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

[&x, Add, Adjoint, BackwardSubstitute, BandMatrix, Basis, BezoutMatrix, BidiagonalForm, BilinearForm, CARE, CharacteristicMatrix, CharacteristicPolynomial, Column, ColumnDimension, ColumnOperation, ColumnSpace, CompanionMatrix, CompressedSparseForm, ConditionNumber, ConstantMatrix, ConstantVector, Copy, CreatePermutation, CrossProduct, DARE, DeleteColumn, DeleteRow, Determinant, Diagonal, DiagonalMatrix, Dimension, Dimensions, DotProduct, EigenConditionNumbers, Eigenvalues, Eigenvectors, Equal, ForwardSubstitute, FrobeniusForm, FromCompressedSparseForm, FromSplitForm, 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, ProjectionMatrix, QRDecomposition, RandomMatrix, RandomVector, Rank, RationalCanonicalForm, ReducedRowEchelonForm, Row, RowDimension, RowOperation, RowSpace, ScalarMatrix, ScalarMultiply, ScalarVector, SchurForm, SingularValues, SmithForm, SplitForm, 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]);
```

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

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

(2)

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

Define reciprocal lattice translation

```
> G1 := Vector(3, [2·Pi/a, 0, 0]); G2 := Vector(3, [0, 2·Pi/a, 0]);
  G3 := Vector(3, [0, 0, 2·Pi/a]);
```

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

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

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

```
> tau := Vector(3, [0.5·a, 0.5·a, 0.5·a]);
```

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

```
>
```

```
> η := 4/a^2; Ω := a^3; con1 := 4·Pi/Omega; con2 := sqrt(η/Pi);
```

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

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

$$con1 := \frac{4\,\pi}{a\sim^3} \quad (5)$$

$$con2 := \frac{2}{a\sim\sqrt{\pi}} \tag{5}$$

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

```
>
```

```
> tot := -evalf(con2·2);
```

$$tot := -\frac{2.256758334}{a\sim} \tag{6}$$

```
> 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);
```

$$-\frac{2.256758334}{a\sim} + \frac{0.0003951360355 + 1.907345200 \times 10^{-24}\,I}{a\sim} \tag{7}$$

```
> 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);
```

$$-\frac{4.071118106}{a\sim} + \frac{0.0003951360355 + 1.907345200 \times 10^{-24}\,I}{a\sim} \tag{8}$$

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

$$-\frac{4.070722970}{a\sim} \tag{9}$$

```
>
```