Supporting Information

for

Calculation of the effect of tip geometry on noncontact atomic force microscopy using a qPlus sensor

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Further details of the presented theoretical model
Appendix A

The boundary conditions in Equations 6–9 allow us to form four simultaneous equations for the factors $b_1..4$ of $\Phi_i(x)$ from Equation 4.

$$b_1 + b_3 = 0$$ (36)

$$b_2 + b_4 = 0$$ (37)

$$b_1 \left( -\cos(\beta_i L) + \frac{J \beta_i^2}{\gamma_i} \sin(\beta_i L) \right) + b_2 \left( -\sin(\beta_i L) - \frac{J \beta_i^2}{\gamma_i} \cos(\beta_i L) \right) + b_3 \left( \cosh(\beta_i L) - \frac{J \beta_i^2}{\gamma_i} \sinh(\beta_i L) \right) + b_4 \left( \sinh(\beta_i L) - \frac{J \beta_i^2}{\gamma_i} \cosh(\beta_i L) \right) = 0$$ (38)

$$b_1 (\gamma_i \sin(\beta_i L) + \cos(\beta_i L)) + b_2 (-\gamma_i \cos(\beta_i L) + \sin(\beta_i L)) + b_3 (\gamma_i \sinh(\beta_i L) + \cosh(\beta_i L)) + b_4 (\gamma_i \cosh(\beta_i L) + \sinh(\beta_i L)) = 0$$ (39)

where $\gamma_i$ is a dimensionless parameter defined as

$$\gamma_i = \frac{EI \beta_i^3}{m_{tip} \omega_i^2}.$$ (40)

Writing Equations 36, 37, 38, and 39 as a matrix equation in the form

$$D \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$ (41)

it becomes clear that if $\det(D) \neq 0$, then the solution would trivially be $b_{1..4} = 0$, a stationary beam. Hence, $\det(D) = 0$, giving the following condition for $\beta_i$:

$$1 + m^* \beta_i^4 J L^2 - \left(1 + m^* \beta_i^4 J L^2 \right) \cos(\beta_i L) \cosh(\beta_i L) + m^* \beta_i L \left[ (1 - J \beta_i^2) \cos(\beta_i L) \sinh(\beta_i L) - (1 + J \beta_i) \cosh(\beta_i L) \sin(\beta_i L) \right] = 0$$ (42)
using

\[ \gamma_i = \frac{\rho A}{\beta_i m_{\text{tip}}} = \frac{1}{\beta_i L m^*}, \]  

from Equations 5 and 40, where \( m^* \) is the ratio of the tip mass to the mass of the tine. Equation 42 can be numerically solved simply and quickly by using the Newton-Raphson method.

**Appendix B**

Equation 12 can be expanded to give

\[
W = \frac{EI}{2} \left[ \sum_{i=1}^{\infty} \mathcal{T}_i^2(t) \int_{0}^{L} \left( \frac{d^2 \Phi_i(x)}{dx^2} \right)^2 dx \right. \\
+ \sum_{i=1}^{\infty} \sum_{k=1, k \neq i}^{\infty} \mathcal{T}_i(t) \mathcal{T}_k(t) \int_{0}^{L} \frac{d^2 \Phi_i(x)}{dx^2} \frac{d^2 \Phi_k(x)}{dx^2} dx \right]. 
\]  

(44)

Butt and Jaschke [1] use

\[ \frac{d^4 \Phi_i(x)}{dx^4} = \beta_i^4 \Phi_i(x) \]  

(45)

(which is clearly still true for our boundary conditions from the general form of \( \Phi \) given in Equation 4) to show that the integral with mixed (\( \Phi_i(x) \) and \( \Phi_k(x) \)) second derivatives can be written as

\[
\int_{0}^{L} \frac{d^2 \Phi_i(x)}{dx^2} \frac{d^2 \Phi_k(x)}{dx^2} dx = \frac{1}{\beta_i^4 - \beta_k^4} \left[ \beta_i^4 \frac{d^2 \Phi_k(x)}{dx^2} \frac{d \Phi_i(x)}{dx} - \beta_i^4 \frac{d^3 \Phi_k(x)}{dx^3} \Phi_i(x) \right. \\
- \beta_k^4 \frac{d^2 \Phi_i(x)}{dx^2} \frac{d \Phi_k(x)}{dx} + \beta_k^4 \frac{d^3 \Phi_i(x)}{dx^3} \Phi_k(x) \left. \right]_0^L. 
\]  

