SFT calculations and asymptotics

This document explores and benchmarks the exact integration of the Fourier transform on the ARM sphere of a simple but suitable model of a molecular orbital which works well for simple di- and tri-atomic molecules. The form factor $R(\boldsymbol{p})$ of the ARM formalism can be expressed in terms of such a transform, which can be written as

$$\mathrm{SFT}\,(\boldsymbol{q}) = \int \frac{d\Omega}{2\pi}\, e^{-i\,\boldsymbol{q}\cdot\hat{\boldsymbol{r}}}\, F(\hat{\boldsymbol{r}}),$$

where $F(\hat{\boldsymbol{r}})$ is the angular part of the Dyson orbital, i.e. $\langle \boldsymbol{r} \mid n_D\rangle = C_\kappa\, \kappa^{3/2}\, e^{-\kappa\, r} (\kappa\, r)^{\frac{Q}{\kappa}-1}\, F(\hat{\boldsymbol{r}})$. This angular dependence can be modelled well, by all accounts, as

$$F(\hat{\boldsymbol{r}}) = \cosh(b\cos(\theta))\,\left(1 + c\cos^2(\theta)\right)\cos^{N_z}(\theta)\sin^{N_x+N_y}(\theta)\cos^{N_x}(\phi)\sin^{N_y}(\phi).$$

This model is taken from a paper by Murray et al. (PRL **106** 173001), which cites in turn A.A. Radzig and B. M. Smirnov, *Reference data on atoms, molecules and ions* (Springer-Verlag, Berlin, 1985), as a source for that form.

This integral can be done exactly, as explained in the thesis, by turning the cosh into exponentials and using standard special-functions theory (specifically, Gegenbauer's finite integral, in Watson's Bessel functions book, p. 50, or formulas 7.333.1 and .2 in Gradshteyn and Ryzhik). It comes out to the very nice form

$$\mathrm{SFT}(\boldsymbol{q}) = (-i)^{N_{\mathrm{xyz}}} \sum_\pm \frac{q_x^{N_x}\, q_y^{N_y} (q_z \pm i\, b)^{N_z}}{\left(q_x^2+q_y^2+(q_z\pm i\, b)^2\right)^{N_{\mathrm{xyz}}/2}} \left[\left(1 + c\,\frac{N_z+1/2}{N_{\mathrm{xyz}}+3/2}\right) j_{N_{\mathrm{xyz}}}\!\left(\sqrt{q_x^2+q_y^2+(q_z\pm i\, b)^2}\right) - c\left(\frac{(q_z\pm i\, b)^2}{q_x^2+q_y^2+(q_z\pm i\, b)^2} - \frac{N_z+1/2}{N_{\mathrm{xyz}}+3/2}\right) j_{N_{\mathrm{xyz}}+2}\!\left(\sqrt{q_x^2+q_y^2+(q_z\pm i\, b)^2}\right)\right],$$

where the js are spherical Bessel functions and $N_{\mathrm{xyz}} = N_x + N_y + N_z$.

One curious feature is that $\mathrm{SFT}(\boldsymbol{q})$ is only a function of the transverse momentum. This is because, by definition, $\boldsymbol{q} = a(\boldsymbol{p} + \boldsymbol{A}(t_s))$, and t_s itself is a function of the momentum, through the saddle-point equation $\frac{1}{2}(\boldsymbol{p} + \boldsymbol{A}(t_s)) + I_p = 0$, which can also be written as $p_\parallel + A(t_s) = -i\sqrt{\kappa^2 + p_\perp^2}$, and therefore $\boldsymbol{q} = a\left(\boldsymbol{p}_\perp - i\sqrt{\kappa^2 + p_\perp^2}\;\hat{\boldsymbol{n}}\right)$.

This document also contains some derived functions which help make sense of this solution.

- An approximation to SFT in the case of large a and small tunnelling angles, which to leading order reads

$$\mathrm{SFT}(\boldsymbol{q}) \simeq (-i)^{N_{\mathrm{xyz}}} \frac{e^{\kappa a}}{\kappa a} \frac{v_x^{n_x} v_y^{n_y} v_z^{n_z}}{\kappa^{n_x+n_y+n_z}} \cos\left(b\left(\frac{p_o}{\kappa} \sin(\theta) + i\left(1 + \frac{p_\perp^2}{2\kappa^2}\right)\cos(\theta)\right)\right) \times \left(1 + c\left(\frac{p_o^2}{\kappa^2}\cos(2\theta) + \left(1 + \frac{p_y^2}{\kappa^2}\right)\cos^2(\theta) - \frac{i}{2}\sqrt{1 + \frac{p_\perp^2}{2\kappa^2}}\ \frac{p_o}{\kappa}\sin(2\theta)\right)\right).$$

- Systematic refinements of this asymptotic approximation to higher order in $1/\kappa a$.

- Restricted versions of SFT for the case of on-axis ionization, or slight variations. Specifically, there are simpler expressions available for the case of $\mathrm{SFT}(p_\perp = 0)$, and for its derivatives with respect to p_o and $p_y$there. These are useful because they can be used to approximate it as $\mathrm{SFT}(q) = \mathrm{SFT}(p_\perp = 0) + q_o \frac{\partial}{\partial q_o}\mathrm{SFT}\ |_{p_\perp=0} + q_y \frac{\partial}{\partial q_y}\mathrm{SFT}\ |_{p_\perp=0}$, which is the corresponding version of the small-angle approximation that is given in the original single-electron ARM paper (Torlina et al, PRA **86** 043409).

Initialization

```
Needs["ARMSupport`"]
$ARMSupportVersion
```

```
ARMSupport v1.0.15, Tue 7 Jun 2016 22:14:23
```

Old definitions

Preliminaries

This assigns the value 1 to the formally undefined expression 0^0, which in this context is always a special case of r^n for real r and integer n. However, it is important to note that this is (in principle) dangerous, and it can potentially cause errors in other notebooks that are running on the same kernel.

```
Unprotect[Power];
Power[0, 0] = 1;
Power[0. + 0. ⅈ, 0] = 1;
Power[0., 0] = 1;
Protect[Power];
```

Some functions for support. The velocity vector **vel** at t_s as a function of alignment angle and transverse momentum and the corresponding $\boldsymbol{q}$ vector.

```
vel[θ_, po_, py_, κ_] :=
  (po {Cos[θ], 0, -Sin[θ]} + py {0, 1, 0} - ⅈ Sqrt[κ^2 + po^2 + py^2] {Sin[θ], 0, Cos[θ]});
qvec[a_, θ_, po_, py_, κ_] := a vel[θ, po, py, κ];
```

SFTnumeric

Old version - not working for some reason

Uses parallelized memoization as per mm.se/q/1259

```
SFTnumeric[qx_, qy_, qz_, b_, c_, nx_, ny_, nz_] :=
  With[{result = SFTnumericParallelized[qx, qy, qz, b, c, nx, ny, nz]},
   (SFTnumeric[qx, qy, qz, b, c, nx, ny, nz] = result) /; result =!= Null];
SFTnumeric[qx_, qy_, qz_, b_, c_, nx_, ny_, nz_] :=
 SFTnumericParallelized[qx, qy, qz, b, c, nx, ny, nz] =
  SFTnumeric[qx, qy, qz, b, c, nx, ny, nz] = NIntegrate[
    1/(2 π) ⅇ^(-ⅈ (qx Sin[θ] Cos[ϕ]+qy Sin[θ] Sin[ϕ]+qz Cos[θ])) Cosh[b Cos[θ]]
     (1 + c Cos[θ]^2) Cos[θ]^nz Sin[θ]^(nx+ny+1) Cos[ϕ]^nx Sin[ϕ]^ny
    , {θ, 0, π}, {ϕ, 0, 2 π}
    , Method → "MultidimensionalRule"
   ]
SetSharedFunction[SFTnumericParallelized];
SFTnumeric[{qx_, qy_, qz_}, b_, c_, nx_, ny_, nz_] :=
 SFTnumeric[qx, qy, qz, b, c, nx, ny, nz]
```

