```
> 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]);
```

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

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

$$T3 := \begin{bmatrix} 0 \\ 0 \\ a\sim \end{bmatrix}$$

(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 := $Vector(3, [0.5\cdot a, 0.5\cdot a, 0.5\cdot a])$;

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

>

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

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

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

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

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

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

>

> $tot := -evalf(con2\cdot 2)$;

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

> **for** n **from** -8 **by** 1 **while** $n < 8$ **do**
for l **from** -8 **by** 1 ***while l < 8 do***

then $g := (n\cdot G1 + m\cdot G2 + l\cdot G3)$;

for m **from** -8 **by** 1 **while** $m < 8$ **do**
if $(n \neq 0$ **or** $m \neq 0$ **or** $l \neq 0)$

$tot := tot + evalf\left(2\cdot con1\cdot(1-\exp(-I\right.$

$$\cdot DotProduct(g, \tau)\,)\,)\cdot\frac{\exp\left(-\frac{DotProduct(g,g)}{eta}\right)}{DotProduct(g,g)}\Bigg)$$ **end if end do end do end do;**

$$evalf(tot);$$

$$-\frac{2.256758334}{a\sim}+\frac{0.0003951360355+1.906745200\,10^{-24}\,I}{a\sim} \tag{7}$$

> **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*** $t := (n\cdot T1+m\cdot T2+l\cdot T3)$ **;**

$$tot := tot - evalf\left(\frac{2\cdot\left(erfc\left(\frac{\mathrm{sqrt}(eta)}{2}\cdot VectorNorm(\tau+t,2)\right)\right)}{VectorNorm(\mathrm{tau}+t,2)}\right);$$

if $(n\neq 0$ **or** $m\neq 0$ **or** $l\neq 0)$ **then** $tot := tot$

$$+evalf\left(\frac{2\cdot erfc\left(\frac{sqrt(eta)}{2}\cdot VectorNorm(t,2)\right)}{VectorNorm(t,2)}\right)$$ **end if end do end do end do;**

$$evalf(tot);$$

$$-\frac{4.071118106}{a\sim}+\frac{0.0003951360355+1.906745200\,10^{-24}\,I}{a\sim} \tag{8}$$

> $\mathrm{Re}(\%);$

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

>