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EFFECT OF MAGNETIC FIELD ORIENTATION ON POSITRON ANNIHILATION IN POTASSIUM †

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The angular correlation of positron annihilation radiation in potassium metal is found to be dependent on the magnetic field orientation. The experimental results are interpreted using the spin-density-wave model of the electronic structure of potassium metal.

It has been proposed by Overhauser that the electronic ground state of potassium metal is a spin-density-wave (SDW) state[1] and that the wave vector, $\vec{Q}$, of the SDW will tend to align itself with a sufficiently large magnetic field.[2] A SDW distorts the spherical Fermi surface to a lemon shape having conical points with the major axis of the lemon along the $\vec{Q}$ direction. At an angle θ the coincidence rate $N(\theta)$ is approximately proportional to the cross-sectional area $A(\vec{k})$ of the Fermi surface, where $\vec{k}=mc\theta\hat{k}/\hbar$. Thus one would expect that the angular correlation of positron annihilation radiation from a SDW state would differ from the nearly parabolic angular correlation obtained from a spherical Fermi surface. In particular, if areas perpendicular to $\vec{Q}$ are measured, the angular correlation should show a smearing of the break at the "Fermi angle" caused by the electrons in the conical points for which $\vec{k}$ is larger than the free-electron $\vec{k}_F$. If areas parallel to $\vec{Q}$ are measured, the angular correlation at zero angle should be larger than the free-electron value, since the extremal area parallel to $\vec{Q}$ through the conical points is larger than the corresponding free-electron extremal area. This approximate view is slightly modified when the wave functions appropriate to a SDW are considered. If the electron wave function is[1]

$$\psi_k = \sin\varphi \exp(i\vec{k}\cdot\vec{r}) - \cos\varphi \exp[i(\vec{k}+\vec{Q})\cdot\vec{r}],$$

where $\sin\varphi$ is slightly less than one everywhere in the Fermi surface except near the points where $\sin\varphi \to 2^{-1/2}$, and $\cos\varphi$ is nearly zero except near the points where $\cos\varphi \to 2^{-1/2}$, then $N(\theta)\propto A(\vec{k})$ when $\vec{Q}$ is parallel to the axis of the apparatus, and $N(\theta)\propto A(\vec{k})\sin^2\varphi$ when $\vec{Q}$ is perpendicular to the axis. Thus, the difference in the coincidence rates near zero angle is somewhat larger than predicted by the simple approximation where $N(\theta)\propto A(\vec{k})$ for both orientations of $\vec{Q}$. Near θ_F, however, the smearing of the break when $\vec{Q}$ is perpendicular to the axis is about half that expected from the approximate model. In addition, there will be a small contribution to the angular correlation beyond θ_F. Both of these effects are due to the substantial mixing of states $\vec{k}$ and $\vec{k}+\vec{Q}$ near the points of the Fermi surface. Figure 1 shows the angular correlations calculated on the basis of a SDW model for $\vec{Q}$ parallel and perpendicular to the axis of the apparatus.[3] At zero angle the coincidence rate for $\vec{Q}$ parallel is 2.4% larger that that for $\vec{Q}$ perpendicular.

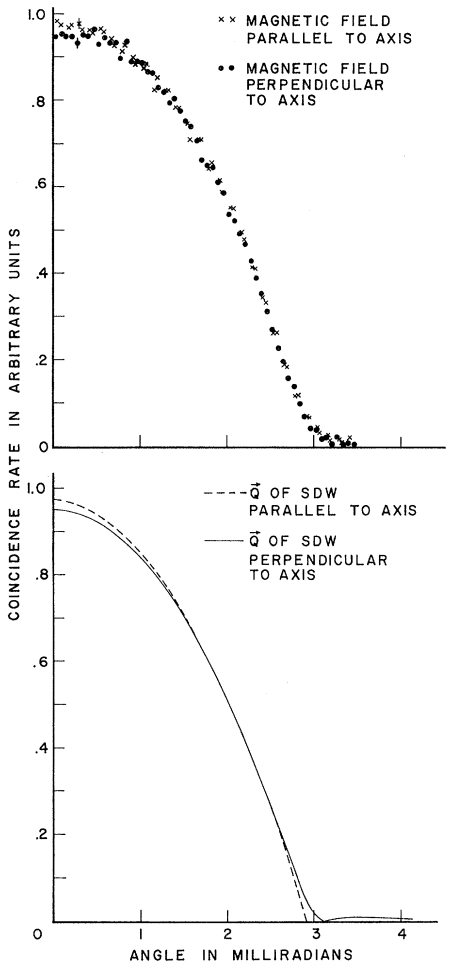

FIG. 1. Experimental and calculated SDW[3] angular correlations of positron annihilation radiation in potassium metal. Experimental points are shown with a Gaussian background subtracted. Errors of the two points shown are representative of the errors of all points.

