BEM in a Nutshell

We want to solve the exterior Dirichlet problem

$$\begin{cases} -\Delta u - k^2 u = 0 & \text{on } \mathbb{R}^3 \setminus \overline{\Omega} \\ \gamma u = g & \text{on } \Gamma \end{cases}$$

We know that the solution can be written in terms of Boundary operators:

$$u = -S_k \gamma \frac{\partial u}{\partial n} + D_k \gamma u \qquad x \in \mathbb{R}^3 \setminus \overline{\Omega}$$

Taking traces we obtain

$$\gamma u = -V_k \gamma \frac{\partial u}{\partial n} + \left(\frac{1}{2} + K_k\right) \gamma u \qquad \text{on } \Gamma$$

$\Rightarrow$ Call $\gamma \frac{\partial u}{\partial n}$ our unknown t then we must solve the problem

$$V_k t = \left(\frac{1}{2} + K_k\right) \gamma u = \left(\frac{1}{2} + K_k\right) g$$

In variational form this is

$$\langle V_k t, \tau \rangle_\Gamma = \left\langle \left(\frac{1}{2} + K_k\right) g, \tau \right\rangle_\Gamma \quad \forall \tau \in H^{-1/2}(\Gamma)$$

Let $S_h^0(\Gamma) = \text{span}\{\varphi_k^0\}_{k=1}^N \subset H^{-1/2}(\Gamma)$ $\varphi_k^0 = \begin{cases} 1 & \tau_k \\ 0 & \end{cases}$

be the trial space of pw. constant basis φ_k^0.

the operator V_k is elliptic in $H^{-1/2}(\Gamma)$ for $k=0$

and $S_h^0(\Gamma) \subset H^{-1/2}(\Gamma)$ therefore there exists a unique solution $t_h \in S_h^0(\Gamma)$ of the Galerkin variational formulation satisfying

$$\|t_h\|_{H^{-1/2}(\Gamma)} \le \frac{1}{c_1^V} \left\| \left(\frac{1}{2} I + K_h\right) g \right\| \le \frac{c_2}{c_1^V} \|g\|_{H^{1/2}(\Gamma)}$$

as well as the error estimate

$$\|t - t_h\|_{H^{-1/2}(\Gamma)} \le \frac{c_2^V}{c_1^V} \inf_{\tilde{t}_h \in S_h^0(\Gamma)} \|t - \tilde{t}_h\|_{H^{-1/2}(\Gamma)}$$

Error bounds:

Let $u \in H^s(\Gamma)$, $s \in [0,1]$, and let $Q_h u \in S_h^0(\Gamma)$ where Q_h is the L^2-projector on S_h^0:

$$\langle Q_h u, v_h \rangle_{L^2(\Gamma)} = \langle u, v_h \rangle_{L^2(\Gamma)} \quad \forall v_h \in S_h^0(\Gamma)$$

then,

$$\|u - Q_h u\|_{L_2}^2 \le c \sum_{k=1}^{N} h_k^{2s} |u|_{H^s(\tau_k)}^2$$

and

$$\|u - Q_h u\| \le c\, h^s |u|_{H^s(\Gamma)}$$

Also for $\sigma \in [-1, 0)$

$$\|u - Q_h u\| \le c\, h^{s-\sigma} |u|_{H^s(\Gamma)}$$

and

$$\|u - Q_h u\|_{L_2}^2 \le c\, h^{-2\sigma} \sum_{k=1}^{N} h_k^{2s} |u|_{H^s(\tau_k)}^2$$

Hence, for Lipschitz boundary Γ we get

$$\| t - t_h \|_{H^{-1/2}(\Gamma)} \le C h^{1+1/2} |t|_{H^1_{pw}(\Gamma)}$$

$\Rightarrow$ When considering higher order the regularity decreases due to corners and edges.

Discretization. Boundary operator matrices.

From

$$\langle V_h t_h, s_h \rangle = \langle (\tfrac{1}{2} + K_h) g, s_h \rangle \quad \forall \varphi_h^i \in S_h^0$$

we need to compute terms N

$$\langle V_h t_h, s_h \rangle \quad \text{writing } t_h = \sum_{i=0}^{N} \alpha_i \varphi_h^i$$

$$\Rightarrow \quad \underline{\alpha} \left[\langle V \varphi_h^j, \varphi_h^k \rangle^N \right]_{j,k=1} \beta$$

$$\Rightarrow \quad \iint_{\tau_i \, \tau_k} \frac{1}{\| x - y \|} \, ds. \qquad \text{How do we do this?}$$

$\Rightarrow$ Quadrature formulas too expensive

$\Rightarrow$ Full matrices

$\Rightarrow$ Loop formulae.

