

## Green's Functions of the Face-Centered-Cubic Heisenberg Ferromagnet with Second-Neighbor Interactions\*

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Green's functions for a fcc Heisenberg ferromagnet with both first- and second-neighbor interactions are given in terms of accurate but simple polynomial approximants. These polynomial approximations greatly simplify the application of sophisticated theory to real physical systems of interest. Our procedure for the calculation of the lattice Green's functions is described. We have computed 24 Green's functions (corresponding to 24 values of the lattice vector  $\vec{R}$ ), each for a range of values of the first- and second-neighbor exchange constants ( $J_1 > 0$ ,  $0 > J_2 > -J_1$ ), and each as a function of energy within the spin-wave band. This enormous quantity of data is condensed by fitting the functions to polynomials in the energy variable, and we tabulate the coefficients of these polynomials. The polynomials not only provide compact representations of the Green's functions (without which Green's-functions theories are useless for applications), but they provide representations which permit Green's-functions theories often to be evaluated analytically. As the polynomials have been formulated to have the rigorously correct analytic behavior at band edges and at Van Hove singularities, results obtained by use of our polynomial approximants are similarly rigorous at the crucial regions of the spectrum, and are highly accurate ( $\sim 0.2\%$ ) everywhere.

### I. INTRODUCTION

An extremely useful tool in the study of the propagation of particles or excitations in crystals is the lattice Green's function<sup>1</sup>

$$G_{\vec{R}}(E) \equiv \frac{1}{N} \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{R}}}{E - E(\vec{k}) + i\delta}. \quad (1)$$

These functions are also prominent in the theory of thermodynamic properties<sup>2</sup> and in the theory of impurities.<sup>1,3,4</sup> Unfortunately, the explicit applications of all of these theories are severely hampered because extensive numerical evaluations of the Green's function have been confined mainly to the simple cubic lattices and to systems with nearest-neighbor interactions only.<sup>5-8</sup>

In this paper we describe a general procedure for accurate calculation of the lattice Green's function. We apply the technique to a fcc lattice with a Heisenberg exchange interaction between both first and second neighbors. We have carried out extensive numerical calculations of the Green's function for 24 lattice vectors  $\vec{R}$ , over ranges of values of the exchange constants  $J_1$  and  $J_2$  and as a function of the energy  $E$  inside the spin-wave band.<sup>9</sup> Rather than tabulate this immense collection of data, we have fit our calculated results to simple polynomials in the energy and we tabulate the coefficients of these polynomials. They provide not only a convenient and compact representation of the numerical data, but we believe that the polynomial approximations will be very useful in facilitating explicit theories involving Green's functions.

The polynomial approximations to the Green's functions introduce an error of not more than 0.2%,

whereas the underlying numerical calculations of the Green's function are accurate to better than six significant figures.

We also give rather detailed analytic descriptions of the behavior of the Green's functions at Van Hove singularities and at the band edges.

In our specific calculations we have restricted our attention to positive values of the nearest-neighbor exchange constant ( $J_1 > 0$ ) and to negative values of the next-nearest-neighbor exchange constant ( $J_2 < 0$ ), such that the ratio  $J_2/J_1$  is between 0 and -1:

$$J_1 > 0, \quad -1 < J_2/J_1 < 0. \quad (2)$$

Through this range of values the system is ferromagnetically ordered.<sup>10</sup>

The excitation energy  $E(\vec{k})$ , which appears in the denominator of the Green's function, is given by

$$E(\vec{k}) = 8SJ_1[3 - \cos(\frac{1}{2}k_1a)\cos(\frac{1}{2}k_2a) - \cos(\frac{1}{2}k_2a)\cos(\frac{1}{2}k_3a) - \cos(\frac{1}{2}k_3a)\cos(\frac{1}{2}k_1a)] + 4SJ_2(3 - \cos k_1a - \cos k_2a - \cos k_3a). \quad (3)$$

The quantities  $J_1$  and  $J_2$  are simple constants in standard spin-wave theory, but in other theories<sup>4,11,12</sup>  $J_1$  and  $J_2$  are considered as self-consistent functions.

We define dimensionless quantities. The ratio of the exchange constants will be defined as

$$\gamma \equiv J_2/J_1, \quad (4)$$

which will be limited to the range -1 to 0 [Eq. (2)].

Dimensionless vectors in real space are mea-

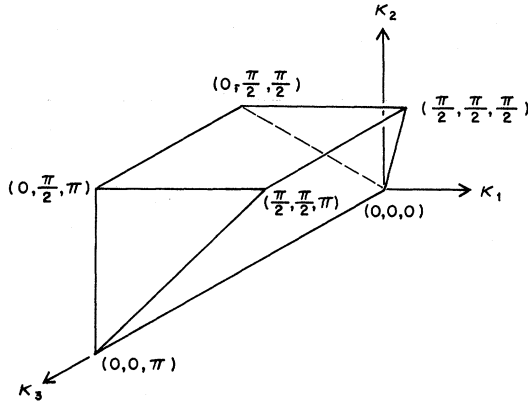


FIG. 1. Volume of integration. This region has the volume of  $\frac{1}{48}$  the Brillouin zone (see Ref. 13).

sured in units of half the lattice constant

$$\vec{r} = 2\vec{R}/a, \quad (5)$$

and the corresponding dimensionless vectors in reciprocal space are

$$\vec{k} = \frac{1}{2}\vec{ka}. \quad (6)$$

The natural unit of energy is the maximum excitation energy  $E_m$  which, in the range  $-1 < \gamma < 0$ , is given by

$$E_m = 32SJ_1. \quad (7)$$

Then a convenient dimensionless energy variable is

$$\omega = E/E_m \quad (8)$$

and the dimensionless Green's function is

$$g(\vec{r}, \omega) \equiv E_m G_{\vec{r}a/2}(E_m \omega) \equiv g_R(\vec{r}, \omega) + i g_I(\vec{r}, \omega). \quad (9)$$

Finally, the excitation energies of Eq. (3) become

$$\omega(\vec{k}) = \frac{3}{4}(1 + \gamma) - \frac{1}{4}(\cos k_1 \cos k_2 + \cos k_2 \cos k_3 + \cos k_3 \cos k_1) - \frac{1}{4}\gamma(\cos^2 k_1 + \cos^2 k_2 + \cos^2 k_3). \quad (10)$$

Since the vectors  $\vec{k}$  are quasidense in reciprocal space, the summation which defines the Green's function [Eq. (1)] can be expressed as an integral over the Brillouin zone:

$$g(\vec{r}, \omega) = \frac{1}{4\pi^3} \iiint d^3k \frac{e^{i\vec{k}\cdot\vec{r}}}{\omega - \omega(\vec{k}) + i\delta}. \quad (11)$$

The range of integration can be contracted drastically by invoking the point-group symmetry:

$$g(\vec{r}, \omega) = \frac{12}{\pi^3} \iiint d^3k \frac{f(\vec{r}, \vec{k})}{\omega - \omega(\vec{k}) + i\delta}, \quad (12)$$

where

$$f(\vec{r}, \vec{k}) \equiv \frac{1}{48} \sum_{\phi} e^{i\vec{r}\cdot\phi\vec{k}}. \quad (13)$$

Here  $\phi$  is an element of the point group and the sum is over the 48 elements of the cubic group. The integral in Eq. (12) is over  $\frac{1}{48}$  of the Brillouin zone, or over the alternate volume region suggested by Andersen<sup>13</sup> and shown in Fig. 1. The advantages of the latter volume region will become evident subsequently.

## II. METHOD OF NUMERICAL CALCULATION OF GREEN'S FUNCTION

We first calculate the imaginary part of the Green's function, later to calculate the real part by a dispersion relation.

Taking the imaginary part of Eq. (12) and letting  $\delta \rightarrow 0$ ,

$$g_I(\vec{r}, \omega) = (-12/\pi^2) \iiint d^3k f(\vec{r}, \vec{k}) \delta(\omega - \omega(\vec{k})). \quad (14)$$

The  $\delta$  function defines a surface of constant energy within the volume of integration. Denoting the element of area on this surface by  $dS$ , the integral normal to the surface is eliminated by the  $\delta$  function, giving

$$g_I(\vec{r}, \omega) = (-12/\pi^2) \iint dS f(\vec{r}, \vec{k}) |\nabla_{\vec{k}} \omega(\vec{k})|^{-1}. \quad (15)$$

It is now advantageous to project the surface of integration onto some convenient plane. For example, if the chosen plane is the  $\kappa_1 - \kappa_2$  plane, the surface element  $dS$  projects onto an element  $d\kappa_1 d\kappa_2$  for which

$$d\kappa_1 d\kappa_2 = \frac{|\hat{k}_3 \cdot \nabla_{\vec{k}} \omega(\vec{k})|}{|\nabla_{\vec{k}} \omega(\vec{k})|} dS. \quad (16)$$

Then the integral becomes

$$g_I(\vec{r}, \omega) = (-12/\pi^2) \iint d\kappa_1 d\kappa_2 f(\vec{r}, \vec{k}) |\hat{k}_3 \cdot \nabla_{\vec{k}} \omega(\vec{k})|^{-1}. \quad (17)$$

The area of integration is the projection of the surface of constant energy onto the  $\kappa_1 - \kappa_2$  plane. For any integration point  $(\kappa_1, \kappa_2)$  the function  $f(\vec{r}, \vec{k})$  is to be evaluated on the surface of constant energy (at that point  $\vec{k}$  which projects to the point  $\kappa_1, \kappa_2$ ); similarly with the last factor in Eq. (17).

Returning to the area of integration, the shape of the projected area is considerably simplified by choosing the alternate Brillouin zone of Fig. 1 in place of the more familiar one.

The choice of projection planes over which the integrals are to be performed is subject to one important restriction. Clearly the factor  $|\hat{k}_3 \cdot \nabla_{\vec{k}} \omega(\vec{k})|^{-1}$  diverges if the constant energy surface is anywhere orthogonal to the  $\kappa_1 - \kappa_2$  plane; it is therefore necessary to choose a projection plane which is nowhere orthogonal to the energy surface. Furthermore, since the shape of the constant energy

surface depends upon the energy, it is sometimes necessary to use different projection planes for different energy regions. The natural projection planes are the coordinate planes (such as the  $\kappa_1 - \kappa_2$  plane) or the planes bounding the zone of Fig. 1. Providing the chosen plane satisfies the restriction that it be nowhere orthogonal to the energy surface, there is little to choose between one plane or another.

In our calculations we carried out the integrals by successive one-dimensional Gaussian quadrature. The order of integration is important to ensure that the intermediate integrand is smoothly varying. A net of as few as 16 points (four-point one-dimensional Gaussian quadrature) is sufficient to give the Green's function to within 1%. We used 100 points, giving an accuracy which is considerably beyond 1 ppm.

Because the areas of integration and the denominators of the integrands are the same for all  $\vec{r}$ , many Green's functions can be evaluated simultaneously. We have evaluated the 24 Green's functions which are needed for a solution of the impurity problem in the fcc lattice.

The 24 Green's functions which we have computed are not all independent.<sup>4</sup> Nevertheless, we chose to compute each directly, invoking the relations among them only as a check of the consistency of the calculations.

The dispersion relation which yields the real part of the Green's function is

$$g_{\vec{R}}(\vec{r}, \omega) = (1/\pi) \int_0^1 g_I(\vec{r}, \omega') (\omega' - \omega)^{-1} d\omega'. \quad (18)$$

Before performing this integration numerically it is necessary to remove the singularity analytically when  $\omega$  is between 0 and 1. Therefore, we used the formula

$$g_{\vec{R}}(\vec{r}, \omega) = \frac{1}{\pi} g_I(\vec{r}, \omega) \ln \left( 1 - \frac{1}{\omega} \right)$$

TABLE I. Types of Van Hove singularities for the fcc lattice. The energies  $\omega \equiv E/32S_1$  are given in column 1 as a function of  $\gamma \equiv J_2/J_1$ . The same information is given in column 2 in terms of the alternate variables  $\omega' \equiv \omega/(1+\gamma)$  and  $\xi \equiv \gamma/(1+\gamma)$ . The type (0, 1, 2, 3) of each singularity is then given in each range of  $\gamma$  (or of  $\xi$ ) in which the singularity exists; dots imply that the singularity does not exist in the relevant range of  $\gamma$ . The types of singularities are defined in Table II. The top of the band is always a type-3 singularity, and in each range of  $\gamma$  the top of the band is determined by that unique Van Hove point which is of type 3.

