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Many-Electron Correlation Effects on the Metallic Interionic Potential*

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The self-consistent treatment of electron correlations in the electron liquid recently given by Singwi *et al.* is applied to calculations of the interatomic force constants in alkali metals. With the Ashcroft form of the pseudopotential, in which the only parameter is the core radius, reasonably good agreement with the force constants derived from neutron inelastic scattering data is obtained, confirming the results of a previous analysis of the phonon dispersion curves. The longitudinal sound velocities for the three main symmetry directions are calculated in the same scheme. Results for the effective interionic potential are presented and discussed.

I. INTRODUCTION

The essential ingredients entering the estimation of the effective interionic potential in simple metals are the form of the pseudopotential and the treatment of the screening. Several forms of the pseudopotential are available – some of which include nonlocal corrections – as well as various forms of the screening function, ranging from simple Hartree screening to more complicated forms incorporating exchange and correlation effects. Recent work of Singwi, Sjölander, Tosi, and Land[1] has presented an improved self-consistent treatment of correlations in the homogeneous electron liquid, which yields a reasonably accurate dielectric function through the whole range of wave vector and electron density of interest in the theory of metals. This screening function has been used in calculations of the lattice dynamics of the alkali metals by Price, Singwi, and Tosi.[2] It was found that good agreement with the phonon dispersion curves, as determined by neutron inelastic scattering experiments,[3–6] could be obtained with the one-parameter local pseudopotential suggested by Ashcroft,[7] with values for the parameter which are in good agreement (for Na and K) or consistent (for Li and Rb) with those derived from Fermi-surface and liquid-resistivity data.

In this paper we consider again the information which can be extracted from the neutron scattering data. The emphasis is now put on the interionic potential in r space, which is the basic starting point for the study of other properties of metals, such as lattice defects and liquid dynamics. As is well known, the potential enters the lattice dynamics through interatomic force constants for various orders of neighbors, and these can be obtained from the phonon data by a Born–von Kàrmàn analysis. We analyze directly these force con-

TABLE I. Interatomic force constants for sodium metal (dyn/cm) ($m^*/m = 1.00$, $r_c = 1.694$).

				Hubbard – Sham				
Shell	Type of atoms	Force constant	Hartree	$\xi = 1$	$\xi = 1 + \frac{2}{\pi k_F a_0}$	$\xi = 1 + \frac{4}{\pi k_F a_0}$	Singwi *et al.*	Experiment[a]
1	$\frac{1}{2}a(1, 1, 1)$	k_{xx}	1311	1299	1250	1243	1199	1178
		k_{xy}	1922	1306	1534	1621	1350	1320
2	$\frac{1}{2}a(2, 0, 0)$	k_{xx}	1507	389	822	992	453	472
		k_{yy}	-121	242	60	1	120	104
3	$\frac{1}{2}a(2, 2, 0)$	k_{xx}	3	-139	-58	-33	-66	-38
		k_{zz}	-9	39	7	-1	-2	0
		k_{xy}	12	-178	-65	-33	-64	-65
4	$\frac{1}{2}a(3, 1, 1)$	k_{xx}	35	-46	12	24	39	52
		k_{yy}	3	4	2	3	2	-7
		k_{xy}	12	-19	4	8	14	14
		k_{yz}	4	-6	1	3	5	3
5	$\frac{1}{2}a(2, 2, 2)$	k_{xx}	10	-9	5	8	13	17
		k_{xy}	10	-16	3	7	13	33

[a] From Woods *et al.*, Ref. 3. The experimental data refer to $T = 90$ °K.

stants in the alkali metals[3–6] in the same theoretical scheme used by Price *et al.*[2]; we also calculate the longitudinal sound velocities for the three main symmetry directions, and present the results for the interionic potential. The procedures for studying these properties have been discussed by Shyu and Gaspari.[8,9] Their work used the Hubbard-Sham approximation[10,11] to account for the exchange and correlation effects among the conduction electrons, but it was realized[9] that these effects are extremely important in determining the potential. This point is illustrated in this paper by analyzing the interatomic force constants in Na and K with the dielectric function of Singwi *et al.*[1] and with earlier dielectric functions.

II. THEORETICAL SCHEME AND RESULTS

Following Shyu and Gaspari,[8,9] the interionic potential $V(r)$ is derived from the total energy of the crystal which depends on the ionic configuration,

TABLE II. Interatomic force constants for potassium metal (dyn/cm) ($m^*/m = 0.93$,[a] $r_c = 2.226$).

