# Kinetic phenomena in the Hubbard model

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Scattering of a delocalized vacancy (vacancion) by spin fluctuations in a completely polarized system is considered within the framework of the Hubbard model involving an almost half-filled band. An exact value of the scattering amplitude is obtained for a simple cubic or plane square lattice. For "inelastic" scattering involving a shift of the flipped spin, the cross section in the long-wave limit of the three-dimensional problem does not depend on the quasimomentum of the vacancion. In the two-dimensional case the "$v^{-1}$ law" is satisfied. It is shown that bound states may exist in the case of scattering of a vacancion by an isotopic impurity. The temperature dependences of spin diffusion are ascertained for both the case of thermally activated vacancies and the case of low temperatures with a specified vacancy density.

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## 1. INTRODUCTION

The Hubbard model has invariably attracted the attention of the theoreticians for two reasons. First, its simplicity makes possible a sufficiently complete theoretical investigation, including the derivation of a number of exact results. Second, there are real physical systems, such as quantum Fermi crystals, the solid phases of $He^3$, dense layers of $He^3$ on various substrates) and some magnetic dielectrics (semiconductors) which are well described by this model, thus permitting its experimental verification.

The Hubbard model comprises a system of fermions localized in lattice sites, with repulsion between two particles situated in one site. Its Hamiltonian is[1]

$$\hat{\mathcal{H}}=-\sum_{ij\sigma} t_{ij}c_{i\sigma}{}^{+}c_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{1.1}$$

where $c_{i\sigma}^{+}$ and $c_{i\sigma}$ are the creation and annihilation operators of a particle with spin $\sigma = \pm 1/2$ at site $i$; $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$ is the operator of the activation number in site $i$, $U$ is the repulsion potential, and $t_{ij} > 0$ is the matrix element of the transition from site $j$ to site $i$.

Interesting results were obtained for this model, in the limit of the almost half-filled band, when the number of particles $N_e$ is somewhat smaller than the number of sites $N$ in the lattice so that $N - N_e \ll N$. In particular, it was shown[2] that when the repulsion is infinite and the transition of the particles (bounded by the nearest neighbors) are possible only as a result of vacancy motion, the ground state for a primitive cubic (pc), body centered cubic lattice (bcc), and planar quadratic and hexagonal lattices is a state with fermagnetic ordering of the spins. The excited states are magnons—spin fluctuations moving exclusively on account of vacancion transitions. The width of their band is proportional to the density of the vacancies $x$. The ground state for a planar triangular (pt) and hexagonal close-packed (hcp) lattice is an unsaturated ferromagnet.[3]

Because the spin motion is effected only via vacancion transitions, there is a close connection between the magnetic structure of a system and the character of the vacancy motion. By itself, a vacancy that violates the spatial symmetry of the lattice becomes delocalized in the form of a Bloch wave and moves as a quasiparticle—vacancion—with a band width proportional to $t_{ij} = t$. However, in a lattice of particles with spin it violates also the magnetic symmetry. The rearrangement of the spins, which takes place when a vacancion moves, leads to indirect exchange via the vacancion and to establishment of the aforementioned magnetic ground-state structures. In turn, it is found[4] that the bandwidth in the case of vacancion motion through a paramagnetic or antiferromagnetic ordered lattice is much narrower than in the case of ferromagnetic ordering. It is clear from the foregoing that in a magnetically polarized ideal lattice the vacancion scattering center can be any magnetic defect, such as a magnon or localized spin fluctuation. In Ref. 5 was considered the problem of renormalization of the effective mass of the vacancion on account of scattering by centers of the second type. The obtained narrowing of the vacancion band agrees qualitatively with the results of Refs. 4 and 6.