New version

```
Quit
```

```
SFTnumeric[qx_?NumericQ, qy_?NumericQ, qz_?NumericQ, b_, c_, nx_, ny_, nz_] := With[
  {result = SFTnumericParallelized[qx, qy, qz, b, c, nx, ny, nz]},
  If[ (result === Null && $KernelID > 0) ||
    (Head[result] === SFTnumericParallelized && $KernelID == 0),
   SFTnumericParallelized[qx, qy, qz, b, c, nx, ny, nz] = NIntegrate[
     1/(2 π) ⅇ^(-ⅈ (qx Sin[θ] Cos[ϕ]+qy Sin[θ] Sin[ϕ]+qz Cos[θ]))
      Cosh[b Cos[θ]] (1 + c Cos[θ]^2) Cos[θ]^nz Sin[θ]^(nx+ny+1) Cos[ϕ]^nx Sin[ϕ]^ny
     , {θ, 0, π}, {ϕ, 0, 2 π}
     , Method → "MultidimensionalRule"
    ]
   , result
  ]
 ]
SetSharedFunction[SFTnumericParallelized];
```

```
AbsoluteTiming[
 SFTnumeric[3 + ⅈ, 0, 15, 2.5, 1, 0, 0, 0]
]
{0.93595, 0.337514 - 0.281196 ⅈ}

Column@AbsoluteTiming@Block[{b = 2.5, c = 1, nx = 0, ny = 0, nz = 0, part = Re[ⅇ^ⅈ #] &},
   ParallelTable[
    part[SFTnumeric[qx, 0, qz, b, c, nx, ny, nz]]
    , {qx, -15, 15, 5}, {qz, -15, 15, 5}
   ]
  ]
$Aborted
```

SFTanalytic

```
SFTanalytic[qx_, qy_, qz_, b_, c_, nx_, ny_, nz_] := With[
  {ss = Function[s, Sqrt[qx^2 + qy^2 + (qz + s ⅈ b)^2]], j = SphericalBesselJ, n = nx + ny + nz},
  Sum[(-ⅈ)^(nx+ny+nz) qx^nx qy^ny (qz + s ⅈ b)^nz ((1 + c (nz + 1/2)/(n + 3/2)) j[n, ss[s]]/ss[s]^n -
      c ((qz + s ⅈ b)^2/(qx^2 + qy^2 + (qz + s ⅈ b)^2) - (nz + 1/2)/(n + 3/2)) j[n + 2, ss[s]]/ss[s]^n), {s, {1, -1}}]
 ]
SFTanalytic[{qx_, qy_, qz_}, b_, c_, nx_, ny_, nz_] :=
 SFTanalytic[qx, qy, qz, b, c, nx, ny, nz]
```

SFTasymptotic

AsymptoticBesselI

```
AsymptoticBesselI[n_, σ_, order_: 1] := Block[{n1, σ1},
  AsymptoticBesselI[n1_, σ1_, order] =
   Normal[Delete[Series[BesselI[n1, σ1], {σ1, ∞, order}], {2, 2}]];
  AsymptoticBesselI[n, σ, order]
 ]
```

This provides an appropriate asymptotic series for the spherical Bessel functions of the exact analytic SFT, which are in the modified-Bessel-function regime of the form $j_n(i\,\sigma)$.

It is important to note that the precise phrasing of this code is very important and it is overall very finick-y.This is because the naive command for the asymptotic series of the Bessel function gets the polyno-mial part correctly, but it returns subexponential terms which are not desired and in general not particu-larly correct:

```
Series[BesselI[n, σ], {σ, ∞, 1}]
```

$$e^{-\sigma}\left(e^{2\sigma}\left(\frac{\sqrt{\frac{1}{\sigma}}}{\sqrt{2\pi}}+O\left[\frac{1}{\sigma}\right]^{3/2}\right)+\left(\frac{i\, e^{i n \pi}\sqrt{\frac{1}{\sigma}}}{\sqrt{2\pi}}+O\left[\frac{1}{\sigma}\right]^{3/2}\right)\right)$$

Leaving aside the weird factorization, the $e^{-\sigma}e^{2\sigma}$ factor is correct but the pure exponential-decay factor in $e^{-\sigma}\times\text{poly}(\sigma)$ is not what we want for large σ. In some ways this is understandable as the half-integer modified Bessel functions come out in terms of hyperbolic sines and cosines,

```
BesselI[1 / 2, σ]
BesselI[11 / 2, σ]
```

$$\frac{\sqrt{\frac{2}{\pi}}\ \mathrm{Sinh}[\sigma]}{\sqrt{\sigma}}$$

$$\frac{\left(2+\frac{1890}{\sigma^4}+\frac{210}{\sigma^2}\right)\mathrm{Cosh}[\sigma]+\left(-\frac{1890}{\sigma^5}-\frac{840}{\sigma^3}-\frac{30}{\sigma}\right)\mathrm{Sinh}[\sigma]}{\sqrt{2\pi}\ \sqrt{\sigma}}$$

but in the asymptotic regime these go away, and they are explicitly ignored in e.g. DLMF 10.40.1. Moreover, it is apparently impossible to get Mathematica to produce the asymptotic series without those terms, even by providing suitable **Assumptions**. To deal with this the code uses a **Delete** statement on the offending terms, but that relies on the to-be-deleted terms being in part ⟦2,2⟧ of the outputof **Series**, which is liable to break if the output is reordered through whatever reason.

So: the above code as stated works, just be very careful with these things when modifying it.

SFTasymptotic

```
ClearAll[SFTasymptotic];
SFTasymptotic[poo_, pyy_, θθ_, bb_, cc_, κκ_, aa_, nx_, ny_, nz_, order_] :=
 Block[{po, py, θ, b, c, κ, a},
  SFTasymptotic[po_, py_, θ_, b_, c_, κ_, a_, nx, ny, nz, order] = Block[
    {n = nx + ny + nz, qx, qy, qz, σ, s, κa},
```

$$\sigma = \kappa a \sqrt{\left(1 + \frac{b^2}{\kappa a^2} - 2\, s\, \frac{b}{\kappa a} \sqrt{1 + \frac{po^2}{\kappa^2} + \frac{py^2}{\kappa^2}}\, \mathrm{Cos}[\theta] + 2\, s\, i\, \frac{b}{\kappa a}\, \frac{po}{\kappa}\, \mathrm{Sin}[\theta]\right)};$$

$$\{qx, qy, qz\} = \left\{\kappa a\, \frac{po\, \mathrm{Cos}[\theta] - i \sqrt{po^2 + py^2 + \kappa^2}\, \mathrm{Sin}[\theta]}{\kappa},\right.$$

$$\left.\kappa a\, \frac{py}{\kappa},\ \kappa a\, \frac{-i \sqrt{po^2 + py^2 + \kappa^2}\, \mathrm{Cos}[\theta] - po\, \mathrm{Sin}[\theta]}{\kappa}\right\};$$

$$e^{\kappa\, a}\, \mathrm{ExpToTrig}\Big[\mathrm{Sum}\Big[$$
$$\quad \mathrm{Normal}\Big[\mathrm{Series}\Big[$$
$$\quad\quad (-i)^n\, e^{-\kappa a}\, qx^{nx}\, qy^{ny}\, (qz + s\, i\, b)^{nz} \sqrt{\frac{\pi}{2}} \left(\left(1 + c\, \frac{nz + 1/2}{n + 3/2}\right) \frac{1}{\sigma^{n+1/2}}\right.$$
$$\quad\quad\quad \mathrm{AsymptoticBesselI}[n + 1/2, \sigma, order + 1] - c\left((qz + s\, i\, b)^2 + \frac{nz + 1/2}{n + 3/2}\, \sigma^2\right)$$
$$\quad\quad\quad \left.\frac{1}{\sigma^{n+5/2}} \mathrm{AsymptoticBesselI}[n + 5/2, \sigma, order + 1]\right)$$
$$\quad\quad , \{\kappa a, \infty, order + 1\}\Big]\Big]\ /.\ \{\kappa a \to \kappa\, a\}$$
$$\quad , \{s, \{1, -1\}\}\Big]\Big]$$

```
   ];
  SFTasymptotic[poo, pyy, θθ, bb, cc, κκ, aa, nx, ny, nz, order]
 ]
```