				Hubbard – Sham				
Shell	Force constant	Hartree	$\xi = 1$	$\xi = 1 + \frac{2}{\pi k_F a_0}$	$\xi = 1 + \frac{4}{\pi k_F a_0}$	Singwi *et al.*		Experiment[b]
1	k_{xx}	782	829	793	787	784	797[c]	786
	k_{xy}	1128	876	1002	1044	914	916	895
2	k_{xx}	886	382	626	710	430	400	432
	k_{yy}	-58	135	27	-4	68	77	29
3	k_{xx}	-10	-96	-45	-32	-57	-59	-41
	k_{zz}	-4	22	3	-0	-0	-1	12
	k_{xy}	-6	-118	-49	-32	-57	-59	-54
4	k_{xx}	21	-22	13	18	27	31	2
	k_{yy}	1	1	1	1	1	1	-4
	k_{xy}	8	-9	5	7	10	11	1.8
	k_{yz}	3	-3	2	2	3	4	0.6
5	k_{xx}	7	-2	6	7	11	12	6
	k_{xy}	7	-5	6	7	12	13	4

[a] From Shaw, Ref. 16.

[b] From Cowley *et al.*, Ref. 4. The experimental data refer to 9 °K.

[c] Values in this column are calculated with $m^*/m = 1.00$ and $r_c = 2.242$.

TABLE III. Interatomic force constants for lithium metal (dyn/cm).

Shell	Type of atoms	Force constant	Singwi *et al.* $m^*/m = 1.00$ $r_c = 1.320$	$m^*/m = 1.09$[a] $r_c = 1.356$	$m^*/m = 1.19$[b] $r_c = 1.386$	$m^*/m = 1.30$ $r_c = 1.415$	Experiment[c]
1	$\frac{1}{2}a(1, 1, 1)$	k_{xx}	1894	2006	2103	2212	2320 ± 32
		k_{xy}	2229	2316	2385	2473	2520 ± 58
2	$\frac{1}{2}a(2, 0, 0)$	k_{xx}	893	870	827	807	678 ± 71
		k_{yy}	130	166	202	235	153 ± 48
3	$\frac{1}{2}a(2, 2, 0)$	k_{xx}	- 70	- 91	- 110	- 130	- 285 ± 28
		k_{zz}	1	- 0	- 2	- 4	110 ± 40
		k_{xy}	- 72	- 91	- 108	- 126	- 152 ± 46
4	$\frac{1}{2}a(3, 1, 1)$	k_{xx}	36	49	63	78	185 ± 33
		k_{yy}	4	4	4	4	- 116 ± 22
		k_{xy}	12	17	22	28	22 ± 27
		k_{yz}	4	6	7	9	- 113 ± 34
5	$\frac{1}{2}a(2, 2, 2)$	k_{xx}	10	15	21	26	158 ± 20
		k_{xy}	9	15	21	27	- 89 ± 57
6	$\frac{1}{2}a(4, 0, 0)$	k_{xx}	- 21	- 22	- 23	- 23	- 266 ± 63
		k_{yy}	1	1	1	2	8 ± 38
7	$\frac{1}{2}a(3, 3, 1)$	k_{xx}	- 3	- 5	- 7	- 9	- 3 ± 18
		k_{zz}	- 1	- 1	- 1	- 1	- 8 ± 12
		k_{xy}	- 2	- 4	- 7	- 9	- 22 ± 13
		k_{xz}	- 1	- 2	- 2	- 3	30 ± 27

[a] From Shaw, Ref. 16.
[b] From Weaire, Ref. 17.
[c] From Smith *et al.*, Ref. 5. The experimental data refer to 98 °K.

$$V(r) = \frac{Z^2e^2}{r} - \frac{2Z^2e^2}{\pi}\int_0^\infty G(q)\,\frac{\sin qr}{qr}\,dq\ , \tag{1}$$

where the second term represents the ion-electron-ion contribution. The function $G(q)$, introduced by Cochran,[12] is given in terms of the bare-ion pseudopotential form factor $w(q)$ and of the dielectric function[13] $\epsilon(q)$ as follows:

$$G(q) = \left|\frac{w(q)}{-4\pi Ze^2/\Omega q^2}\right|^2\left(1 - \frac{1}{\epsilon(q)}\right). \tag{2}$$

TABLE IV. Interatomic force constants for rubidium metal (dyn/cm).