In the Hubbard model with finite repulsion, the existence of magnons is due to two independent causes: the motion of the spins over the lattice on account of exchange with a vacancy (vacancion magnons) and their tunneling proper. As $U \to \infty$ there remain only the vacancion magnons. The purpose of the present paper is to obtain several exact relations for the transport processes in the Hubband model with infinite repulsion. By way of illustration of the results we confine ourselves to polarized quantum crystals, without specifying in greater detail the polarization method. The width of the vacancion band is here $\Delta_v \gg J$, where $J$ is the exchange integral of the $He^3$ atoms in the crystal. This inequality makes the Hubbard model applicable. The existence of the magnetic polarons predicted in this model, which are formed by the vacancies,[7,8] is apparently confirmed by the experimental data.[9] We note that similar phenomena take place in magnetic semiconductors of the type EuTe, EuSe (ferrons—see Ref. 10).

The kinetic coefficients of the considered problem contain the cross section for scattering of a vacancion by a flipped spin (spin diffusion) or by an impurity. It is necessary to distinguish, generally speaking, between two cases. In

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thermal activation of vacancies, the activation potential (the bottom of the energy band) is high enough and the vacancion gas obeys Boltzmann statistics. Scattering of vacancions by a flipped spin (impurity) is rare, and there is no correlation between the scattering acts. Under these conditions one can consider the initial states to be prepared in the form of a plane wave—vacancion and a localized scattering center, whose motion as a result of numerious scatering acts is Brownian. In the other case, if the vacancy density is regarded as specified and constant ("frozen-in vacancies"), degeneracy of the Fermi gas of the vacancions takes place when the temperature is lowered. Only vacancions with momenta in the region of the thermal smearing of the Fermi surface can be scattered with change of momentum. On the other hand, the influence of the filled Fermi background manifests itself in the fact that the localized scattering center (flipped spin or impurity) is transformed into a quasistatic excitation with a lifetime limited by the successive collisions with vacancions with energy $\varepsilon \sim \varepsilon_F \pm \delta$ ($\varepsilon_F$ is the Fermi energy and $\delta \sim T$). In particular, at the temperature $T=0$ such magnons move without damping. Their spectrum is determined in Ref. 2. By way of the initial state, it is now natural to choose two plane waves corresponding to a magnon (impurity quasiparticle) and a vacancion, and consider their scattering by each other. The problem of the mobility of the magnon (impurity) is then reduced to the problem of the mobility of Boltzmann particles in a Fermi gas, which was considered earlier by a number of workers.[11-13]

In Sec. 2 we obtain exact amplitudes of the described scattering by a flipped spin (magnon) for primitive cubic and planar quadratic lattices. On their basis, the temperature dependences of the spin-diffusion coefficient are obtained and the limits of applicability of the previously obtained results[11-24] to our case are discussed. The scattering by an isotopic impurity is considered in the conclusion.

It must be noted that with increasing temperature, as the Fermi degeneracy of the vacancions is lifted, the magnon band is destroyed. Therefore at $T \gg \varepsilon_F$ the vacancion scattering center is certainly well localized. The transition from the magnon picture to scattering by the localized spin fluctuations is described by the change of the real part of the mass operator of the vacancion magnon, and will be studied in a separate article.

Of physical interest from the point of view of applications to quantum crystals is the temperature $T \ll \Delta_v$. The vacancions are in this case close to the bottom of the band, where their spectrum is quadratic. The exposition is carried out in a system of units with $\hbar = 1$.

## 2. SCATTERING AMPLITUDE

We consider a Hubbard model with infinite repulsion. The Hamiltonian (1.1) reduces to the tunnel Hamiltonian

$$\hat{H} = -tP \sum_{ij\sigma}{}' c_{i\sigma}^{+} c_{j\sigma} P, \tag{2.1}$$

where the prime denotes summation over the nearest neighbors; $P$ is a projection operator that selects states with not more than one particle per site. A state with one vacancy in a system is described by the wave function $\Psi(\mathbf{r}_v, \alpha_{\mathbf{r}_v})$,[2-4] where $\alpha_{\mathbf{r}_v}$ denotes the set of spin configurations of the system with vacancy at the point $\mathbf{r}_v$. For the case when all but one of the spins are ferromagnetically polarized, the spin configuration is specified by indicating the coordinate of the flip spin $\mathbf{r}_i$, i.e.,

$$\Psi(\mathbf{r}_v, \mathbf{r}_i) = c_{v\uparrow} c_{i\downarrow}^{+} c_{i\uparrow} |f\rangle,$$

where $|f\rangle$ is a fully ferromagnetic state.

