Free Energy of an Anharmonic Crystal*

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The perturbation techniques of statistical physics have been applied to obtain two formulas for the free energy of an anharmonic crystal. One involves an integration over the coupling constant and the other involves the exact Green's function; both are exact parallels of the fermion case. The anharmonic crystal differs from the interacting fermions in the structure of the phonon interaction, the effect of which on the perturbation series is carefully considered. The stationary property of the free energy with respect to the variation of the proper self-energy is proved. Expressions for the internal energy and entropy are also derived.

1. INTRODUCTION

THE perturbation techniques of quantum-field theory have been applied to the problem of lattice dynamics.[1] The lattice Hamiltonian is expanded in powers of displacements from equilibrium positions of the ions; the harmonic part is analyzed in terms of free phonons and the anharmonic terms constitute the interaction between phonons and are treated as perturbation. Now in the case of fermions or bosons interacting through a two-body potential, the free energy is first obtained as a series in terms of the unperturbed propagators, which can then be resummed as a series in terms of the full propagators, known as the Luttinger-Ward[2] formula. The phonons in an anharmonic crystal are different in that their interaction does not conserve the number of particles. This makes it impossible to relate the full phonon propagator to the unperturbed one by a self-energy part. Therefore, one is forced to expand the perturbation series in terms of some other Green's function of the unperturbed system,[3] namely that of the ionic displacements, rather than that of the phonon creation and annihilation operators [see Eq. (5) below]. Here, we address ourselves to the problem of partially summing the series for the free energy in terms of the unperturbed Green's functions to yield a series in terms of the full Green's functions. We find it possible to derive two expressions for the free energy, one involving an integral over the coupling constant and the other being an exact parallel of the Luttinger-Ward formula. The stationary property of the free energy with respect to variation of the proper self-energy part also holds. As an application, we derive the expressions for the internal energy and the entropy.

2. THE PROPER SELF-ENERGY PART AND THE FREE ENERGY

We start with the Hamiltonian for the anharmonic crystal,[3]

$$H=H_0+H_1, \tag{1}$$

where the harmonic Hamiltonian is

$$H_0=\tfrac{1}{4}\sum_Q \hbar\omega_Q(A_QA_{-Q}-B_QB_{-Q}), \tag{2}$$

and the anharmonic part is

$$H_1=\sum_{n=3}^{\infty}\lambda^n\sum_{Q_1,\cdots,Q_n}V^{(n)}(Q_1\cdots Q_n)A_{Q_1}\cdots A_{Q_n}. \tag{3}$$

Q denotes a four-vector $(\mathbf{q},j)$ as the phonon wave vector reduced to the first Brillouin zone and the mode of polarization; $-Q\equiv(-\mathbf{q},j)$; ω denotes the phonon frequency; A and B are given in terms of phonon creation and annihilation operators as

$$\begin{aligned}A_Q&=a_Q+a_{-Q}^{\dagger},\\ B_Q&=a_{-Q}^{\dagger}-a_Q.\end{aligned} \tag{4}$$

We introduce a power of the coupling constant λ^n into the $V^{(n)}$ term in the anharmonic perturbation to characterize the structure of that term which has n operators A. It is merely a convenient formal device and has nothing to do with the usual parameter of smallness[4] ϵ, which is the ratio of the mean ionic displacement to the lattice parameter. The $V^{(n)}$ term is of order ϵ^{n-2}. In the final results, we shall put λ equal to unity.

We define the proper self-energy part via the thermodynamic Green's function

$$D_{QQ'}(\tau-\tau')=\langle T\tilde{A}_Q(\tau)\tilde{A}_{Q'}^{\dagger}(\tau')\rangle, \quad |\tau-\tau'|\leq\beta, \tag{5}$$

where the Heisenberg representation is used:

$$\tilde{A}(\tau)=\exp(H\tau)A\exp(-H\tau). \tag{6}$$

T is the ordering operator and $1/\beta$ is the product of Boltzmann constant and the temperature. It is straightforward to obtain the equation of motion by differentiating D twice,[5]

$$\begin{aligned}&\partial^2D_{QQ'}(\tau-\tau')/\partial\tau^2\\ &\quad=-2\hbar\omega_Q\delta(\tau-\tau')\delta_{Q,Q'}+(\hbar\omega_Q)^2D_{QQ'}(\tau-\tau')\\ &\qquad+\hbar\omega_Q\langle T[\tilde{H}_1(\tau),\tilde{B}_Q(\tau)]\tilde{A}_{Q'}^{\dagger}(\tau')\rangle,\end{aligned} \tag{7}$$

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[1] See the review articles by R. A. Cowley, Advan. Phys. **12**, 421 (1963); and A. A. Maradudin (to be published).