Chapter 2

▶ Implementation of the algorithm

In this chapter, we will collect all necessary parts to implement the algorithm we derived in the first part of this thesis.

2.1 A boundary element method

The main question is how to calculate integrals of the form

$$(A)_{i,j} = \langle V_\kappa \phi_i, \phi_j \rangle = \frac{1}{4\pi} \int_\Gamma \int_\Gamma \frac{\cos(\kappa \|x-y\|)}{\|x-y\|} \phi_i dS_y \phi_j dS_x$$

which have to be evaluated for $i, j = 1 \ldots N$. Fortunately, the integral is symmetric with regard to exchange of x and y. This ensures a symmetric stiffness matrix A. In contrast to the finite element method, our matrix A will be much smaller but dense. Each matrix element calculation is a very costly procedure as we will now see and partly compensates the benefit of the much smaller matrix.

2.1.1 Panelization of the domain

Definition 2.1: *(taken from [6]) A* ***panelization*** $\mathcal{G}$ *of the boundary* Γ *is a subdivision of* Γ *into open, disjoint elements* $\tau \subset \Gamma$*. Of course it has to hold that*

$$\Gamma = \overline{\bigcup_{\tau \in \mathcal{G}} \tau}$$

We look at the discretization of the unit cube $[0,1]^3$, for which it is reasonable to create a simple *triangular panelization* of the boundary, shown in figure 2.1. As we use *piecewise constant basisfunctions* ϕ_i, that are 1 on $\triangle_i$ and 0 elsewhere, the integral

$$\int_\Gamma \int_\Gamma f(\kappa, x, y) \phi_i dS_y \phi_j dS_x$$

simplifies to:

$$\iint_{\triangle_j} \iint_{\triangle_i} f(\kappa, x, y) dS_y dS_x$$

As we want to compute this integral using a Gauss-Legendre quadrature rule, we need to calculate the n Gauss points and n weights on each triangle. By determining the locations of the points in barycentric coordinates, a simple multiplication with the vertices (P_1, P_2, P_3) of our triangle $\triangle_i$ directly yields the corresponding Gauss points x_k^i in $\triangle_i$. The weights w_k^i have to be scaled by

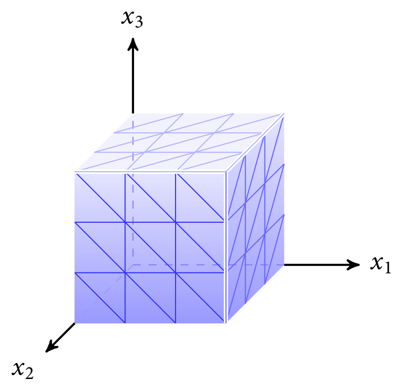

Figure 2.1: *A panelization of the cube into 108 triangles.*

the area of the triangle such that the integral over $f(x) = 1$ equals the area of $\triangle_i$:

$$\iint_{\triangle_i} 1 \, dS_x \approx \sum_{k=1}^{n} w_k \stackrel{!}{=} \text{Area}(\triangle_i)$$

The values of the Gauss-Legendre points and weights in barycentric coordinates can be found ready to use in the literature, see [3] With the points and weights transformed for each triangle, we can now integrate numerically:

$$\iint_{\triangle_j} \iint_{\triangle_i} f(\kappa, x, y) \, dS_y \, dS_x \approx \sum_{m=1}^{n} \sum_{k=1}^{n} w_m^j \, w_k^i \, f(\kappa, x_m^j, x_k^i)$$

In the framework, $n = 7$ and $n = 13$ are supported.