$\omega$	$\omega' = \frac{\omega}{1+\gamma}$	$-1 < \gamma < 0$ $\xi < 0$	$0 < \gamma < \frac{1}{2}$ $0 < \xi < \frac{1}{3}$	$\frac{1}{2} < \gamma < 1$ $\frac{1}{3} < \xi < \frac{1}{2}$	$\gamma > 1$ $\frac{1}{2} < \gamma < 1$
0	0	0	0	0	0
$\omega_A = \frac{3}{4}(1+\gamma)$	$\omega'_A = \frac{3}{4}$	1	1	3	3
$\omega_B = 1 + \frac{1}{4}\gamma$	$\omega'_B = 1 - \frac{3}{4}\xi$	2	3	1	0
$\omega_C = 1$	$\omega'_C = 1 - \xi$	3	1	1	0
$\omega_D = \frac{1}{2} + \frac{1}{4}\gamma + \frac{1}{4}\gamma^2$	$\omega'_D = \frac{1}{2} - \frac{1}{4}\xi + \frac{1}{4}[\xi^2/(1-\xi)]$	...	...	...	...
$\omega_E = \frac{3}{4} + \frac{1}{2}\gamma - \frac{1}{4}[\gamma/(1+2\gamma)]$	$\omega'_E = \frac{3}{4} - \frac{1}{4}\xi + \frac{1}{4}\xi(1-\xi)/(1+\xi)$	...	2	2	2

$$+ \frac{1}{\pi} \int_0^1 \frac{g_I(\vec{r}, \omega') - g_I(\vec{r}, \omega)}{\omega' - \omega} d\omega'. \quad (19)$$

The integration of Eq. (19) was carried out by six-point Gaussian quadrature, using the polynomial approximations for the imaginary parts of the Green's functions. The accuracy of the polynomial approximations thereby determined the accuracy of the integration, as the Gaussian quadrature had a much higher precision.

The integrand in Eq. (19) is strongly peaked when  $\omega$  is near a Van Hove singularity. The regions of integration therefore must be chosen carefully, according to considerations which we now review.

### III. VAN HOVE SINGULARITIES

Green's functions are nonanalytic at a few particular values of the energy. These singularities were first investigated by Van Hove<sup>14</sup>; a clear and elementary discussion can be found in Weinreich's text.<sup>15</sup>

The integrand of Eq. (15) has a singularity when the gradient of the energy vanishes:

$$\nabla_{\vec{\kappa}} \omega(\vec{\kappa}) = 0. \quad (20)$$

The solutions of this equation, determining the energies of the Van Hove singularities for an fcc lattice with first- and second-neighbor interactions, are given in the first column of Table I.

Van Hove singularities can be classified in four "types"<sup>14,15</sup> according to the functional behavior of the Green's functions. These four types are listed in Table II, and the six Van Hove singularities of  $(-1/\pi)g_I(0, \omega)$  (the density-of-states function) are classified in Table I. It will be noted from Table I that a particular singularity may change type as a function of  $\gamma$ .

Classification of the singularities is based on expansion of the energy  $\omega$  as a function of  $\vec{\kappa}$ , in the

TABLE II. Types of Van Hove singularities (Refs. 13 and 14).

Type of Van Hove singularity [number of negative coefficients in Eq. (21)]	Functional form of density of states ( $-1/\pi$ ) $g_I(0, \omega)$	
	$\omega \lesssim \omega_c$	$\omega \gtrsim \omega_c$
0	$\pm(\omega_c - \omega)$	$(\omega - \omega_c)^{1/2}$
1	$-(\omega_c - \omega)^{1/2}$	$\pm(\omega - \omega_c)$
2	$\pm(\omega_c - \omega)$	$-(\omega - \omega_c)^{1/2}$
3	$(\omega_c - \omega)^{1/2}$	$\pm(\omega - \omega_c)$

vicinity of a root of Eq. (20). Choosing local axes so as to eliminate cross terms, and carrying the expansion to second order,

$$\omega - \omega_c = A(\Delta\kappa_1)^2 + B(\Delta\kappa_2)^2 + C(\Delta\kappa_3)^2. \quad (21)$$

The number of negative coefficients on the right-hand side of this equation determines the functional behavior of the density-of-states function near the critical point. The type of singularity is therefore designated in Table II by the number of negative coefficients in Eq. (21) (from 0 to 3). The functional behavior of  $g_I(0, \omega)$  just below the singularity ( $\omega \lesssim \omega_c$ ) and just above ( $\omega \gtrsim \omega_c$ ) is given in Table II.

Under very special conditions one or more of the coefficients in Eq. (21) may vanish. If one coefficient vanishes the next term in the expansion dominates, and the singularity may be "stronger" than the simple square-root behavior. If two coefficients vanish the density of states becomes infinite; such infinities occur in our model for  $\gamma = -1, 0$ , and  $\frac{1}{2}$ . This effect can be seen in Fig. 2. As  $\gamma \rightarrow 0$  the spectral weight shifts toward the top of the band presaging a divergence in the limit  $\gamma = 0$ . Similarly, the spectral weight is seen to shift to the bottom

of the band as  $\gamma \rightarrow 1$ , again forecasting a divergence for  $\gamma = 1$ .

Another effect requiring special comment is the "suppression" of the square-root singularity at a Van Hove point under certain conditions. This suppression of the square-root behavior at  $\omega_A$  occurs in 13 of the 24 Green's functions which we evaluated. The effect originates in the numerator of the integrand in Eq. (19), which may vanish at a Van Hove point. The Van Hove point at  $\omega_A$  arises from the point  $\vec{k} = (\frac{1}{2}\pi, \frac{1}{2}\pi, \frac{1}{2}\pi)$  and we observe that the numerator  $f(\vec{r}, \vec{k})$  does vanish at that  $\vec{k}$  whenever  $\vec{r}$  has one or more odd-integral coordinates. Thus the Green's function  $g(\vec{r}, \omega)$  do not have square-root singularities at  $\omega_A$  if  $\vec{r}$  has an odd-integral coordinate.

The rules above permit one to form at least a qualitative picture of the Green's functions based solely on the location and type of the Van Hove singularities. In Fig. 3 we give such a schematic representation of  $-(1/\pi)g_I(0, \omega)$  for a much wider range of  $\gamma$ . The behavior for large  $\gamma$  is interesting, and it can be understood by considering the limit  $\gamma \rightarrow \infty$  (or  $J_1 \rightarrow 0$ ). In that limit the fcc lattice reduces to independent interpenetrating simple cubic lattices with nearest-neighbor interactions. The two lowest-energy Van Hove singularities are both of type 0. In the limit  $\gamma \rightarrow 0$  they coalesce to form a single Van Hove singularity at the bottom of the band. This leads to an infinity of the derivative of the ferromagnetic Curie temperature with respect to  $J_1$  at  $J_1 = 0$ .<sup>12</sup>

Finally, we consider the appearance of the Van Hove singularities in the real parts of the Green's functions. From the dispersion relation [Eq. (18)] we see that the singularity in the real part arises from the integral over the corresponding singularity in the imaginary part. The relevant integrals are of the form (for small  $\omega$ )

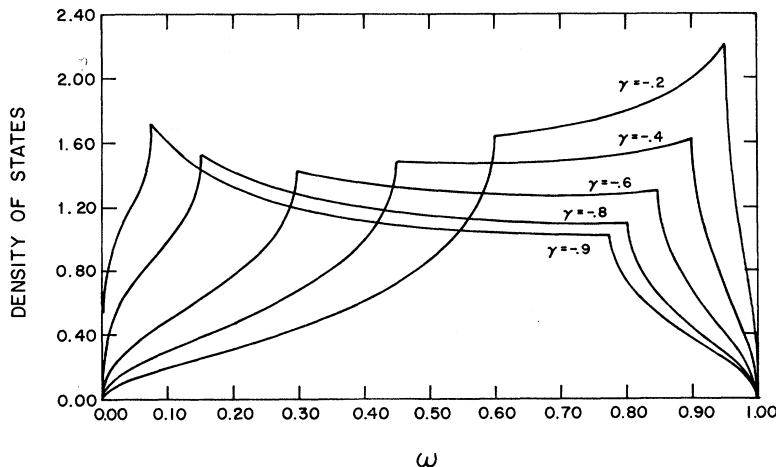


FIG. 2. Density of states,  $(-1/\pi) \times g_I(0, \omega)$ , for the pure fcc ferromagnet for various values of  $\gamma = J_2/J_1$ .

TABLE III. Green's functions for  $J_2/J_1 = -0.10$ . The Green's function is listed in column 1, by number and by the vector  $\bar{i}$ . The energy region is specified in column 2, along with the particular function ( $G \equiv g_I, H, J, \text{ or } K$ ) being tabulated [Eq. (28)]. The coefficients  $c_0 \dots c_5$  for this function and the values of  $g_I(\omega_A)$  and  $g_I(\omega_B)$  are listed. The last six columns give the coefficients for  $g_R(\bar{i}, \omega)$ .