Shell	Force constant	Singwi *et al.* $m^*/m = 1.00$ $r_c = 2.470$	$m^*/m = 0.89$[a] $r_c = 2.450$	$m^*/m = 2.430$ $r_c = 2.430$	Experiment[b]
1	k_{xx}	674	659	644	614 ± 8
	k_{xy}	764	767	763	741 ± 9
2	k_{xx}	324	372	395	455 ± 19
	k_{yy}	72	59	51	1 ± 12
3	k_{xx}	- 54	- 52	- 49	- 33 ± 6
	k_{zz}	- 1	- 0	1	6 ± 7
	k_{xy}	- 53	- 52	- 49	- 39 ± 6
4	k_{xx}	29	24	20	...
	k_{yy}	1	0	0	...
	k_{xy}	11	9	8	...
	k_{yz}	4	3	3	...
5	k_{xx}	12	10	9	...
	k_{xy}	13	11	10	...

[a] From Shaw, Ref. 16.
[b] From Copley *et al.*, Ref. 6. The experimental data refer to 120 °K.

TABLE V. Interatomic force constants for cesium metal (dyn/cm).

Shell	Force constant	Singwi *et al.* $m^*/m = 1.00$ $r_c = 2.70$	$m^*/m = 0.85$ $r_c = 2.65$	$m^*/m = 0.78$ $r_c = 2.60$
1	k_{xx}	578	543	512
	k_{xy}	666	639	604
2	k_{xx}	313	327	305
	k_{yy}	57	46	41
3	k_{xx}	- 49	- 43	- 38
	k_{zz}	- 1	0	0
	k_{xy}	- 48	- 43	- 38
4	k_{xx}	25	19	17
	k_{yy}	0	0	0
	k_{xy}	10	7	6
	k_{yz}	3	3	2
5	k_{xx}	10	8	7
	k_{xy}	12	9	8

TABLE VI. Sound velocities in the alkali metals (10^5 cm/sec).

Direction of propagation			[100]		[110]		[111]	
Metal	m^*/m	r_c	Theory	Experiment	Theory	Experiment	Theory	Experiment
Li	1.00	1.320	5.283	...	6.823	6.69^a	7.264	...
	1.09	1.356	5.360		6.943		7.395	
	1.19	1.386	5.423		7.047		7.511	
Na	1.00	1.694	2.771	2.895^b	3.576	3.628^b	3.807	...
K	1.00	2.242	2.161	2.185^c	2.733	2.71^c	2.899	...
	0.93	2.226	2.164		2.723		2.885	
Rb	1.00	2.470	1.488	1.360^d	1.865	1.645^d	1.974	1.710^d
	0.89	2.450	1.494		1.856		1.961	
	0.82	2.430	1.500		1.851		1.954	
Cs	1.00	2.70	1.176	1.092^e	1.470	1.41^e	1.556	...
	0.85	2.65	1.154		1.435		1.517	
	0.78	2.60	1.123		1.400		1.480	

[a] From Nash and Smith, Ref. 19. The experimental values refer to 78 °K.

[b] From Diederich and Trivisonno, Ref. 21. The experimental values refer to 78 °K.

[c] From Marquardt and Trivisonno, Ref. 20. The experimental values refer to 4.2 °K.

[d] From Roberts and Meister, Ref. 22. The experimental data refer to 80 °K.

[e] From Kollarits and Trivisonno, Ref. 23. The experimental data refer to 78 °K.

A detailed discussion of these functions has been given previously.[2] We adopt the analytic form suggested by Ashcroft[7] for the bare-ion pseudopotential,

$$w(q) = -(4\pi Z e^2/\Omega q^2)\cos q r_c a_0 , \tag{3}$$

where $r_c a_0$ is an adjustable parameter representing an effective radius of the ion core. On the other hand, the dielectric function is given by the expression

