Table 1
Equations for all dTMM solvers of electron structure

Solver type	Equation	p/q	q_{pq}
Parabolic	$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d\psi_n(z)}{dz}+U_{\mathrm{eff}}(z)\psi_n(z)=E_n\psi_n(z)$	$\sqrt{\frac{2m_{i/i+1}(U_{i/i+1}-E)}{\hbar^2}}$	$\frac{m_{i+1}}{m_i}\frac{p}{q}$
Two band	$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)\left(1+\alpha(E-U_{\mathrm{eff}}(z))\right)}\frac{d\psi_n(z)}{dz}+U_{\mathrm{eff}}(z)\psi_n(z)=E_n\psi_n(z)$	$\sqrt{\frac{2m_{i/i+1}\left(1+\alpha_{i/i+1}(E-U_{i/i+1})\right)(U_{i/i+1}-E)}{\hbar^2}}$	$\frac{m_{i+1}\left(1+\alpha_{i+1}(E-U_{i+1})\right)}{m_i\left(1+\alpha_i(E-U_i)\right)}\frac{p}{q}$
Taylor	$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{\left(1-\alpha(E-U_{\mathrm{eff}}(z))\right)}{m(z)}\frac{d\psi_n(z)}{dz}+U_{\mathrm{eff}}(z)\psi_n(z)=E_n\psi_n(z)$	$\sqrt{\frac{2m_{i/i+1}(U_{i/i+1}-E)}{\left(1-\alpha_{i/i+1}(E-U_{i/i+1})\right)\hbar^2}}$	$\frac{m_{i+1}\left(1-\alpha_i(E-U_i)\right)}{m_i\left(1-\alpha_{i+1}(E-U_{i+1})\right)}\frac{p}{q}$
14 **k·p**	$\frac{d^2}{dz^2}\alpha^E(z)\frac{d^2\psi_n(z)}{dz^2}-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d\psi_n(z)}{dz}+U_{\mathrm{eff}}(z)\psi_n(z)=E_n\psi_n(z)$	$\sqrt{\frac{\hbar^2\left[1-\sqrt{1-16\lvert\alpha^E_{i/i+1}\rvert(E-U_{i/i+1})\left(\frac{m_{i/i+1}}{\hbar^2}\right)^2}\right]}{4\lvert\alpha^E_{i/i+1}\rvert m_{i/i+1}}}$	$\frac{2\alpha_i^E p^2-\frac{\hbar^2}{2m_i}}{2\alpha_{i+1}^E q^2-\frac{\hbar^2}{2m_{i+1}}}\frac{p}{q}$

Table 2
Derivatives for all dTMM solvers of electron structure

Solver type	$\frac{dp}{dE}$	$\frac{dq}{dE}$	$\frac{dq_{pq}}{dE}$
Parabolic	$-\frac{m_i}{\hbar^2 p}$	$-\frac{m_{i+1}}{\hbar^2 q}$	$\frac{m_{i+1}}{m_i}\frac{\frac{dp}{dE}q-\frac{dq}{dE}p}{q^2}$
Two band	$-\frac{m_i\left(1+2\alpha_i(E-U_i)\right)}{\hbar^2 p}$	$-\frac{m_{i+1}\left(1+2\alpha_{i+1}(E-U_{i+1})\right)}{\hbar^2 q}$	$\frac{m_{i+1}\left(1+\alpha_{i+1}(E-U_{i+1})\right)}{m_i\left(1+\alpha_i(E-U_i)\right)}\frac{\frac{dp}{dE}q-\frac{dq}{dE}p}{q^2}+\frac{p}{q}\frac{m_{i+1}\left(\alpha_{i+1}-\alpha_i+\alpha_i\alpha_{i+1}\left(U_{i+1}-U_i\right)\right)}{m_i\left(1+\alpha_i(E-U_i)\right)^2}$
Taylor	$-\frac{m_i}{\left(1-\alpha_i(E-U_i)\right)^2\hbar^2 p}$	$-\frac{m_{i+1}}{\left(1-\alpha_{i+1}(E-U_{i+1})\right)^2\hbar^2 q}$	$\frac{m_{i+1}\left(1-\alpha_i(E-U_i)\right)}{m_i\left(1-\alpha_{i+1}(E-U_{i+1})\right)}\frac{\frac{dp}{dE}q-\frac{dq}{dE}p}{q^2}+\frac{p}{q}\left(\frac{\alpha_{i+1}m_{i+1}\left(1-\alpha_i(E-U_i)\right)}{m_i\left(1-\alpha_{i+1}(E-U_{i+1})\right)^2}-\frac{m_{i+1}\alpha_i}{m_i\left(1-\alpha_{i+1}(E-U_{i+1})\right)}\right)$
14 **k·p**	$\frac{m_i}{\hbar^2}\frac{1}{p+\frac{4\lvert\alpha_i^E\rvert m_i}{\hbar^2}p^3}$	$\frac{m_{i+1}}{\hbar^2}\frac{1}{q+\frac{4\lvert\alpha_{i+1}^E\rvert m_{i+1}}{\hbar^2}q^3}$	$\frac{6\alpha_i^E p^2-\frac{\hbar^2}{2m_i}}{2\alpha_{i+1}^E q^3-\frac{\hbar^2}{2m_{i+1}}q}\frac{dp}{dE}-\frac{\left(2\alpha_i^E p^3-\frac{\hbar^2}{2m_i}p\right)\left(6\alpha_{i+1}^E q^2-\frac{\hbar^2}{2m_{i+1}}\right)}{\left(2\alpha_{i+1}^E q^3-\frac{\hbar^2}{2m_{i+1}}q\right)^2}\frac{dq}{dE}$