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts							
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
# 1 (000)	8.2004	2.0511	0.4032	0.0982	0.0276	0.0085	-5.5972	-8.7440	-2.44906	-0.6738	-0.1322	-0.0285	-0.0072	-0.0026
2-G	-6.6407	-1.3736	-0.4456	-0.1612	-0.0638	-0.0228			1.0684	4.3812	1.0718	0.8681	0.3096	0.1994
3-K	161.3701	-50.5581	13.0639	-6.4701	3.0184	-1.2966			9.9136	0.4679	-0.0604	0.0458	-0.0053	-0.0063
# 2 (110)	-1.0135	0.5955	0.1546	0.0493	0.0170	0.0056	-0.1472	2.8261	0.2589	0.8444	0.0847	0.0146	0.0011	-0.0013
2-J	1.1769	1.4432	0.1348	0.0639	0.0227	0.0081			0.6732	-1.0003	-0.6206	-0.2536	-0.1380	-0.0591
3-K	-51.1900	18.1329	-4.8152	2.3426	-1.0981	0.4703			-2.1796	-0.2544	0.0211	-0.0149	0.0015	0.0024
# 3 (200)	-6.8192	-1.5915	-0.7661	-0.3736	-0.1872	-0.0792	2.6536	-4.6859	0.4057	0.6377	-0.1139	-0.0131	0.0050	0.0151
2-G	-0.1409	-3.3795	-0.7585	-0.2385	-0.0898	-0.0314			-1.2059	-0.4533	1.3142	0.3051	0.3078	0.0842
3-K	2.2619	-50.2009	8.8351	-5.3308	2.3330	-1.0297			2.5435	1.6293	0.0700	0.0324	0.0052	-0.0065
# 4 (211)	-0.1540	1.1467	-0.2400	-0.0655	-0.0215	-0.0068	0.5302	-0.7767	0.0255	-0.0266	-0.3718	-0.0335	-0.0038	0.0016
2-J	-0.2107	-0.8218	0.0938	0.0840	0.0346	0.0129			-0.2346	0.5771	0.4914	0.1431	0.0626	0.0177
3-K	94.0470	11.4195	2.0979	0.1755	0.1084	-0.0106			0.6574	-0.9236	-0.1181	0.0056	-0.0076	0.0007
# 5 (220)	3.8596	4.1814	0.7046	0.3897	0.2090	0.0920	-1.3141	-1.0495	-0.1631	-0.3437	-0.4268	0.0944	-0.0104	-0.0191
2-G	-0.2264	-0.4326	-0.8254	-0.2406	-0.0984	-0.0355			-0.2833	-0.7466	0.2228	0.2228	0.0478	0.0617
3-K	-142.3332	-44.6981	1.0594	-2.9883	1.0053	-0.5043			0.1991	2.2027	0.2275	0.0943	0.0141	-0.0043
# 6 (310)	-0.1811	0.6353	-0.7104	-0.0516	-0.0222	-0.0080	-0.3016	2.4601	-0.1827	-0.3841	-0.3473	0.0829	0.0127	0.0060
2-J	-0.0810	1.2692	1.0886	0.1398	0.0450	0.0134			0.2425	0.9494	-0.4684	-0.4525	-0.1698	-0.0826
3-K	-40.6470	23.6075	-6.6167	3.0099	-1.4514	0.6137			-1.0226	-0.4893	0.0145	-0.0125	0.0006	0.0037
# 7 (400)	4.2475	2.8135	-0.0051	0.8051	0.3766	0.1628	-1.8121	-3.4815	-0.1107	-0.1681	0.0078	0.2114	-0.0402	-0.0347
2-G	-0.3637	-0.0905	-2.0248	-0.6362	-0.2044	-0.0679			-0.0448	-1.5195	-0.4249	0.8372	0.2727	0.2204
3-K	66.7729	-154.8953	3.0236	-7.6171	2.6694	-1.3017			0.9446	0.8278	0.6084	0.1065	0.0003	-0.0033
# 8 (321)	-0.3303	0.2520	-0.7015	0.2478	0.0528	0.0154	-0.3526	-0.6291	-0.0153	-0.0140	0.0578	0.2495	0.0310	-0.0053
2-J	-0.1124	-0.0734	-0.4243	-0.0407	-0.0043	0.0034			0.1477	-0.1822	0.1469	0.2320	0.0371	0.0416
3-K	87.9037	9.7978	4.1307	-0.2200	0.4129	-0.1196			0.2550	-0.7780	-0.1765	-0.0004	-0.0076	-0.0005
# 9 (222)	-3.1344	-2.0097	-2.4144	-0.7137	-0.3165	-0.1317	0.8273	2.1937	0.0044	0.0022	0.0145	0.2584	0.0507	0.0336
2-G	0.4037	0.8080	1.2189	-0.0649	-0.0780	-0.0332			-0.1051	0.1070	-0.7361	-0.9236	-0.1750	-0.1184
3-K	-273.5264	-34.3112	-9.9277	0.4092	-0.9047	0.2548			-1.1537	2.4665	0.3971	-0.0078	0.0218	0.0001
#10 (411)	-0.3331	0.1463	-0.6055	0.4128	0.0113	0.0058	-0.2868	-0.9384	0.0326	0.0931	0.1758	0.2334	-0.0513	-0.0060
2-J	-0.0031	-0.2223	-0.7255	-0.1249	0.0510	0.0246			-0.0127	-0.7005	0.0110	0.2933	0.0955	0.0088
3-K	0.4405	99.8410	12.5272	0.8793	0.6684	-0.0952			0.3885	0.3522	-0.6142	-0.0862	-0.0010	-0.0059
#11 (422)	2.0887	2.7304	1.1809	1.6450	0.3123	0.1352	-0.6198	1.9762	-0.0008	-0.0055	-0.0138	-0.0614	-0.2107	-0.0333
2-G	0.1948	0.4079	0.4008	0.9111	0.1116	0.0055			0.1314	0.1007	0.3933	0.1691	-0.5066	-0.0886
3-K	-165.5817	-117.0000	-25.0415	-0.0479	-2.0375	0.5036			-0.6462	1.0239	0.8729	0.1035	0.0174	0.0093
#12 (332)	-0.1543	0.4323	-0.2920	0.4939	-0.1561	-0.0463	0.1471	-0.9437	0.0031	0.0078	0.0121	-0.0055	-0.1719	-0.0012
2-J	-0.1366	-0.2663	-0.3558	-0.3446	0.0827	0.0282			-0.0480	0.0319	-0.0442	0.3115	0.2298	0.0228
3-K	94.1998	16.7828	3.8791	-0.6507	0.4408	-0.1658			0.4017	-0.7502	-0.1836	0.0034	-0.0056	-0.0005

TABLE III. (Continued)

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts								
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	
#13 (420)	1-H 2-G 3-K	-3.8226 0.2062 -54.8929	-2.6198 -0.3117 138.0549	-2.0060 0.1829 -9.7704	0.0395 -0.4389 -4.2146	-0.2295 -0.1057 0.5499	-0.1106 -0.0413 -0.4916	1.0659	-0.5883	0.1158 -0.1597 -0.0212	0.2405 -0.2504 1.0033	0.2530 -0.2315 0.7419	0.2125 -0.2569 0.1022	-0.0681 0.1869 0.0093	0.0210 0.0132 0.0020
#14 (330)	1-J 2-J 3-K	-0.2778 0.2529 -19.0749	0.2852 -0.2664 37.3474	-0.4553 0.4649 -10.2766	0.5052 0.9347 3.4569	0.0453 0.1949 -2.0067	0.0169 0.0590 0.7889	1.6685		0.1094 0.2873 -0.2638	0.2246 0.2391 -0.6903	0.2391 0.9208 -0.0534	0.2370 -0.0587 0.0001	-0.0640 -0.3140 0.0019	-0.0146 -0.1167 0.0060
#15 (440)	1-H 2-G 3-K	2.7157 -0.1925 52.5885	3.2321 0.1056 -207.2395	1.3570 -0.3300 -22.8136	1.2536 -0.2255 -7.9392	-0.1981 -0.3963 0.3403	0.0969 -0.0371 -0.7824	-0.7649	-1.1138	-0.0816 -0.0490 0.1410	-0.1735 -0.0354 -0.0757	-0.1883 -0.2168 1.0436	-0.1948 -0.0425 0.2255	-0.1616 0.0916 0.0154	0.0481 0.2155 0.0077
#16 (431)	1-J 2-J 3-K	-0.0941 0.0595 -19.7332	0.4948 -0.0202 84.1952	-0.1707 0.2394 16.4008	0.5048 -0.2295 1.6021	-0.2487 -0.1646 0.9996	-0.0260 -0.0430 -0.1086	0.3445	-0.1665	0.0173 -0.1713 -0.0474	0.0241 0.0171 0.4220	-0.0083 -0.2966 -0.5023	-0.0736 -0.2701 -0.1080	-0.1803 0.0117 -0.0064	0.0227 0.0377 -0.0075
#17 (620)	1-H 2-G 3-K	3.1264 -0.0754 -80.5864	3.0519 0.3844 -52.5065	1.0185 -0.1984 -74.1165	0.8069 0.0923 -11.2752	-0.3786 -0.3038 -0.7404	0.2540 -0.0491 -0.7008	-1.0137	-0.2599	-0.0898 -0.0373 -0.0951	-0.1833 -0.2812 0.6960	-0.1768 -0.2498 0.2595	-0.1420 -0.1837 0.4442	-0.0467 0.1593 0.0755	0.0840 0.1251 0.0020
#18 (521)	1-J 2-J 3-K	-0.0800 -0.0989 84.5490	0.4695 -0.1675 10.1740	0.1583 0.0140 5.4841	0.4327 -0.2272 -0.3301	-0.3447 0.0599 0.7833	0.0039 -0.0396 -0.2122	0.2322	-0.5935	-0.0049 -0.0678 0.1987	-0.0221 0.2476 -0.7056	-0.0590 -0.0641 -0.1387	-0.1225 -0.0355 -0.0035	-0.1597 0.0977 -0.0086	0.0535 0.0476 -0.0024
#19 (600)	1-H 2-G 3-K	-3.1643 -0.0746 23.5678	-1.4362 -0.1542 -77.2378	-1.0621 0.0559 -59.5107	-0.1399 -1.4293 -15.4290	-0.9742 -0.5605 2.4532	-0.1685 -0.1747 -1.8156	1.1442	-2.5664	-0.0064 -0.4976 0.3192	-0.0300 0.1207 -0.7248	-0.0826 -1.2400 0.1441	-0.1316 -0.4947 0.4536	-0.0797 0.4999 0.0655	0.1325 0.2201 -0.0086
#20 (530)	1-J 2-J 3-K	-0.1065 -0.1886 -3.3955	0.3645 0.2602 52.6559	-0.2679 -0.2601 -9.4815	0.2455 0.1028 2.5916	-0.4606 0.6652 -2.4748	0.0454 0.1654 0.7931	-0.2272	0.9082	-0.0814 0.0871 0.0512	-0.1675 0.3603 -0.6359	-0.1726 0.0701 -0.1723	-0.1648 0.6855 -0.0054	-0.1046 0.0974 0.0070	0.0964 -0.2103 0.0090
#21 (800)	1-H 2-G 3-K	1.6851 0.1082 33.7099	1.6572 -0.0734 -124.0149	0.5785 0.0851 0.1500	0.9509 0.1864 -65.8009	0.4071 -1.0369 -1.9086	0.7485 -0.4320 -2.9584	-0.6119	-1.7408	0.0412 -0.0909 -0.0660	0.0842 -0.5890 0.8079	0.0913 -0.0506 0.0539	0.0841 -0.9610 0.1145	0.0269 -0.4889 0.3368	-0.0413 0.3977 0.0341
#22 (611)	1-J 2-J 3-K	-0.0746 -0.0970 11.7905	0.3928 0.2150 2.8766	-0.2127 -0.0753 77.7348	0.2414 -0.5873 7.1395	-0.4504 -0.2003 1.9988	0.1137 0.0096 0.0150	-0.0028	-0.6230	-0.0586 -0.1945 -0.0090	-0.1282 0.0873 0.7197	-0.1477 -0.6148 -0.0681	-0.1475 -0.1308 -0.4304	-0.0658 0.2149 -0.0642	0.1078 0.0873 -0.0055
#23 (710)	1-J 2-J 3-K	-0.1943 -0.1137 -9.4468	0.0867 0.2004 42.0946	-0.4188 -0.3550 -9.5713	0.0613 0.5333 4.7698	-0.3577 0.7286 -2.5095	0.3008 0.1704 0.9947	-0.5057	1.2674	-0.0482 0.2727 0.0126	-0.0852 0.1690 -0.7457	-0.0441 0.4917 -0.0652	-0.0432 0.7432 -0.0120	0.0291 -0.0512 -0.0031	0.1376 -0.2444 0.0084
#24 (510)	1-J 2-J 3-K	-0.1370 -0.2781 -25.3131	0.4271 -0.2925 32.3782	-0.1554 0.8087 -8.5366	0.6092 0.8798 3.8457	-0.1552 0.1656 -1.9594	0.0076 0.0420 0.8105	0.5182	1.8936	0.1169 0.1848 -0.3620	0.2219 0.5459 -0.6742	0.1728 0.8319 -0.0144	0.0380 -0.2097 -0.0111	-0.1533 -0.3269 -0.0004	0.0125 -0.1202 0.0058

TABLE IV. Green's functions for  $J_B/J_I = -0.30$ . The Green's function is listed in column 1, by number and by the vector  $\bar{r}$ . The energy region is specified in column 2, along with the particular function ( $G \equiv g_I, H, J$ , or  $K$ ) being tabulated [Eq. (28)]. The coefficients  $c_0 \dots c_5$  for this function and the values of  $g_I(\omega_A)$  and  $g_I(\omega_B)$  are listed. The last six columns give the coefficients for  $g_R(\bar{r}, \omega)$ .

