Efficient calculation of first- and second-order derivatives of thermodynamic potentials

F. Sandin*
IFPA, Département AGO, Université de Liège, Sart Tilman, 4000 Liège, Belgium

Derivatives of thermodynamic potentials are needed to calculate various physical quantities, and to solve, *e.g.*, gap and charge neutrality equations. Standard numerical derivation is inefficient if several first- and second-order derivatives of the potential are needed. Here a more efficient method is described. This method is implemented in the mean-field Polyakov-loop Nambu–Jona-Lasinio model of the 3FCS; http://3fcs.pendicular.net. As far as I know the derivation of second-order terms is original. See my Ph.D. thesis for background information, in particular appendices E/F and related chapters; http://epubl.ltu.se/1402-1544/2007/05/index.html.

I. CALCULATION OF DERIVATIVES

After Matsubara summation the thermodynamic potential for fermions is on the form

$$\Omega(T,x,y) = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left\{\frac{\lambda_i(p,x,y)}{2} + T\ln\left[1+e^{-\lambda_i(p,x,y)/T}\right]\right\} + \cdots, \tag{1}$$

where $\lambda_i = \lambda_i(p,x,y)$ are dispersion relations and γ is the degeneracy factor. The variables "x" and "y" are symbols for any variable, other than the momentum, p, that appears in the matrix operator used to calculate the dispersion relations. These variables could represent, *e.g.*, chemical potentials or gaps. The non-trivial parts of the first- and second-order derivatives of the potential are

$$\frac{\partial\Omega}{\partial x} = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left[\frac{\partial\lambda_i}{\partial x}\left(\frac{1}{2}-\frac{1}{1+e^{\lambda_i/T}}\right)\right] + \cdots, \tag{2}$$

$$\frac{\partial^2\Omega}{\partial x^2} = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left[\frac{\partial^2\lambda_i}{\partial x^2}\left(\frac{1}{2}-\frac{1}{1+e^{\lambda_i/T}}\right) + \left(\frac{\partial\lambda_i}{\partial x}\right)^2\frac{e^{\lambda_i/T}}{T\left(1+e^{\lambda_i/T}\right)^2}\right] + \cdots. \tag{3}$$

$$\frac{\partial^2\Omega}{\partial x\partial y} = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left[\frac{\partial^2\lambda_i}{\partial x\partial y}\left(\frac{1}{2}-\frac{1}{1+e^{\lambda_i/T}}\right) + \frac{\partial\lambda_i}{\partial x}\frac{\partial\lambda_i}{\partial y}\frac{e^{\lambda_i/T}}{T\left(1+e^{\lambda_i/T}\right)^2}\right] + \cdots, \tag{4}$$

$$\frac{\partial^2\Omega}{\partial x\partial T} = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left[\frac{\partial\lambda_i}{\partial x}\frac{\lambda_i}{T^2}\frac{-e^{\lambda_i/T}}{\left(1+e^{\lambda_i/T}\right)^2}\right] + \cdots. \tag{5}$$

In order to evaluate these expressions the first- and second-order derivatives of the dispersion relations are needed. The dispersion relations are calculated by solving eigenproblems. For a given momentum, p, one or several eigenvalue problems of this type are solved:

$$(A-\lambda_i I)\,v_i = 0. \tag{6}$$

The matrix A, the eigenvalues λ_i and the right eigenvectors v_i are functions of x and y. The left eigenvectors, u_i^T, are defined as $u_i^T\,(A-\lambda_i I) = 0$. To calculate the first-order derivatives of the eigenvalues with respect to x I use the derivative of the eigenvalue equation (6)

$$\frac{\partial\lambda_i}{\partial x}v_i = \frac{\partial A}{\partial x}v_i + (A-\lambda_i I)\frac{\partial v_i}{\partial x}. \tag{7}$$

*Electronic address: fredrik.sandin@gmail.com

The second term on the right-hand side of (7) includes the derivative of an eigenvector, which is unknown. This term is cancelled by multiplying the corresponding left eigenvector, u_i^T, from the left-hand side. By solving for the derivative I get

$$\frac{\partial \lambda_i}{\partial x} = \frac{u_i^T \frac{\partial A}{\partial x} v_i}{u_i^T v_i}, \tag{8}$$

where the matrix derivative $\partial A/\partial x$ typically is a sparse matrix. Sparse (complex) matrices are supported by the 3FCS common library.