2.1.2 The singular integrals

The big problem in evaluating these integrals, however, is the **singularity of f at the point** $x = y$. This happens in 3 cases:

1. both panels $\triangle_i$ and $\triangle_j$ are identical
2. $\triangle_i$,$\triangle_j$ share one edge
3. $\triangle_i$,$\triangle_j$ share one point in the corner

Of these 3 cases, the first is the most important, while the other introduce more or less small errors depending on the choice of integration points. E.g., with the Gauss-Legendre quadrature rule, all points lie in the interior of the triangle, whereas the Gauss-Lobatto rule defines points directly on the edge or corner. Notice that we can split the integral

$$\iint_{\triangle_i} \iint_{\triangle_j} \frac{\cos(\kappa\|x-y\|)}{\|x-y\|} dS_y dS_x$$

into a singular part given by the electrostatic kernel integral and a nonsingular rest:

$$= \iint_{\triangle_i} \iint_{\triangle_j} \frac{1}{\|x-y\|} dS_y dS_x + \iint_{\triangle_i} \iint_{\triangle_j} \frac{\cos(\kappa\|x-y\|) - 1}{\|x-y\|} dS_y dS_x$$

A Taylor expansion of the cosine around zero immediately reveals the nonsingularity of the second term for $\|x-y\| \to 0$:

$$\begin{aligned}\frac{\cos(\kappa\|x-y\|)-1}{\|x-y\|} &= \frac{1-\frac{1}{2}(\kappa\|x-y\|)^2+O(\kappa\|x-y\|)^4-1}{\|x-y\|}\\ &= \kappa\,\frac{-\frac{1}{2}(\kappa\|x-y\|)^2+O(\kappa\|x-y\|)^4}{\kappa\|x-y\|}\\ &= -\kappa\,\frac{1}{2}(\kappa\|x-y\|)^1+\kappa\, O(\kappa\|x-y\|)^3 \longrightarrow 0\end{aligned}$$

Therefore, direct integration with a Gauss-Legendre quadrature rule poses no problem for the second term. For the electrostatic kernel integral, however, we have to apply a trick shown below.

2.1.3 Solving the inner integral analytically

The method goes back to A.T. de Hoop [4] (also mentioned in [1]) and was shown to the author in helpful discussions with C. J. Hanckes, which we will closely follow in this section. The idea is to solve the inner integral analytically as a function $F(x)$ depending on the outer integration variable x:

$$\iint_{\triangle_i}\iint_{\triangle_j}\frac{1}{\|x-y\|}dS_y dS_x = \iint_{\triangle_i}F(x)dS_x\ ,\quad \text{with } F(x)=\iint_{\triangle_j}\frac{1}{\|x-y\|}dS_y$$

With this, the integral can be evaluated very accurately and efficiently now using not two, but only one quadrature rule for the outer integral:

$$\iint_{\triangle_j}F(x)dS_x \approx \sum_{m=1}^{n} w_m^j\,F(x)$$

The analytic solution is quite tricky to find and requires a clever reformulation of the integral over the triangle as a contour integral over the boundary of the triangle. We will here go through the most important steps. In the first part, we already used the following relation:

$$\Delta\|x-y\| = \frac{2}{\|x-y\|}$$

using this, we can write for $F(x)$:

$$F(x)=\iint_{\triangle_j}\frac{1}{\|x-y\|}dS_y = \frac{1}{2}\iint_{\triangle_j}\Delta\|x-y\|dS_y$$

With clever use of vector identities not discussed into detail in this short overview, this can be transformed into the seemingly more complicated relation:

$$\begin{aligned} F(x) &= \frac{1}{2}\iint_{\triangle_j} \Delta\|x-y\| dS_y \\ &= \frac{1}{2}\iint_{\triangle_j}\left(\frac{\partial^2}{\partial\vec{n}^2}\|x-y\| - \vec{n}\cdot\nabla\times\nabla\times(\|x-y\|\vec{n})\right)dS_y \\ &= \underbrace{\frac{1}{2}\iint_{\triangle_j}\frac{\partial^2}{\partial\vec{n}^2}\|x-y\|dS_y}_{F_1(x)} - \underbrace{\frac{1}{2}\iint_{\triangle_j}\vec{n}\cdot\nabla\times\nabla\times(\|x-y\|\vec{n})\,dS_y}_{F_2(x)} \\ &= F_1(x) - F_2(x) \end{aligned}$$

Let us now first look at $F_1(x)$ and simplify the integrand:

$$\frac{\partial^2}{\partial\vec{n}^2}\|x-y\| = \frac{\partial}{\partial\vec{n}}(\nabla\|x-y\|\cdot\vec{n}) = \frac{\partial}{\partial\vec{n}}\left(\frac{(y-x)}{\|x-y\|}\cdot\vec{n}\right)$$