SFTrestricted

Benchmarking

SFTnumeric vs SFTanalytic

Pre-computation of SFTnumeric values

```
LaunchKernels[16];
```

```
Column@AbsoluteTiming@Block[{b = 2.5, c = 1, nx = 0, ny = 0, nz = 0, part = Re[e^i #] &},
   ParallelTable[
     part[SFTnumeric[qx, 0, qz, b, c, nx, ny, nz]]
     , {qx, -15, 15, 1}, {qz, -15, 15, 1}
    ];
  ]
```

NIntegrate::slwcon :
Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

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Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

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Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

```
298.658
```

About 300s=5min on 16 cores. Click on button to restore the data from the cal

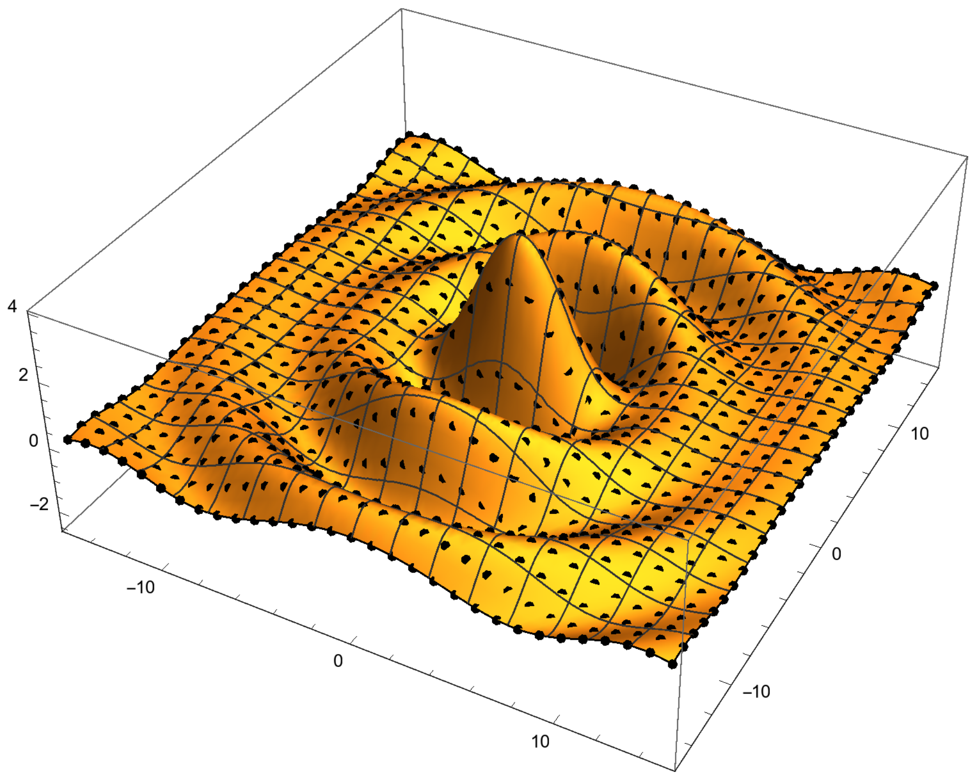
```
With[{data = Compress[ToString[InputForm[FullDefinition[SFTnumeric]]]]},
 Button["Restore calculation data", ToExpression[Uncompress[data]]]
]
```

Restore calculation data

SFTnumeric vs SFTanalytic

Comparing the numeric integration with the explicit analytical integration.

```
Block[{b = 2.5, c = 1, nx = 0, ny = 0, nz = 0, part = Re[ⅇ^ⅈ #] &},
 Show[{
   Plot3D[
    part[SFTanalytic[qx, 0, qz, b, c, nx, ny, nz]]
    , {qx, -15, 15}, {qz, -15, 15}
    , PlotRange → Full
    , PlotPoints → 50
    , ImageSize → 500
   ],
   DiscretePlot3D[
    part[SFTnumeric[qx, 0, qz, b, c, nx, ny, nz]]
    , {qx, -15, 15, 1}, {qz, -15, 15, 1}
    , Filling → None
    , PlotStyle → Black
   ]
  }]
]
```



SFTanalytic vs SFTasymptotic

Precomputation of asymptotics

```
Quit
```

```
DateString[]
AbsoluteTiming[
 Table[AbsoluteTiming[SFTasymptotic[po, py, θ, b, c, κ, a, nx, ny, nz, order];
   {nx, ny, nz, order}] , {nx, 0, 1}, {ny, 0, 1}, {nz, 0, 1}, {order, 0, 2}]]
(*re-run to check memoization*)
AbsoluteTiming[
 Table[AbsoluteTiming[SFTasymptotic[po, py, θ, b, c, κ, a, nx, ny, nz, order];
   {nx, ny, nz, order}] , {nx, 0, 1}, {ny, 0, 1}, {nz, 0, 1}, {order, 0, 2}]]
DateString[]
```

```
Thu 2 Jun 2016 19:51:59

$Aborted

$Aborted

Thu 2 Jun 2016 20:08:15
```

?????

```
With[{data = Compress[ToString[InputForm[FullDefinition[SFTasymptotic]]]]},
 Button["Restore memoization data", ToExpression[Uncompress[data]]]
]
```

Restore memoization data

For a given situation and specific order, **SFTasymptotic** returns the correct asymptotic behaviour in an analytic form, which is symbolically calculated once (slow) and then used from cache.

```
SFTasymptotic[po, py, θ, b, 0, κ, a, 0, 0, 0, 0]
```

```
$Aborted
```

This goes to higher orders,

```
SFTasymptotic[po, py, θ, b, 0, κ, a, 0, 0, 0, 1]
```

More complex molecular shapes,

```
SFTasymptotic[po, py, θ, b, c, κ, a, 1, 0, 0, 0]
```

Or both (with an obvious price on the length and complexity of the resulting expression).

```
SFTasymptotic[po, py, θ, b, c, κ, a, 1, 0, 0, 2]
```

```
SFTasymptotic[1, 1, 15 °, 2.5, 0, 1, 10, 0, 0, 0, 0]
```

```
$Aborted
```