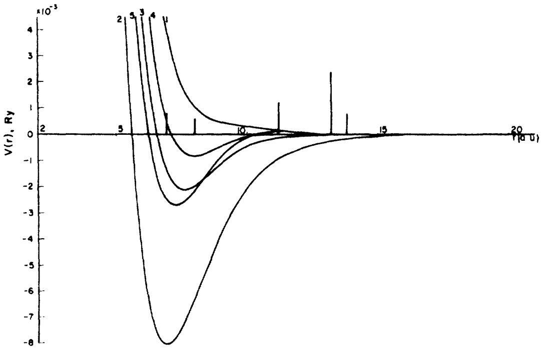

FIG. 1. Interionic potential $V(r)$ as a function of the interionic separation r in sodium metal ($m^*/m = 1.00$, $r_c = 1.694$). Curve 1, Hartree screening; curve 2, Hubbard-Sham screening (HS) with $\xi = 1$; curve 3, HS with $\xi = 1 + 2/\pi k_F a_0$; curve 4, HS with $\xi = 1 + 4/\pi k_F a_0$; curve 5, self-consistent screening. The vertical bars indicate the positions of the first few shells of neighbors.

$$\epsilon(q) = 1 + \frac{Q_0(q)}{1 - f(q)Q_0(q)} , \tag{4}$$

where $Q_0(q)$ is the Lindhard electron polarizability times $-4\pi e^2/q^2$,

$$Q_0(q) = \frac{k_{FT}^2}{q^2} F\left(\frac{q}{k_F}\right), \tag{5}$$

with

$$F(x) = \frac{1}{2} + \frac{4 - x^2}{8x} \ln \left| \frac{2 + x}{2 - x} \right| \tag{6}$$

and

$$k_{FT}^2 = \frac{m^*}{m} \frac{4k_F}{a_0 \pi} . \tag{7}$$

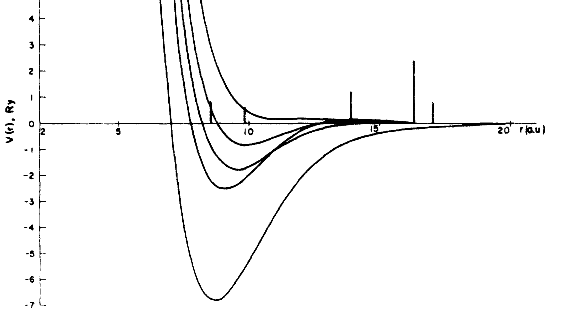

FIG. 2. Interionic potential for potassium metal ($m^*/m = 0.93$, $r_c = 2.226$). The curves are labeled as in Fig. 1.

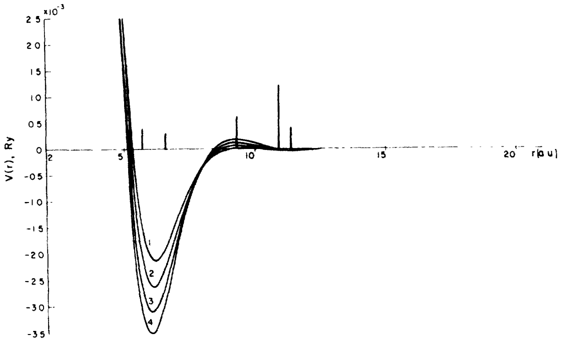

FIG. 3. Interionic potential for lithium metal, based on self-consistent screening. Curve 1, $m^*/m = 1.00$ and $r_c = 1.320$; curve 2, $m^*/m = 1.09$ and $r_c = 1.356$; curve 3, $m^*/m = 1.19$ and $r_c = 1.386$; curve 4, $m^*/m = 1.30$ and $r_c = 1.415$.

Here we have included band-structure effects on the conduction electrons by introducing an effective mass m^*. The function $f(q)$ in Eq. (4) accounts for exchange and correlation effects among the conduction electrons; it has been evaluated by Singwi *et al.*[1] in a self-consistent treatment, and the values appropriate to the electron density and the effective mass for each metal can be obtained from Ref. 1 by the procedure discussed previously.[2] For purposes of comparison, in Na and K we have considered also the Hartree approximation $[f(q) = 0]$, as well as the approximation of Hubbard-Sham, where

$$f(q) = \tfrac{1}{2} q^2 / (q^2 + \xi k_F^2). \tag{8}$$

Several alternative values for the parameter ξ have been considered; specifically, $\xi = 1$ as in the original work of Hubbard,[10] $\xi = 1 + 4/\pi k_F a_0$ as in the work of Sham,[11] and $\xi = 1 + 2/\pi k_F a_0$ as suggested by Animalu.[14] The latter value is not very different for Na and K from the value $\xi \simeq 2$ obtained by Geldart and Vosko[15] by requiring that the compressibility sum rule be satisfied for the homogeneous electron liquid.