Close inspection reveals that for all $y \in \triangle_j$

$$(y-x)\cdot\vec{n} = \text{dist}(x,\triangle_j) = const$$

with $\text{dist}(x,\triangle_j)$ being the distance of point x from the triangle $\triangle_j$. This makes it possible to move it outside the integral:

$$\begin{aligned} F_1(x) &= \frac{1}{2}\text{dist}(x,\triangle_j)\iint_{\triangle_j}\frac{\partial}{\partial\vec{n}}\left(\frac{1}{\|x-y\|}\right)dS_y \\ &= \frac{1}{2}\text{dist}(x,\triangle_j)\iint_{\triangle_j}\text{grad}\left(\frac{1}{\|x-y\|}\right)\cdot\vec{n}\,dS_y \\ &= -\frac{1}{2}\text{dist}(x,\triangle_j)\iint_{\triangle_j}\frac{(y-x)}{\|x-y\|^3}\cdot\vec{n}\,dS_y \end{aligned}$$

This integral is nothing else than the definition of the solid angle $\Omega(x,\triangle_j)$ which the triangle $\triangle_j$ covers when viewed from point x. $F_1(x)$ thus simplifies to:

$$F_1(x) = -\frac{1}{2}\text{dist}(x,\triangle_j)\,\Omega(x,\triangle_j)$$

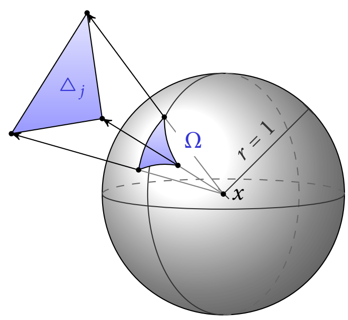

Figure 2.2: *The solid angle $\Omega(x,\triangle_j)$ is the area of the projection of $\triangle_j$ onto the unit sphere centered around x.*

The solid angle can be calculated very efficiently using the *Oosterom and Strackee* algorithm [8].

For $F_2(x)$, we will use Stoke's theorem to convert the surface integral over $\triangle_j$ into a contour integral along its boundary $\partial \triangle_j$:

$$\iint_{\triangle_j} \vec{n} \cdot \nabla \times \nabla \times (\|x-y\|\vec{n})\, dS_y = \oint_{\partial\triangle_j} \nabla \times (\|x-y\|\vec{n})\, d\vec{l}$$
$$= \oint_{\partial\triangle_j} \nabla\|x-y\| \times \vec{n}\, d\vec{l}$$
$$= \oint_{\partial\triangle_j} \frac{(y-x)}{\|x-y\|} \times \vec{n}\, d\vec{l}$$

To simplify this term, we introduce the following notations: Let C_1, C_2, C_3 be the edges of the triangle, τ_1, τ_2, τ_3 the normalized tangent vectors to the edges:

$$\tau_i = \frac{P_{i+1} - P_i}{\|P_{i+1} - P_i\|}$$

and v_1, v_2, v_3 the outward oriented normal vectors to the edges (see Figure 2.3):

$$v_i = \tau_i \times \vec{n}$$

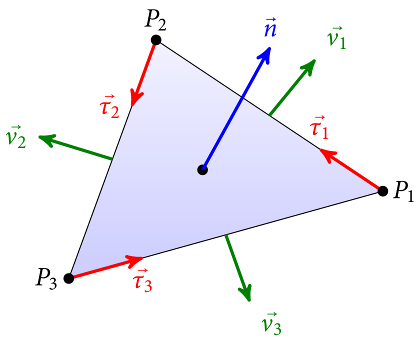

Figure 2.3: *The triangle with its vertices and the corresponding normal and tangent vectors.*

Using these notations, the integral can be written as a sum of three contour integrals, each along one edge of the triangle:

$$\oint_{\partial\triangle_j} \frac{(y-x)}{\|x-y\|} \times \vec{n}\, d\vec{l} = \sum_{k=1}^{3} \int_{C_k} \frac{(y-x)}{\|x-y\|} \times \vec{n} \cdot \tau_k\, dC_k$$
$$= -\sum_{k=1}^{3} \int_{C_k} \frac{(y-x)}{\|x-y\|} \cdot v_k\, dC_k$$