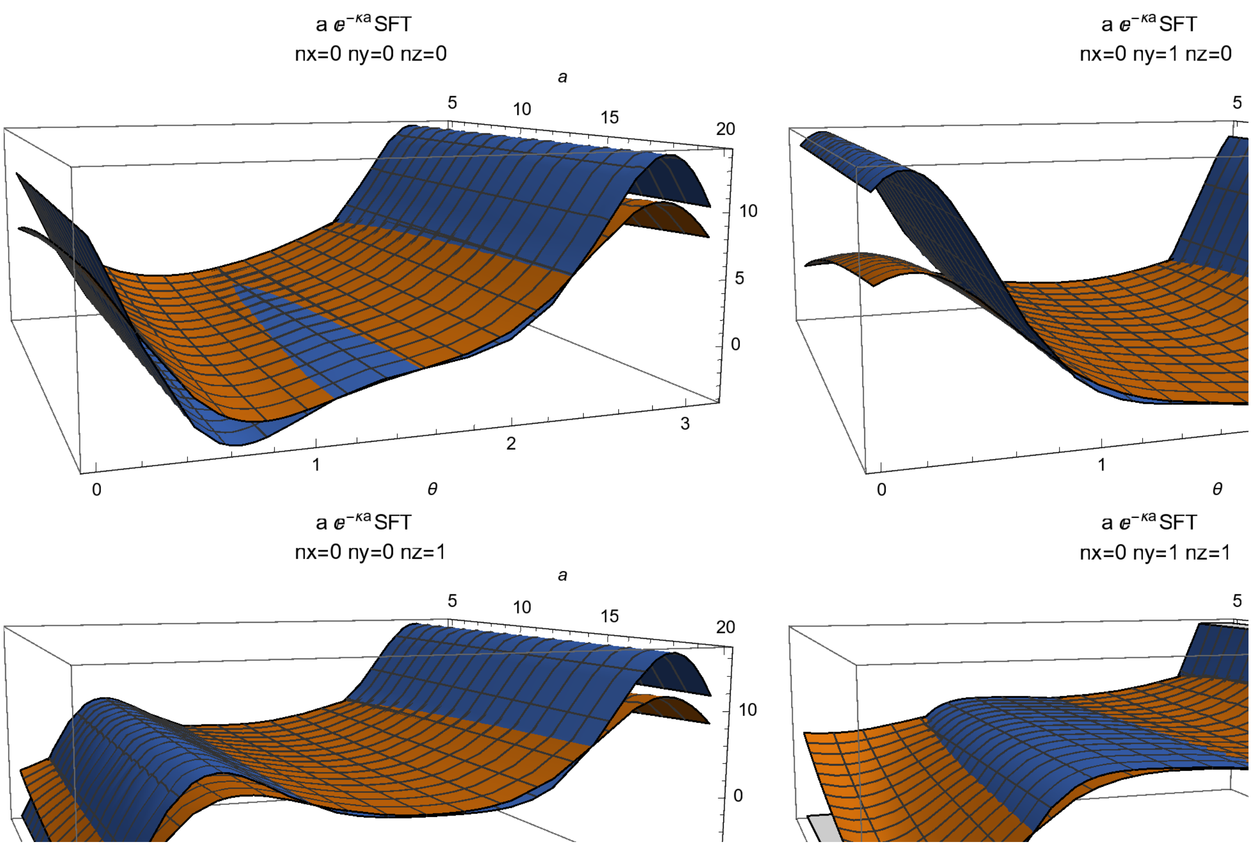
```
?? SFTasymptotic
```

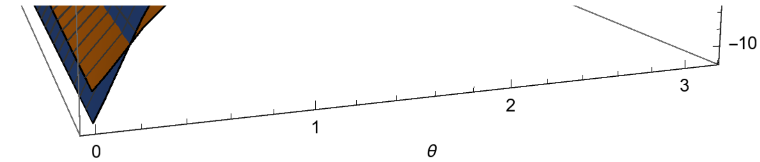
```
ARMSupport`SFTasymptotic
```

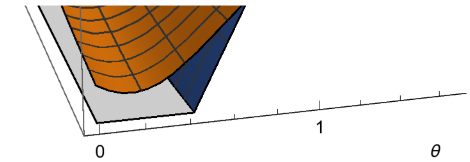
Asymptotics with a for fixed momentum

```
Column[Table[
  Column[
   AbsoluteTiming[Block[{κ = 1, c = 1, b = 2.5, po = -0.5, py = 0.15, part = Re[ⅇ^ⅈ #] &},
     Labeled[Grid[Transpose[Flatten[Table[
           Plot3D[
            {Tooltip[a ⅇ^(-κ a) part[SFTanalytic[
                  qvec[a, θ, po, py, κ], b, c, nx, ny, nz]], "Analytic"],
             Tooltip[a ⅇ^(-κ a) part[SFTasymptotic[po, py, θ, b, c, κ,
                  a, nx, ny, nz, order]], "Asymptotic"]}
            , {a, 5, 20}, {θ, 0, π}
            , ImageSize → 400
            , AxesLabel → {"a", "θ"}
            , PlotLabel → "a ⅇ^(-κa) SFT \n nx=" <>
              ToString[nx] <> " ny=" <> ToString[ny] <> " nz=" <> ToString[nz]
            , ViewPoint → {2, -0.7, Scaled[0.0005]}
           ]
           , {nx, {0, 1}}, {ny, {0, 1}}, {nz, {0, 1}}], {1, 2}]]],
      Style["order=" <> ToString[order], 20], {Top, Left}]
    ]]]
  , {order, 0, 2}], Spacings → Scaled[0.1]]
```

