COMMENTS AND ADDENDA

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Calculation of Watson-Like Sums (Integrals)*

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We find that the semianalytic method recently proposed by Flax and Raich for the evaluation of Watson-like integrals suffers from shortcomings in its scope of application and also in accuracy. In its place we propose simple expansions for both the high and low temperatures which cover much of the range of interest, and we provide evidence that a method involving direct numerical integration leads not only to good results for all temperatures but accommodates more general integrands than are practical with any of the expansions. The results are illustrated by the bcc case of the generalized Watson integrals for which Flax and Raich's work is simplest.

In a recent series of papers, Flax and Raich[1] have put forward, and used in several applications,[1,2] a new semianalytic method for evaluating the Watson-like integrals which arise in the theory of cooperative phenomena in lattice systems, particularly in the theory of magnetism. Our investigations into the evaluation of such integrals give reason to doubt the usefulness of their method, which is limited in application and approximates poorly the low-temperature behavior of the generalized Watson integrals considered in their first paper.

The form of generalized Watson integral that they consider is

$$\phi(\alpha,\eta)=\frac{1}{N}\sum_{\vec{k}}(e^{\alpha\omega_{\vec{k}}}-1)^{-1}\,, \tag{1}$$

where the integrand has the form of the Planck (or Bose-Einstein) distribution function (α may be inversely proportional to temperature) and the dispersion function $\omega_{\vec{k}}$ is given by

$$\omega_{\vec{k}}=1-\eta\gamma_{\vec{k}}/\gamma_0,\quad 0<\eta<1\,. \tag{2}$$

In (2) the structure factor $\gamma_{\vec{k}}$ is defined by

$$\gamma_{\vec{k}}=\sum_{\vec{\delta}}^{nn} e^{i\vec{k}\cdot\vec{\delta}}\,, \tag{3}$$

where the sum is over all nearest-neighbor vectors.

In (1) the sum is taken over the N distinct $\vec{k}$ vectors of a lattice with N primitive cells. This sum can be replaced by an integral and the region of integration is often taken as the first Brillouin zone of the reciprocal lattice; i.e., we are dealing with Brillouin-zone sums or integrals.

The results of Flax and Raich's procedure are simplest in the bcc case of (1), giving[3]

$$\phi_{\rm bcc}(\alpha,\eta)=\frac{W(\eta)}{\alpha}-\frac{1}{2}+\frac{1}{\alpha}\left[\frac{\alpha}{2}\coth\left(\frac{\alpha}{2}\right)-1-\frac{1}{8}\eta^2+\frac{1}{8}\left(\frac{\alpha}{2}\right)^3\eta^2\,\mathrm{csch}^2\left(\frac{\alpha}{2}\right)\coth\left(\frac{\alpha}{2}\right)\cdots\right]\,, \tag{4}$$

where $W(\eta)$ is the extended Watson integral defined by

$$W(\eta)=\frac{1}{N}\sum_{\vec{k}}(\omega_{\vec{k}})^{-1}\,. \tag{5}$$

In our comparisons with other methods we shall consider the most demanding case which occurs for $\eta=1$ in (2), for then $\omega_{\vec{k}}\propto k^{-2}$ for small $\vec{k}$, causing a strong singularity in the integrands of (1) and (5). Table I gives a tabulation of Flax and Raich's formula (4) for a wide range of α, 10^2–10^{-2}. To give a feeling for the physical significance of the magnitude of α in the context of magnetism, we note that in spin-wave theory[4] (for the bcc structure and spin $\frac{1}{2}$) the critical temperature corre-

TABLE I. Comparison of the results obtained for $\phi(\alpha, 1)$ on a bcc lattice with a nearest-neighbor dispersion function by the four methods discussed in the text. Four figures are given in column (a) while up to four figures are listed in columns (b) and (c), depending on the accuracy, and the results of column (d) are estimated to be good to 1% or better.

