Double dissociation.
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Problem Statement: A chemical species A becomes a positively charged cation (A^+, the protonated form of A) in an acid solution; it becomes a negatively charged anion (A^-, the deprotonated form of A) in an alkaline solution. The dissociation constants for these steps are K_1 and K_2, which are defined as:

$A^+ \longrightarrow A + H^+ \qquad K_1 = 10^{-pK_1} = \frac{A_{neutral} \cdot H}{A_{cation}}$

$A \longrightarrow A^- + H^+ \qquad K_2 = 10^{-pK_2} = \frac{A_{anion} \cdot H}{A_{neutral}}$

Conservation of mass (i.e., all fractions add up to unity): $A_{cation} + A_{neutral} + A_{anion} = 1$

For glutamic acid, $pK_1 := 2.10 \qquad pK_2 := 9.47 \qquad K_1 := 10^{-pK_1} \qquad K_2 := 10^{-pK_2}$

We can solve these three equations in the linear form:

$$K_1 \cdot A_{cation} - H \cdot A_{neutral} = 0$$
$$K_2 \cdot A_{neutral} - H \cdot A_{anion} = 0 \qquad \text{or} \qquad \begin{bmatrix} K_1 & -H & 0 \\ 0 & K_2 & -H \\ 1 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} A_{cation} \\ A_{neutral} \\ A_{anion} \end{bmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$
$$A_{cation} + A_{neutral} + A_{anion} = 1$$

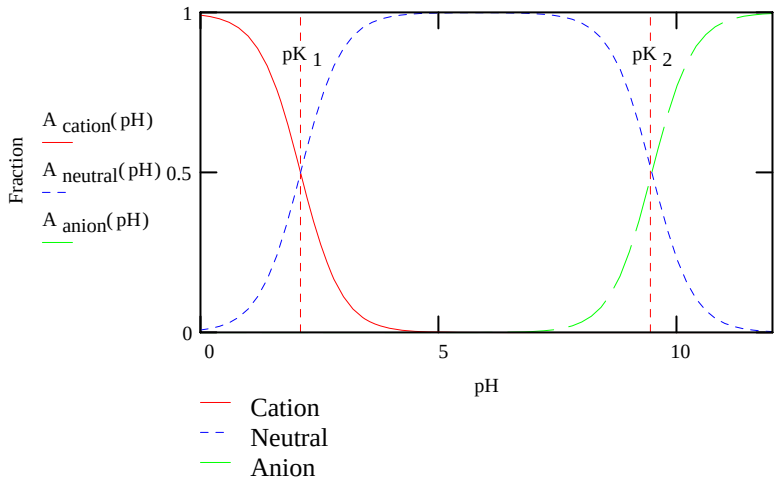
In the standard A·x=b format, the matrix A is:

$$A(pH) := \begin{bmatrix} K_1 & -10^{-pH} & 0 \\ 0 & K_2 & -10^{-pH} \\ 1 & 1 & 1 \end{bmatrix} \qquad b := \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad fraction(pH) := A(pH)^{-1} \cdot b$$

Solution of the linear equations.

$A_{cation}(pH) := fraction(pH)_0 \qquad A_{neutral}(pH) := fraction(pH)_1 \qquad A_{anion}(pH) := fraction(pH)_2$

Table and plot $pH := 0, 0.2 .. 12$



pH	$A_{cation}(pH)$	$A_{neutral}(pH)$	$A_{anion}(pH)$
0	0.992	0.008	0.000
0.2	0.988	0.012	0.000
0.4	0.980	0.020	0.000
0.6	0.969	0.031	0.000
0.8	0.952	0.048	0.000
1	0.926	0.074	0.000
1.2	0.888	0.112	0.000
1.4	0.834	0.166	0.000
1.6	0.760	0.240	0.000
1.8	0.666	0.334	0.000
2	0.557	0.443	0.000
2.2	0.443	0.557	0.000
2.4	0.334	0.666	0.000
2.6	0.240	0.760	0.000
2.8	0.166	0.834	0.000
3	0.112	0.888	0.000
3.2	0.074	0.926	0.000
3.4	0.048	0.952	0.000
3.6	0.031	0.969	0.000
3.8	0.020	0.980	0.000
4	0.012	0.988	0.000
4.2	0.008	0.992	0.000
4.4	0.005	0.995	0.000
4.6	0.003	0.997	0.000
4.8	0.002	0.998	0.000
5	0.001	0.999	0.000
5.2	0.001	0.999	0.000
5.4	0.001	0.999	0.000

5.6	0.000	1.000	0.000
5.8	0.000	1.000	0.000
6	0.000	1.000	0.000
6.2	0.000	0.999	0.001
6.4	0.000	0.999	0.001
6.6	0.000	0.999	0.001
6.8	0.000	0.998	0.002
7	0.000	0.997	0.003
7.2	0.000	0.995	0.005
7.4	0.000	0.992	0.008
7.6	0.000	0.987	0.013
7.8	0.000	0.979	0.021
8	0.000	0.967	0.033
8.2	0.000	0.949	0.051
8.4	0.000	0.922	0.078
8.6	0.000	0.881	0.119
8.8	0.000	0.824	0.176
9	0.000	0.747	0.253
9.2	0.000	0.651	0.349
9.4	0.000	0.540	0.460
9.6	0.000	0.426	0.574
9.8	0.000	0.319	0.681