The operator (2.1) acts on the functions $\Psi(\mathbf{r}_v, \mathbf{r}_i)$ in the following manner:

$$\hat{H}\Psi(\mathbf{r}_v, \mathbf{r}_i) = -t \sum_{\rho} \Psi(\mathbf{r}_v+\rho, \mathbf{r}_i), \quad \mathbf{r}_v+\rho \neq \mathbf{r}_i, \quad \mathbf{r}_v \neq \mathbf{r}_i,$$
$$H\Psi(\mathbf{r}_v, \mathbf{r}_i) = -t\Psi(\mathbf{r}_i, \mathbf{r}_v), \ \mathbf{r}_v+\rho = \mathbf{r}_i, \tag{2.2}$$

where $\rho$ is the lattice translation vector. To eliminate from the equations the unphysical situation $\mathbf{r}_v = \mathbf{r}_i$, we must add the following condition:

$$H\Psi(\mathbf{r}_v, \mathbf{r}_i) = 0, \ \mathbf{r}_v = \mathbf{r}_i. \tag{2.3}$$

The stationary Schrödinger equation

$$H\Psi(\mathbf{r}_v, \mathbf{r}_i) = (E-E_0)\Psi(\mathbf{r}_v, \mathbf{r}_i), \tag{2.4}$$

where $E_0$ is the energy of the localized vacancy, is written in the following form:

$$\sum_{\rho} \{\Psi(\mathbf{r}_v+\rho, \mathbf{r}_i)(1-\delta_{\mathbf{r}_v, \mathbf{r}_i})$$
$$+[\Psi(\mathbf{r}_i, \mathbf{r}_v) - \Psi(\mathbf{r}_v+\rho, \mathbf{r}_i)]\delta_{\mathbf{r}_v-\mathbf{r}_i+\rho, 0}\} = -\lambda\Psi(\mathbf{r}_v, \mathbf{r}_i), \tag{2.5}$$

where $\lambda = (E-E_0)/t$ and $\delta_{ij}$ is the Kronecker delta. Equation (2.5) does not determine the function $\Psi(\mathbf{r}, \mathbf{r})$ at $\lambda = 0$. It must be additionally defined by the condition

$$\Psi(\mathbf{r}, \mathbf{r}) = 0, \ \lambda = 0. \tag{2.6}$$

We shall consider the stationary problem of scattering for the Hamiltonian (2.1). It is convenient to seek the solution in the momentum representation. Separating the relative motion of the vacancion and of the flip spin, we introduce the Fourier transform of the function $\Psi(\mathbf{r}_v, \mathbf{r}_i)$ from the following relation:

$$\Psi(\mathbf{r}_v, \mathbf{r}_i) = \left(\frac{a}{2\pi}\right)^{2d} \iint \Psi_{\mathbf{q}}(\mathbf{k}) \exp[i\mathbf{k}(\mathbf{r}_v-\mathbf{r}_i)] \exp(i\mathbf{q}\mathbf{r}_i)\, d^d k\, d^d q. \tag{2.7}$$