α	(a) Flax and Raich [Eq. (4)]	(b) High-temperature expansion [Eq. (7)]	(c) Low-temperature expansion [Eq. (8)]	(d) Numerical integration
100	0.2682×10^{-2}	···	0.6671×10^{-3}	0.669×10^{-3}
50	0.5364×10^{-2}	···	0.190×10^{-2}	0.190×10^{-2}
10	0.2715×10^{-1}	···	0.23×10^{-1}	0.225×10^{-1}
5	0.7124×10^{-1}	···	···	0.714×10^{-1}
1	0.9747	0.9729	···	0.975
0.5	0.2328×10^{1}	0.2328×10^{1}	···	0.233×10^{1}
0.1	0.1344×10^{2}	0.1344×10^{2}	···	0.134×10^{2}
0.05	0.2737×10^{2}	0.2737×10^{2}	···	0.273×10^{2}
0.01	0.1388×10^{3}	0.1388×10^{3}	···	0.139×10^{3}

sponds to $\alpha\sim4$, whereas in the random-phase approximation (RPA)[1] it occurs at $\alpha=0$; in both cases the large α limit gives the low-temperature region.

For high temperatures (small α), we can find a simple expansion in powers of α by first expanding the integrand of (1) for small $\alpha\omega_{\vec{k}}$ and then integrating exactly over the odd powers of $\omega_{\vec{k}}$ to give

$$\phi(\alpha,\eta)=\frac{W(\eta)}{\alpha}-\frac{1}{2}+\frac{\alpha}{12}-\frac{\alpha^3}{360}\left(1+\frac{3\eta^2}{8}\right)+\frac{\alpha^5}{15120}\times\left(1+\frac{5}{4}\eta^2+\frac{135}{512}\eta^4\right)-\frac{\alpha^5}{604800}\times\left(1+\frac{21}{8}\eta^2+\frac{945}{512}\eta^4+\frac{875}{4096}\eta^6\right)\cdots,\quad \alpha<\pi\ . \tag{6}$$

Table I shows good agreement between the results obtained from (6) and those from (4).

The low-temperature expansion (α large) is well known as it occurs in the low-temperature magnetization of noninteracting spin waves in ferromagnets. Taken from Dyson's work[5] and translated to our present notation, we have for $\eta=1$ that

$$\phi(\alpha,1)=a_0\theta^{3/2}+a_1\theta^{5/2}+a_2\theta^{7/2}+O(\theta^{9/2})\cdots\ , \tag{7}$$

where $\theta=3/(2\pi\nu\alpha)$ and ν, a_0, a_1, a_2 are given by Dyson for the three cubic lattices—more terms could be found if required. (For $\eta<1$, one requires the inclusion of an external magnetic field.) Equation (7) contains the first few terms of an asymptotic expansion and consequently has to be treated with some care; however, experience with spin-wave theory suggests that (7) should be reliable for temperatures $\lesssim\frac{1}{3}T_c$ or $\alpha\gtrsim12$, so that the poor agreement with Flax and Raich in this region requires a further check.

This is conveniently provided by direct numerical integration of (1) using procedures developed recently by Loly and Huett,[6] which may be readily implemented on a computer for all the cubic lattices. An accuracy rather better than 1% was obtained with a sample of 10^4 points in the Brillouin zone distributed with a strong increase in density toward the zone center to take care of the singularity in the integrand. As shown in Table I the results obtained in this way give good agreement with the results of (6) and (7) in the high- and low-temperature regimes and fill in the gap where they fail. If necessary the accuracy could be improved by using more sampling points.

It is clear from Table I that Flax and Raich's formula (4) becomes increasingly inadequate as α is increased beyond 5, so that their claim that (4) is valid for all values of α is unfounded. Though agreement may be improved by calculating more terms which contribute to (4) it appears that there is a weakness at low temperatures which renders null their claim to four-place accuracy; e.g., for $\alpha=100$ they are out by a factor of 4. However all of the series methods require a great deal of algebraic work which has to be done for each new function attempted and becomes impractical for dealing with any but the simplest functions, e.g., nearest-neighbor dispersion laws such as (2). On the other hand, the great advantage of our numerical integration scheme is that once the procedures are established, complicated functions arising in problems with many-neighbor interactions are handled with no further difficulty.

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[1]L. R. Flax and J. C. Raich, Phys. Rev. 185, 797 (1969).