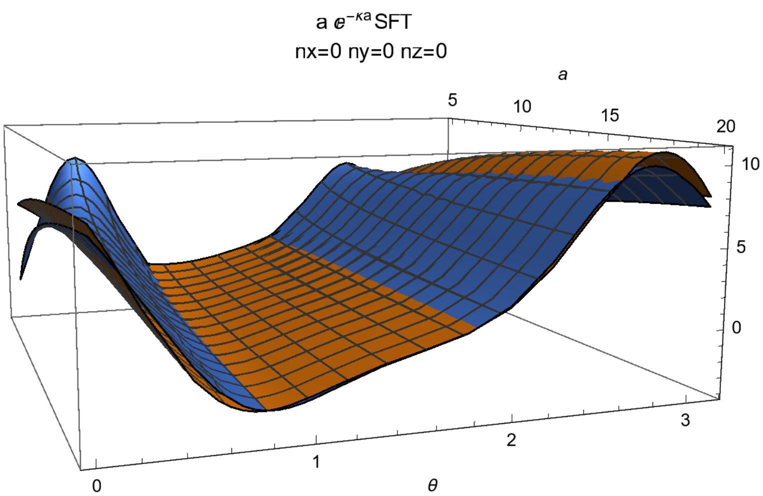
11.9478

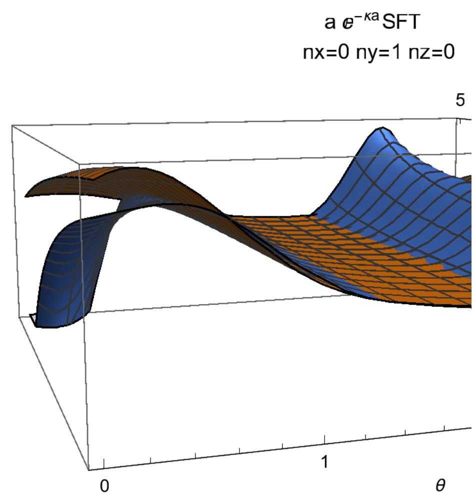


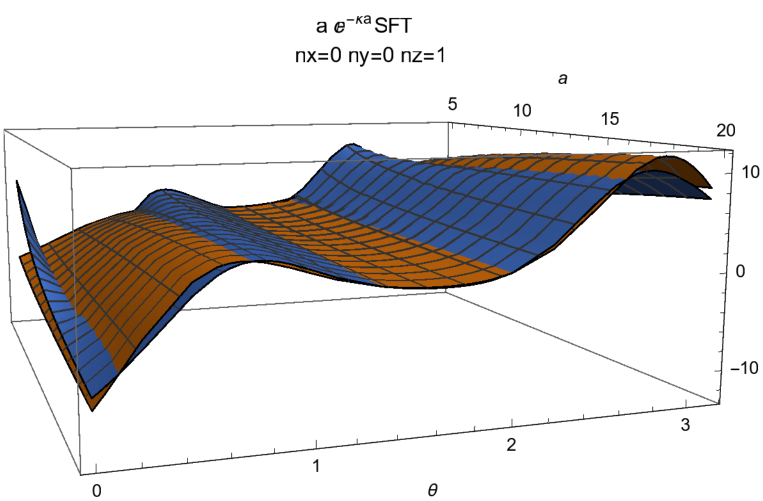


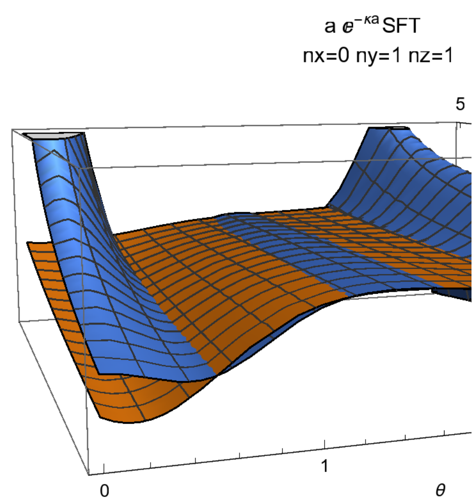


27.1358

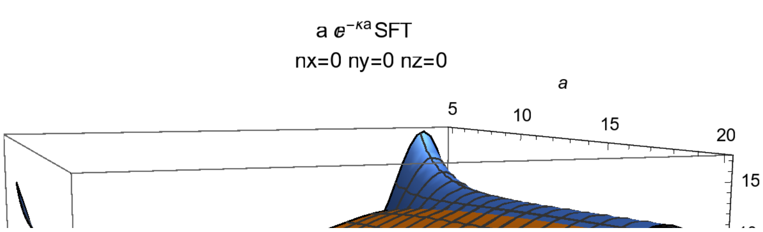


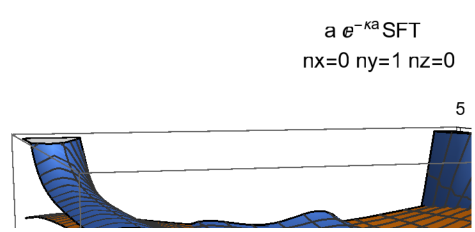


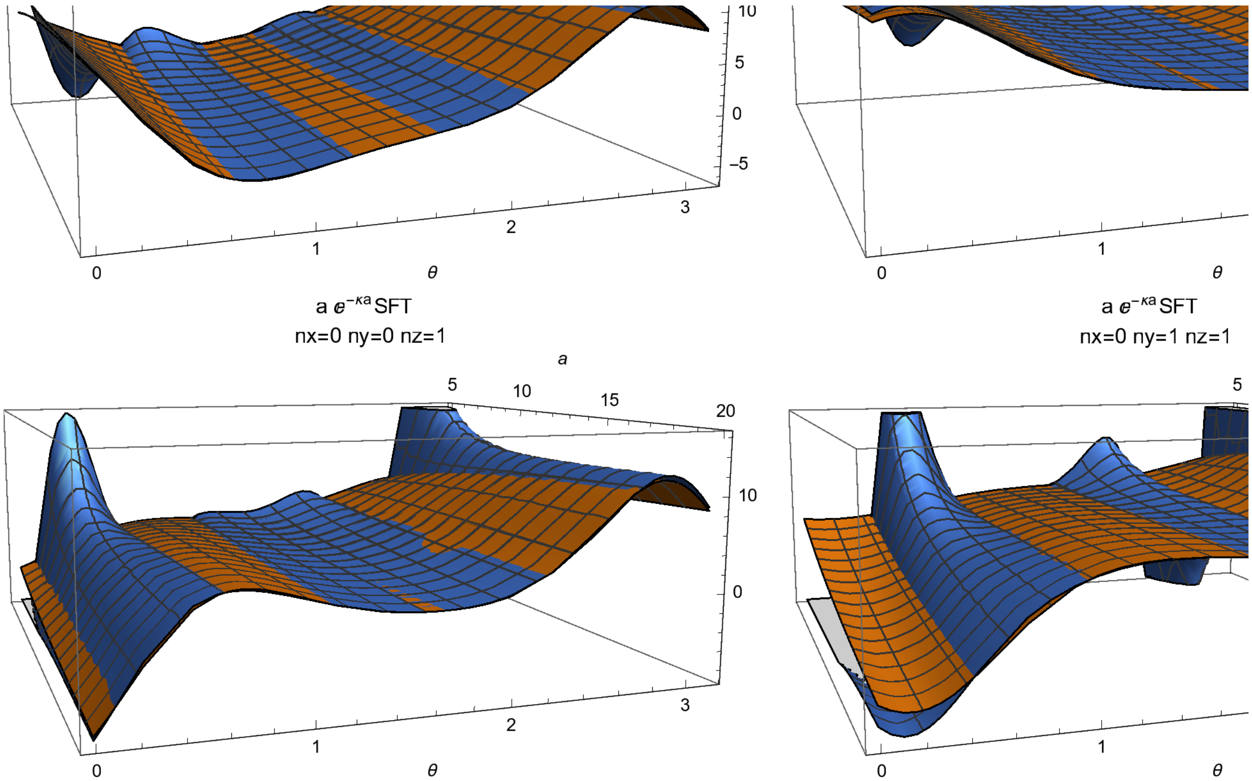




50.073



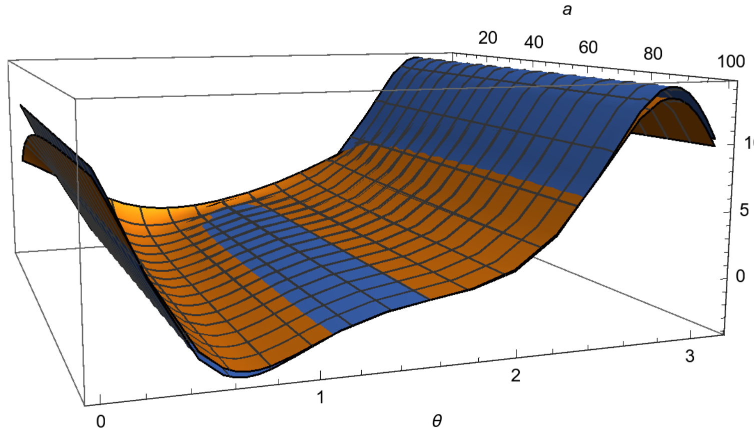




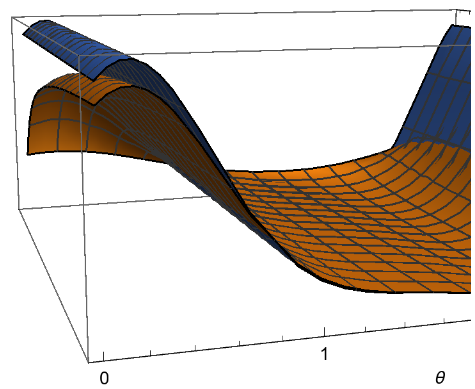
Long-range asymptotics for a fixed momentum.

```
Column[Table[
  Column[
   AbsoluteTiming[Block[{κ = 1, c = 1, b = 2.5, po = -0.5, py = 0.15, part = Re[ⅇ^ⅈ #] &},
     Labeled[Grid[Transpose[Flatten[Table[
          Plot3D[
           {Tooltip[a ⅇ^(-κ a) part[SFTanalytic[
                qvec[a, θ, po, py, κ], b, c, nx, ny, nz]], "Analytic"],
            Tooltip[a ⅇ^(-κ a) part[SFTasymptotic[po, py, θ, b, c, κ,
                a, nx, ny, nz, order]], "Asymptotic"]}
           , {a, 5, 100}, {θ, 0, π}
           , ImageSize → 400
           , AxesLabel → {"a", "θ"}
           , PlotLabel → "a ⅇ^(-κa)SFT \n nx=" <>
             ToString[nx] <> " ny=" <> ToString[ny] <> " nz=" <> ToString[nz]
           , ViewPoint → {2, -0.7, Scaled[0.0005]}
          ]
          , {nx, {0, 1}}, {ny, {0, 1}}, {nz, {0, 1}}], {1, 2}]]],
      Style["order=" <> ToString[order], 20], {Top, Left}]
    ]]]
  , {order, 0, 2}], Spacings → Scaled[0.1]]
11.9678
```