Here $a$ is the lattice constant, $d$ is the dimensionality of the problem; the integration is over the first Brillouin zone. Using the Fourier expansion of the Kronecker delta and taking into account the conditions (2.3) and (2.6), we obtained from (2.5) after a number of changes in notation the Schrödinger equation in the momentum representation:

$$\Psi_{\mathbf{q}}(\mathbf{k})[\lambda+\lambda(\mathbf{k})] = \sum_{\rho} [1-e^{i(\mathbf{k}-\mathbf{q})\rho}]\Psi_{\mathbf{q}}(\rho), \quad \lambda(\mathbf{k}) = \sum_{\rho} e^{i\mathbf{k}\rho}, \tag{2.8}$$

where $\Psi_{\mathbf{q}}(\rho)$ is the Fourier transform of the function $\Psi(\mathbf{r}_v - \mathbf{r}_i = \mathbf{R}, \mathbf{r}_i)$ with respect to the variable $\mathbf{r}_i$. A general solution of (2.8) with account taken of the continuity of the spectrum in the considered problem can be written in the form

$$\Psi_{\mathbf{q}}(\mathbf{k})=[\lambda+\lambda(\mathbf{k})]^{-1}\sum_{\rho}[1-\exp i(\mathbf{k}-\mathbf{q})\rho]\Psi_{\mathbf{q}}(\rho)+A_{\mathbf{q}}\delta(\mathbf{k}-\mathbf{k}_0). \tag{2.9}$$

The second term in (2.9) is the solution of Eq. (2.8) without the right-hand side, $A_{\mathbf{q}}$ is an arbitrary constant, and $\mathbf{k}_0$ is the root of the equation

$$\lambda=-\lambda(\mathbf{k}). \tag{2.10}$$

The scattering amplitude is determined from the comparison of the asymptotic form of the coordinate wave function $\Psi(\mathbf{R}, \mathbf{r}_i)$ as $R\to\infty$ with the boundary condition as $R\to\infty$ (see the Appendix).

In the high-temperature case $T \gg \varepsilon_F$ we choose for scattering by a localized center the constant $A_{\mathbf{q}}$ in the form

$$A_{\mathbf{q}}=(2\pi/a)^d\exp(-i\mathbf{q}\mathbf{r}_0). \tag{2.11}$$

Substituting the solution (2.9) of the Schrödinger equation in (2.7) and taking (2.11) into account, we write the coordinate wave function for $R \gg \rho$ in the following manner:

$$\Psi(\mathbf{r}_0, \mathbf{r}_i)=\Psi(\mathbf{R}, \mathbf{r}_i-\mathbf{r}_0=\mathbf{r})=\delta_{\mathbf{r},0}e^{i\mathbf{k}_0\mathbf{R}}+G(\mathbf{R})I_d(\mathbf{r}), \tag{2.12}$$

where

$$I_d(\mathbf{r})=(a/2\pi)^d\int d^dq e^{i\mathbf{q}\mathbf{r}}\sum_{\rho}(1-e^{-i\mathbf{q}\rho})[\varphi_{\mathbf{q}}(\rho)]_d, \tag{2.13}$$

$$\varphi_{\mathbf{q}}(\mathbf{r})=e^{i\mathbf{q}\mathbf{r}_0}\Psi_{\mathbf{q}}(\mathbf{r}), \tag{2.14}$$

$$G(\mathbf{R})=\left(\frac{a}{2\pi}\right)^d\int\frac{e^{i\mathbf{k}\mathbf{R}}}{\lambda+\lambda(\mathbf{k})}d^dk; \tag{2.15}$$

$G(\mathbf{R})$ is the Green's function that describes, in the asymptotic limit $R\to\infty$, the scattered wave with a wave vector $\mathbf{k}'_0=k_0\mathbf{n}'$ (the circuiting around the poles $k=\pm k_0$ is specified by the asymptotic behavior, see the Appendix). The direction $\mathbf{n}$ of the wave vector of the incident wave $\mathbf{k}_0=k_0\mathbf{n}$ is specified as a boundary condition. On the other hand, the scattering direction $\mathbf{n}'$ is determined by the form of the equal-energy surface (2.10).[15-17] The explicit asymptotic form of the function $G(\mathbf{R})$ is written out in the Appendix. When writing the asymptotic form (2.12) we have neglected $\mathbf{k}'_0\cdot\boldsymbol{\rho}$ in comparison with $\mathbf{k}'_0\cdot\mathbf{R}$. The index $d$ denotes the dimensionality for which it is necessary to write out the functions that enter in the integrand.