[2] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

[3] A. A. Maradudin and A. E. Fein, Phys. Rev. **128**, 2589 (1962).

[4] L. van Hove, N. M. Hugenholtz and L. P. Howland, *Quantum Theory of Many-Particle Systems* (W. A. Benjamin, Inc., New York, 1961).

[5] A. A. Abriskosov, L. P. Gorkov and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963), Chap. 3.

with boundary conditions

$$D(\tau-\tau')=D(\tau-\tau'+\beta), \quad \tau\leq\tau'$$

and

$$\partial D(\tau-\tau')/\partial\tau=\partial D(\tau-\tau'+\beta)/\partial\tau, \quad \tau\leq\tau'. \quad (8)$$

The proper self-energy part M is defined by

$$\sum_{Q''}\int_0^\beta d\tau'' M_{QQ''}(\tau-\tau'')D_{Q''Q'}(\tau''-\tau') = -\tfrac{1}{2}\langle T[\tilde{H}_1(\tau),\tilde{B}_Q(\tau)]\tilde{A}_{Q'}{}^\dagger(\tau')\rangle. \quad (9)$$

Hence, we have the Dyson equation in term of the Green's function in the harmonic crystal:

$$D_{QQ'}{}^{(0)}(\tau-\tau')=\langle T\tilde{A}_Q(\tau)\tilde{A}_{Q'}(\tau')\rangle_0, \quad (10)$$

the subscript denoting averaging over the canonical ensemble of the harmonic system H_0. Taking the Fourier components, we get

$$D_{QQ'}(i\omega_n)=D_{QQ'}{}^{(0)}(i\omega_n) + \sum_{Q_1Q_2} D_{QQ_1}{}^{(0)}(i\omega_n)M_{Q_1Q_2}(i\omega_n)D_{Q_2Q'}(i\omega_n) \quad (11)$$

where

$$D_{QQ'}(i\omega_n)=\beta^{-1}\int_0^\beta d\tau\,\exp(i\hbar\omega_n\tau)D_{QQ'}(\tau), \quad (12)$$

$$M_{QQ'}(i\omega_n)=\beta\int_0^\beta d\tau\,\exp(i\hbar\omega_n\tau)M_{QQ'}(\tau), \quad (13)$$

and

$$\omega_n=2n\pi/\hbar\beta, \quad n \text{ integer}. \quad (14)$$

The term "proper self-energy part" is adopted merely because of the analogy between (11) and the usual Dyson equation. It is somewhat misleading because, strictly speaking, it is not the proper self-energy of the phonon in the anharmonic field, which, in fact, cannot be defined.

For the perturbation expansion starting from H_0, we need to work in the interaction representation

$$\hat{A}(\tau)=\exp(H_0\tau)A\,\exp(-H_0\tau), \quad (15)$$

and use the development operator

$$\mathcal{S}(\beta)=T\exp\left\{-\int_0^\beta \hat{H}_1(\tau)d\tau\right\}. \quad (16)$$

The free energy is given by

$$F=F_0-\beta^{-1}\ln\langle\mathcal{S}(\beta)\rangle_0. \quad (17)$$

F_0 is the free energy in the harmonic approximation and F depends on λ through $\mathcal{S}$.

Since

$$\frac{\partial\mathcal{S}}{\partial\lambda}=-\frac{1}{2\lambda}\sum_Q T\left\{\int_0^\beta d\tau[\hat{H}_1(\tau),\hat{B}_Q(\tau)]\hat{A}_Q{}^\dagger(\tau)\mathcal{S}(\beta)\right\}, \quad (18)$$

we have

$$\frac{\partial F}{\partial\lambda}=\frac{1}{2\lambda\beta}\sum_Q\left\langle T\int_0^\beta d\tau[\hat{H}_1(\tau),\hat{B}_Q(\tau)]\hat{A}_Q{}^\dagger(\tau)\mathcal{S}(\beta)\right\rangle_0\Big/ \langle\mathcal{S}(\beta)\rangle_0. \quad (19)$$