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts							
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
# 1 (000)	7.7553	1.7706	0.3822	0.1366	0.0604	0.0249	-4.8677	-5.8658	-2.6113	-0.3839	-0.0584	-0.0046	-0.0009	-0.0024
2-G	-5.1999	-0.4605	-0.1550	-0.0346	-0.0105	-0.0030			0.6645	3.3191	0.4440	0.5222	0.1071	0.1057
3-K	44.8840	-9.5558	2.9980	-1.3290	0.6470	-0.2729			5.8885	-0.0664	-0.0541	0.0364	-0.0173	0.0035
# 2 (110)	-1.4533	0.7870	0.0920	0.0322	0.0089	0.0030	-0.3789	1.8291	0.1714	0.8500	0.0181	0.0065	-0.0008	-0.0007
2-J	0.7402	1.1860	-0.0532	0.0248	0.0020	0.0012			0.6721	-0.7219	-0.4129	-0.1201	-0.0691	-0.0251
3-K	-13.6854	3.7620	-1.2382	0.5451	-0.2646	0.1115			-1.0627	-0.1111	0.0221	-0.0119	0.0054	-0.0007
# 3 (200)	-7.8590	-0.8491	-0.6181	-0.2554	-0.1289	-0.0533	2.3416	-2.7967	0.5150	0.7892	-0.1322	-0.0031	-0.0005	0.0069
2-G	0.1959	-2.4944	-0.4029	-0.0690	-0.0185	-0.0046			-0.9357	-0.6569	1.0093	0.0952	0.1814	0.0126
3-K	3.5471	-8.9984	2.8084	-1.2579	0.6116	-0.2579			1.0305	1.0192	-0.0115	0.0107	-0.0024	-0.0028
# 4 (211)	-0.3324	1.5094	-0.3537	-0.0330	-0.0142	-0.0034	0.5541	-0.6212	0.0862	0.0946	-0.3634	0.0019	-0.0015	0.0015
2-J	-0.0522	-0.7640	0.1013	0.0553	0.0093	0.0028			-0.1749	0.3394	0.3740	0.0734	0.0370	0.0135
3-K	21.1382	5.5277	0.2649	-0.0817	0.0386	-0.0158			0.3566	-0.5803	-0.0464	0.0121	-0.0075	0.0029
# 5 (220)	3.7483	4.8473	0.3310	0.3236	0.1544	0.0680	-1.0556	-0.2434	-0.1412	-0.2889	-0.4385	0.0387	-0.0060	-0.0089
2-G	-0.0346	0.5152	-0.5818	-0.1000	-0.0304	-0.0073			-0.2202	-0.6164	-0.5677	0.1951	-0.0775	0.0336
3-K	-31.4303	-6.7350	0.9842	-0.5206	0.2544	-0.1082			-0.1698	1.3821	0.0926	-0.0121	0.0101	-0.0058
# 6 (310)	-0.1566	1.1332	-0.8514	0.0113	-0.0251	-0.0052	0.0625	1.3627	-0.1528	-0.3757	-0.4091	0.0874	-0.0011	0.0040
2-J	-0.1634	0.6610	0.9064	0.0032	0.0080	0.0008			0.0792	0.9463	-0.2720	-0.3190	-0.0772	-0.0397
3-K	-9.1044	5.9783	-2.0374	0.8758	-0.4283	0.1806			-0.3048	-0.3405	0.0153	-0.0097	0.0042	0.0011
# 7 (400)	5.3033	3.5715	-0.7468	0.6898	0.1958	0.1032	-1.7900	-1.7687	-0.2370	-0.4036	-0.1310	0.2176	-0.0366	-0.0095
2-G	-0.2971	0.4858	-1.3928	-0.4536	-0.0835	-0.0184			-0.0071	-0.9766	-0.6129	0.6333	0.1634	0.1323
3-K	16.0591	-35.3984	3.3965	-1.8606	0.9051	-0.3844			0.1694	0.4876	0.4021	0.0462	-0.0151	0.0010
# 8 (321)	-0.4194	0.4938	-0.9395	0.3321	0.0208	0.0116	-0.3467	-0.5649	-0.0420	-0.0734	-0.0102	0.2477	-0.0191	-0.0018
2-J	-0.1595	-0.0407	-0.3783	-0.0188	0.0034	0.0042			0.0736	-0.1090	0.0926	0.1889	0.0566	0.0273
3-K	19.5385	0.7748	1.0072	-0.3022	0.1556	-0.0650			0.1933	-0.4504	-0.0742	0.0069	-0.0068	0.0016
# 9 (222)	-3.7916	-1.5654	-2.7007	-0.4756	-0.2455	-0.1013	0.8500	1.8605	0.0258	0.0196	-0.0336	0.2452	0.0122	0.0172
2-G	0.3600	0.6071	1.0487	-0.0882	-0.0491	-0.0115			-0.0777	0.2292	-0.5197	-0.7128	-0.0658	-0.0895
3-K	-60.9490	-2.9244	-2.2087	0.7494	-0.3684	0.1538			-0.7160	1.4450	0.2205	-0.0294	0.0207	-0.0059
# 10 (411)	-0.4437	0.2448	-0.9474	0.4915	-0.0353	0.0106	-0.4863	-0.3554	-0.0452	-0.0496	0.1001	0.2528	-0.0571	0.0034
2-J	-0.0419	0.2235	-0.5477	-0.0884	0.0642	0.0133			0.0065	-0.5319	-0.1821	0.1866	0.0342	-0.0109
3-K	-3.5256	20.3576	1.6145	-0.1988	0.1208	-0.0489			0.0230	0.3283	-0.3954	-0.0334	0.0077	-0.0050
# 11 (422)	2.3976	3.0664	0.7937	1.9086	0.1478	0.1239	-0.6643	1.3608	-0.0127	-0.0176	0.0059	-0.0101	-0.1973	-0.0034
2-G	0.1045	0.3073	0.2103	0.7267	0.0433	-0.0156			0.1893	0.1100	0.3980	-0.0607	-0.3913	-0.0273
3-K	-31.9277	-22.0800	-5.5643	1.0833	-0.6328	0.2627			-0.2870	0.3800	0.5732	0.0430	0.0061	0.0040
# 12 (332)	-0.2386	0.6015	-0.4893	0.6375	-0.2292	-0.0297	0.1333	-0.7665	-0.0061	-0.0101	0.0047	0.0212	-0.1749	0.0132
2-J	-0.1151	-0.1802	-0.2894	-0.3206	0.0957	0.0095			-0.0631	-0.0229	-0.1087	0.2314	0.1680	0.0040
3-K	20.3789	2.5842	1.1946	-0.5022	0.2320	-0.0984			0.2193	-0.3735	-0.1292	0.0099	-0.0055	0.0008

TABLE IV. (Continued)

Green's Region- function type	Coefficients for imaginary parts					Coefficients for real parts									
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	
#13 (420)	1-H 2-G 3-K	-3.9213 0.1803 -9.7656	-2.5700 -0.0687 -29.3081	-2.5953 0.2247 -0.6694	0.3005 -0.3100 -0.5359	-0.2402 -0.0451 0.2217	-0.0743 -0.0177 -0.0976	0.7527	-0.0483	0.0893 -0.0276 -0.1448	0.1935 -0.1368 0.4834	0.2426 -0.1691 0.4892	0.2499 -0.2096 0.0420	-0.0783 0.1585 -0.0040	0.0195 -0.0096 0.0015
#14 (330)	1-J 2-J 3-K	-0.4426 0.1121 -3.1656	0.3495 -0.3074 9.5533	-0.7473 0.1477 -3.0712	0.6148 0.7475 1.0707	-0.0021 0.0388 -0.5676	0.0206 0.0092 0.2395	-0.1093	0.7192	0.0883 0.2376 0.0369	0.1925 0.0465 -0.4280	0.2254 0.7489 -0.0444	0.2694 -0.0304 0.0021	-0.0687 -0.2450 0.0042	-0.0028 -0.0451 0.0027
#15 (440)	1-H 2-G 3-K	2.3307 -0.1323 17.9939	3.6101 -0.0056 -43.4618	1.3982 -0.1807 -3.4950	1.7449 -0.1651 -1.5736	-0.3751 -0.3094 0.4871	0.1436 0.0076 -0.2298	-0.4564	-0.7912	-0.0507 -0.0350 0.1027	-0.1175 0.0817 -0.2287	-0.1520 -0.1049 0.6404	-0.1872 -0.0433 0.1437	-0.1867 0.0997 -0.0088	0.0598 0.1709 0.0056
#16 (431)	1-J 2-J 3-K	-0.1899 0.1289 -8.0980	0.6263 -0.0248 16.7545	-0.3275 0.2929 2.9013	0.7034 -0.1336 0.0471	-0.3154 -0.1145 0.1095	0.0057 -0.0069 -0.0393	0.3424	0.1431	0.0442 -0.1005 -0.1141	0.0792 -0.0167 0.3230	0.0490 -0.1765 -0.3023	-0.0232 -0.2473 -0.0617	-0.1835 0.0038 0.0042	0.0342 0.0157 -0.0050
#17 (620)	1-H 2-G 3-K	2.8881 -0.0221 -17.1170	3.6370 0.3030 -9.1198	1.2672 0.0217 -15.9334	1.3131 0.1612 -1.3282	-0.6580 -0.2070 0.0957	0.2877 -0.0252 -0.0765	-0.6501	0.2015	-0.0705 -0.0272 -0.1355	-0.1542 -0.0083 0.2919	-0.1800 -0.1356 0.1558	-0.1942 -0.1670 0.2920	-0.1055 0.0852 -0.0048	0.0992 0.0852 -0.0048
#18 (521)	1-J 2-J 3-K	-0.1703 -0.0327 18.4436	0.5855 -0.2818 1.7513	-0.2794 0.0330 1.7768	0.6719 -0.2068 -0.4595	-0.4135 -0.0525 0.3042	0.0412 -0.0279 -0.1243	0.2880	-0.6097	0.0341 -0.0711 0.1628	0.0597 -0.0583 -0.3398	0.0262 -0.0198 -0.1122	-0.0711 -0.0207 0.0017	-0.1752 0.0860 -0.0076	0.0596 0.0361 -0.0002
#19 (600)	1-H 2-G 3-K	5.0832 0.1810 2.7902	-1.9498 -0.2345 -17.4123	-1.0118 0.5706 -11.2825	0.6927 -0.8529 -2.8610	-0.9257 -0.4621 1.1514	-0.0271 -0.1122 -0.5063	1.4720	-0.9580	0.1227 -0.3352 -0.0928	0.2074 0.0685 0.4106	0.0833 -0.6828 0.0882	-0.0999 -0.7002 0.3037	-0.1467 0.3007 0.0154	0.1004 0.1396 -0.0104
#20 (530)	1-J 2-J 3-K	-0.1123 -0.1539 -0.3547	0.6227 0.0795 13.0948	-0.2841 -0.2199 -2.3654	0.4819 -0.1068 0.7155	-0.5699 0.5335 -0.6080	0.0835 0.0745 0.2418	0.0922	0.2194	-0.0591 -0.0377 0.1206	-0.1291 0.2618 -0.2920	-0.1533 -0.0772 -0.1441	-0.1799 0.5179 -0.0065	-0.1494 0.1007 0.0094	0.0986 0.1542 0.0039
#21 (800)	1-H 2-G 3-K	3.7691 -0.0068 6.3346	2.6246 0.2710 -29.5816	0.1233 -0.1491 2.3451	0.4530 0.6028 -14.4876	-0.2183 -0.4841 0.8411	0.8703 -0.3940 -0.5967	-1.2077	-0.4322	-0.0610 0.1230 -0.1390	-0.1005 -0.3787 0.2850	-0.0307 0.1939 0.1060	0.0703 -0.3445 0.0596	0.1102 -0.6518 0.2164	0.0521 0.2023 0.0036
#22 (611)	1-J 2-J 3-K	-0.0752 0.0779 0.2556	0.6604 0.0572 -4.1202	-0.1538 0.3477 16.2997	0.5382 -0.3515 0.4954	-0.5608 0.1652 0.1798	0.1463 0.0380 -0.0543	0.3818	0.0392	0.0139 -0.1326 -0.1461	0.0020 0.1358 0.3791	-0.0698 -0.3248 0.0443	-0.1591 -0.2551 -0.2792	-0.1253 0.1320 -0.0232	0.1083 0.0534 0.0022
#23 (710)	1-J 2-J 3-K	-0.1373 -0.2303 -0.0551	0.3961 -0.2077 11.9638	-0.4052 -0.4282 -2.1638	0.1505 -0.0490 1.3058	-0.6091 0.5712 -0.7139	0.3298 0.1403 0.2959	-0.2694	0.2272	-0.1017 0.0276 0.1467	-0.2062 0.1708 -0.3311	-0.1935 -0.0312 -0.0994	-0.1183 0.6274 -0.0173	0.0431 0.1401 0.0014	0.1639 -0.1565 0.0051
#24 (510)	1-J 2-J 3-K	-0.3482 0.1666 -3.5271	0.3221 -0.4454 9.2189	-0.4633 0.2204 -2.6050	0.8026 0.7280 1.1738	-0.1949 0.0815 -0.6063	0.0367 0.0070 0.2568	0.1302	0.7305	0.1275 -0.2022 -0.0496	0.2700 0.0918 -0.4239	0.2782 0.7794 -0.0308	0.1401 -0.0203 -0.0093	-0.1423 -0.2369 0.0033	0.0241 -0.0606 0.0031



TABLE V. Green's functions for  $J_2/J_1 = -0.50$ . The Green's function is listed in column 1, by number and by the vector  $\bar{r}$ . The energy region is specified in column 2, along with the particular function ( $G \equiv g_I, H, J$ , or  $K$ ) being tabulated [Eq. (28)]. The coefficients  $c_0 \dots c_5$  for this function and the values of  $g_I(\omega_A)$  and  $g_I(\omega_B)$  are listed. The last six columns give the coefficients for  $g_R(\bar{r}, \omega)$ .