(46)
If we combine Equations 40 and 43 to give

$$\beta_i^4 L m^* = \frac{m_{tip} \omega_t^2}{EI}$$  \hspace{1cm} (47)$$
then we can rewrite boundary conditions Equations 8 and 9 as

$$\frac{\partial^2 \Phi_i(L)}{\partial x^2} = \beta_i^4 J L m^* \frac{\partial \Phi_i(L)}{\partial x}$$  \hspace{1cm} (48)$$
$$\frac{\partial^3 \Phi_i(L)}{\partial x^3} = -\beta_i^4 L m^* \Phi_i(L).$$  \hspace{1cm} (49)$$

From these conditions it becomes clear that the first and third terms in the square brackets of Equation 46 cancel, as do the second and fourth. Thus,

$$\int_0^L \frac{d^2 \Phi_i(x)}{dx^2} \frac{d^2 \Phi_k(x)}{dx^2} dx = 0,$$  \hspace{1cm} (50)$$

and

$$W = \frac{EI}{2} \sum_{i=1}^{\infty} \mathcal{R}_i^2(t) \int_0^L \left( \frac{\partial^2 \Phi_i(x)}{\partial x^2} \right)^2 dx.$$  \hspace{1cm} (51)$$

**Appendix C**

To solve $\Lambda_i$ we first integrate by parts twice to give

$$\Lambda_i = \left[ \frac{d \Phi_i(x)}{dx} \frac{d^2 \Phi_i(x)}{dx^2} - \Phi_i(x) \frac{d^3 \Phi_i(x)}{dx^3} \right]_0^L + \int_0^L \Phi_i(x) \frac{d^4 \Phi_i(x)}{dx^4} dx.$$  \hspace{1cm} (52)$$

The square brackets can be evaluated using boundary conditions from Equations 6, 7, 48, and 49. Furthermore, with Equation 45 the integral can be written in terms of $\Phi_i(x)$ only:

$$\Lambda_i = \beta_i^4 L J m^* \left( \frac{d \Phi_i(L)}{dx} \right)^2 + \beta_i^4 L m^* \Phi_i^2(L) + \beta_i^4 \int_0^L \Phi_i(x)^2 dx.$$  \hspace{1cm} (53)$$
The integral can be solved by substituting in $\zeta = x/L$, and writing $\beta_i L$ as $\alpha_i$,

$$
\int_0^L \Phi_i^2 dx = L \int_0^1 \left\{ \sin(\alpha_i) + \sinh(\alpha_i) - \frac{J \beta_i^2}{\gamma_i} \left( -\cos(\alpha_i) + \cosh(\alpha_i) \right) \right\} 
	imes \left( \cos(\alpha_i \zeta) - \cosh(\alpha_i \zeta) \right) 
	imes \left( \sin(\alpha_i \zeta) - \sinh(\alpha_i \zeta) \right) \, d\zeta
$$

$$
= L \left( \frac{1}{\alpha_i} \right) \left( \frac{3L}{\alpha_i} \right) \left( 1 + \cos(\alpha_i) \cosh(\alpha_i) \right) 
	imes \left( -\cosh(\alpha_i) \sin(\alpha_i) + \cos(\alpha_i) \sinh(\alpha_i) \right) 
	imes \left( \frac{1}{\alpha_i} \right) \left( -4 + \cos(2\alpha_i) + \left( 1 + 2\cos(2\alpha_i) \right) \cosh(2\alpha_i) \right) 
	imes \left( -2(\cos(\alpha_i) - \cosh(\alpha_i)) (\sin(\alpha_i) + \sinh(\alpha_i)) \right) 
	imes \left( \frac{J \beta_i^2}{\gamma_i} \right) 
	imes \left( \cos(\alpha_i) - \cosh(\alpha_i) \right)^2 
+ \left( \frac{J \beta_i^4}{\gamma_i^2} \right) \left( -1 + \cos(\alpha_i) \cosh(\alpha_i) \right) 
	imes \left( \cosh(\alpha_i) \sin(\alpha_i) + \cos(\alpha_i) \sinh(\alpha_i) \right) \right) .
$$