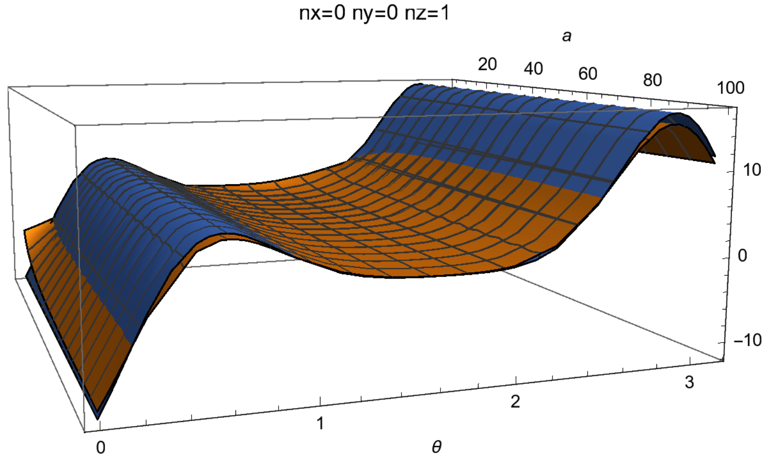
$a\,e^{-\kappa a}$ SFT
nx=0 ny=0 nz=0



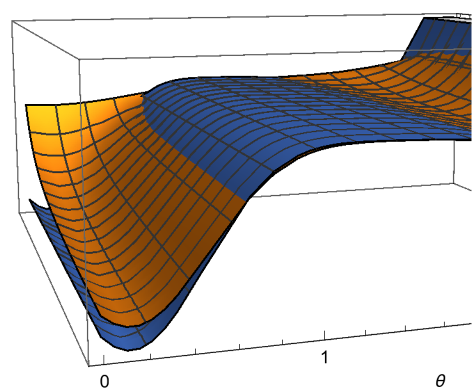
$a\,e^{-\kappa a}$ SFT
nx=0 ny=1 nz=0



$a\,e^{-\kappa a}$ SFT
nx=0 ny=0 nz=1

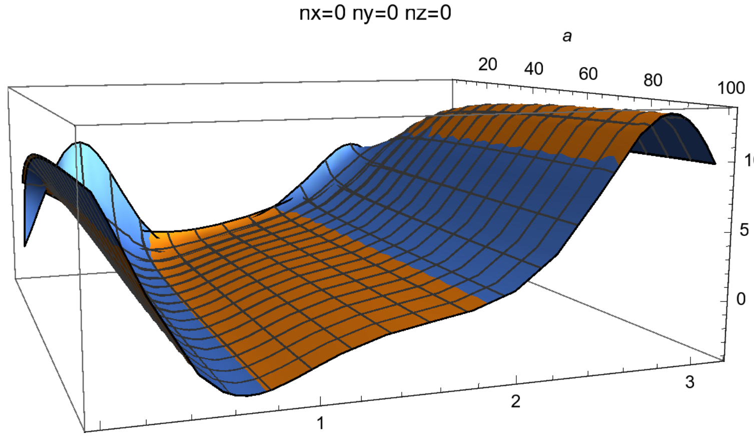


$a\,e^{-\kappa a}$ SFT
nx=0 ny=1 nz=1

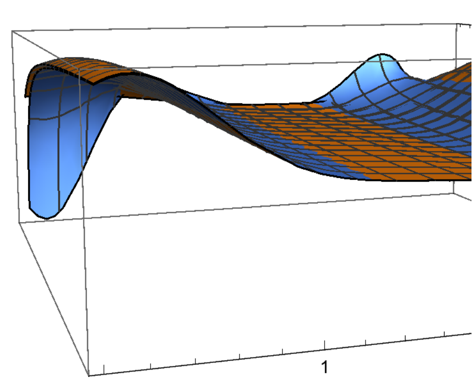


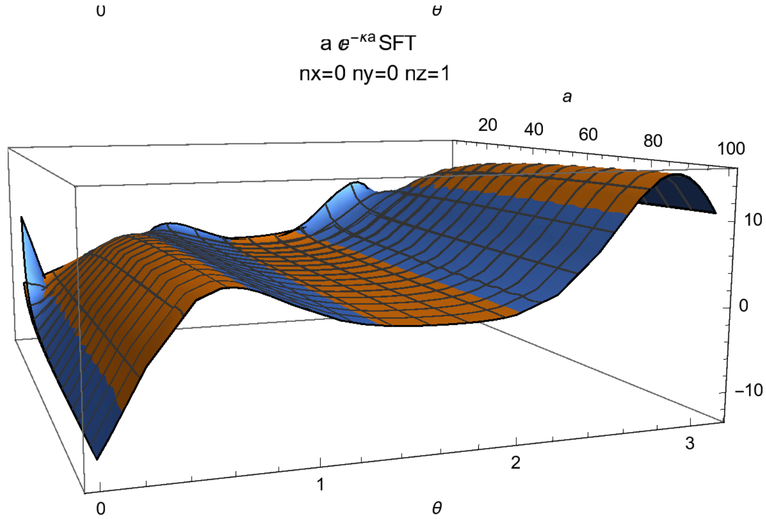

```
23.9256
```

$a\,e^{-\kappa a}$ SFT
nx=0 ny=0 nz=0

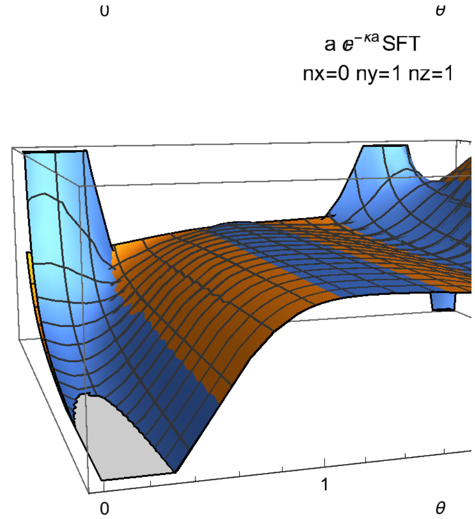


$a\,e^{-\kappa a}$ SFT
nx=0 ny=1 nz=0



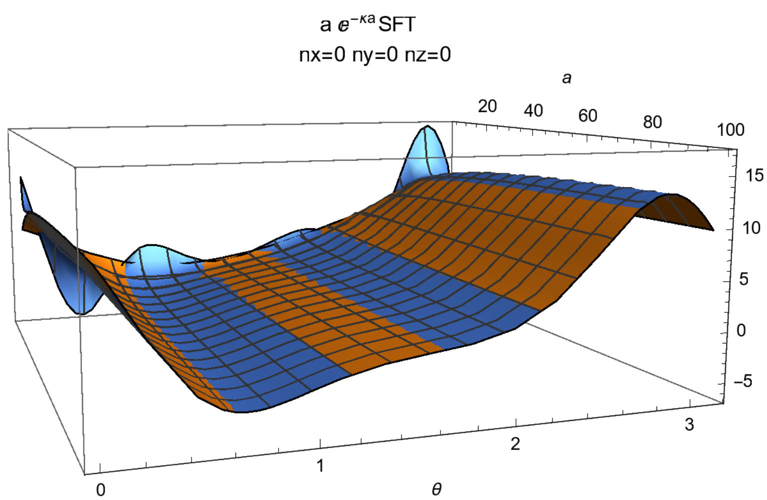


a $e^{-\kappa a}$ SFT
nx=0 ny=0 nz=1
a
20 40 60 80 100
10
0
−10
0 1 2 3
θ

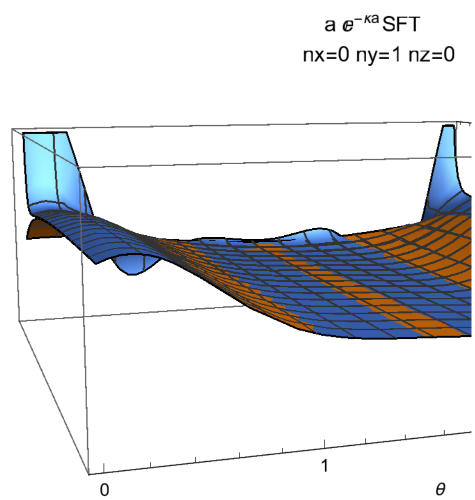


a $e^{-\kappa a}$ SFT
nx=0 ny=1 nz=1
0 1
θ

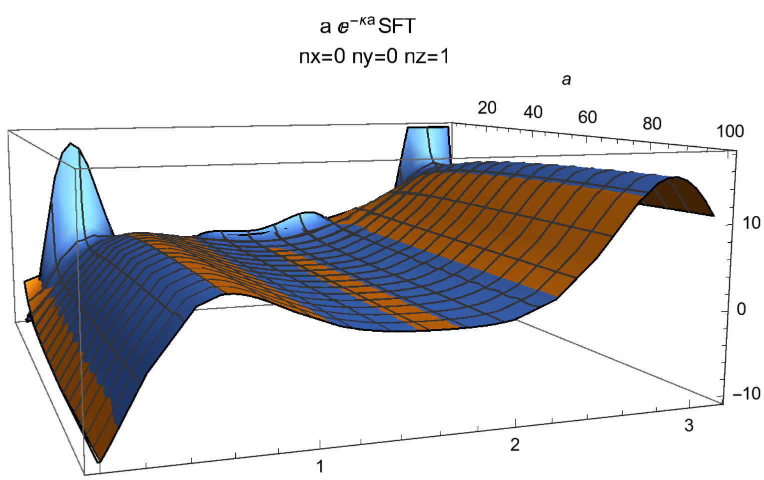
45.9839



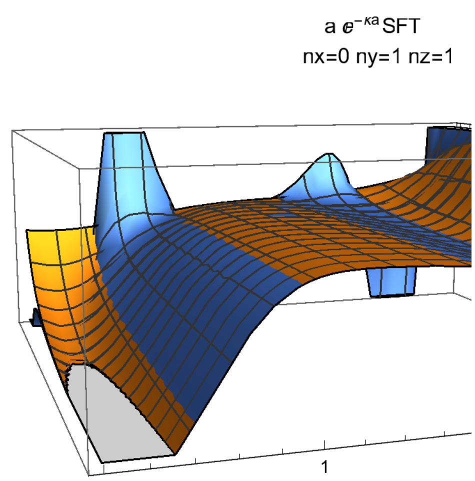
a $e^{-\kappa a}$ SFT
nx=0 ny=0 nz=0
a
20 40 60 80 100
15
10
5
0
−5
0 1 2 3
θ