The expression inside the summation sign is just the perturbation expression[5] for

$$\int_0^\beta d\tau \lim_{\tau'\to\tau-0}\langle T[\tilde{H}_1(\tau),\tilde{B}_Q(\tau)]\tilde{A}_Q{}^\dagger(\tau')\rangle.$$

Hence, by the definition of the proper self-energy part [Eq. (9)], we have

$$\frac{\partial F}{\partial\lambda}=-\frac{1}{\lambda\beta}\int_0^\beta d\tau\int_0^\beta d\tau'\sum_{QQ'}M_{QQ'}(\tau-\tau')D_{Q'Q}(\tau'-\tau). \quad (20)$$

Integrating over the coupling constant, we get

$$F=F_0-\beta^{-1}\int_0^1\frac{d\lambda}{\lambda}\sum_{QQ'n}M_{QQ'}(i\omega_n)D_{Q'Q}(i\omega_n), \quad (21)$$

where M and D depend on λ. This is analogous to the formula for interacting fermions.[2] A similar result was obtained by Marinchuck and Moskalenko[6] including only cubic and quartic anharmonic terms. They introduced a coupling constant which multiplies the whole anharmonic perturbation and hence there appeared factors $1/n$, which are automatically included in our formalism.

3. THE LUTTINGER-WARD FORMULA FOR THE FREE ENERGY

The derivation of the Luttinger-Ward expression for the free energy of the system of interacting phonons follows closely that in Ref. 2 for the fermions interacting through two-body potentials. The only difference is in the counting of Feynman diagrams since the phonon interaction has a very different structure.

We start with the examination of the perturbation series for the phonon Green's function, Eq. (5). The rules for constructing the Feynman diagrams and establishing the contribution of a single term corresponding to a diagram in terms of the harmonic Green's function, Eq. (10), are given in Ref. 3. We shall consider only the counting procedure for a diagram to determine the numerical factor to the contribution of the diagram. Take an unlabeled diagram with ν vertices.

[6] A. E. Marinchuk and V. A. Moskalenko, Fiz. Tver. Tela **5**, 575 (1963) [English transl.: Soviet Phys.—Solid State **5**, 418 (1963)].

All the terms which this diagram represents come from

$$\frac{(-1)^\nu}{\nu!}\left\langle T\hat{A}_Q(\tau)\hat{A}_{Q'}{}^\dagger(\tau')\left\{\int_0^\beta \hat{H}_1(\tau'')d\tau''\right\}^\nu\right\rangle_0. \quad (22)$$

The numerical factor is then, apart from $(-\beta)^\nu$, $1/\nu!$ times the number of different terms which this diagram represents. Suppose there are r different kinds of vertices. (joining different numbers of phonon lines), the ith kind having m_i in number such that

$$\sum_{i=1}^{r} m_i=\nu. \quad (23)$$

There are

$$\nu!/\prod_{i=1}^{r}(m_i)!$$

ways of picking out such a combination of vertices from (22). In each combination there are

$$\prod_{i=1}^{r}(m_i)!$$

different arrangements of vertices of the same kinds, which correspond to distinct terms in the contraction of Eq. (22) but to the same diagram topologically. To each arrangement of ν vertices, there are still a number of ways of contracting equivalent operators which belong to the same vertex, $V^{(n)}(Q_1\cdots Q_n)A_{Q_1}\cdots A_{Q_n}$. This is precisely the number of ways of labeling the momenta carried by the phonon lines in the diagram. In conclusion, the number of different terms corresponding to the same diagram is $\nu!$ times the number of ways of labeling momenta in the diagram, and the numerical factor we have sought for is just the number of ways of labeling the momenta.

It is easy to see that the proper self-energy part defined by Eq. (9) is given by all the diagrams for the Green's function (with the two end lines removed) which cannot be separated into two parts by cutting a single propagator. Now we can perform partial summation and see that M, the proper self-energy part, is given by the sum of all skeleton diagrams, i.e., those with no self-energy insertions—with each line, however, now representing the anharmonic Green's function $D(\tau)$.

