \partial_i\mathcal{H}_f |l\rangle \langle l| \partial_j\mathcal{H}_f |n\rangle - \langle n| \partial_j\mathcal{H}_f |l\rangle \langle l| \partial_i\mathcal{H}_f |n\rangle] \tag{13}$$

$$= 2i\sum_{j=1}^{5}\sum_{l\neq n} \frac{\frac{\partial r_j}{\partial t}}{(E_n - E_l)^2} \operatorname{Im}[\langle n| \partial_i\mathcal{H}_f |l\rangle \langle l| \partial_j\mathcal{H}_f |n\rangle]. \tag{14}$$

Equation 12 can be used for something similar when evaluating the synthetic electric potential:

$$\Phi = \sum_{i=1}^{5}\sum_{l\neq n} \frac{\hbar^2}{2m_i}(\langle \partial_i n|l\rangle \langle l|\partial_i n\rangle) = \sum_{i=1}^{5}\sum_{l\neq n} \frac{\hbar^2}{2m_i} \frac{\langle n| \partial_i\mathcal{H}_f |l\rangle \langle l| \partial_i\mathcal{H}_f |n\rangle}{(E_n - E_l)^2} \tag{15}$$

$$= \frac{\hbar^2}{2m}\sum_{l\neq n} \frac{\langle n| \vec{\boldsymbol{\nabla}}\mathcal{H}_f |l\rangle \cdot \langle l| \vec{\boldsymbol{\nabla}}\mathcal{H}_f |n\rangle}{(E_n - E_l)^2}. \tag{16}$$

Note however that no simple form to the derivative of the electric potential Φ has been found, which might not be easily described analytically.

The problem has thus been reduced to evaluating, per equations 13 and 15,

$$m\frac{\partial^2\vec{\mathbf{r}}}{\partial t^2} = \vec{\mathbf{F}}^A - \frac{\partial\Phi}{\partial\vec{\mathbf{r}}} - \frac{\partial E_n}{\partial\vec{\mathbf{r}}}. \tag{17}$$

2.4 Differentiation of the Hamiltonian

In order to easily evaluate equations 13 and 15 derivatives of $\mathcal{H}_f$ from equation 6 are to be found. Writing any of the coordinates x, y, z as r the derivatives can be written:

$$\partial_r\mathcal{H}_f = \gamma B\hbar\begin{pmatrix} -\dot{\vartheta}_B\sin(\vartheta_B) & \Omega & 0 \\ \Omega^* & 0 & \Omega \\ 0 & \Omega^* & \dot{\vartheta}_B\sin(\vartheta_B)\end{pmatrix} + \frac{\dot{B}}{B}\mathcal{H}_f \tag{18}$$

$$\frac{1}{\gamma B\xi\hbar}\partial_{\vartheta_r}\mathcal{H}_f = \begin{pmatrix} -\sin(2\vartheta_r) & -\sqrt{2}e^{-i\varphi_r}\cos(2\vartheta_r) & e^{-2i\varphi_r}\sin(2\vartheta_r) \\ -\sqrt{2}e^{i\varphi_r}\cos(2\vartheta_r) & 2\sin(2\vartheta_r) & \sqrt{2}e^{-i\varphi_r}\cos(2\vartheta_r) \\ e^{2i\varphi_r}\sin(2\vartheta_r) & \sqrt{2}e^{i\varphi_r}\cos(2\vartheta_r) & -\sin(2\vartheta_r)\end{pmatrix} \tag{19}$$

$$\frac{1}{\gamma B\xi\hbar}\partial_{\varphi_r}\mathcal{H}_f = \begin{pmatrix} 0 & i\frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & -2ie^{-2i\varphi_r}\sin^2(\vartheta_r) \\ -i\frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & 0 & -i\frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) \\ 2ie^{2i\varphi_r}\sin^2(\vartheta_r) & i\frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & 0\end{pmatrix}. \tag{20}$$

Here $(i\dot{\varphi}_B\sin(\vartheta_B) - \dot{\vartheta}_B\cos(\vartheta_B))\frac{e^{-i\varphi_B}}{\sqrt{2}}$ is introduced as a means of compressing the rather lengthy expressions for the derivative with respect to r, and asterisks signify the complex conjugate.

