[2]P. K. Hansma and H. P. Broida, Appl. Phys. Lett. 32, 545 (1978).
[3]R. K. Jain, S. Wagner, and D. H. Olson, Appl. Phys. Lett. 32, 62 (1978).
[4]S. L. McCarthy and J. Lambe, Appl. Phys. Lett. 30, 427 (1977).
[5]S. L. McCarthy and J. Lambe, Appl. Phys. Lett. 33, 858 (1978).

Exact Solution of Some Nonseparable Band Problems

Bill Sutherland
Department of Physics, University of Utah, Salt Lake City, Utah 84112
(Received 22 November 1978)

In this paper I introduce and solve a series of band problems in higher dimensions which are generalizations of the one-dimensional Kronig-Penney model. These problems are nonseparable, in contrast to the three-dimensional model in the original Kronig-Penney work. In two dimensions the band problem is on a triangular lattice, while in three dimensions the band problem is on a body-centered-cubic lattice.

In an early and classic paper,[1] Kronig and Penney illustrated the Bloch theory of electrons in periodic potentials by a simple one-dimensional model. The potential assumed was a regular array of δ-function potentials. The resulting calculation is manageable and instructive, for it illustrates the expected band structure. Undoubtedly this simple and transparent example has helped to introduce generations of solid state physicists to an understanding of the three-dimensional band theory.

In fact, the original Kronig and Penney paper also introduced a three-dimensional band problem, by taking as a potential the sum of one-dimensional potentials in three orthogonal directions. The resulting potential then has cubic symmetry. Since this potential is separable, one easily constructs the solution from the corresponding one-dimensional solution.

In this paper I introduce and solve a series of band problems—generalizations of the Kronig-Penney model—which are not separable. The potentials are again δ functions; but in two dimensions, the lattice is a triangular lattice, while in three dimensions the lattice is bcc. To my knowledge, this is the first example of the exact solution of a nonseparable (higher-dimensional) band problem.

I wish to consider certain band problems in d dimensions,

$$-\sum_{\alpha=1}^{d}\frac{\partial^2\Phi}{\partial y_\alpha^{\,2}}+V(\vec{y})\Phi=\epsilon\Phi. \tag{1}$$

The potential V is periodic, $V(\vec{y}+\vec{\varphi})=V(\vec{y})$, with $\vec{\varphi}=n_\alpha\vec{\varphi}_\alpha$. $\vec{\varphi}_\alpha$ are the primitive lattice vectors, and repeated Greek indices are summed from 1 to d. The overhead arrow will always designate a d-component vector.

The particular problems I wish to consider will be derived from a corresponding periodic one-dimensional N-body system, where $N=d+1$:

$$-\sum_{j=1}^{N}\frac{\partial^2\Psi}{\partial x_j^{\,2}}+V\Psi=E\Psi. \tag{2}$$

The potential V is a sum of pair potentials,

$$V=\sum_{i>j=1}^{N}v(x_i-x_j), \tag{3}$$

each periodic with period unity, i.e., $v(x+n)=v(x)$ for integer n.

To exhibit the correspondence, I make a change of variables from x's to new variables y's, where

$$y_N=\sum_{j=1}^{N}x_j/\sqrt{N}$$

is the center-of-mass coordinate. I assume that the change of variables is given by an orthogonal transformation Λ: $y=\Lambda^{-}x$, $x=\Lambda y$ ($\Lambda^{\dagger}=\Lambda^{-1}$). Note also that $\Lambda_{jN}=N^{-1/2}$. Thus

$$\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^{\,2}}=\frac{\partial^2}{\partial y_N^{\,2}}+\sum_{\alpha=1}^{d}\frac{\partial^2}{\partial y_\alpha^{\,2}}. \tag{4}$$

The particle separations are

$$\begin{aligned}x_i-x_j&=(\Lambda_{ik}-\Lambda_{jk})y_k\\&=(\Lambda_{i\alpha}-\Lambda_{j\alpha})y_\alpha\equiv\lambda_{ij}{}^{\alpha}y_\alpha.\end{aligned} \tag{5}$$

(Repeated Latin indices are to be summed from 1 to N.)