a $e^{-\kappa a}$ SFT
nx=0 ny=1 nz=0
0 1
θ



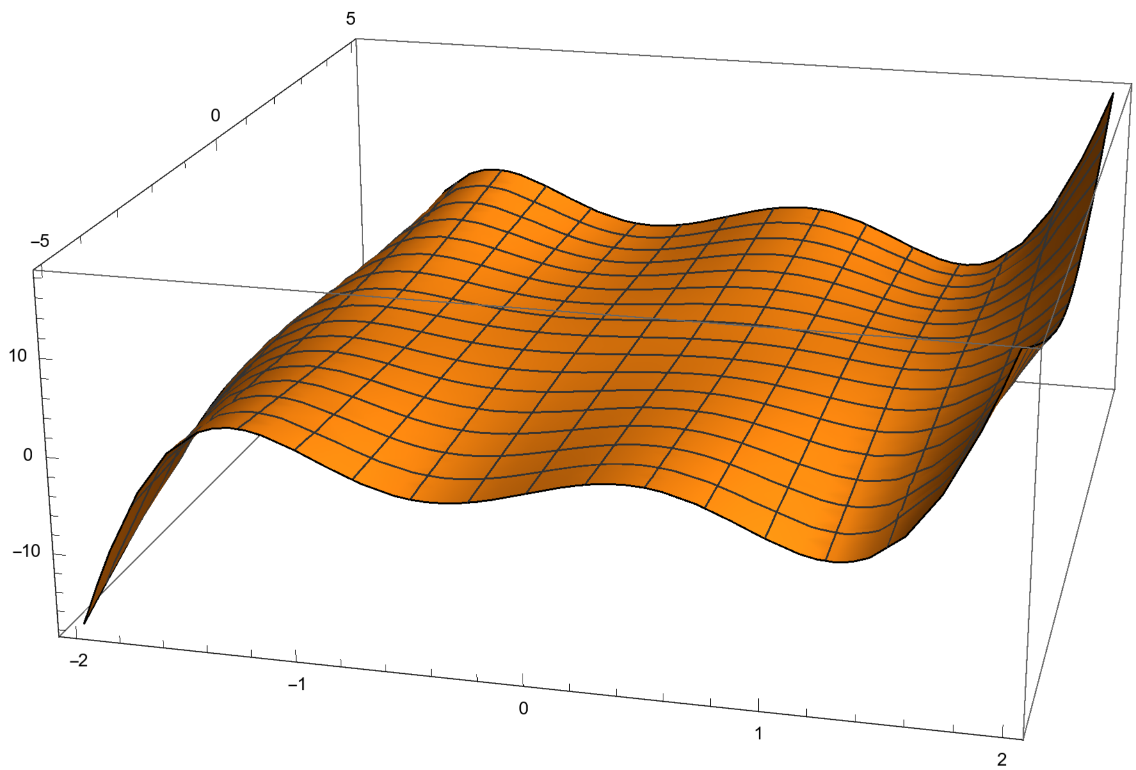
a $e^{-\kappa a}$ SFT
nx=0 ny=0 nz=1
a
20 40 60 80 100
10
0
−10
1 2 3



a $e^{-\kappa a}$ SFT
nx=0 ny=1 nz=1
1

Momentum dependence of the exact SFTanalytic

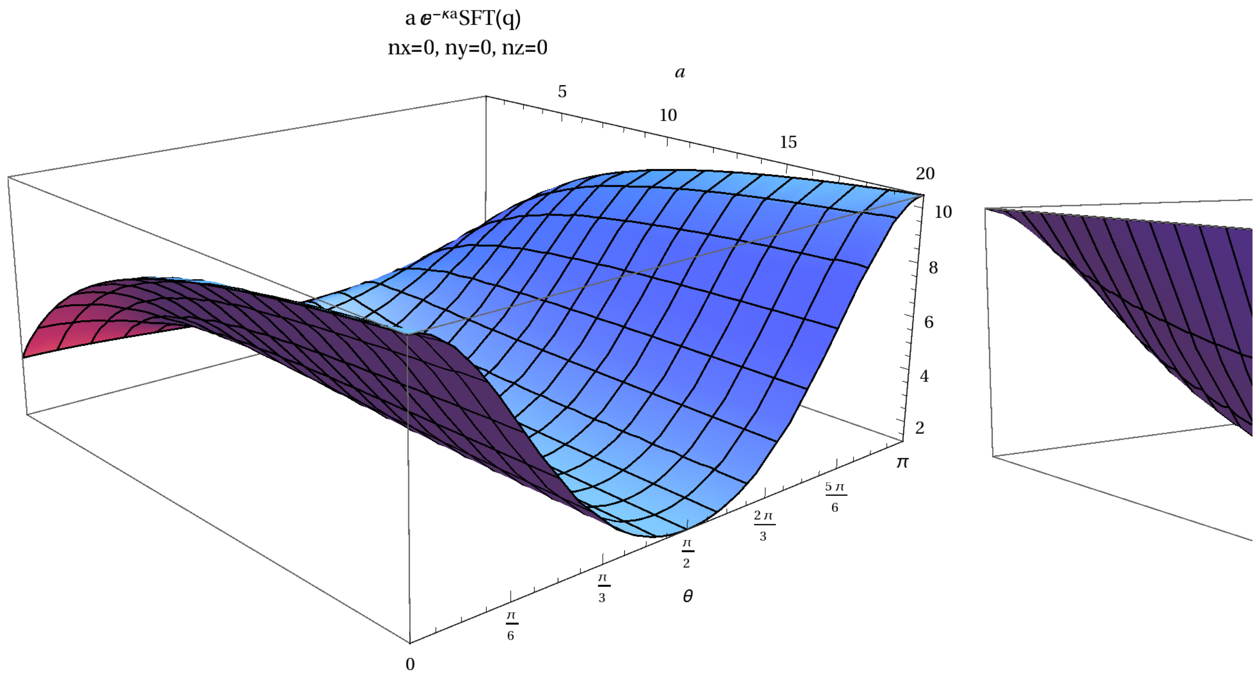
```
Block[{κ = 1, c = 1, b = 2.5, θ = 90 °, part = Re[ⅇ^ⅈ #] &, nx = 1, ny = 0, nz = 1, a = 15},
 Plot3D[
  Tooltip[a ⅇ^(-κ a) part[SFTanalytic[qvec[a, θ, po, py, κ], b, c, nx, ny, nz]], "Analytic"]
  , {po, -2, 2}, {py, -5, 5}
  , PlotRange → Full
 ]
]
```