2.5 Solution of the fast subsystem

The usage of the Born-Oppenheimer approximation requires a solution to the fast subsystem, i.e. that the eigenvalues and eigenvectors to $\mathcal{H}_f$ are found. Unfortunately this is not possible analytically for the present system, but we note that it is the same as solving the following transcendental characteristic equation, which follows from equation 6, for the eigenvalues $\lambda_n = \frac{E_n}{J\hbar}$:

$$\begin{vmatrix} \lambda_n - \cos^2(\vartheta_r) + \xi\cos(\vartheta_B) & -\frac{\xi e^{-i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) + \frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) & -e^{-2i\varphi_r}\sin^2(\vartheta_r) \\ \frac{e^{i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) - \xi\frac{e^{i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) & \lambda\cos(2\vartheta_r) & -\xi\frac{e^{-\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) - \frac{e^{-i\varphi_r}}{\sqrt{2}}\sin(2\vartheta_r) \\ -e^{2i\varphi_r}\sin^2(\vartheta_r) & -\xi\frac{e^{i\varphi_B}}{\sqrt{2}}\sin(\vartheta_B) - \frac{e^{i\varphi_r}}{\sqrt{2}}\sin(\vartheta_r) & \lambda + \cos^2(\vartheta_r) - \xi\cos(\vartheta_B)\end{vmatrix}$$
$$= 0 = \lambda^3 + \lambda^2\cos(2\vartheta_r) + \lambda(2\cos^2(\vartheta_r)[\xi\cos(\vartheta_B) - \sin^2(\vartheta_r)) - 1 - \xi^2) + \dots$$
$$+ \cos(2\vartheta_r)(-1 + 2\xi\cos^2(\vartheta_r)\cos(\vartheta_B) + \dots$$
$$- \xi^2\cos^2(\vartheta_B)(1 + 2\cos^2(\vartheta_B)(1 + 2\cos^2(\vartheta_B)(1 + 2\cos(\varphi_r - \varphi_B)\sin(\vartheta_B)\sin(2\vartheta_r)] + \dots$$
$$+ \frac{\xi}{2}\cos(\varphi_r - \varphi_B)\sin(\vartheta_B)\sin(2\vartheta_r) + \frac{1}{2}\cos(\varphi_r - \varphi_B)\sin(\vartheta_B)\sin(2\vartheta_r) + \dots$$
$$+ \frac{\xi}{2}\cos(2(ph_r - ph_B))\sin^2(\vartheta_B) + \frac{3}{2}\xi\cos(\varphi_r - \varphi_B)\sin(\vartheta_B)\sin(2\vartheta_r) + \dots$$
$$- \frac{1}{2}\cos(\varphi_r - \varphi_B)\sin(\vartheta_B)\sin(2\vartheta_r) - \frac{\xi}{2}\cos(2(\varphi_r - \varphi_B))\sin^2(\vartheta_B) + \frac{1}{2}\sin^2(2\vartheta_r) + \dots$$
$$- 2\xi^2\cos(\vartheta_B)\cos(\varphi_r - \varphi_B)\sin(\vartheta_B)\sin(2\vartheta_r). \tag{21}$$

This is rather messy, and unfortunately does not bring much clarity to the behaviour of the eigenvalues.

Solving for the eigenvectors as a function of the eigenvalues does not yield any strikingly useful relation neither, so the calculation of eigenvalues and eigenvectors may be left to numerics from the onset. Equation 21 could in principle be differentiated implicitly to receive the derivatives of the energies also needed, but since many other quantities must also be calculated numerically the derivatives of the energies will be done so likewise for practicality's sake.