One then sees that Eq. (2) separates, and I

write a solution as

$$\Psi(x)=\exp(iky_N)\Phi(\vec{y}). \tag{6}$$

Thus, I make the identification with corresponding quantities in the band problem of Eq. (1):

$$V(\vec{y})=\sum_{i>j=1}^{N} v(\lambda_{ij}{}^{\alpha}y_{\alpha}),\quad \epsilon=E-k^2. \tag{7}$$

Recall now that the original V was periodic in the x's, so that $V(x_j+n_j)=V(x_j)$, with n_j integers. But if $x_j\to x_j+n_j$, then the y's are transformed as $y_\alpha\to y_\alpha+n_j\Lambda_{j\alpha}$. As a function of the y's, then, $V(y)$ is periodic with primitive lattice vectors $[\vec{\varphi}_j]_\alpha=\Lambda_{j\alpha}$.

These N lattice vectors are of course not all independent, since

$$\sum_{j=1}^{N}\vec{\varphi}_j=0.$$

Also, one sees that

$$\begin{aligned}&\vec{\varphi}_j\cdot\vec{\varphi}_k=-1/N,\quad j\neq k;\\ &\vec{\varphi}_j\cdot\vec{\varphi}_k=1-1/N,\quad j=k.\end{aligned} \tag{8}$$

Thus, I conclude that in d dimensions, the $d+1$ lattice vectors point to the corners of a regular "$(d+1)$-ahedron"; that is, a line segment, equilateral triangle, tetrahedron, etc.

Recall that the potential is a sum of $N(N-1)/2=d(d+1)/2$ terms, each periodic, and each the identical function of different variables as in Eq. (7). Define the planes of the potential to be the $(d-1)$-dimensional surfaces given by $x_i-x_j=\text{integer}=\vec{\lambda}_{ij}\cdot\vec{y}$. Thus the planes are perpendicular to the vectors $\vec{\lambda}_{ij}$. But one sees that $\vec{\varphi}_k\cdot\vec{\lambda}_{ij}=\delta_{ki}-\delta_{kj}$. Thus all the $d-1$ independent $\vec{\varphi}_k$ $(k\neq i,j)$ lie within the $\vec{\lambda}_{ij}$ potential plane, or parallel to it. This is sufficient to determine the plane.

In d dimensions, then, the volume of space bounded by potential planes is an irregular $(d+1)$-ahedron with vertices at the points

$$\sum_{j=1}^{k}\vec{\varphi}_j,\quad k=1,\ldots,N.$$

For $d=2$, the potential planes form a triangular lattice. For $d=3$ the potential planes form a body-centered-cubic lattice; the intersections of potential planes are lines connecting all nearest and next-nearest neighbors.

I finally remark that although the many-body system of Eq. (2) is periodic, the wave functions Ψ are not to be chosen periodic. This would be the case, for instance, if the particles were charged and confined to a loop threaded by a magnetic flux. By Bloch's theorem, one may choose wave functions so that

$$\Psi(x_j+n_j)=\exp(i\lambda_j n_j)\Psi(x_j), \tag{9}$$

or

$$\Phi(\vec{y}+\vec{\varphi})=\exp(in_j\lambda_j)\Phi(\vec{y})\equiv e^{i\vec{\varphi}\cdot\vec{\kappa}}\Phi(\vec{y}). \tag{10}$$

The reciprocal lattice vector $\vec{\kappa}$ is given by $\vec{\kappa}=\lambda_j\vec{\varphi}_j$.