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts							
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
# 1 (000)	8.0976	2.1667	0.4581	0.2293	0.1006	0.0444	-4.5399	-4.5549	-2.8815	-0.0813	-0.0332	0.0122	0.0026	-0.0007
2-G	-4.4260	0.0034	-0.1159	-0.0096	-0.0051	-0.0010			0.4781	2.8105	0.1528	0.4223	0.0402	0.0037
3-K	22.1895	-4.3210	1.3188	-0.5824	0.2836	-0.1197			4.3720	-0.1588	-0.0318	0.0258	-0.0136	0.0034
# 2 (110)	-2.2755	1.2552	-0.0275	0.0408	0.0010	0.0031	-0.6110	1.3850	0.0627	0.9262	-0.0554	0.0122	-0.0031	0.0003
2-J	0.4456	1.1890	-0.1973	0.0481	-0.0067	0.0019			0.6491	-0.6034	-0.3269	-0.0645	-0.0516	-0.0149
3-K	-6.5819	1.8006	-0.5938	0.2613	-0.1266	0.0533			-0.6904	-0.0854	0.0160	-0.0085	0.0042	-0.0006
# 3 (200)	-10.4911	0.3327	-0.7172	-0.1540	-0.1099	-0.0377	2.0959	-2.0513	0.6411	0.9702	-0.1883	0.0106	-0.0098	0.0021
2-G	0.3069	-2.0546	-0.2753	-0.0175	-0.0086	-0.0013			-0.7026	-0.7378	0.8991	0.0112	0.1446	-0.0051
3-K	1.8215	-4.0428	1.4097	-0.6264	0.3044	-0.1283			0.6240	0.7917	-0.0199	0.0074	-0.0019	-0.0023
# 4 (211)	-0.7184	2.2175	-0.6039	0.0371	-0.0218	0.0006	0.5542	-0.4829	0.1491	0.2387	-0.3902	0.0402	-0.0067	0.0027
2-J	0.0685	-0.7580	0.1285	0.0452	-0.0027	0.0020			-0.1075	0.1829	0.3311	0.0343	0.0280	0.0108
3-K	9.7441	-0.0956	0.1307	-0.0516	0.0237	-0.0097			0.2371	-0.4322	0.0262	0.0091	-0.0056	0.0022
# 5 (220)	3.8750	6.7544	-0.2712	0.3922	0.1036	0.0612	-0.8964	-0.0498	-0.1291	-0.2230	-0.4772	0.0833	-0.0087	0.0001
2-G	0.0336	0.4751	-0.4895	-0.0495	-0.0165	-0.0018			-0.1633	-0.5358	-0.4731	0.1887	-0.0826	0.0307
3-K	-14.7501	-2.8510	0.5208	-0.2458	0.1221	-0.0520			-0.2053	1.0476	0.0617	-0.0101	0.0075	-0.0046
# 6 (310)	-0.2076	2.0145	-1.1902	0.1309	-0.0508	0.0024	0.4179	0.9244	-0.0810	-0.3211	-0.4825	0.1135	-0.0163	0.0065
2-J	0.0976	0.2452	0.9206	-0.0915	0.0120	-0.0009			-0.0252	0.8754	-0.1725	-0.2804	-0.0354	-0.0299
3-K	-3.8733	3.1039	-1.0540	0.4609	-0.2248	0.0949			-0.1331	-0.2739	0.0067	-0.0067	0.0030	0.0011
# 7 (400)	6.7299	5.5444	-2.0074	0.8043	-0.0110	0.0772	-1.5608	-1.1459	-0.3529	-0.6500	-0.2961	0.2395	-0.0457	0.0106
2-G	0.2996	0.6364	-1.0240	-0.4226	-0.0284	-0.0057			-0.0638	-0.5205	-0.7183	0.5406	0.1294	0.0953
3-K	7.0252	-16.8741	2.0130	-0.9613	0.4775	-0.2030			0.0280	0.3605	0.3220	0.0257	-0.0113	0.0001
# 8 (321)	-0.6151	1.0052	-1.3934	0.5210	-0.0421	0.0204	-0.2992	-0.4821	-0.0574	-0.1159	-0.0873	0.2662	-0.0437	0.0062
2-J	0.1689	-0.0144	-0.3423	-0.0028	0.0092	0.0035			0.0221	-0.0516	0.0544	0.1654	0.0386	0.0201
3-K	9.0761	0.2668	0.5187	-0.1848	0.0905	-0.0381			0.1535	-0.3238	-0.0591	0.0053	-0.0048	0.0011
# 9 (222)	-5.4577	-0.8064	-3.6263	-0.1371	-0.2607	-0.0798	0.9248	1.5303	0.0687	0.0689	-0.0933	0.2506	-0.0258	0.0117
2-G	0.3321	0.4294	0.9324	-0.1239	-0.0356	-0.0025			-0.0745	0.2636	-0.4079	-0.6008	-0.0061	-0.0761
3-K	-28.1904	-0.8498	-1.1536	0.4578	-0.2196	0.0920			-0.5263	1.0441	0.1671	-0.0229	0.0150	-0.0042
# 10 (411)	-0.5755	0.6370	-1.5243	0.6997	-0.1213	0.0313	-0.5207	-0.1474	-0.1243	-0.2160	-0.0042	0.2836	-0.0746	0.0159
2-J	0.1308	0.4499	-0.4592	-0.1025	0.0841	-0.0012			-0.0177	-0.3077	-0.2797	0.1627	0.0180	-0.0167
3-K	-2.3675	8.9415	0.5676	-0.1222	0.0600	-0.0250			-0.0380	0.2599	-0.2920	-0.0186	0.0063	-0.0038
# 11 (422)	3.1704	4.1991	0.0787	2.6373	-0.1481	0.1678	-0.7407	1.0315	-0.0454	-0.0696	-0.0017	0.0438	-0.2001	0.0277
2-G	0.0384	0.2854	0.0998	0.6265	0.0113	-0.0244			0.1911	0.0955	0.3515	-0.0153	-0.3419	-0.0029
3-K	-13.7488	-9.7864	-2.7999	0.6828	-0.3588	0.1521			-0.1744	0.1978	0.4456	0.0326	0.0029	0.0038
# 12 (332)	-0.3936	1.0043	-0.8695	0.9280	-0.3761	0.0112	0.1505	-0.6125	-0.0154	-0.0349	-0.0182	0.0556	-0.1885	0.0346
2-J	0.1031	-0.1192	-0.2316	-0.3208	0.1290	-0.0102			-0.0706	-0.0180	-0.1390	0.1964	0.1363	-0.0109
3-K	9.1654	1.0992	0.7246	-0.3068	0.1455	-0.0614			0.1469	-0.2383	-0.1060	0.0062	-0.0039	0.0001

TABLE V. (Continued)

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts							
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
#13 (420)	1-H 2-G 3-K	-4.6240 0.1230 -4.2926	-2.4846 0.0317 -13.5990	-4.0106 0.2138 -0.1906	0.8128 -0.2565 -0.2140	-0.3700 -0.0226 0.1044	-0.0200 -0.0130 -0.0452	0.0730	0.0560 0.0101 -0.1304	0.1216 -0.0492 0.3123	0.2076 -0.1547 0.3863	0.2956 -0.1737 0.0270	-0.1016 0.1385 -0.0038	0.0249 -0.0167 0.0011
#14 (330)	1-J 2-J 3-K	-0.7502 0.0375 -1.1773	0.5719 -0.2115 4.7449	-1.2737 -0.0503 -1.4706	0.8658 0.7302 0.5578	-0.0915 -0.0530 -0.2867	0.0420 0.0054 0.1223	0.4274	0.0555 0.2083 0.0675	0.1469 -0.0592 -0.3059	0.1977 0.6324 -0.0443	0.3144 -0.0134 0.0015	-0.0859 -0.2240 0.0026	0.0120 -0.0136 0.0022
#15 (440)	1-H 2-G 3-K	1.9547 -0.0785 9.2988	4.6311 -0.0964 -19.6926	1.4142 -0.0867 -1.5921	2.8705 -0.1297 -0.7746	-0.7572 -0.2727 0.2927	0.2780 0.0376 -0.1290	-0.6345	-0.0055 -0.0205 0.0919	-0.0318 0.0816 -0.2261	-0.0920 -0.0209 0.4780	-0.1639 -0.0809 0.1133	-0.2218 0.1100 -0.0075	0.0810 0.1446 0.0032
#16 (431)	1-J 2-J 3-K	-0.3944 0.1458 -4.2418	0.8944 -0.0561 7.4212	-0.6824 0.2845 1.2091	1.0668 -0.0835 0.0070	-0.4711 -0.1137 0.0329	0.0633 0.0142 -0.0138	0.1829	0.0624 -0.0459 -0.0975	0.1198 -0.0528 0.2408	0.0986 -0.0844 -0.2197	0.0361 -0.2274 -0.0444	-0.1988 0.0081 -0.0034	0.0551 0.0156 -0.0034
#17 (620)	1-H 2-G 3-K	2.6480 0.0120 -7.5295	4.6608 0.1577 -3.9752	1.4887 0.0770 -7.5667	2.4967 -0.1841 -0.4375	-1.1676 -0.1647 0.0396	0.4525 -0.0190 -0.0230	0.2305	-0.0270 -0.0076 -0.0869	0.0675 0.0406 0.1419	-0.1134 -0.0187 0.1263	-0.2048 -0.1483 0.2296	-0.1690 0.1494 -0.0186	0.1199 0.0687 -0.0037
#18 (521)	1-J 2-J 3-K	-0.3708 -0.0022 8.2976	0.7747 -0.2520 0.9127	-0.6337 -0.0744 1.0676	1.0776 -0.1731 -0.3114	-0.5827 -0.0482 0.1831	0.1086 -0.0775	-0.5262	0.0453 -0.0398 0.1146	0.0961 -0.0647 -0.1991	0.1024 -0.0019 -0.1017	-0.0036 0.0119 -0.0015	-0.1976 0.0740 -0.0052	0.0783 0.0290 -0.0006
#19 (600)	1-H 2-G 3-K	7.2846 0.2651 0.7904	-3.1472 -0.3614 -8.3505	-1.7632 0.6036 -5.1293	2.0351 -0.4702 -1.2464	-1.0844 -0.4611 0.5977	0.2027 -0.0785 -0.2584	-0.5133	0.2483 -0.1428 -0.0973	0.4713 -0.0748 0.2465	0.3348 -0.1981 0.0869	0.0078 -0.7557 0.2358	-0.1972 0.1924 0.0059	0.0917 0.1280 -0.0085
#20 (530)	1-J 2-J 3-K	-0.1852 -0.0762 -0.3141	1.0422 -0.0315 6.2371	-0.4290 -0.0930 -0.9346	0.9090 -0.2391 0.3708	-0.7957 0.5113 -0.2843	0.1612 0.0247 0.1197	0.0893	-0.0206 -0.0755 0.0861	-0.0604 0.2114 -0.1623	-0.1033 -0.1263 -0.1221	-0.1710 0.3989 -0.0095	-0.1977 0.1101 0.0068	0.1159 -0.1405 0.0027
#21 (800)	1-H 2-G 3-K	5.7939 -0.1483 3.6037	5.1550 0.4062 -13.7455	0.4014 -0.3122 0.8814	0.3003 0.4825 -6.6806	-1.4579 -0.1022 0.5414	1.0849 -0.3981 -0.2794	-0.2536	-0.1978 0.0474 -0.0599	-0.3820 -0.0586 0.0874	-0.3116 -0.0298 0.1042	-0.1204 0.1280 0.0515	0.0967 -0.6278 0.1674	0.1464 0.0770 -0.0022
#22 (611)	1-J 2-J 3-K	-0.2528 0.1904 0.0574	0.8713 -0.1893 -2.7218	-0.2998 0.4656 7.1850	1.0516 -0.1823 0.1234	-0.7745 -0.2014 0.0479	0.2273 0.0625 -0.0188	0.1504	0.1028 -0.0407 -0.1066	0.1846 0.0841 0.2110	0.0926 -0.0471 0.0702	-0.1087 -0.3043 -0.2099	-0.1777 0.0932 -0.0126	0.1242 0.0553 0.0022
#23 (710)	1-J 2-J 3-K	-0.0680 -0.1058 -0.2427	0.9975 0.0105 5.9018	-0.2651 -0.0745 -0.6439	0.5553 -0.4078 0.6071	-0.9745 -0.4943 -0.3304	0.4267 0.1562 0.1401	0.0602	-0.0398 -0.1044 0.0897	-0.1166 0.2356 -0.1495	-0.2043 -0.2185 -0.1014	-0.2374 0.3966 -0.0223	-0.0554 0.2579 0.0012	0.1921 -0.1190 0.0036
#24 (510)	1-J 2-J 3-K	-0.6781 0.0388 -1.0799	0.2511 -0.2109 4.8360	-1.0972 -0.1869 -1.2338	1.1399 0.7197 0.5962	-0.3126 0.0457 -0.3087	0.0856 -0.0137 0.1320	0.3712	0.0584 0.2179 0.0836	0.1793 -0.1419 -0.2875	0.3186 0.6321 -0.0450	0.2406 0.0952 -0.0076	-0.1477 -0.2213 0.0023	0.0428 -0.0403 0.0027

TABLE VI. Green's functions for  $J_2/J_1 = -0.70$ . The Green's function is listed in column 1, by number and by the vector  $\vec{r}$ . The energy region is specified in column 2, along with the particular function ( $G \equiv g_I, H, J$ , or  $K$ ) being tabulated [Eq. (28)]. The coefficients  $c_0 \dots c_5$  for this function and the values of  $g_I(\omega_A)$  and  $g_I(\omega_B)$  are listed. The last six columns give the coefficients for  $g_{\vec{r}}(\vec{r}, \omega)$ .