Additionally, we have for all $y \in C_k$:

$$(y-x)\cdot v_k = (P_k - x)\cdot v_k = R_k \cdot v_k\,, \quad \text{with } R_k = P_k - x$$

We have finally found an easy expression for $F_2(x)$:

$$F_2(x) = -\frac{1}{2}\sum_{k=1}^{3} R_k \cdot v_k \int_{C_k} \frac{1}{\|x-y\|}\, dC_k$$

Now, the only remaining integrations in $F_2(x)$ are the integrals along the edges of the triangle, which can be solved analytically. The entire (tedious) derivation is shown in the appendix, as it does not yield much insight into the problem. Instead, we just show the result here:

$$F_2(x) = -\frac{1}{2}\sum_{k=1}^{3} R_k \cdot \nu_k \;\log\left(\frac{\|R_{k+1}\| + R_{k+1}\cdot \tau_k}{\|R_k\| + R_k \cdot \tau_k}\right)$$

Combined with F_1, we have found the following analytical expression for $F(x)$:

$$\boxed{F(x) = -\frac{1}{2}\,\mathrm{dist}(x, \triangle_j)\,\Omega(x, \triangle_j) + \frac{1}{2}\sum_{k=1}^{3} R_k \cdot \nu_k \;\log\left(\frac{\|R_{k+1}\| + R_{k+1}\cdot \tau_k}{\|R_k\| + R_k \cdot \tau_k}\right)}$$

This can now be used to quickly evaluate the electrostatic kernel integral. The other non-singular integrals pose no problem for direct numerical integration, so we now have everything we need for the setup of the system matrix.

2.2 Implementing the Newton method

We start from the **linear operator equation:**

Given (t_h^n, κ^n), find $(t_h^{n+1}, \kappa^{n+1}) \in S_0^h \times \mathbb{R}$ s.t.:

$$\langle V_{\kappa^n} t_h^{n+1}, \varphi_h\rangle - \kappa^{n+1}\langle A_{\kappa^n} t_h^n, \varphi_h\rangle = -\kappa^n \langle A_{\kappa^n} t_h^n, \varphi_h\rangle \quad \forall \varphi_h \in S_0^h$$

we derived earlier, to which we will add the normalization condition from the paper:

$$\|t\|_S^2 = \langle St, t\rangle_\Gamma = \frac{1}{4\pi}\int_\Gamma t(x)\int_\Gamma \frac{1}{\|x-y\|} t(y)\, dSy\, dSx \overset{!}{=} 1$$

Where $S : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is the standard single layer potential for the laplacian. Including this condition into our Newton scheme we arrive at our iteration:

$$\langle V_{\kappa^n} t_h^{n+1}, \varphi_h\rangle - \kappa^{n+1}\langle A_{\kappa^n} t_h^n, \varphi_h\rangle = -\kappa^n \langle A_{\kappa^n} t_h^n, \varphi_h\rangle \quad \forall \varphi_h \in S_0^h$$
$$2\langle St_h^n, t_h^{n+1}\rangle_\Gamma = \langle St_h^n, t_h^n\rangle_\Gamma + 1$$

This is a saddle point problem which can be written as a $(n+1)\times(n+1)$ system of linear equations:

$$\begin{bmatrix} \mathbf{A} & -\mathbf{B}\underline{t_n} \\ 2\underline{t_n}^T\mathbf{C} & 0 \end{bmatrix}\begin{bmatrix} \underline{t_{n+1}} \\ \kappa_{n+1} \end{bmatrix} = \begin{bmatrix} -\kappa_n \mathbf{B}\underline{t_n} \\ \underline{t_n}^T\mathbf{C}\underline{t_n} + 1 \end{bmatrix}$$