I henceforth restrict myself in this paper to a particular two-body potential—the δ-function potential—given by $v(x)=2c\delta(x)$. Thus the potential V vanishes everywhere except on the potential planes. It then is convenient to partition the whole space into regions designated by $n=(n_1,\ldots,n_N)$, n_j an integer; where

$$n_j-n_k+1>x_j-x_k>n_j-n_k-1.$$

Note that the regions are overlapping, and n and $n+\alpha$ represent the same region.

Designate the region $0=(0,\ldots,0)$ as the fundamental region (f.r.), and observe that in the f.r. $|x_j-k_k|<1$ and $|x_j-\Sigma x_l/N|<1$. Any other region n may be mapped one-to-one onto the f.r. by $x\to x'=x-n$. I here use the vector notation $x=(x_1,\ldots,x_N)$. The wave function $\Psi(x)$ in region n will be denoted by $\Psi(x;n)$. The f.r. is further partitioned into $N!$ sectors labeled by a permutation Q of N objects—$Q=(Q1,Q2,\ldots,QN)$—where $x_{Q1}<x_{Q2}<\ldots<x_{QN}$. The sector (n,Q) of the region n will be defined as that portion of the region n mapped onto the sector Q of the f.r. by the previous mapping. In each sector Q of the f.r. I seek a solution $\Psi_{0Q}(x)$ in a form known as Bethe's *Ansatz*[2]:

$$\begin{aligned}\Psi_{0Q}(x)\sum_P A_0(Q,P)\exp\Big[i\sum_{j=1}^{N}x_{Qj}k_{Pj}\Big]\\ \equiv\sum_P A_0(Q,P)\exp(ix_Qk_P).\end{aligned} \tag{11}$$

Here $P=(P1,\ldots,PN)$ is a permutation of N objects.

It has been shown by McGuire[3] and by Yang[4] that it is possible to satisfy consistently the boundary conditions imposed by the δ-function potential *within* the f.r. There remain $N!$ free parameters, which may be chosen to be either $A_0(Q,I)$ or $A_0(I,P)$, or possibly some other convenient choice. Such a solution I designate $\Psi_0(x|A_0)$.

In any other region n, I seek a solution of the form

$$\Psi(x;n)=\Psi_0(x-n|A_n). \tag{12}$$

Clearly this choice for the wave function satisfies Eq. (4) with energy

$$E=\sum_{j=1}^{N} k_j^2$$

within the region n. It then remains to match the wave function in the overlap region.

I now look at the region of overlap by considering a point x in sector Q of the f.r.; by definition $x_{Q1}<\ldots<x_{QN-1}<x_{QN}$. The point x' of the region $n_j=-\delta_{j,QN}$, mapped onto this point under the inverse map $x'\to x=x'-n$, is given by $x_{Q1},\ldots,x'_{QN-1},x_{QN}'=x_{Q1},\ldots,x_{QN-1},x_{QN}^{-1}$.

Clearly the point x' lies within the region n; I claim that it also lies within the f.r. For $1>x_{QN}-x_{Qj}>0$ $(j\neq N)$; but then

$$0>x_{QN}-1-x_{Qj}=x_{QN}'-x_{Qj}'>-1 \quad (j\neq N).$$

Thus x' lies within the f.r. I determine the sector Q' by noting that

$$x_{QN}'<x_{Q1}'<\ldots<x_{QN-1}'$$
$$\equiv x_{Q'1}<x_{Q'2}<\ldots<x_{Q'N}.$$

Thus, $(Q'1,Q'2,\ldots,Q'N)=(QN,Q1,\ldots,QN-1)$, and Q' is a cyclic permutation of Q.

If one then equates terms in the wave functions for the two overlapping regions in the region of overlap, one finds

$$\exp(ik_{PN})A_n(Q,P)\exp(ik_P x_Q)$$
$$=A_0(Q',P')\exp(ik_{P'}x_{Q'}). \quad (13)$$

Q and Q' are related as before.