Comparing (2.12) with the boundary conditions (A1) and taking Eqs. (A3)–(A8) into account, we obtain the amplitude for the scattering of a vacancion by a localized flipped spin. We write down this amplitude in the long-wave limit $k_0 a\to 0$. As already indicated, it is precisely this limit which corresponds to the real physical situation. The expressions for the scattering amplitude in the general case are written in the Appendix. From Eqs. (A5) and (A8) it can be seen that near the bottom of the vacancion band the scattering is isotropic. As $k_0 a\to 0$ we have:

in the case $d=3$

$$f(\mathbf{r})=\frac{a}{4\pi}I_3(\mathbf{r}), \tag{2.16}$$

in the case $d=2$

$$f(\mathbf{r})=\frac{1}{2}\left(\frac{i}{2\pi k_0}\right)^{1/2}I_2(\mathbf{r}). \tag{2.17}$$

The scattering amplitudes (2.16), (2.17), (A9), and (A10) contain under the integral sign of (2.13) the unknown functions $\varphi_{\mathbf{q}}(\boldsymbol{\rho})$. Determination of these functions completes the calculation of the exact scattering amplitude. Substituting in the expression

$$\Psi_{\mathbf{q}}(\rho)=\left(\frac{a}{2\pi}\right)^d\int\Psi_{\mathbf{q}}(\mathbf{k})e^{i\mathbf{k}\rho}d^dk \tag{2.18}$$

the solution (2.9) with the constant (2.11) and recalling the connection (2.14), we obtain the system of equations for $\varphi_{\mathbf{q}}(\boldsymbol{\rho})$:

$$\varphi_{\mathbf{q}}(\rho)=e^{i\mathbf{k}_0\rho}+\sum_{\rho'}\varphi_{\mathbf{q}}(\rho')[G(\rho)-G(\rho+\rho')e^{-i\mathbf{q}\rho'}]. \tag{2.19}$$

The solutions of the system (2.19) for a primitive cubic and for a planar quadratic lattice are given in the Appendix. Substitution of these solutions in the wave function (2.12) makes this asymptotic solution of the Schrödinger equation (2.5) self-consistent.

Of physical interest is the long-wave limit. Taking its importance into account, we write down with the aid of (A17) the integral $I_d(\mathbf{r})$ as $k_0 a\to 0$ in explicit form:

$$I_d(\mathbf{r})=\left(\frac{a}{2\pi}\right)^d\int d^dq e^{i\mathbf{q}\mathbf{r}}\left[\frac{F_1-F_0}{1+G_\perp F_1-GF_0}\right]_d. \tag{2.20}$$

The function $F_i$ and $G_i$ are determined in the Appendix. We need the values of this integral for the case of scattering without a shift of the flipped spin. Numerical integration of (2.20) with $\mathbf{r}=0$ yields

$$I_3(0)|_{k_0a\to 0}=-0.843,\quad I_2(0)|_{k_0a\to 0}=-0.547+0.193i. \tag{2.21}$$