Appendix B
Further proofs

B.1 Solving the contour integral

We want to solve the integral:

$$I(x) = \int_{C_k} \frac{1}{\|x-y\|}\, dC_k$$

For simplicity, we take $k = 1$, as the other cases are completely analogous. C_1 is the edge of the triangle connection the endpoints P_1 and P_2. Given a parametrisation of the path, we can write

$$I(x) = \int_0^1 \frac{1}{\|x-\phi(t)\|} \|\phi'(t)\|\, dt$$

such a parametrisation is given by

$$\phi(t) = P_1 + (P_2 - P_1)t, \quad \phi'(t) = P_2 - P_1$$

$$\phi(0) = P_1, \quad \phi(1) = P_2$$

Therefore,

$$I(x) = \|P_2 - P_1\| \int_0^1 \frac{1}{\|P_1 - x + (P_2 - P_1)t\|}\, dt$$

Splitting the norm in the denominator:

$$\begin{aligned} I(x) &= \|P_2 - P_1\| \int_0^1 \frac{1}{\sqrt{\|P_1 - x + (P_2 - P_1)t\|^2}} \\ &= \|P_2 - P_1\| \int_0^1 \frac{1}{\sqrt{\|P_1 - x\|^2 + 2\langle P_1 - x, P_2 - P_1\rangle t + \|P_2 - P_1\|^2 t^2}} \end{aligned}$$

This is an integral of the kind

$$\int \frac{1}{\sqrt{ax^2 + bx + c}} dx$$

whose solution can be found in the standard integral tables, e.g. *Bronstein* [2]*, integral No. 241:*

$$X = ax^2 + bx + c$$

$$\int \frac{1}{\sqrt{X}}\, dx = \frac{1}{\sqrt{a}} \log(2\sqrt{aX} + 2ax + b) + C \quad \text{for } a > 0$$

This leads to

$$\begin{aligned} I(x) = \frac{\|P_2 - P_1\|}{\|P_2 - P_1\|} \log\Big(2\sqrt{\|P_2 - P_1\|^2(\|P_2 - P_1\|^2 t^2 + 2\langle P_1 - x, P_2 - P_1\rangle t + \|P_1 - x\|^2)} \\ + 2\|P_2 - P_1\|^2 t + 2\langle P_1 - x, P_2 - P_1\rangle\Big)\Big|_0^1 \end{aligned}$$

$$
\begin{aligned}
&= \log\Big(2\|P_2 - P_1\|\sqrt{(\|P_2 - P_1\|^2 + 2\langle P_1 - x, P_2 - P_1\rangle + \|P_1 - x\|^2)} \\
&\qquad + 2\|P_2 - P_1\|^2 + 2\langle P_1 - x, P_2 - P_1\rangle\Big) \\
&\qquad - \log\big(2\|P_2 - P_1\|\|P_1 - x\| + 2\langle P_1 - x, P_2 - P_1\rangle\big)
\end{aligned}
$$

$$
\begin{aligned}
&= \log\Big(2\|P_2 - P_1\|\|P_2 - P_1 + (P_1 - x)\| + 2\langle P_1 - x, P_2 - P_1\rangle + \langle P_2 - P_1, P_2 - P_1\rangle\Big) \\
&\qquad - \log\big(2\|P_2 - P_1\|\|P_1 - x\| + 2\langle P_1 - x, P_2 - P_1\rangle\big)
\end{aligned}
$$

$$
\begin{aligned}
&= \log\big(2\|P_2 - P_1\|\|P_2 - x\| + 2\langle P_2 - x, P_2 - P_1\rangle\big) \\
&\qquad - \log\big(2\|P_2 - P_1\|\|P_1 - x\| + 2\langle P_1 - x, P_2 - P_1\rangle\big)
\end{aligned}
$$

$$
= \log\left(\frac{2\|P_2 - P_1\|\|P_2 - x\| + 2\langle P_2 - x, P_2 - P_1\rangle}{2\|P_2 - P_1\|\|P_1 - x\| + 2\langle P_1 - x, P_2 - P_1\rangle}\right)
$$

$$
= \log\left(\frac{\|P_2 - x\| + \langle P_2 - x, \frac{P_2 - P_1}{\|P_2 - P_1\|}\rangle}{\|P_1 - x\| + \langle P_1 - x, \frac{P_2 - P_1}{\|P_2 - P_1\|}\rangle}\right)
$$

Recalling that

$$
R_i = P_i - x \qquad \text{and} \qquad \tau_i = \frac{P_{i+1} - P_i}{\|P_{i+1} - P_i\|}
$$

we can finally obtain the simple formula:

$$
I(x) = \log\left(\frac{\|R_2\| + \langle R_2, \tau_1\rangle}{\|R_1\| + \langle R_1, \tau_1\rangle}\right)
$$