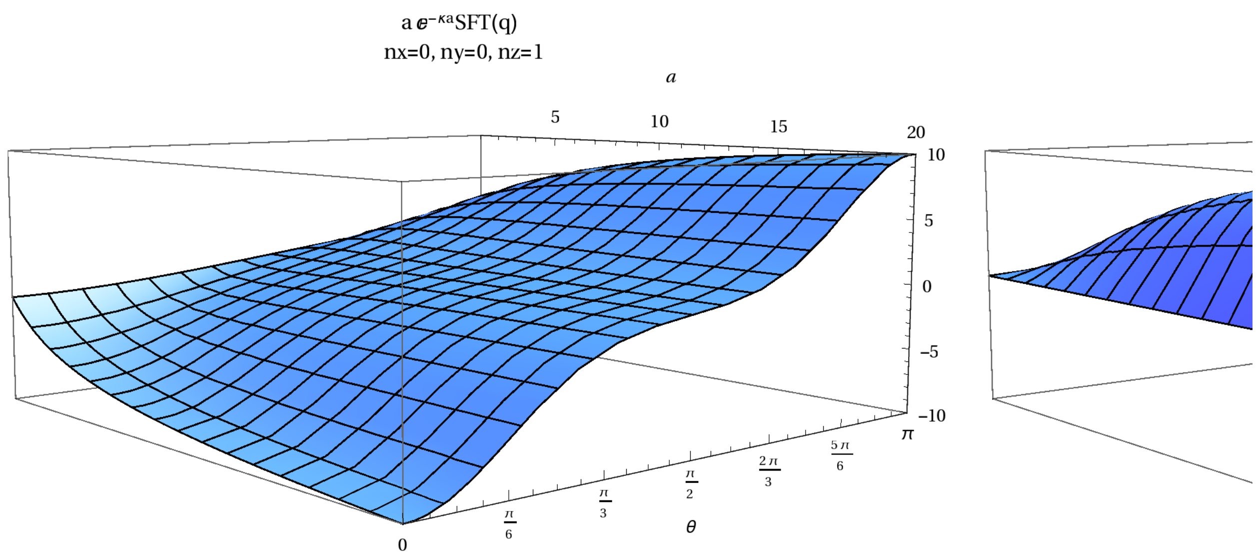


Long-range dependence of the exact SFTanalytic

```
Column[AbsoluteTiming[Block[{κ = 1, c = 1, b = 2.5, po = 0, py = 0, part = Re[#] &},
   Grid[Transpose[Flatten[Table[
        Plot3D[
         Tooltip[
          a ⅇ^(-κ a) part[SFTanalytic[qvec[a, θ, po, py, κ], b, c, nx, ny, nz]], "Analytic"]
         , {a, 1, 20}, {θ, 0, π}
         , ImageSize → 500
         , AxesLabel → {"a", "θ"}
         , PlotLabel → "a ⅇ^(-κa)SFT(q) \n nx=" <>
           ToString[nx] <> ", ny=" <> ToString[ny] <> ", nz=" <> ToString[nz]
         , ViewPoint → {2, -1.7, Scaled[0.0005]}
         , PlotRangePadding → None
         , PlotTheme → "Classic"
         , Ticks → {Automatic,
           Join[{#, #} & /@ Range[0, π, π / 6], {#, "", {0.01, 0}} & /@ Range[0, π, π / 24]]
           , Automatic}
        ]
        , {nx, {0, 1}}, {ny, {0}}, {nz, {0, 1}}], {1, 2}]]]
  ]]]
```

```
3.68851
```

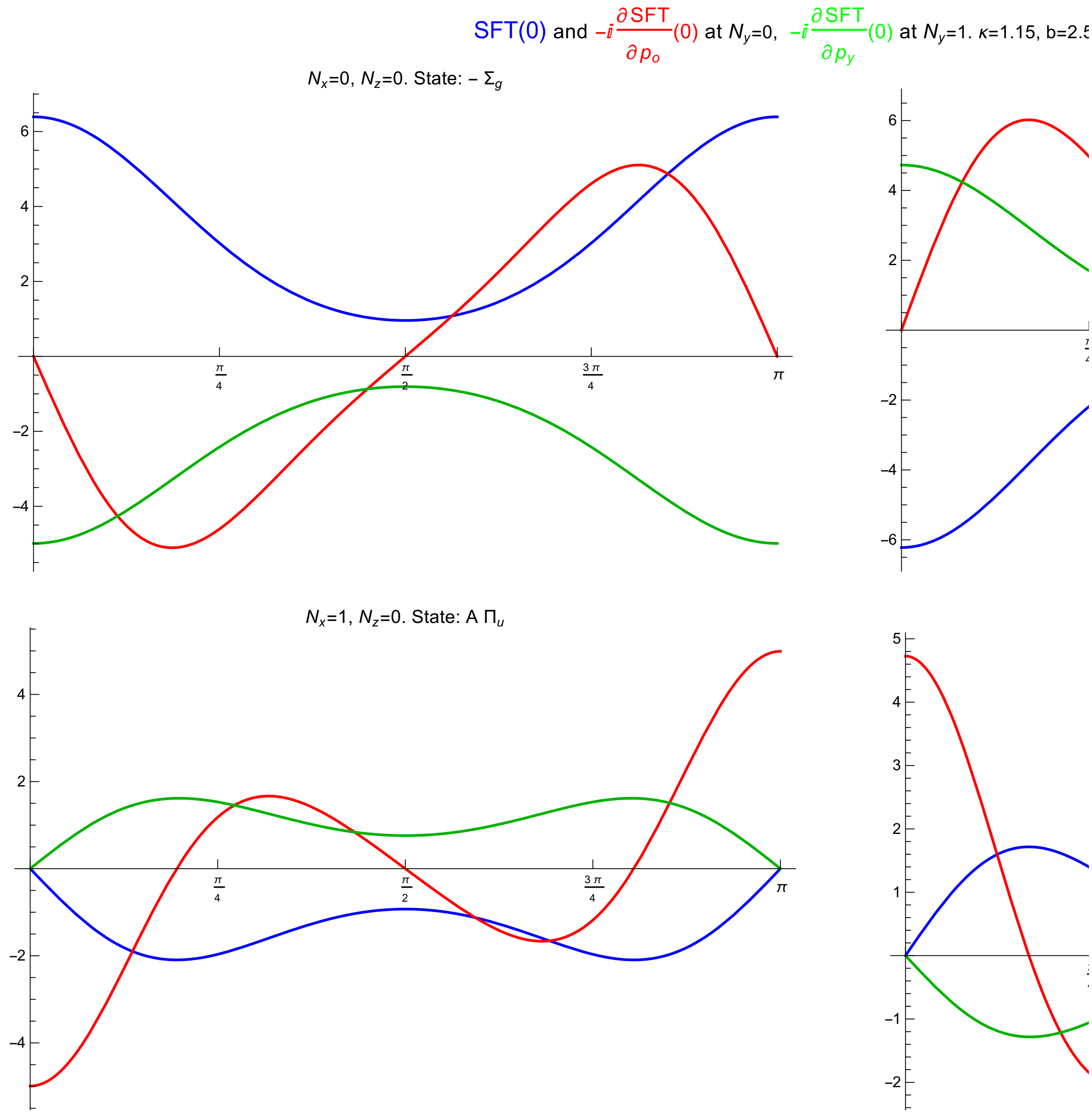

a $e^{-\kappa a}$SFT(q)
nx=0, ny=0, nz=0
a
5
10
15
20
10
8
6
4
2
π
5π/6
2π/3
π/2
π/3
π/6
0
θ


a $e^{-\kappa a}$SFT(q)
nx=0, ny=0, nz=1
a
5
10
15
20
10
5
0
−5
−10
π
5π/6
2π/3
π/2
π/3
π/6
0
θ

SFTrestricted

Plots of SFT and its derivatives on axis

```
Block[{κ = 1.15, b = 2.5, c = 0.3, a = 30},
 GraphicsGrid[
  Table[
   Plot[{
     a ⅇ^(-κ a) SFTrestricted[θ, κ, a, b, c, nx, 0, nz]
     , Evaluate[a ⅇ^(-κ a) Im[SFTderivative[θ, κ, a, b, c, nx, 0, nz]]]
     , Evaluate[a ⅇ^(-κ a) Im[SFTpy[θ, κ, a, b, c, nx, 1, nz]]]
    }, {θ, 0, π / 1}
    , PlotRange → Full
    , PlotLabel → "N_x=" <> ToString[nx] <> ", N_z=" <>
      ToString[nz] <> ". State: " <> Piecewise[{{"X Π_g", 2 nz + nx == 3},
        {"A Π_u", 2 nz + nx == 1}, {"B Σ_u", 2 nz + nx == 2}, {"- Σ_g", 2 nz + nx == 0}}]
    , PlotStyle → {Blue, Red, Darker[Green, 0.3]}
    , Ticks → {π/4 Range[0, 4], Automatic}
   ]
   , {nx, 0, 1}, {nz, 0, 1}]
  , ImageSize → 1000, PlotLabel →
   "SFT(0) and -ⅈ ∂SFT/∂p_o(0) at N_y=0,   -ⅈ ∂SFT/∂p_y(0) at N_y=1. κ=1.15, b=2.5, c=0.3, a=30"]
]
```


SFT(0) and −i ∂SFT/∂p_o (0) at N_y=0, −i ∂SFT/∂p_y (0) at N_y=1. κ=1.15, b=2.5
N_x=0, N_z=0. State: − Σ_g
6
4
2
−2
−4
π/4
π/2
3π/4
π
N_x=1, N_z=0. State: A Π_u
5
4
3
2
1
−1
−2
−4
−6