From the expressions (2.16), (2.17), (A9), and (A10) obtained for the scattering amplitude it is clear that we can classify the scattering channels in accord with the shift of the flipped spin. Taking the properties of Im $G_i$ into account (see the Appendix), as well as the fact that the integrand in (2.20) has no pole with respect to $k$, we find that in the limit of small $k_0$ the scattering amplitude, depending on the dimensionality of the problem, takes the form:

$$f(\mathbf{r})=[b_{\mathbf{r}}'+ikb_{\mathbf{r}}'']_{(3)},\quad d=3, \tag{2.22}$$

$$f(\mathbf{r})=(i/k)^{1/2}[\beta_{\mathbf{r}}'+i\beta_{\mathbf{r}}'']_{(2)},\quad d=2, \tag{2.23}$$

where $b'_{\mathbf{r}}$, $b''_{\mathbf{r}}$, $\beta'_{\mathbf{r}}$, and $\beta''_{\mathbf{r}}$ are constants that depend on the parameter $\mathbf{r}$ and are analogous in their physical meaning to the scattering length. It can be seen from (2.20) that the amplitude of scattering with a shift is isotropic along the direction $\mathbf{r}$ and decrease exponentially with increasing $r$. For cross sections in the input channel, corresponding to "elastic" scattering without a shift of the flipped spin, we obtain

$$\sigma_e=(\pi/k^2)|1-S_{00}|^2=c_1a^2,\quad d=3, \tag{2.24}$$

$$\sigma_e=(\pi^{1/2}/k)|1-S_{00}|^2=c_2/k,\quad d=2, \tag{2.25}$$

where

$$S_{0\mathbf{r}}=1+(2ik)^{(d-1)/2}f(\mathbf{r}) \tag{2.26}$$

is the scattering-matrix element corresponding to zero angular momentum (isotropic $s$-scattering), with a shift of the flipped spin by an amount $\mathbf{r}$.

The total cross section of all the processes with a shift is given by the equations

$$\sigma_i=(\pi/k^2)\,(1-|S_{00}|^2)=c_3a^2,\ d=3, \tag{2.27}$$

$$\sigma_i=(\pi^{1/2}/k)\,(1-|S_{00}|^2)=c_4/k,\ d=2, \tag{2.28}$$

where $c_i$ are constants whose numerical values can be easily obtained with the aid of Eqs. (2.21) and (2.26). We have, in particular, $c_1=0.057$, $c_2=0.047$, and $c_4=0.143$. In the two-dimensional case we used Eqs. (A23)–(A26). We point out that in the three-dimensional case, for "inelastic" scattering of slow particles with a shift of the flipped spin, the "$v^{-1}$ law" for cross sections is not satisfied. The behavior of the cross sections as functions of $k$ does not depend on the scattering channel.

We note that our definition of the Hamiltonian in the wave function in terms of the operators $c_i$ and $c_i^+$, which specifies the bottoms of the vacancion band in the limit as $k_0 a \to 0$, was chosen from convenience considerations. The definition under which the energy is a minimum on the boundaries of the Brillouin zone (the opposite sign of the spectrum) multiplies our solution (2.4) by an inessential phase factor without changing the results obtained for the cross sections.

We write down also equations for the case when the vacancions are scattered by a vacancion magnon. In this case, of course, the foregoing distinction between elastic and inelastic processes becomes meaningless. Assuming that the vacancions are located near the bottom of the band, we neglect umklapp processes. If we choose the constant $A_{\mathbf{q}}$ in (2.9) in the form

$$A_{\mathbf{q}}=(2\pi/a)^{2d}\delta(\mathbf{q}-\mathbf{Q}), \tag{2.29}$$

and introduce in place of the relation (2.14) the function $\varphi_{\mathbf{q}}(\boldsymbol{\rho})$ defined by

$$\Psi_{\mathbf{q}}(\boldsymbol{\rho})=(2\pi/a)^{d}\delta(\mathbf{q}-\mathbf{Q})\,\varphi_{\mathbf{q}}(\boldsymbol{\rho}), \tag{2.30}$$

the asymptotic form of the coordinate wave function now becomes [cf. (2.12)]:

$$\Psi(\mathbf{R},\mathbf{r}_i)=\exp(i\mathbf{Q}\mathbf{r}_i)\left\{e^{i\mathbf{k}_0\mathbf{R}}+G(\mathbf{R})\left[\sum_{\boldsymbol{\rho}}(1-e^{-i\mathbf{q}\boldsymbol{\rho}})\varphi_{\mathbf{q}}(\boldsymbol{\rho})\right]\right\}, \tag{2.31}$$