The experimental interatomic force constants are various linear combinations of the radial force constant $d^2V(r)/dr^2$ and the tangential force constant $(1/r)\, dV(r)/dr$, with $V(r)$ given in Eq. (1). The results of this calculation are reported in Tables I–V for the various alkali metals. The core radius was adjusted so as to give best agreement between the force constants calculated with the dielectric function of Singwi *et al.*[1] and the experimental force constants. For Li and Rb, the calculations were repeated for a number of values of m^*, varying r_c in each case. The following remarks can be made:

(i) The force constants calculated with the self-consistent dielectric function and the optimized values of r_c are in reasonably good agreement with the experimental values, especially for the first few shells of neighbors, with some notable exceptions (e.g., $k_{yy}^{(2)}$ for potassium and rubidium). The degree of agreement is very sensitive to the value of r_c and, to a lesser extent, to the value of m^* (see, e.g., the last two columns of calculated force constants in Table II). It is rewarding, in this respect, that closest agreement in Li metal is found for $m^*/m \simeq 1.3$, in good agreement with the value calculated recently by Shaw and Smith.[18]

(ii) The optimized values of r_c agree closely with those obtained by Price *et al.*[2] by fitting the phonon dispersion curves. This should obviously be so, but, since the two calculations were carried out independently, it gives us confidence in the internal self-consistency of the analysis of the data. The comparison of these values of r_c with those obtained from other metallic properties has already been discussed by Price *et al.*[2] We may here recall their suggestion that the Ashcroft pseudopotential appears to be rather a good concept for Na and K but less so for the other alkali metals.

(iii) While we have not optimized r_c separately for the various dielectric functions, the discrepancies illustrated in Tables I and II and the variation of the results with r_c are such that the agreement with the experimental force constants for the first few shells would remain poorer. Furthermore, since at the density of metallic sodium the self-consistent $f(q)$ is quite close to the expression of Eq. (8) with $\xi = 1 + (2/\pi k_F a_0)$ for $q \lesssim k_F$, the large wave-vector behavior of $f(q)$ appears to play a relevant role.

With the values of r_c determined above, we have calculated the longitudinal sound velocity in

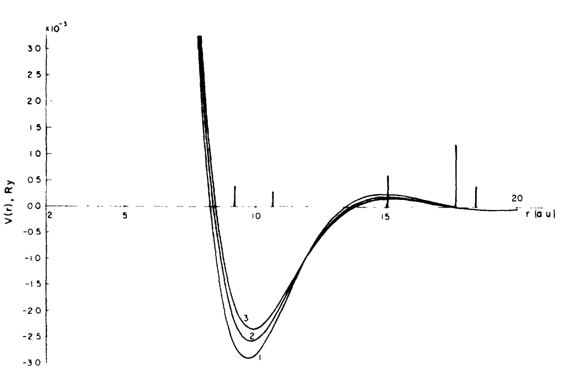

FIG. 4. Interionic potential for rubidium metal, based on self-consistent screening. Curve 1, $m^*/m = 1.00$ and $r_c = 2.470$; curve 2, $m^*/m = 0.89$ and $r_c = 2.450$; curve 3, $m^*/m = 0.82$ and $r_c = 2.430$.

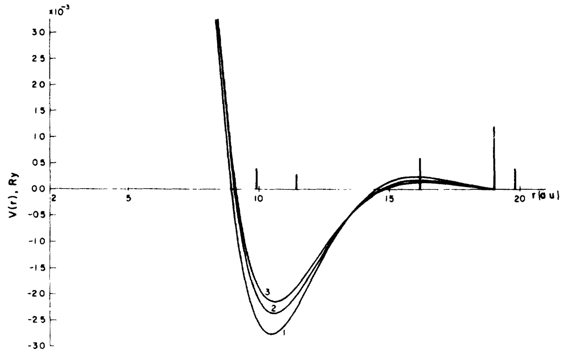

FIG. 5. Interionic potential for cesium metal, based on self-consistent screening. Curve 1, $m^*/m = 1.00$ and $r_c = 2.70$; curve 2, $m^*/m = 0.85$ and $r_c = 2.65$; curve 3, $m^*/m = 0.78$ and $r_c = 2.60$.

alkali metals for the three main symmetry directions, following Shyu and Gaspari.[8] The results are reported in Table VI and compared with the available experimental values.[19-23] Good agreement is obtained.