Green's Region-		Coefficients for imaginary parts						Coefficients for real parts							
function	type	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
# 1	1-H	8.9323	4.8548	0.3718	0.5821	0.1337	0.1018	-4.5658	-3.7561	-3.4480	0.3482	-0.0772	0.0453	0.0001	0.0046
(000)	2-G	-3.9765	0.3844	-0.1744	0.0193	-0.0094	0.0010			0.3492	2.5295	-0.0639	0.4095	-0.0108	0.0807
	3-K	13.4357	-2.4960	0.7368	-0.3241	0.1579	-0.0667			3.5231	-0.1822	-0.0194	0.0193	-0.0107	0.0029
# 2	1-J	-4.3657	2.6780	-0.4611	0.1670	-0.0446	0.0170	-0.9524	1.1198	-0.1316	1.1390	-0.1788	0.0457	-0.0143	0.0058
(110)	2-J	0.1165	1.4526	-0.4544	0.1520	-0.0445	0.0129			0.6352	-0.5437	-0.2808	-0.0233	-0.0514	-0.0040
	3-K	-3.8988	1.0858	-0.3563	0.1565	-0.0757	0.0318			-0.4987	-0.0766	0.0128	-0.0066	0.0033	-0.0004
# 3	1-H	-18.2183	4.0975	-1.7284	0.2305	-0.2027	0.0098	1.8448	-1.6298	0.8156	1.2628	-0.3166	0.0481	-0.0325	0.0030
(200)	2-G	0.3433	-1.7568	-0.2215	0.0177	-0.0132	0.0015			-0.4989	-0.8306	0.8685	-0.0535	0.1330	-0.0143
	3-K	1.0619	-2.3569	0.8621	-0.3843	0.1866	-0.0786			0.4396	0.6569	-0.0208	0.0057	-0.0013	-0.0021
# 4	1-J	-1.8615	4.0828	-1.3531	0.2953	-0.1021	0.0264	0.5110	-0.3882	0.2250	0.4765	-0.4821	0.1049	-0.0276	0.0120
(211)	2-J	0.1805	-0.8048	0.1660	-0.0430	-0.0183	0.0074			-0.0290	0.0362	0.3342	-0.0015	0.0280	0.0100
	3-K	5.6610	-0.1694	0.0856	-0.0351	0.0162	-0.0066			0.1750	-0.3462	-0.0171	0.0070	-0.0043	0.0017
# 5	1-H	3.7087	12.9434	-2.2111	1.0136	-0.1044	0.1209	-0.8096	0.0257	-0.1337	-0.0940	-0.5717	0.1625	-0.0284	0.0162
(220)	2-G	0.0679	0.4293	-0.4419	-0.0137	-0.0166	0.0018			-0.1052	-0.5095	-0.3895	0.1784	-0.0854	0.0324
	3-K	-8.7433	-1.6336	0.3245	-0.1485	0.0739	-0.0315			-0.2015	0.8525	0.0482	-0.0082	0.0060	-0.0038
# 6	1-J	-0.5964	4.1932	-2.1834	0.5038	-0.1810	0.0438	0.8332	0.6850	0.0760	-0.1783	-0.6129	0.1789	-0.0470	0.0209
(310)	2-J	0.0881	-0.2462	1.1116	-0.2442	0.0532	-0.0100			-0.0745	0.7738	-0.0781	-0.2871	0.0044	-0.0337
	3-K	-2.0821	1.9655	-0.6572	0.2903	-0.1417	0.0598			-0.0647	-0.2294	0.0011	-0.0048	0.0021	0.0011
# 7	1-H	8.6897	12.1623	-5.6278	1.7522	-0.5937	0.1606	-1.0251	-0.8251	-0.4246	-0.9046	-0.5298	0.3071	-0.0769	0.0400
(400)	2-G	-0.2591	0.5780	-0.6962	-0.4692	0.0304	-0.0085			-0.1725	-0.1229	-0.8083	0.4804	0.1244	0.0632
	3-K	3.8816	-10.0810	1.3079	-0.5994	0.2990	-0.1274			-0.0146	0.2839	0.2730	0.0163	-0.0084	-0.0005
# 8	1-J	-1.2217	2.4777	-2.5767	1.0743	-0.2508	0.0833	-0.1955	-0.4185	-0.0544	-0.1264	-0.2107	0.3247	-0.0868	0.0298
(321)	2-J	-0.1516	-0.0254	-0.3008	-0.0005	0.0175	0.0001			-0.0155	-0.0070	0.0273	0.1495	0.0276	0.0151
	3-K	5.3281	0.1572	0.3239	-0.1234	0.0598	-0.0252			0.1271	-0.2531	-0.0509	0.0042	-0.0036	0.0007
# 9	1-H	-10.5932	2.0655	-6.7533	0.9430	-0.5931	0.0190	1.0682	1.2956	0.1623	0.1930	-0.2025	0.2890	-0.0810	0.0215
(222)	2-G	0.3324	0.2716	0.8719	-0.1609	-0.0202	0.0023			-0.0673	0.2564	-0.3250	-0.5401	0.0388	-0.0732
	3-K	-16.4838	-0.4001	-0.7302	0.3051	-0.1462	0.0613			-0.4202	0.8214	0.1390	-0.0181	0.0114	-0.0029
#10	1-J	-0.8531	2.0282	-2.9333	1.3301	-0.3827	0.1184	-0.3356	-0.0537	-0.1823	-0.4081	-0.1709	0.3550	-0.1153	0.0455
(411)	2-J	-0.1954	0.5443	-0.3434	-0.1828	0.1448	-0.0327			-0.0842	-0.0755	-0.3677	0.1596	0.0143	-0.0298
	3-K	-1.6245	5.0450	0.2716	-0.0747	0.0356	-0.0149			-0.0508	0.2080	-0.2307	0.0119	0.0049	-0.0030
#11	1-H	4.8072	8.2487	-2.4161	5.0318	-1.1279	0.4533	-0.8083	0.8307	-0.1060	-0.1788	-0.0564	0.1280	-0.2305	0.0759
(422)	2-G	-0.0140	0.2919	0.0265	0.5599	-0.0034	-0.0310			0.1665	0.1119	0.2859	0.0241	-0.3185	0.0111
	3-K	-7.6684	-5.6308	-1.7537	0.4602	-0.2335	0.1002			-0.1201	0.1154	0.3684	0.0283	0.0014	0.0037
#12	1-J	-0.8226	2.2539	-1.9047	1.7015	-0.7839	0.1486	0.2429	-0.5074	-0.0131	-0.0598	-0.0798	0.1200	-0.2243	0.0795
(332)	2-J	0.0851	-0.1069	-0.1510	-0.3741	0.1995	-0.0490			-0.0858	0.0133	-0.1674	0.1783	0.1188	-0.0324
	3-K	5.2393	0.6328	0.5018	-0.2070	0.0996	-0.0420			0.1081	-0.1682	-0.0915	0.0038	-0.0030	-0.0002

TABLE VI. (Continued)

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts							
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
#13 (420) 1-H 2-G 3-K	-7.2476 0.0805 -2.4577	-1.2551 0.0733 -8.0138	-8.4561 0.2119 -0.1041	2.5054 -0.2340 -0.1139	-1.0138 -0.0042 0.0594	0.1939 -0.0144 -0.0258	0.4645	0.1129	0.0293 -0.0012 -0.1103	0.0207 0.0476 0.2238	0.1219 -0.1711 0.3237	0.3762 -0.1395 0.0205	-0.1535 0.1208 -0.0032	0.0471 -0.0209 0.0009
#14 (1330) 1-J 2-J 3-K	-1.5613 -0.0545 -0.5885	1.4212 -0.0271 2.9009	-2.5962 -0.2872 -0.8532	1.5779 0.8306 0.3439	-0.3646 -0.1713 -0.1752	0.1348 0.0322 0.0750	-0.6478	0.2886	-0.0092 0.1854 0.0686	0.0775 -0.1103 -0.2346	0.1306 0.5411 -0.0427	0.3969 0.0162 0.0005	-0.1292 -0.2254 0.0018	0.0439 0.0189 0.0020
#15 (440) 1-H 2-G 3-K	1.3562 -0.0381 5.7531	7.7540 -0.1550 -11.3766	0.6315 -0.0383 -0.9800	6.3235 -0.0844 -0.4769	-2.0535 -0.2731 0.1929	0.7914 0.0707 -0.0837	-0.1956	-0.5342	0.0504 0.0188 0.0847	0.0944 0.0113 -0.2108	0.0038 0.0832 0.3844	-0.1048 -0.1400 0.0957	-0.2866 0.1288 -0.0055	0.1273 0.1327 0.0018
#16 (431) 1-J 2-J 3-K	-0.9753 0.1361 -2.5991	1.7161 -0.0523 4.2373	-1.7274 0.2381 0.6583	1.9885 -0.0177 0.0055	-0.9204 -0.1476 0.0126	0.2300 0.0435 -0.0057	0.1168	0.1793	0.0653 -0.0048 -0.0800	0.1381 -0.0900 0.1879	0.1323 -0.0166 -0.1726	0.1299 -0.2121 -0.0351	-0.2410 0.0078 0.0036	0.1017 0.0261 -0.0026
#17 (620) 1-H 2-G 3-K	2.8636 0.0162 -4.1499	7.3526 0.0947 -2.2407	0.7876 0.0433 -4.5642	6.1205 -0.2196 -0.2019	-2.7716 -0.1466 0.0143	1.0790 -0.0162 -0.0079	-0.3800	0.2002	-0.0067 0.0369 -0.0532	0.0041 -0.0176 0.0692	0.0178 0.0821 0.1067	-0.1561 -0.1288 0.1925	-0.2608 -0.1461 0.0134	0.1669 0.0612 -0.0027
#18 (521) 1-J 2-J 3-K	-0.8573 -0.0384 4.7020	1.4257 -0.1146 0.5867	-1.7509 -0.1613 0.7434	2.0744 -0.1234 -0.2225	-1.0724 -0.0515 0.1251	0.2968 -0.0115 -0.0534	0.0138	-0.4478	0.0109 -0.0169 0.0821	0.0435 -0.1182 -0.1260	0.1545 -0.0152 -0.0923	0.1057 0.0225 -0.0038	-0.2459 0.0576 -0.0009	0.1255 0.0269 -0.0009
#19 (600) 1-H 2-G 3-K	-9.3746 0.2066 0.4128	-5.8539 -0.2539 -4.9767	5.8837 0.3697 -3.0544	5.4041 -0.1064 -0.6969	-2.1248 -0.5097 0.3613	0.8075 -0.0472 -0.1567	0.4923	-0.3378	0.2522 0.0524 -0.0739	0.5741 -0.3268 0.1535	0.6204 0.1481 0.0833	0.2042 -0.7212 0.1956	-0.2658 0.0763 0.0026	0.1162 0.1512 -0.0070
#20 (530) 1-J 2-J 3-K	-0.5082 0.0169 -0.3075	2.0382 -0.1720 3.6774	-1.0849 0.0782 -0.4423	1.9741 -0.3888 0.2312	-1.4026 0.5482 -0.1659	0.3817 -0.0242 0.0714	0.5877	0.0503	0.0402 -0.0740 0.0598	0.0439 0.1564 -0.0971	-0.0146 -0.1212 -0.1048	-0.1194 0.2941 -0.0114	-0.2705 0.1338 0.0048	0.1669 -0.1453 0.0021
#21 (800) 1-H 2-G 3-K	4.0271 -0.0938 2.5572	10.7228 0.1961 -7.8993	3.0349 -0.1115 0.3298	2.7471 0.1099 -3.9206	-4.3895 0.2108 0.3563	2.0165 -0.3990 -0.1655	-0.0846	-0.2278	-0.1479 -0.1118 -0.0179	-0.3520 0.2708 0.0110	-0.4848 -0.2807 0.0861	-0.4292 0.3275 0.0490	-0.0443 -0.4614 0.1387	0.2473 -0.0507 -0.0039
#22 (611) 1-J 2-J 3-K	-0.8965 0.1953 0.1651	1.0864 -0.2184 -1.8111	-1.2185 0.3245 4.0240	2.2602 0.0800 0.0559	-1.3570 -0.3220 0.0137	0.4600 0.1152 -0.0061	0.1104	0.1561	0.1257 0.0730 -0.0707	0.2911 -0.0817 0.1210	0.3129 0.1697 0.0749	0.0202 -0.3060 -0.1680	-0.2506 0.0438 -0.0079	0.1732 0.0831 0.0019
#23 (710) 1-J 2-J 3-K	-0.3664 0.1598 -0.4279	1.8187 -0.4327 3.4794	-0.3413 0.3840 -0.1638	1.8094 -0.6247 0.3523	-1.7899 0.3687 -0.1871	0.7242 0.2329 0.0804	0.7862	0.0386	0.1438 -0.0844 0.0517	0.2389 0.1488 -0.0671	0.0359 -0.1044 -0.0892	-0.2664 0.1037 -0.0264	-0.1909 0.3645 0.0011	0.2525 -0.0718 0.0026
#24 (510) 1-J 2-J 3-K	-1.2449 -0.1954 -0.4823	0.6469 0.2618 3.0343	-2.7221 -0.6114 -0.6916	2.0175 0.7868 0.3580	-0.6804 0.0246 -0.1864	0.2298 -0.0351 0.0802	-0.8398	0.2172	-0.1173 0.1799 0.0759	-0.1196 -0.1618 -0.2036	0.2663 0.4119 -0.2036	0.3756 0.2255 -0.0068	-0.1840 -0.2406 0.0015	0.0834 -0.0302 0.0024