Second-order derivatives are calculated in a similar way. The starting point is the second-order derivative of the eigenvalue equation (6)

$$\frac{\partial^2 \lambda_i}{\partial x^2} v_i = 2\left(\frac{\partial A}{\partial x} - \frac{\partial \lambda_i}{\partial x} I\right)\frac{\partial v_i}{\partial x} + (A - \lambda_i I)\frac{\partial^2 v_i}{\partial x^2}. \tag{9}$$

In this expression the term including the factor $\partial^2 A/\partial x^2$ is omitted, because I limit this discussion to matrices A that are at most bilinear in x and y. The second term on the right-hand side of (9) is cancelled by multiplying the left eigenvector, u_i^T, because the second-order derivative of the eigenvector is an unknown quantity. By solving for the second-order derivative I get

$$\frac{\partial^2 \lambda_i}{\partial x^2} = \frac{2u_i^T \left(\frac{\partial A}{\partial x} - \frac{\partial \lambda_i}{\partial x} I\right)\frac{\partial v_i}{\partial x}}{u_i^T v_i}. \tag{10}$$

To evaluate this expression, first calculate the first-order derivative (8) and then the first-order derivative of the eigenvector with the help of (7). The latter equation can be written

$$(A - \lambda_i I)\frac{\partial v_i}{\partial x} = -\left(\frac{\partial A}{\partial x} - \frac{\partial \lambda_i}{\partial x} I\right) v_i. \tag{11}$$

This is a system of linear equations for the vector $\partial v_i/\partial x$. The matrix $A - \lambda_i I$ is rank deficient by construction, *i.e.*, it does not have an inverse. This is to be expected, because the norm of an eigenvector is arbitrary and the derivative is defined only when the norm is fixed. I therefore require that

$$\frac{\partial |v_i|}{\partial x} = 0 \quad \rightarrow \quad v_i^\dagger \frac{\partial v_i}{\partial x} = 0. \tag{12}$$

This condition means that the derivative of v is perpendicular to v itself, *i.e.*, the change in the direction of v is accounted for, but not the change of its norm. The two equations (11) and (12) give a unique solution for $\partial v_i/\partial x$, provided that the matrix A has no degenerate eigenvalues. In order to understand this, consider the eigendecomposed analogue of (11). Define V as the matrix with columns equal to the eigenvectors of A, and Λ as the diagonal matrix of eigenvalues. Presuming that the eigenvectors are linearly independent, which typically is the case here, the eigendecomposition of A is $A = V\Lambda V^{-1}$. Equation (11) can therefore be written

$$(\Lambda - \lambda_i I)\, d_i = -V^{-1}\left(\frac{\partial A}{\partial x} - \frac{\partial \lambda_i}{\partial x} I\right) v_i, \tag{13}$$

where $d_i = V^{-1}\partial v_i/\partial x$ is the unknown vector. This is a linear system of equations. If the eigenvalues are nondegenerate the diagonal matrix $\Lambda - \lambda_i I$ has exactly one vanishing diagonal element. Consequently, it is trivial to solve for all elements of d_i except for the one that multiplies the vanishing diagonal element of the matrix. This remaining element is determined by (12) and the unique solution for the derivative is

$$\frac{\partial v_i}{\partial x} = V d_i. \tag{14}$$

If several derivatives are needed it is worthwhile to calculate V^{-1}, because (13) is then trivial to solve. If only a few eigenvector derivatives are needed it could be more efficient to multiply (13) with V from the left-hand side and solve the non-trivial system of equations. Mixed second-order derivatives can be obtained from the derivative of (7) with respect to y. The result is

$$\frac{\partial^2 \lambda_i}{\partial x \partial y} = \frac{u_i^T \frac{\partial^2 A}{\partial x \partial y} v_i + u_i^T \left(\frac{\partial A}{\partial x} - \frac{\partial \lambda_i}{\partial x} I\right)\frac{\partial v_i}{\partial y} + u_i^T \left(\frac{\partial A}{\partial y} - \frac{\partial \lambda_i}{\partial y} I\right)\frac{\partial v_i}{\partial x}}{u_i^T v_i}, \tag{15}$$

where I have kept the derivative $\partial^2 A/\partial x\partial y$, because some elements of the matrix may contain bilinear terms. The mixed derivatives can be calculated practically for free, because all quantities needed appear also in the expressions (8) and (10). This is fortunate, because many mixed derivatives are needed when solving for the physical minima of a potential.

The derivatives of the thermodynamic potential with respect to T are more simple. They can be calculated with these expressions

$$\frac{\partial \Omega}{\partial T} = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left\{\ln\left[1+e^{-\lambda_i(p,x)/T}\right]+\frac{\lambda_i(p,x)/T}{1+e^{\lambda_i(p,x)/T}}\right\}+\cdots\,, \tag{16}$$

$$\frac{\partial^2 \Omega}{\partial T^2} = -\frac{\gamma}{2}\int \frac{d^3p}{(2\pi)^3}\sum_{i=1}^{N}\left\{\frac{\lambda_i^2(p,x)\,e^{-\lambda_i(p,x)/T}}{T^3\left[1+e^{-\lambda_i(p,x)/T}\right]^2}\right\}+\cdots\,. \tag{17}$$

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