The detailed behavior of the interionic potential $V(r)$ in the alkali metals is illustrated in Figs. 1–5. Our neglect of Born-Mayer terms[24] in Eq. (1) is justified *a posteriori*, by noting that the potential becomes positive at distances much larger than the Born-Mayer diameter (3.3 Å in Na metal, as compared with a Born-Mayer diameter of 2.5 Å for Na^+ in sodium halides[25]). In the case of Na and K, we show the results obtained with the different dielectric functions. The influence of the exchange and correlation effects on the nature and the behavior of the interionic potential is clearly a major one,[9] e.g., in the Hartree approximation one fails to reproduce the minimum of the potential in the region between first and second neighbors that the neutron scattering data indicate. The discrepancies between the potentials based on the Hubbard-Sham approximation and those obtained from the self-consistent approximation would, of course, be somewhat less dramatic if the core radius were optimized in each case.

III. DISCUSSION

We have here determined the interionic potential in alkali metals by a fitting of the force constants derived from the neutron scattering data, based on the self-consistent dielectric function of Singwi *et al.*[1] and the one-parameter pseudopotential of Ashcroft.[7] The results of the fitting of the phonon dispersion curves[2] are fully confirmed, and good agreement is found with the sound velocities determined by ultrasonic techniques.

A relevant question concerns the validity and the reliability of the interionic potential determined from the neutron scattering data. The theoretical analysis of the lattice-dynamics problem shows that the phonon curves are affected by secondary effects,[2] namely, anharmonic effects, solid-state effects in the screening function, and possible nonlocal corrections to the pseudopotential. Thus, the potential obtained by fitting these data is not necessarily applicable to the study of other metallic properties. Even if one overlooks these difficulties, it appears that such a potential is, in certain aspects, not very reliable. To test its reliability, one may compare its two gross features, namely, the depth of the minimum and the repulsive-part intercept of the r axis, for different fittings of the phonon dispersion curves. A four-parameter fit of the measured dispersion curves along the three main symmetry directions in Na has been given by Schneider and Stoll,[26] using the Hubbard-Sham dielectric function with $\xi = 1 + 2/\pi k_F a_0$. The quality of the fit is comparable with that of the one-parameter fit obtained by Price *et al.*,[2] using the self-consistent dielectric function, for those and other directions. Yet, while the potentials obtained from these two fits cross the r axis at approximately the same distance, the potential of Schneider and Stoll[27] is deeper at the minimum by about 1×10^{-3} Ry. On the other hand, the potential derived by Cochran[28] is shallower than ours, again by about 1×10^{-3} Ry. A sizable uncertainty in the depth of the potential well is perhaps not surprising, since the neutron scattering data yield only the first and the second derivative of the potential at the positions of the first few neighbors.

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Compton Scattering and Electron Momentum Density in Beryllium*

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Compton-scattered x-ray spectra were measured for three orientations of a beryllium single crystal. The reduced profiles were analyzed in terms of the electron momentum distribution. Observed anisotropies can be explained qualitatively in terms of the geometry of the Fermi surface and are in qualitative agreement with earlier positron and x-ray data. The present results show high-momentum components among the valence electrons which are not revealed in the positron experiment nor accounted for by available calculations. In the process of reducing the data to obtain the momentum distribution of the valence electrons, detailed consideration was given to the effects of binding upon the Compton scattering by the core electrons.

I. INTRODUCTION

The energy distribution of inelastically scattered (Compton) x rays is of interest, in part because of its close relationship to the momentum-space electron wave functions in the scatterer. A measurement of the scattered x-ray energy spectrum provides a direct insight into the electron momentum distribution and (with single crystals) its anisotropies.

Earlier Compton work[1] and a positron annihilation study[2] on beryllium had indicated the existence of a number of anomalies, that is, of characteristics in the momentum profiles which were not predicted by the then available theoretical representations. These were variously attributed to such circumstances as (a) grossly altered 1*s* electron wave functions (compared to the free-atom state), (b) unexpectedly large high-momentum components among the conduction electrons, (c) inaccuracy of the scattering models, (d) uncertainties in the positron wave functions, (e) many-body effects, (f) experimental inaccuracies, and (g) inaccuracy in the data-reduction procedures. We have undertaken a repetition of the Compton measurements, striving for an accuracy which would allow a narrowing of the uncertainties.

II. EXPERIMENTAL TECHNIQUE

Measurements were made for three crystallographic directions on a single cube-shaped beryllium crystal; the x-ray scattering vector, $\vec{k}=\vec{k}_f$