TABLE VII. Green's functions for  $J_2/J_1 = -0.90$ . The Green's function is listed in column 1, by number and by the vector  $\hat{i}$ . The energy region is specified in column 2, along with the particular function ( $G \equiv g_I, H, J$ , or  $K$ ) being tabulated [Eq. (28)]. The coefficients  $c_0 \dots c_5$  for this function and the values of  $g_I(\omega_A)$  and  $g_I(\omega_B)$  are listed. The last six columns give the coefficients for  $g_R(\hat{i}, \omega)$ .

Green's Region- function type	Coefficients for imaginary parts						Coefficients for real parts							
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
# 1 (000)	-2.8021	43.6451	-11.1583	8.3784	-2.5837	1.6407	-5.4584	-3.2090	-5.1970	1.4686	-0.4471	0.2334	-0.0998	0.0594
2-G	-3.8178	0.9348	-0.4273	0.1495	-0.0664	0.0235			0.2013	2.4623	-0.3432	0.5215	-0.1196	0.1252
3-K	9.0699	-1.6284	0.4666	-0.2044	0.0997	-0.0421			2.9703	-0.1873	-0.0115	0.0151	-0.0086	0.0024
# 2 (110)	-16.6576	13.2347	-5.1237	2.3875	-1.1026	0.4482	-1.8916	0.9411	-0.8313	1.9453	-0.6158	0.2576	-0.1171	0.0869
2-J	-0.7513	2.8173	-1.5444	0.8268	-0.4109	0.1697			0.6316	-0.4999	-0.2759	0.0583	-0.0966	0.0751
3-K	-2.5837	0.7339	-0.2402	0.1052	-0.0508	0.0214			-0.3783	-0.0764	0.0134	-0.0067	0.0033	-0.0006
# 3 (200)	-75.6049	47.5276	-20.0793	9.3577	-4.2885	1.7813	1.2547	-1.3552	1.0675	2.1009	-0.7807	0.2698	-0.1550	0.0776
2-G	0.3009	-1.4427	-0.2737	0.1008	-0.0561	0.0204			-0.2716	-1.0183	0.9358	-0.1420	0.1444	-0.0166
3-K	0.6817	-1.5598	0.5864	-0.2623	0.1273	-0.0536			0.3374	0.5636	-0.0196	0.0045	-0.0008	-0.0019
# 4 (211)	-10.1878	16.0039	-7.2755	3.1404	-1.4597	0.5749	0.1812	-0.3213	0.2747	1.2192	-0.8794	0.3594	-0.1539	0.1144
2-J	0.2521	-0.8033	0.1144	0.1419	-0.1143	0.0584			0.0970	-0.1806	0.4152	-0.0612	0.0410	0.0244
3-K	3.7093	-0.1625	0.0625	-0.0257	0.0118	-0.0049			0.1389	-0.2908	-0.0112	0.0051	-0.0032	0.0013
# 5 (220)	-12.6051	69.1899	-25.8815	12.6710	-5.3924	2.3296	-0.9526	0.0607	-0.2576	0.4548	-0.9536	0.4292	-0.1771	0.1087
2-G	0.0688	0.4279	-0.4513	0.0471	-0.0436	0.0161			-0.0101	-0.5798	0.2683	0.1432	-0.0807	0.0403
3-K	-5.8376	-1.0800	0.2239	-0.1011	0.0530	-0.0214			-0.1893	0.7216	0.0406	-0.0071	0.0050	-0.0032
# 6 (310)	-5.4382	17.2001	-9.1942	3.9074	-1.8368	0.7127	1.4166	0.5353	0.5667	0.4135	-1.0433	0.4538	-0.1911	0.1438
2-J	0.6565	-1.3880	1.8820	-0.7587	0.2959	-0.1031			-0.0296	0.5403	0.1167	-0.3998	0.0975	-0.0915
3-K	-1.2720	1.3747	-0.4529	0.2012	-0.0983	0.0415			-0.0328	-0.1950	-0.0035	-0.0030	0.0012	0.0013
# 7 (400)	-0.8725	74.4839	-39.8330	16.7927	-8.6953	3.0790	0.4346	-0.6336	-0.1401	-0.9773	-1.0968	0.5925	-0.2540	0.1656
2-G	0.0712	0.2040	-0.2130	-0.6772	0.1661	-0.0506			-0.2878	0.1903	-0.8393	0.3717	0.1908	-0.0144
3-K	2.4433	-6.7579	0.9127	-0.4112	0.2055	-0.0877			-0.0298	0.2326	0.2380	0.0117	-0.0066	-0.0008
# 8 (321)	-6.3341	12.9578	-10.1788	5.2383	-2.2718	0.9120	0.0395	-0.3694	0.0320	0.1217	-0.6031	0.5857	-0.2534	0.1767
2-J	0.0407	-0.2038	-0.1489	-0.0751	0.0660	-0.0216			-0.0221	-0.0141	0.0421	0.1101	0.0374	-0.0021
3-K	3.5277	0.1140	0.2234	-0.0882	0.0426	-0.0179			0.1078	-0.2070	-0.0456	0.0036	-0.0029	0.0005
# 9 (222)	-53.3401	40.6743	-37.2980	15.3232	-7.3943	2.7309	1.3003	1.1241	0.4523	0.7045	-0.5952	0.5146	-0.2579	0.1323
2-G	0.3646	0.1018	0.8632	-0.2072	-0.0002	0.0041			-0.0169	0.1587	-0.1972	-0.5493	0.1031	-0.0879
3-K	-10.8818	-0.2446	-0.5074	0.2175	-0.1044	0.0437			-0.3515	0.6783	0.1205	-0.0149	0.0091	-0.0021
#10 (411)	-3.5333	12.7835	-11.4585	5.9403	-2.6731	1.0676	0.5199	-0.0062	0.0069	-0.4964	-0.6375	0.6455	-0.2875	0.2089
2-J	0.0171	0.0711	0.2473	-0.6717	0.4851	-0.2016			-0.1724	0.1371	-0.4318	0.1172	0.0580	-0.1162
3-K	-1.1689	3.2425	0.1506	-0.0483	0.0231	-0.0097			-0.0543	-0.1738	-0.1923	-0.0070	0.0032	-0.0022
#11 (422)	2.1940	51.1972	-31.6451	27.9325	-12.5576	4.9750	-0.6297	0.6952	-0.1751	-0.3446	-0.3508	0.3995	-0.4131	0.2439
2-G	-0.0313	0.2588	0.0190	0.4732	0.0172	-0.0510			0.1067	0.1889	0.1856	0.0751	-0.3096	0.0118
3-K	-4.8878	-3.6904	-1.2208	0.3307	-0.1675	0.0713			-0.0892	0.0712	0.3151	0.0259	0.0005	0.0036
#12 (332)	-4.4020	11.7771	-9.0299	6.7415	-3.6491	1.3232	0.6562	-0.4327	0.1295	0.0520	-0.3615	0.3787	-0.3807	0.2771
2-J	0.0818	-0.4090	0.2146	-0.7000	0.4741	-0.1974			-0.1070	0.0483	-0.1875	0.1417	0.1337	-0.1087
3-K	3.3953	0.4204	0.3716	-0.1495	0.0725	-0.0306			0.0815	-0.1227	-0.0831	0.0035	-0.0030	-0.0001

TABLE VII. (Continued)