with the function $\varphi_{\mathbf{q}}(\boldsymbol{\rho})$ solutions of the system (2.19) as before. Comparing expressions (2.31) and (A2) and again taking (A3)–(A8) into account, we find that the amplitude for scattering by a magnon takes the following form (for the sake of brevity we write it in the limit as $k_0 a \to 0$):

$$f_{\mathbf{Q}}=\frac{a}{4\pi}\left[\frac{F_1(\mathbf{Q})-F_0(\mathbf{Q})}{1+G_\perp F_1(\mathbf{Q})-GF_0(\mathbf{Q})}\right]_{(3)},\quad d=3, \tag{2.32}$$

$$f_{\mathbf{Q}}=\frac{1}{2}\left(\frac{i}{2\pi k_0}\right)^{1/2}\left[\frac{F_1(\mathbf{Q})-F_0(\mathbf{Q})}{1+G_\perp F_1(\mathbf{Q})-GF_0(\mathbf{Q})}\right]_{(2)},\quad d=2. \tag{2.33}$$

The cross sections are determined by Eqs. (2.24)–(2.26) but with other constants $c_i$.

### 3. SPIN DIFFUSION

Spin diffusion in the case of a Boltzmann gas of vacancions will be calculated following Ref. 14. The average velocity of the flipped spin as a result of vacancion scattering by it is written the following form:

$$\mathbf{v}=\sum_{\boldsymbol{\rho}}\boldsymbol{\rho}W_{\rho}, \tag{3.1}$$

where $W_\rho$ is the probability of displacing the flipped spin by the vector $\boldsymbol{\rho}$. Assuming that the flipped spin is acted upon by a force $\mathbf{F}$, we obtain

$$W_\rho=\int_{\varepsilon_0}^{\varepsilon_0+\Delta_v}\frac{d\varepsilon}{(2\pi)^3}[n(\varepsilon)-n(\varepsilon+\mathbf{F}\boldsymbol{\rho})]\int\sigma_i(\boldsymbol{\rho})\,ds, \tag{3.2}$$

where $n(\varepsilon)$ is the vacancion (Boltzmann) distribution function, $\varepsilon_0$ is the bottom of the vacancion energy band, and $ds$ is an element of the equal-energy surface. At a temperature $T \ll \varepsilon_0$ the Boltzmann factors cut off the integration in (3.2) near the bottom of the band. Under these conditions, taking (2.27) and (2.28) into account, we find that the integral with respect to $ds$ is proportional to $\varepsilon-\varepsilon_0$ for $d=3$ and is a constant for $d=2$. Restricting the summation in (3.1) by the condition $\mathbf{F}\cdot\boldsymbol{\rho}>0$ (the remaining shifts are taken into account in (3.2) as inverse processes) we obtain in the limit as $\mathbf{F}\cdot\boldsymbol{\rho}/T\to 0$ for the average velocity $\mathbf{v}=\mu\mathbf{F}$, where $\mu$ is the mobility coefficient. We calculate the spin-mobility coefficient $D$ by using the Einstein relation. We obtain