We are now in a position to investigate the perturbation expansion for the free energy, given by[5]

$$F=F_0-\beta^{-1}\langle S(\beta)-1\rangle_{0\text{ connected}}. \quad (24)$$

The subscript "connected" means that only connected vacuum-fluctuation diagrams are included. Consider a diagram with m phonon lines $[D^{(0)}(\tau)]$. This represents terms of order λ^{2m}. We can count the number of terms which contribute to the same unlabeled diagram by cutting each line and counting the contributions to the resulting proper or improper self-energy diagram. There are m ways of cutting the free-energy diagram and for each cut there are two distinct self-energy terms. If we count all possible (proper or improper) self-energy diagrams which can be joined up by a phonon line to give the free-energy diagram, we have counted each contribution to the free energy $2m$ times over. This factor $1/2m$ is guaranteed by the coupling-constant integration as in Eq. (21). The integrand in the coupling-constant integral obtained in this way by summing over all diagrams is $M_iD^{(0)}$ where M_i is the improper self-energy part. Since $M_iD^{(0)}\equiv MD$, we recover Eq. (21) by diagrammatic considerations. We shall illustrate the counting by an example in the Appendix.

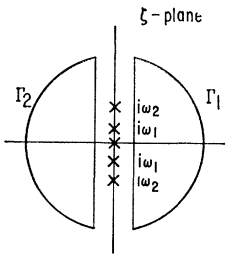

FIG. 1. Semicircular contours Γ_1 and Γ_2 with radii tending to infinity.

Let Y' be $-1/\beta$ times the sum of all connected skeleton free-energy diagrams. Each diagram is evaluated as before except that a line now represents the anharmonic Green's function $D(i\omega_n)$. It is well known that unlike the case for the proper self-energy part, Y' does not give the free energy. We shall show that Y gives the free energy, where

$$Y=F_0+(2\beta)^{-1}\sum_n \mathrm{Tr}[\ln\{1-\mathbf{D}^{(0)}(i\omega_n)\cdot\mathbf{M}(i\omega_n)\}+\mathbf{M}(i\omega_n)\cdot\mathbf{D}(i\omega_n)]+Y'. \quad (25)$$

For convenience, we sometimes represent $M_{QQ'}(i\omega_n)$ by the matrix $\mathbf{M}(i\omega_n)$. Tr denotes the trace.

Consider differentiation of Eq. (25) with respect to an element $M_{Q_1Q_2}(i\omega_{n_1})$. Take Y' first. A connected skeleton free-energy diagram (F diagram) with m phonon lines may be formed by closing one or more proper self-energy diagrams (M diagrams) with a line $D(i\omega_n)$. If we count all possible M diagrams, we know the contribution is $2m$ times that for the F diagram. Take any one of the M diagrams and close it with D. If this M diagram can be obtained from the F diagram by cutting any one of j equivalent lines, then the contribution of this M diagram closed by D is (i) j times that of the F diagram if the transpose of the M diagram is distinct and (ii) $2j$ times if the transpose is the same as the original M diagram. Hence cutting any of the j lines of the F diagram gives us half the contribution of the sum of the M diagram and its transpose or half the contribution of the M diagram if the transpose is the same. To differentiate Y' with respect to $M_{Q_1Q_2}(i\omega_n)$, we differentiate each phonon line in an F diagram and by the above reasoning we get half of the M diagrams closed by the derivative of D with respect to $M_{Q_1Q_2}(i\omega_{n_1})$, i.e.,

$$\frac{\partial Y'}{\partial M_{Q_1Q_2}(i\omega_{n_1})}=-(2\beta)^{-1}\sum_n \mathrm{Tr}\mathbf{M}(i\omega_n)\cdot\frac{\partial\mathbf{D}(i\omega_n)}{\partial M_{Q_1Q_2}(i\omega_n)}. \quad (26)$$

Now it is not difficult to show that

$$\partial Y/\partial M_{Q_1Q_2}(i\omega_{n_1})=0. \tag{27}$$

By the virtue of this stationary property, for $\partial Y/\partial\lambda$ we need only differentiate the explicit factors of λ in Y'. For an F diagram with m lines, there is a factor λ^{2m}. From similar reasonings as above,

$$\partial Y/\partial\lambda=-(\lambda\beta)^{-1}\sum_n \mathrm{Tr}\mathbf{M}(i\omega_n)\cdot\mathbf{D}(i\omega_n). \tag{28}$$