Green's Region- function type	Coefficients for imaginary parts					Coefficients for real parts								
	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$g_I(\omega_A)$	$g_I(\omega_B)$	$c_0$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
#13 (420) 1-H 2-G 3-K	-33.9939 0.0933 -1.6012	28.2281 0.0077 -5.3286	-48.1420 0.2830 -0.0765	21.4967 -0.2735 -0.0692	-10.4144 0.0415 0.0377	3.9370 -0.0316 -0.0165	0.7401	0.1258	0.1374 -0.0473 -0.0937	-0.0507 0.1658 0.1703	-0.2342 -0.2092 0.2798	0.6607 -0.1122 0.0171	-0.3528 0.1150 -0.0028	0.1880 -0.0370 0.0007
#14 (330) 1-J 2-J 3-K	-7.1036 -0.2986 0.3444	9.3605 0.4815 1.9759	-10.7134 -0.8318 -0.5523	6.4431 1.2426 0.2332	-2.7096 -0.4869 -0.1186	1.1188 0.1649 0.0508	-1.0372	0.2094	-0.2149 0.1567 0.0664	0.0437 -0.1084 -0.1909	-0.1755 0.4423 -0.0390	0.6793 0.0864 -0.0012	-0.3106 -0.2656 0.0018	0.2104 0.0994 0.0016
#15 (440) 1-H 2-G 3-K	-4.3183 -0.0518 3.9363	37.5998 -0.1050 -7.4448	-20.4283 -0.1013 0.6868	35.9404 0.0423 -0.3270	-16.1113 -0.3506 0.1364	6.8502 0.1354 -0.0589	-0.6793	-0.4635	0.0102 0.0943 0.0802	0.2540 -0.1288 -0.1962	0.0986 0.2224 0.3233	0.1424 -0.2101 0.0830	-0.5177 0.1392 -0.0038	0.3151 0.1566 0.0009
#16 (431) 1-J 2-J 3-K	-5.1393 0.0638 -1.7502	8.8890 0.0757 2.7547	-9.1129 0.0734 0.4108	7.6612 0.1526 0.0060	-4.0454 -0.2734 0.0050	1.5371 0.1188 -0.0025	-0.1593	0.1663	0.0157 0.0152 -0.0651	0.1156 -0.0985 0.1507	0.0099 0.0135 -0.1412	0.4283 -0.1757 -0.0296	-0.4202 -0.0139 0.0034	0.3101 0.0658 -0.0022
#17 (620) 1-H 2-G 3-K	5.4928 -0.0533 -2.5798	34.5838 0.1891 -1.4318	-23.5717 -0.0953 -3.0978	37.4084 0.2915 -0.1122	-18.9829 -0.1446 0.0039	7.8986 -0.0178 -0.0024	-0.6591	0.1639	-0.1660 0.0482 -0.0325	0.2956 -0.0262 0.0306	0.1450 0.0784 0.0913	0.1340 -0.0394 0.1672	-0.5313 0.1919 0.0105	0.3666 0.0736 -0.0020
#18 (521) 1-J 2-J 3-K	-3.6049 -0.1495 3.0066	8.2741 0.1274 0.4111	-9.7196 -0.2813 0.5565	8.1040 -0.0993 -0.1669	-4.4141 -0.0138 0.0917	1.7051 -0.0359 -0.0393	-0.0219	-0.3837	-0.0697 -0.0577 -0.0592	0.2703 -0.0354 -0.0821	0.0235 -0.1195 -0.0843	0.4429 0.0856 -0.0049	-0.4370 0.0212 -0.0030	0.3425 0.198 -0.0010
#19 (600) 1-H 2-G 3-K	-8.6609 -0.0413 0.3091	-3.3421 0.2017 -3.3120	-53.7537 -0.1134 -2.0713	33.0118 -0.2964 -0.4432	-15.9127 -0.5855 0.2404	6.8436 -0.0264 -0.1048	-1.0236	-0.2551	-0.2380 0.0981 -0.0544	-0.2439 0.3279 0.0986	0.7066 0.1437 0.0773	0.6980 -0.4477 0.1686	-0.5030 -0.1669 0.0010	0.2947 0.2364 -0.0059
#20 (530) 1-J 2-J 3-K	-3.5025 0.1613 -0.2856	8.8485 -0.4287 2.4277	-7.3134 0.3677 -0.2288	8.3029 -0.6432 0.1591	-5.2159 0.6834 -0.1088	1.9531 -0.1079 0.0474	0.6879	0.0368	0.1577 -0.0491 0.0411	0.1746 0.0820 -0.0588	0.0785 -0.0766 -0.0918	0.1528 0.1829 -0.0120	-0.4840 0.1748 0.0033	0.4036 -0.1740 0.0019
#21 (800) 1-H 2-G 3-K	-17.1678 0.0871 1.9250	27.2609 -0.1918 -5.0929	6.6262 0.1940 0.1146	40.4135 -0.1653 -2.6096	-26.1008 -0.2764 0.2513	12.0504 -0.2704 -0.1111	0.6011	-0.2238	0.2178 -0.0242 0.0068	0.5520 0.0878 -0.0231	0.2615 -0.0527 0.0701	-0.5768 0.0771 0.0454	-0.5085 -0.1074 0.1202	0.5020 -0.1394 -0.0048
#22 (611) 1-J 2-J 3-K	-3.9415 -0.2336 0.2263	4.7917 0.5957 -1.2649	-9.4340 -0.5269 2.5560	9.1665 0.8038 0.0347	-5.1439 -0.7261 0.0017	2.0906 0.2873 -0.0011	-0.8102	0.1374	-0.1952 0.1025 -0.0440	-0.2431 -0.0976 0.0665	0.4471 0.1675 0.0744	0.4356 -0.1342 -0.1406	-0.4787 -0.1080 -0.0049	0.4067 0.1979 0.0014
#23 (710) 1-J 2-J 3-K	-3.9535 0.1068 -0.4749	3.7531 -0.2259 2.2663	-6.0034 0.0847 0.0119	9.5129 -0.0601 0.2345	-6.4100 -0.3221 -0.1199	2.6898 0.6312 0.0520	-0.2999	0.0464	0.0766 0.0843 0.0376	0.3869 -0.1672 -0.0373	0.7033 0.1928 -0.0690	0.0595 -0.1293 -0.0322	-0.5067 0.3699 0.0026	0.5185 0.1497 0.0011
#24 (510) 1-J 2-J 3-K	-3.3496 -0.5207 -0.2802	8.0895 0.8683 2.0917	-12.3663 -0.9935 -0.4263	7.6797 0.7644 0.2363	-3.5215 -0.1560 -0.1239	1.4474 -0.1589 0.0535	-0.6319	0.1406	-0.3637 0.0062 0.0599	-0.8621 0.1122 -0.1456	-0.1271 0.0320 -0.0546	0.7424 0.4237 -0.0053	-0.3705 -0.2922 0.0004	0.2770 -0.0654 0.0024

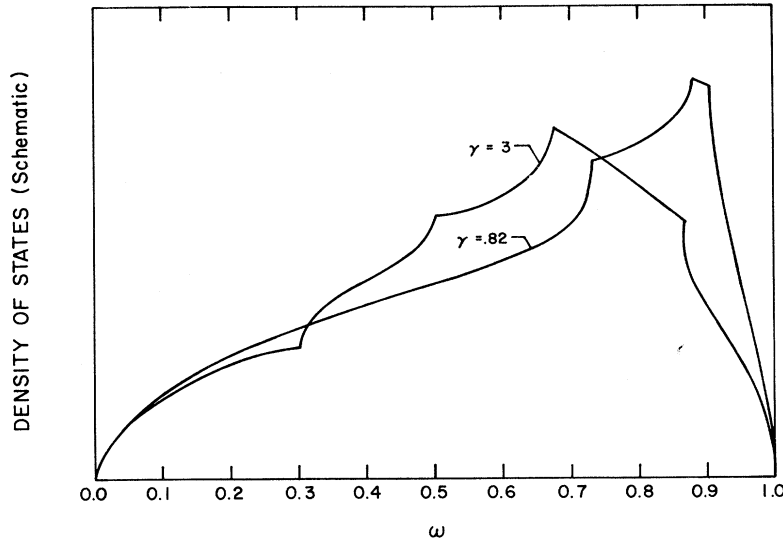


FIG. 3. Density of states,  $(-1/\pi) \times g_I(0, \omega)$ , (schematic) for positive values of  $\gamma = J_2/J_1$ .

$$\int_0^a \frac{(\omega')^{1/2} d\omega'}{\omega' - \omega} = \begin{cases} 2a^{1/2} - \pi |\omega|^{1/2} + \dots, & \omega < 0 \\ 2a^{1/2} - (4/a)\omega + \dots, & \omega > 0. \end{cases} \quad (22)$$

Clearly the square-root singularities appear on opposite sides of the Van Hove point in the real and imaginary parts, and have opposite signs. The factor of  $\pi$  cancels with the factor in Eq. (18), so that the square-root terms have the same coefficient in both real and imaginary parts of the Green's function.

#### IV. APPROXIMATE GREEN'S FUNCTIONS

Reference to Table I reveals that for  $-1 < \gamma < 0$  there are but two Van Hove singularities within the spin-wave band (in addition to the singularities at the bottom and top of the band). These singularities therefore divide the spin-wave band into three energy regions, bounded by singular points. Region 1 is the range  $0 < \omega < \omega_A$ ; region 2 is  $\omega_A < \omega < \omega_B$ ; and region 3 is  $\omega_B < \omega < 1$ .

The square-root singularities of the imaginary parts of the Green's functions fall on the low-energy side of  $\omega_A$  and on the high-energy side of  $\omega_B$  (see Table I). Hence region 1 has square-root singularities of  $g_I(\vec{r}, \omega)$  at each of its limits, as does region 3, but region 2 contains no square-root singularities whatever.

The polynomial approximants for the Green's functions have been calculated separately for each of the three energy regions.

The Green's functions with a square-root singularity at  $\omega_A$  have been approximated by a somewhat different procedure from those in which the singularity is suppressed. Consider those with the square-root singularity at  $\omega_A$  (i. e., those in which  $\vec{r}$  contains no odd coordinates). To improve the accuracy of the polynomial approximation we have

removed the square-root singularities analytically, and the polynomial fit in region 1 has been made to the function

$$H(\vec{r}, \omega) = (\omega_A - \omega)^{-1/2} [\omega^{-1/2} g_I(\vec{r}, \omega) - \omega_A^{-1/2} g_I(\vec{r}, \omega_A)]. \quad (23)$$

Given  $H(\vec{r}, \omega)$  from our tables, then the Green's function is to be computed from the inverse formula

$$g_I(\vec{r}, \omega) = \omega^{1/2} [\omega_A^{-1/2} g_I(\vec{r}, \omega_A) + (\omega_A - \omega)^{1/2} H(\vec{r}, \omega)]. \quad (24)$$

In region 2 the Green's function has been approximated directly, and in region 3 the square-root dependence has again been removed analytically, so that the function which is approximated is

$$K(\vec{r}, \omega) = (\omega - \omega_B)^{-1/2} [(1 - \omega)^{-1/2} g_I(\vec{r}, \omega) - (1 - \omega_B)^{-1/2} g_I(\vec{r}, \omega_B)]. \quad (25)$$

Inversely,

$$g_I(\vec{r}, \omega) = (1 - \omega)^{1/2} [(1 - \omega_B)^{-1/2} g_I(\vec{r}, \omega_B) + (\omega - \omega_B)^{1/2} K(\vec{r}, \omega)]. \quad (26)$$

For the 13 Green's functions with an odd coordinate of  $\vec{r}$  there is no square-root behavior at  $\omega_A$ , and in both regions 1 and 2 we have approximated the function

$$J(\vec{r}, \omega) = \omega^{-1/2} g_I(\vec{r}, \omega). \quad (27)$$

In region 3 we have again approximated the function  $K(\vec{r}, \omega)$ , defined in Eq. (25).

It was found empirically that sufficient accuracy could be obtained if we approximated the real parts of the Green's functions directly in all energy re-

gions, which we have done.

The polynomial approximants which we employ are six-term expansions in a Tchebyshev series:

$$g_I(\vec{r}, \omega) [\text{or } H, J, \text{ or } K] = \sum_{n=0}^5 c_n T_n(\omega), \quad (28)$$

where  $T_n(\omega)$  is the  $n$ th Tchebyshev polynomial:

$$\begin{aligned} T_0(\omega) &= 1, & T_1(\omega) &= \omega, \\ T_2(\omega) &= 2\omega^2 - 1, & T_3(\omega) &= 4\omega^3 - 3\omega, \\ T_4(\omega) &= 8\omega^4 - 8\omega^2 + 1, \\ T_5(\omega) &= 16\omega^5 - 20\omega^3 + 5\omega. \end{aligned} \quad (29)$$

The coefficients  $c_n$  of Eq. (28) are tabulated in Tables III-VII. Additional tables, for intermediate values of  $J_z/J_1$ , can be obtained from Callen.

The various approximation functions can be evaluated from the tabulated coefficients  $c_n$  and the definitions (29) of the Tchebyshev potentials. However, there is a simpler, and extremely convenient, evaluation procedure<sup>16</sup> based on the properties of Tchebyshev polynomials. Given the six coefficients  $c_n$  ( $n = 0, 1, \dots, 5$ ) we form a sequence of numbers  $a_m$  ( $m = 0, 1, \dots, 5$ ) by the rule

$$a_m - 2\omega a_{m+1} + a_{m+2} = c_m, \quad (30)$$

with

$$a_6 = a_7 = 0. \quad (31)$$

Then the sum is simply given by

$$\sum_{n=0}^5 c_n T_n(\omega) = a_0 - a_1 \omega. \quad (32)$$

Now it will be noted that solution of Eq. (30) is quite trivial, since for  $m = 5$  we have  $a_5 = c_5$ ; then  $a_4 = 2\omega c_5 + c_4$ , etc. Hence the  $a$ 's can be evaluated one by one until  $a_1$  and  $a_0$  are obtained.

The derivatives of the Green's functions are also obtainable through a similar algorithm. Again, given the six coefficients in Eq. (28) we form a sequence of numbers  $b_m$  ( $m = 0, 1, \dots, 5$ ) by the rule

$$b_m - 2\omega b_{m+1} + b_{m+2} = (m-1)c_m, \quad (33)$$

with

$$b_6 = b_7 = 0. \quad (34)$$

Then

$$\frac{d}{d\omega} \sum_{n=0}^5 c_n T_n(\omega) = b_1.$$

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