(54)
Returning back to notation without $\alpha_i$ or $\gamma_i$ and using Equation 42 to replace $(1 + \cos(\beta_i L) \cosh(\beta_i L))$ in the second term, after some manipulation gives

\[
= L \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 \\
- 3L m^* \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right)^2 \\
- \beta_i^2 J m^* L \left[ - \frac{5}{2} + \cos(2\beta_i L) + \cosh(2\beta_i L) \right] \\
+ \frac{1}{2} \cos(2\beta_i L) \cosh(2\beta_i L) \\
- 2\beta_i L \left( \cos(\beta_i L) - \cosh(\beta_i L) \right) \left( \sin(\beta_i L) + \sinh(\beta_i L) \right) \\
- 3m^* \beta_i L \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right) \\
\times \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right) \right] \\
+ \beta_i^6 J^2 m^* L^3 \left[ \left( \cos(\beta_i L) - \cosh(\beta_i L) \right)^2 \right] \\
+ 3\beta_i^5 J^2 m^* L^2 \left[ \left( -1 + \cos(\beta_i L) \cosh(\beta_i L) \right) \right] \\
\times \left( \cosh(\beta_i L) \sin(\beta_i L) + \cos(\beta_i L) \sinh(\beta_i L) \right) \right].
\]

(56)
Using Equation 42 again, this time to replace $\beta_i^3 Jm^* L (\cosh(\beta_i L) \sin(\beta_i L) + \cos(\beta_i L) \sinh(\beta_i L))$ in the final term, and rearranging will give

$$
\int_0^L \Phi_i^2 \, dx = L \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2
$$

$$
- 3Lm^* \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right)^2
$$

$$
- \beta_i^2 Jm^* L \left[ \sin^2(\beta_i L) \sinh^2(\beta_i L) \right]
$$

$$
- 2\beta_i L \left( \cos(\beta_i L) - \cosh(\beta_i L) \right) \times \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)
$$

$$
- 6m^* \beta_i L \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right)
$$

$$
\times \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right)
$$

$$
+ \beta_i^6 J^2 m^*^2 L^3 \left[ \left( \cos(\beta_i L) - \cosh(\beta_i L) \right)^2
$$

$$
- 3m^* \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right)^2 \right].
$$

(57)

It can be shown simply that

$$
\left( \frac{d\Phi_i(L)}{dx} \right)^2 = 4\beta_i^2 \sin^2(\beta_i L) \sinh^2(\beta_i L),
$$

(58)

and that

$$
\Phi_i^2(L) = 4 \left[ \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right)^2
$$

$$
- 2\beta_i^3 Jm^* L \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right)
$$

$$
\times \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right)
$$

$$
+ \beta_i^6 J^2 m^*^2 L^3 \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right)^2 \right].
$$

(59)
Note that this form of $\Phi_i^2(L)$ appears in Equation 57, allowing us to reduce it to

$$\int_0^L \Phi_i^2 \, dx = L \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 - \frac{3Lm^*}{4} \Phi_i^2(L)$$

$$- \beta_i^2 Jm^* L \left[ \sin^2(\beta_i L) \sinh^2(\beta_i L) \right.$$  
$$- 2\beta_i L \left( \cos(\beta_i L) - \cosh(\beta_i L) \right) \left( \sin(\beta_i L) + \sinh(\beta_i L) \right) \right]$$

$$+ \beta_i^6 J^2 m^* L^3 \left( \cos(\beta_i L) - \cosh(\beta_i L) \right)^2. \quad (60)$$

Combining Equations 58, 59, and 60 after some manipulation gives

$$\Lambda_i = \frac{\beta_i^4 Lm^*}{4} \Phi_i^2(L) + \beta_i^4 L \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2$$

$$- \beta_i^6 Jm^* L \left[ - 3 \sin^2(\beta_i L) \sinh^2(\beta_i L) \right.$$  
$$- 2\beta_i L \left( \cos(\beta_i L) - \cosh(\beta_i L) \right) \left( \sin(\beta_i L) + \sinh(\beta_i L) \right) \right]$$

$$+ \beta_i^10 J^2 m^* L^3 \left( \cos(\beta_i L) - \cosh(\beta_i L) \right)^2. \quad (61)$$

