```
> restart; assume(a,'positive'); with(LinearAlgebra);
```

[&x, Add, Adjoint, BackwardSubstitute, BandMatrix, Basis, BezoutMatrix, BidiagonalForm, BilinearForm, CARE, CharacteristicMatrix, CharacteristicPolynomial, Column, ColumnDimension, ColumnOperation, ColumnSpace, CompanionMatrix, ConditionNumber, ConstantMatrix, ConstantVector, Copy, CreatePermutation, CrossProduct, DARE, DeleteColumn, DeleteRow, Determinant, Diagonal, DiagonalMatrix, Dimension, Dimensions, DotProduct, EigenConditionNumbers, Eigenvalues, Eigenvectors, Equal, ForwardSubstitute, FrobeniusForm, GaussianElimination, GenerateEquations, GenerateMatrix, Generic, GetResultDataType, GetResultShape, GivensRotationMatrix, GramSchmidt, HankelMatrix, HermiteForm, HermitianTranspose, HessenbergForm, HilbertMatrix, HouseholderMatrix, IdentityMatrix, IntersectionBasis, IsDefinite, IsOrthogonal, IsSimilar, IsUnitary, JordanBlockMatrix, JordanForm, KroneckerProduct, LA_Main, LUDecomposition, LeastSquares, LinearSolve, LyapunovSolve, Map, Map2, MatrixAdd, MatrixExponential, MatrixFunction, MatrixInverse, MatrixMatrixMultiply, MatrixNorm, MatrixPower, MatrixScalarMultiply, MatrixVectorMultiply, MinimalPolynomial, Minor, Modular, Multiply, NoUserValue, Norm, Normalize, NullSpace, OuterProductMatrix, Permanent, Pivot, PopovForm, QRDecomposition, RandomMatrix, RandomVector, Rank, RationalCanonicalForm, ReducedRowEchelonForm, Row, RowDimension, RowOperation, RowSpace, ScalarMatrix, ScalarMultiply, ScalarVector, SchurForm, SingularValues, SmithForm, StronglyConnectedBlocks, SubMatrix, SubVector, SumBasis, SylvesterMatrix, SylvesterSolve, ToeplitzMatrix, Trace, Transpose, TridiagonalForm, UnitVector, VandermondeMatrix, VectorAdd, VectorAngle, VectorMatrixMultiply, VectorNorm, VectorScalarMultiply, ZeroMatrix, ZeroVector, Zip] **(1)**

Define lattice translation

```
> T1 := Vector(3, [a, 0, 0]); T2 := Vector(3, [0, a, 0]); T3 := Vector(3, [0, 0, a]);
```

$$T1 := \begin{bmatrix} a\sim \\ 0 \\ 0 \end{bmatrix}$$

$$T2 := \begin{bmatrix} 0 \\ a\sim \\ 0 \end{bmatrix}$$

$$T3 := \begin{bmatrix} 0 \\ 0 \\ a\sim \end{bmatrix} \quad (2)$$

Define reciprocal lattice translation

> $G1 := Vector\left(3, \left[\frac{2 \cdot Pi}{a}, 0, 0\right]\right); G2 := Vector\left(3, \left[0, \frac{2 \cdot Pi}{a}, 0\right]\right); G3 := Vector\left(3, \left[0, 0, \frac{2 \cdot Pi}{a}\right]\right);$

$$G1 := \begin{bmatrix} \frac{2\pi}{a\sim} \\ 0 \\ 0 \end{bmatrix}$$

$$G2 := \begin{bmatrix} 0 \\ \frac{2\pi}{a\sim} \\ 0 \end{bmatrix}$$

$$G3 := \begin{bmatrix} 0 \\ 0 \\ \frac{2\pi}{a\sim} \end{bmatrix} \quad (3)$$

> $\text{tau} := Vector(3, [0.5 \cdot a, 0.5 \cdot a, 0.5 \cdot a]);$

$$\tau := \begin{bmatrix} 0.5\, a\sim \\ 0.5\, a\sim \\ 0.5\, a\sim \end{bmatrix} \quad (4)$$

>

> $\eta := \frac{4}{a^2}; \Omega := a^3; con1 := \frac{4 \cdot Pi}{Omega}; con2 := \text{sqrt}\left(\frac{\eta}{Pi}\right);$

$$\eta := \frac{4}{a\sim^2}$$

$$\Omega := a\sim^3$$

$$con1 := \frac{4\pi}{a\sim^3}$$

$$con2 := \frac{2}{a\sim\sqrt{\pi}} \quad (5)$$

Initial terms - - Cl- Cl **and** *Cs- Cs*

```
> tot := -evalf(con2·2);
```

$$tot := -\frac{2.256758334}{a\sim} \qquad (6)$$

```
> for n from -8 by 1 while n < 8 do    for m from -8 by 1 while m < 8
     do    for l from -8 by 1 while l < 8 do    if (n ≠ 0 or m
     ≠ 0 or l ≠ 0) then  g := (n·G1 + m·G2 + l·G3) ;    tot := tot
     + evalf( 2·con1·(1-exp( -I·DotProduct(g, τ)))
     · exp( - DotProduct(g, g) / eta ) / DotProduct(g, g) )  end if end do end do end do;  evalf(tot);
```

$$-\frac{2.256758334}{a\sim} + \frac{0.0003951360355 + 1.906745200\ 10^{-24}\ \mathrm{I}}{a\sim} \qquad (7)$$

```
> for n from -8 by 1 while n < 8 do    for m from -8 by 1 while m < 8
     do    for l from -8 by 1 while l < 8 do    t := (n·T1 + m
     ·T2 + l·T3) ;    tot := tot
     - evalf( 2·(erfc( sqrt(eta)/2 ·VectorNorm(τ + t, 2))) / VectorNorm(tau + t, 2) ) ;    if (n ≠ 0
     or m ≠ 0 or l ≠ 0) then    tot := tot
     + evalf( 2·erfc( sqrt(eta)/2 ·VectorNorm(t, 2)) / VectorNorm(t, 2) )  end if end do end do
     end do;  evalf(tot);
```

$$-\frac{4.071118106}{a\sim} + \frac{0.0003951360355 + 1.906745200\ 10^{-24}\ \mathrm{I}}{a\sim} \qquad (8)$$

```
> Re(%);
```

$$-\frac{4.070722970}{a\sim} \qquad (9)$$

```
>
```