By Eq. (20), we have

$$F=Y. \tag{29}$$

It is possible to replace the summation over n in Eq. (25) by an appropriate integral over contours Γ_1 and Γ_2 shown in Fig. 1, where the semicircular arcs are taken to infinity and the straight-line portions near the imaginary axis:

$$F=(2\beta)^{-1}\Big[\frac{1}{2\pi i}\int_{\Gamma_1}d\zeta\,\ln[\exp(\hbar\beta\zeta)-1]\,\mathrm{Tr}\Big\{\frac{\partial\mathbf{D}^{-1}(\zeta)}{\partial\zeta}\cdot\mathbf{D}(\zeta)\Big\}+\frac{1}{2\pi i}\int_{\Gamma_2}d\zeta\,\ln[1-\exp(\hbar\beta\zeta)]\,\mathrm{Tr}\Big\{\frac{\partial\mathbf{D}^{-1}(\zeta)}{\partial\zeta}\cdot\mathbf{D}(\zeta)\Big\}$$
$$-\frac{1}{2\pi i}\int_{\Gamma_1+\Gamma_2}d\zeta\frac{\hbar\beta}{1-\exp(-\hbar\beta\zeta)}\,\mathrm{Tr}\{\mathbf{M}(\zeta)\cdot\mathbf{D}(\zeta)\}\Big]+Y'. \tag{30}$$

Note that this expression involves only the full Green's function D and nowhere involves the harmonic approximation $D^{(0)}$.

4. THE INTERNAL ENERGY AND THE ENTROPY

As a simple application of Eq. (25), we shall derive an expression for the internal energy and hence the entropy. The internal energy is given by

$$E=\partial(\beta F)/\partial\beta. \tag{31}$$

By the stationary property

$$\partial F/\partial M=0, \tag{32}$$

we can neglect the dependence of M on β. An F diagram in $\beta Y'$ with ν vertices has a factor β^ν. Hence

$$\partial(\beta Y')/\partial\beta=-\tfrac{1}{2}\sum_n \mathrm{Tr}\{\mathbf{M}(i\omega_n)\cdot\partial\mathbf{D}(i\omega_n)/\partial\beta\}+E', \tag{33}$$

where we keep in mind that in $\partial\mathbf{D}/\partial\beta$, $\mathbf{M}$ is kept constant, and E' is $-1/\beta$ times the sum of all skeleton F diagrams for which the contributions are evaluated as in Y' except that for a diagram with ν vertices there is now a factor ν. The internal energy is

$$E=E_0-\tfrac{1}{2}\sum_n \mathrm{Tr}[\{\mathbf{D}^{(0)}(i\omega_n)\}^{-1}\cdot\{\partial\mathbf{D}^{(0)}(i\omega_n)/\partial\beta\}\cdot\mathbf{M}(i\omega_n)\cdot\mathbf{D}(i\omega_n)]+E'. \tag{34}$$

It is simple to show in terms of an associated Green's function,

$$C_{QQ'}(\tau-\tau')=\langle T\tilde{B}_Q(\tau)\tilde{A}_{Q'}{}^\dagger(\tau')\rangle, \tag{35}$$

that we have

$$\beta[\partial D_{QQ'}{}^{(0)}(i\omega_n)/\partial\beta]=\{i\hbar\omega_n\beta C_{QQ'}{}^{(0)}(i\omega_n)-1\}D_{QQ'}{}^{(0)}(i\omega_n). \tag{36}$$

Whence,

$$E=E_0+(2\beta)^{-1}\sum_n \mathrm{Tr}[\{-i\hbar\omega_n\beta\mathbf{C}^{(0)}(i\omega_n)+\mathbf{1}\}\cdot\mathbf{M}(i\omega_n)\cdot\mathbf{D}(i\omega_n)]+E'. \tag{37}$$

Or, in terms of contour integrals,

$$E=(2\beta)^{-1}\Big[\frac{1}{2\pi i}\int_{\Gamma_1+\Gamma_2}d\zeta\frac{\hbar\beta}{1-\exp(-\hbar\beta\zeta)}\,\mathrm{Tr}\{\hbar\beta\zeta\mathbf{C}(\zeta)-\mathbf{M}(\zeta)\cdot\mathbf{D}(\zeta)\}\Big]+E'. \tag{38}$$