[2]L. R. Flax and J. C. Raich, Phys. Rev. B 1, 186 (1970); 2, 1338 (1970).

[3]Misprints in Ref. 1, Eq. (16), have been corrected [L. R. Flax (private communication)].
[4]P. D. Loly, J. Phys. C 4, 1365 (1971).
[5]F. J. Dyson, Phys. Rev. 102, 1230 (1956).
[6]P. D. Loly and B. J. S. Huett (unpublished).

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Surface-Plasmon Excitation by Electron Tunneling*†

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The role of various parameters in our theory of inelastic-electron tunneling associated with the excitation of surface plasmons is clarified in order to refute Duke's criticism. It is shown here that our theory involves only one adjustable parameter, which can be determined independently from the random-phase-approximation analysis of surface plasmons. Hence there are no adjustable parameters in fitting theory to experiment. We have fortified the claim of agreement between our theory and experiment by a calculation of the background, and a detailed comparison with raw experimental data. Predictions from both the inelastic surface-plasmon excitation model and the electron–bulk-plasmon interaction model are compared. The surface-plasmon excitation model provides a far superior fit to the experimental data.

Recently carrier-concentration-dependent broad structures in the d^2I/dV^2 characteristics of n-type GaAs–metal tunnel junctions have been observed independently by Tsui[1] and by Duke *et al.*[2] These observations have been interpreted as being caused by the mechanism of inelastic tunneling associated with the excitation of surface plasmons (SP) in the GaAs electron by Tsui.[1] Subsequently, Ngai *et al.*[3] have presented a theory of inelastic-electron surface-plasmon interactions in metal-semiconductor junctions. Their calculated inelastic SP emission structure in d^2I/dV^2 agrees with experiments[1,2] both in magnitude and line shape. A different point of view was taken by Duke *et al.*,[2] who identified such structures with self-energy effects in the GaAs electrode resulting from electron–bulk-plasmon interaction. In a recent paper,[4] Duke has criticized the reliability of the bulk-plasmon (BP) energy as arrived at by Tsui,[1] using values of the electron concentration n obtained from sample suppliers. Such doubts have been removed when Tsui and Barker[5] subsequently made infrared-reflectivity measurements to determine directly the BP energies of the GaAs samples. Their results therefore fortified the interpretation of excitation of surface plasmons in the GaAs electrode by tunneling electrodes. Furthermore, Duke,[4] though acknowledging that the line shapes as calculated by Ngai *et al.*[3] look much better than those calculated by Duke *et al.*,[2] stated that "Ngai *et al.*[3] permitted themselves the luxuries of five adjustable parameters ($\gamma, \alpha, k_{c2}, d$, and ϕ_{eff}) and an arbitrary background subtraction procedure...." One of the purposes of this communication is to refute this statement by clarifying the roles of the parameters and by showing that the theory involves essentially *one* adjustable parameter for determination of the line shape. Moreover, its value as determined by comparison with experiment[1] agrees with the prediction of the random-phase-approximation (RPA) analysis of surface plasmons.[6]

In our treatment of the inelastic current associated with SP emission, we used an average-square-barrier model[7] to represent the tunnel junction at biases in a relatively narrow energy range about the SP energy. ϕ_{eff} and d are *fixed* parameters that enter into this model description of one-electron tunneling. Their chosen values ($\phi_{eff} \approx \frac{1}{2}$ eV, $d \approx 100$ Å) are inferred from independent measurements. γ, α, and k_{c2} are parameters characteristic of SP. Plasmons of small wavelength can decay through energetically possible electron-hole-pair excitations and the result is Landau damping. For SP, Landau damping (LD) plays a vital role. The reason is that an SP oscillation of surface wave vector $\vec{Q}$ cannot be a plane wave along the direction normal to the surface and consequently the eigenfunctions along this direction contain components of very small wavelength, which are responsible for increased damping. The microscopic theory of SP[6] indicates that LD introduces a finite imaginary part to the SP frequency which is linear in Q. Introducing a characteristic wave number Q_c defined by the equation $Q_c = \omega_s/v_F$, where ω_s is the plasma energy and v_F is the Fermi velocity, we expressed[3] this result as