The angular correlations were measured using the standard long-slit apparatus with an angular resolution of 0.25 mrad. (A discussion of similar apparatus is given by Stewart, Shand, and Kim.[4]) The Co^{58} positron source was plated on a 0.000 25-in.-thick copper foil which was held in the center of an aluminum mold. High-purity potassium metal was cast around the foil and slowly cooled below the melting point. The entire assembly was then cooled to 4.2°K and held at that temperature for the duration of the experiment. The potassium sample was essentially strain free since the thermal contraction of potassium is greater than that of either aluminum or copper, and potassium does not adhere readily to either. The angular correlation was first measured with a 12-kG magnetic field perpendicular to the axis of the apparatus, and then it was measured with the magnetic field parallel to the axis. The magnet had large axial holes through the pole caps to avoid attenuation and scattering of the annihilation radiation when the magnetic field was parallel to the axis.

The experimental angular correlations for the two magnetic field orientations are shown in Fig. 1. A Gaussian background has been subtracted from both, and they were normalized at all points between 0 and 3 mrad. Even though the positron source was mounted on a very thin copper foil, a significant part of the annihilations occurred in the foil. The background from these annihilations obscures both the small portion of the angular correlation beyond θ_F and the smearing of the break at θ_F in the case where the magnetic field is perpendicular to the axis. The background has little effect on the shape of the angular correlations near zero angle, since the angular correlation from copper is flat in that region.[5] Near zero angle the angular correlation measured with the magnetic field parallel to the axis is an average of $2.3 \pm 0.8\%$ larger than that measured with the magnetic field perpendicular to the axis. While it is clear that the difference between the two angular correlations is consistent with SDW theory, the close numerical agreement must be regarded as fortuitous, since the normalization depends on the points away from zero angle where differences in the background rates could cause the normalization to be in error. The problems caused by normalization and background can be reduced by examining the ratio of the coincidence rates as a function of angle near zero angle. The smoothed experimental ratios and the expected variations in the ratio for the free-electron and SDW[3] models are shown in Fig. 2. Between 0 and 1.5 mrad, where the ratios are most reliable, there is a clear decrease of the ratio with increasing angle as predicted by the SDW model.

While unknown geometrical effects caused by rotation of the magnet cannot be conclusively ruled out as the cause of the change in the angular correlations, the close agreement between the experimental results and the predictions of SDW theory does provide evidence that the electronic ground state of potassium metal is a magnetically orientable SDW. Further

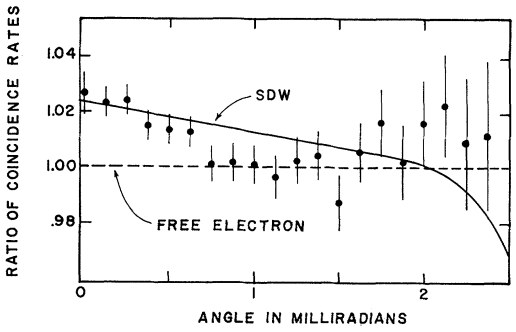

FIG. 2. Experimental and calculated SDW[3] ratios of coincidence rates versus angle. Normalization of the ratios is arbitrary.

work, with the objective of reducing the various backgrounds, is in progress.

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PHASE TRANSITION OF HARD-SQUARE LATTICE WITH SECOND-NEIGHBOR EXCLUSION*

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This report presents some evidences indicating a possible fluid-solid phase transition for a two-dimensionally infinite hard-square "lattice gas." The pair interaction between molecules is an infinite repulsion due to the finite geometrical size of molecules such that the nearest and second-nearest neighbors of a site occupied by the center of a molecule cannot be occupied by other molecules (see the shaded area in the inset of Fig. 1).

Recently, Kramers and Wannier's matrix method has been used rather extensively to investigate occurrence of an order-disorder transition on the square lattice which occurs when the interaction is limited to nearest-neighbor exclusion.[1,2] Bellemans and Nigam[3] applied it also to square-lattice systems with interactions extending up to third neighbors. With second-neighbor exclusion, their studies on semi-infinite strips ($M\times\infty$) with width M ranging from 2 to 12 led to no definite conclusions regarding a thermodynamic phase transition for the limiting $\infty\times\infty$ system, although a first-order phase transition seemed to be ruled out.

In an attempt to determine the location and nature of this transition, therefore, we made similar studies with width extending up to $M=18$ with periodic boundaries. The following thermodynamic variables are calculated: the reduced pressure P^* [$\equiv P/(kT)$; the lattice constant is taken to be the unit of length, k = Boltzmann's constant; T = absolute temperature], the reduced density ρ^* [$\equiv\rho/\rho_0$; ρ_0 = the density at close packing = 0.25], $d\rho/d\mu^*$ [μ^* = the reduced chemical potential $\equiv\mu/(kT)$], and $d^2\rho/d\mu^{*2}$. In the calculation, the quantity $u\equiv z/(1+z)$ [z $\equiv$ activity $=\exp(\mu^*)$] is used as an independent variable. In this way, the interval $(0,\infty)$ for z is mapped onto a finite interval $(0,1)$ for u. Furthermore, equal increments in u give approximately equal increments in the density except at the high-density end.

These thermodynamic variables are expressed exactly in terms of the eigenvalues λ_i and the corresponding eigenvectors Ψ_i of a particular submatrix B of the symmetric Kramers-Wannier matrix A which is required in computing the thermodynamic properties of a finite $M\times N$ system. The use of the CDC 6600 for this stage of the calculation gives an accuracy of 9 digits or better for all the thermodynamic