Finally, the entropy is

$$S=k\beta(E-F)$$
$$=S_0-(k/2\beta)\sum_n \mathrm{Tr}[i\hbar\omega_n\beta\mathbf{C}^{(0)}(i\omega_n)\cdot\mathbf{M}(i\omega_n)\cdot\mathbf{D}(i\omega_n)+\ln\{1-\mathbf{D}^{(0)}(i\omega_n)\cdot\mathbf{M}(i\omega_n)\}]+k\beta(E'-Y'), \tag{39}$$

$$=\frac{k}{2}\Big[\frac{1}{2\pi i}\int_{\Gamma_1+\Gamma_2}d\zeta\frac{(\hbar\beta)^2\zeta}{1-\exp(-\hbar\beta\zeta)}\,\mathrm{Tr}\mathbf{C}(\zeta)-\frac{1}{2\pi i}\int_{\Gamma_1}d\tau\,\ln[\exp(\hbar\beta\zeta)-1]\,\mathrm{Tr}\Big\{\frac{\partial\mathbf{D}^{-1}}{\partial\zeta}\cdot\mathbf{D}(\zeta)\Big\}$$
$$-\frac{1}{2\pi i}\int_{\Gamma_2}d\zeta\,\ln[1-\exp(\hbar\beta\zeta)]\,\mathrm{Tr}\Big\{\frac{\partial\mathbf{D}^{-1}}{\partial\zeta}\cdot\mathbf{D}(\zeta)\Big\}\Big]+\beta k(E'-Y'). \tag{40}$$

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APPENDIX

Consider a free-energy diagram [Fig. 2(a)] which represents some terms from

$$-\beta^{-1}\frac{(-1)^3}{3!}\left\langle T\left\{\int_0^\beta H_1(\tau)d\tau\right\}^3\right\rangle_0,$$

with two $V^{(3)}$ vertices and one $V^{(4)}$ vertex. Let us first get the numerical factor directly. In the cube of H_1, there are 3 terms of the form $V^{(4)}V^{(3)}V^{(3)}$. Now for vertex X in Fig. 2(a), there are 3 ways of choosing an operator to contract with one from Z and the remaining two operators from X can contract with two from Y in 2 ways. For vertex Y, there are $4!/(2!\times 2!)$ ways of picking two operators to contract with X and leaving two to contract with Z. The vertex Z is counted the same way as X. Hence the numerical factor is

$$\frac{1}{3!}\times 3\times 3\times 2\times\frac{4!}{2!\times 2!}\times 2\times 3=108. \tag{A1}$$

To follow the method of counting in Sec. 3, we first note that the possible M diagrams which can be closed to form Fig. 2(a) are given in Figs. 2(b), 2(c), and 2(d). The numerical factor for Fig. 2(b) is just the number of ways of labeling momenta in the figure, which is, following the same reason as in the preceding paragraph

$$3\times 2\times\frac{4!}{2!\times 2!}\times 2\times 3=216. \tag{A2}$$

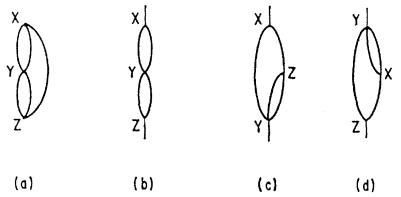

FIG. 2. Free-energy and self-energy diagrams.

Now consider (c). For vertex X, there are 3 ways of choosing an A operator to be the free one, and then 2 ways of choosing one for the contraction XZ, leaving one for XY. For vertex Z, there are 3 ways of choosing an A for XZ, leaving two for YZ which can be formed in 2 ways. In vertex Y, the 4 operators are separated in $4!/(1!1!2!)$ ways for YZ, XY and the free end. The numerical factor for (c) is

$$3\times 2\times 3\times 2\times\frac{4!}{1!\times 1!\times 2!}=432. \tag{A3}$$

The numerical factor for Fig. 2(d) is the same as for Fig. 2(c).

When we count all the self-energy diagrams (b), (c), and (d), we have counted the contributions to the F diagram (a) ten times over. The sum of all self-energy terms divided by 10 does give the correct factor (A1).

Furthermore, note that there is only one line in (a) which we can cut to give (b). (A2) verifies the assertion that since (b) is the same as its transpose, the contribution of this M diagram closed by a line gives twice that to the F diagram. The transpose of (c) is (d) and either can be formed from (a) by cutting any one of four lines. Thus, the M diagram (c) when closed by a line gives four times the contribution to the F diagram. Equation (26) can be verified for these diagrams.