Which for simplicity, can be written as

$$\Lambda_i = \frac{\beta_i^4 Lm^*}{4} \Phi_i^2(L) + \beta_i^4 L \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 + \beta_i^6 Jm^* L f(m^*, J), \quad (62)$$

where

$$f(m^*, J) = 3 \sin^2(\beta_i L) \sinh^2(\beta_i L)$$

$$+ 2\beta_i L \left( \cos(\beta_i L) - \cosh(\beta_i L) \right) \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)$$

$$+ \beta_i^4 Jm^* L^2 \left( \cos(\beta_i L) - \cosh(\beta_i L) \right)^2. \quad (63)$$
By substituting Equation 42 into Equation 59 and rearranging we get

\[ \Phi_2^2(L) = 4 \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 \]

\[- 8 \beta_i L m^* \sin(\beta_i L) \sinh(\beta_i L) \times \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right) \]

\[ + 8 \beta_i^3 L J m^* \left[ - \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right) \right. \]

\[ \left. \times \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right) \right] \]

\[- \sin(\beta_i L) \sinh(\beta_i L) \left( \cosh(\beta_i L) \sin(\beta_i L) + \cos(\beta_i L) \sinh(\beta_i L) \right) \]

\[ + \beta_i L m^* \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right) \sin(\beta_i L) \sinh(\beta_i L) \]

\[ + 4 \beta_i^6 L^2 J^2 m^*^2 \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right)^2 . \] (64)

Initially this form appears to be more complicated. However, as will be demonstrated, because it contains the boundary conditions it produces a final result that is more physically understandable. For simplicity it can be written as

\[ = 4 \left[ \left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 - \beta_i L m^* \left( 2 g + \beta_i^2 J h(m^*, J) \right) \right] , \] (65)

where

\[ g = \sin(\beta_i L) \sinh(\beta_i L) \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right) \] (66)
\[ h(m^*, J) = 2 \left[ - \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right) \right. \]
\[ \times \left( \cosh(\beta_i L) \sin(\beta_i L) - \cos(\beta_i L) \sinh(\beta_i L) \right) \]
\[ - \sin(\beta_i L) \sinh(\beta_i L) \left( \cosh(\beta_i L) \sin(\beta_i L) + \cos(\beta_i L) \sinh(\beta_i L) \right) \]
\[ + \beta_i L m^* \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right) \sin(\beta_i L) \sinh(\beta_i L) \]
\[ + \frac{\beta_i^3 L J m^*}{4} \left( 1 - \cos(\beta_i L) \cosh(\beta_i L) \right)^2 \]  
(67)

Thus, finally we can write

\[ \frac{\Lambda_i L^3}{\Phi_i^2(L)} = \frac{\beta_i^4 L^4}{4} m^* \]
\[ + \frac{\left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 + \beta_i^2 J m^* f(m^*, J)}{\left( \sin(\beta_i L) + \sinh(\beta_i L) \right)^2 - \beta_i L m^* \left( 2g + \beta_i^2 J h(m^*, J) \right)} \]  
(68)

It is clear that in the case of no tip, \( m^* = 0 \), this reduces to just \( \frac{\beta_i^4 L^4}{4} \). Inserting this into Equation 16 yields a result consistent with Melcher et al. [2]. Further consistency with the literature can be shown in the case of the point mass, where \( J = 0 \) but \( m^* \neq 0 \). Inserting Equation 68 into Equation 16 with these conditions, agrees with the results of Lozano et al. [3].

A final test of the accuracy of this equation can be done by considering equipartition theorem with Hooke’s law in terms of the static spring constant:

\[ \frac{1}{2} k_B T = \frac{1}{2} k_{\text{stat}} \sum_{i=1}^{\infty} \langle Z_i^2(L) \rangle \]  
(69)

and inserting Equation 15 we get

\[ \sum_{i=1}^{\infty} \frac{L^3 \Lambda_i}{\Phi_i^2(L)} = 3. \]  
(70)
Using the same model qPlus sensor as described above, this has been plotted in Figure 1, for $i = 1..8$ showing excellent agreement with theory, and faster convergence for larger tips.

Figure S 1: Agreement with $\lim_{N \to \infty} \sum_{i=1}^{N} L^3 \Lambda_i \Phi_i^2(L) = 3$, plotted for $N = 8$ roots to show that the equation is consistent with equipartition theorem. Where $H$ is the length and $D_{\text{tip}}$ is the diameter of a cylindrical tip.

References

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