For equality of the exponential factors, one sees that P' must be the same cyclic permutation of P that Q' is of Q. One finally then concludes that

$$A_0(Q',P')=\exp(ik_{PN})A_n(Q,P), \quad (14)$$

with $Q'j=Qj-1$, $P'j=Pj-1$, and $n_j=-\delta_{jQN}$.

One sees that these two regions overlap in all $(N-1)!$ sectors such that QN is fixed but the other Qj are arbitrary. For consistency, then one must verify that a scattering of particles $Qj-1$ and Qj followed by a cyclic permutation of QN gives the same amplitude as a cyclic permutation of QN followed by a scattering of particles $Q'j=Qj-1$ and $Q'j+1=Qj$. One can easily verify this term by term.

For interpretation as a band problem, it is convenient to choose the wave function to obey Bloch's theorem, $\Psi(x+n)=e^{i\lambda n}\Psi(x)$. With the previous choice for n, we have

$$\Psi_0(x|A_n)=\exp(-i\lambda_{QN})\Psi_0(x|A_0). \quad (15)$$

Upon combining Eqs. (14) and (15), one finds

$$A_0(Q',P')=\exp[i(k_{PN}-\lambda_{QN})]A_0(Q,P). \quad (16)$$

Q,P are related to Q',P' as before.

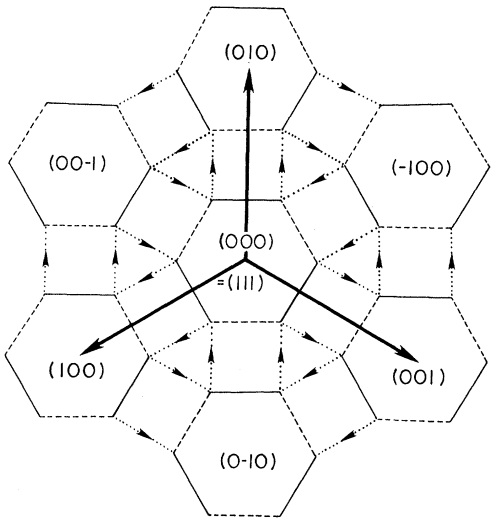

FIG. 1. The connections between amplitudes for the two-dimensional band problem. The solid line indicates a T_{12} scattering, a dashed line indicates a T_{23} scattering, while a dotted line indicates a cyclic permutation.

As an example, consider the case of $N=3$. I treat a band problem, and so I choose the c.m. momentum to be zero: $k_1+k_2+k_3=0$. The sectors (n,Q) I represent as points, and within a region n the sector Q will be connected to sector $Q'=Q1,\ldots,Qj+1,Qj,\ldots,QN$ by an appropriate two-body scattering matrix $T_{j,j+1}$. Further, cyclic permutations of appropriate sectors will connect neighboring regions.

These connections are shown graphically in Fig. 1. One is to imagine the graph extending indefinitely as an infinite tiling of the plane. The consistency relations verify that a determination of a set of amplitudes $A_n(Q,P)$, with P variable, around a closed path leads to an identity.

As promised, I have presented and solved a series of d-dimensional band problems. Explicit determination of the band structure requires determining the eigenvalues of d commuting matrices of size $(d+1)!$ by $(d+1)!$. In a subsequent publication I will present explicit expressions for these eigenvalues in the form of coupled algebraic equations. Such a determination enables

one to treat thermodynamic systems, i.e., systems with finite density of particles, corresponding to mixtures of particles with different charges moving on a loop threaded by a magnetic flux. In this way one can investigate the occurrence of superconductivity.

This work was supported in part by the National Science Foundation under Grant No. DMS77-08474.

[1]R. DeL. Kronig and W. G. Penney, Proc. Roy. Soc. London, Ser. A 130, 499 (1931).
[2]H. Bethe, Z. Phys. 71, 205 (1931).
[3]J. McGuire, J. Math. Phys. (N.Y.) 5, 622 (1964).
[4]C. N. Yang, Phys. Rev. Lett. 19, 1312 (1967).

Specific-Heat Anomalies at the Lower Critical Temperature in Reentrant Ferromagnetic Superconductors

H. B. MacKay, L. D. Woolf, and M. B. Maple
Institute for Pure and Applied Physical Sciences, University of California, San Diego, La Jolla, California 92093

and

D. C. Johnson
Corporate Research Laboratories, Exxon Research and Engineering Company, Linden, New Jersey 07036

(Received 29 January 1979)

A spike-shaped heat-capacity anomaly has been identified at the lower superconducting-to-normal transition temperature T_{c2} of the magnetic superconducting system $(Er_{1-x}Ho_x)$-Rh_4B_4. This anomaly can be distinguished from the feature due to long-range magnetic ordering and indicates that the transition at T_{c2} is thermodynamically of first order.

The discovery of the destruction of superconductivity at a second lower critical temperature T_{c2} in the ternary rare-earth (RE) compounds $ErRh_4B_4$[1] and $Ho_{1.2}Mo_6S_8$[2] and in various pseudo-ternary RE compounds[3-7] due to the onset of long-range ferromagnetic order has prompted recent theoretical[8-13] and experimental[14,15] interest in this new phase transition. In this Letter we present evidence that a spike-shaped anomaly in the heat capacity of these compounds, which can be distinguished from the broader background due to magnetic ordering alone, is associated with the superconducting-to-normal state (SC-N) transition at T_{c2}.

The feature in the heat capacity near T_{c2} for $ErRh_4B_4$ is presented in Fig. 1 which shows much more detail than originally reported in Ref. 1. There is a distinct sharp spike-shaped anomaly that peaks at 0.93 K, within the narrow range of T_{c2} values as inferred from ac electrical resistance and magnetic susceptibility measurements (0.91–0.94 K),[1,16] which appears to be superimposed on a broader feature due to the long-range ordering of the Er^{3+} magnetic moments. The latter feature begins at ~ 1.5 K, close to the onset of precursor scattering at 1.2 K observed in neutron diffraction experiments.[17]

To establish that the heat-capacity spike is as-

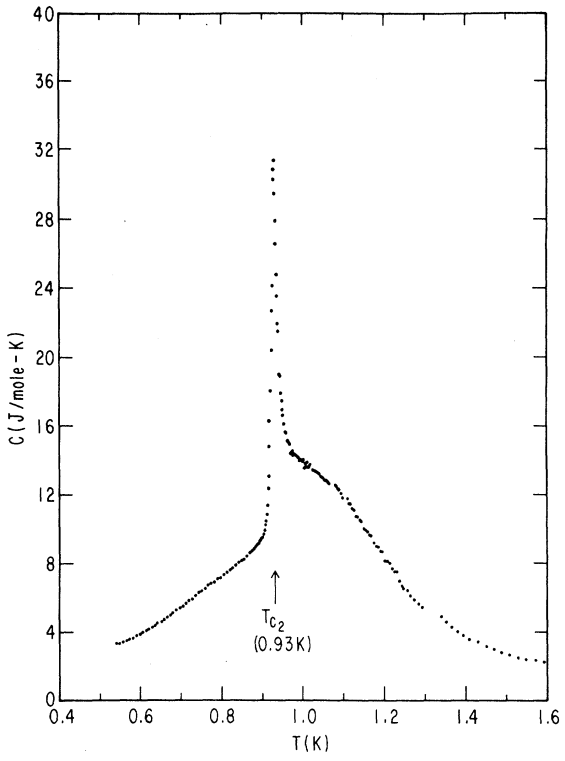

FIG. 1. Heat capacity C vs temperature T near T_{c2} for $ErRh_4B_4$. The arrow indicates the SC-N transition temperature as measured by ac magnetic susceptibility.