$$D=\text{const}\,(Ta)^2\exp(-\varepsilon_0/T),\quad d=3, \tag{3.3}$$

$$D=\text{const}\,a^2\exp(-\varepsilon_0/T),\quad d=2. \tag{3.4}$$

The discrepancy between the result (3.3), recalculated in terms of mobility, and the paper by Andreev and Meĭerovich is due to the fact that the assumption made in Ref. 14, that the $v^{-1}$ law holds for the considered inelastic scattering, is replaced in our case by the exact result (2.27), namely $\sigma=\text{const}$. The $v^{-1}$ law presupposes that the logarithmic derivative of the radial part of the wave function, taken on the boundary of the limit of the action of the scattering potential, is equal to a certain complex constant, and its reciprocal modulus determines the characteristic scale over which the deformation of the wave function takes place in the scattering process (see, e.g., Ref. 18). Although in our case such a boundary condition does not have a direct physical meaning, from the formal point of view the result (2.27) denotes renormalization of the characteristic deformation length by the small factor $k_0 a \ll 1$. Thus, the "reaction zone," which has in the quasiclassical fast-vacancy approximation a dimension $\sim a$, decreases with increasing vacancion wavelength. Physically this means that a slow vacancion can displace a flipped spin localized on a lattice site by merely passing at an infinitely close distance from it. For fast (quasiclassical) vacancions the impact parameter is the lattice constant.

We consider now the case of Fermi degeneracy of a vacancion gas. We confine ourselves to the dimensionality $d=3$. Then $\varepsilon_F\sim x^{2/3}\Delta_v$. As noted in the Introduction (see also Ref. 2) a localized spin fluctuation turns into a magnon with a bandwidth $\Delta_i\sim\Delta_v\,x\sim\varepsilon_F\,x^{1/3}$. In this case, if the polarization is induced by vacancions [Nagaoka ground state with exchange intensity $J_v\sim\Delta_v\,x$ (vacancion ferromagnet)], the energy $J_v$ acquired in the spin flip is offset by the spin

delocalization, and the discussed "vacancion magnon" is a gapless excitation. In the case of polarization by a magnetic field, the fields required for this purpose produce in the magnon spectrum a gap of the order of $\varepsilon_F$. We shall assume equilibrium magnon and vacancion distribution functions. This means that the observed effects receive contributions from thermal excitations. At temperatures needed to flip in a magnetic field a number of spins that is not exponentially small, the vacancion gas is no longer degenerate, and we return to the picture of localized spin fluctuation. The magnetic field has no influence on the localization of an isotopic impurity (see the Conclusion).

For $x \ll 1$ we have a hierarchy of parameters: $\Delta_i \ll \Sigma_F \ll \Delta_v$. Assuming the magnon gas to be rarefied, we arrive at the problem of the mobility of a Boltzmann particle in a Fermi gas, for which the following results can be obtained. At $k \gg q$ we obtain from the solution of the kinetic equation[11,13]

$$\mu \sim (MT)^{-2}\sigma^{-1}, \tag{3.5}$$

where $M$ is the effective mass of the Boltzmann particle (magnon). In the opposite limit $k \ll q$, collisions with Fermi particles (vacancions) lead to a small change of the magnon momentum, and the kinetic equation reduces to a Fokker-Planck equation. The results for the mobility is[12]

$$\mu \sim p_F^{-4}\sigma^{-1}, \tag{3.6}$$

where $p_F$ is the Fermi momentum of the vacancion. We note that in both cases it is necessary to check on the validity of the kinetic equation. The cross sections can be calculated from the amplitude (2.32) for scattering by a vacancion magnon. In our case it is necessary to take into account also the band character of the motion of the vacancion and of the magnon, but at $T \ll \Delta_i$ these restrictions are inessential. From the estimates $k \sim (m\varepsilon_F)^{-1/2}$ and $q \sim (MT)^{1/2}$, where $m$ is the effective mass of the vacancion, we obtain a new parameter $T_0 \sim \Delta_i x^{2/3}$, so that $k \gg q$ at $T \ll T_0$ and vice versa. We note that at $T \gtrsim \Delta_i \gg T_i$ a change takes place in the estimate for $q$; it takes the form $q \sim (M\Delta_i)^{1/2}$. The inequality $k \ll q$ continues to the satisfied in this case.

Thus, at $T \ll T_0$ the result (3.5) is valid. Using again the Einstein relation, we obtain for the spin-diffusion coefficient the expression

$$D \sim (ax\Delta_v)^2 T^{-1}. \tag{3.7}$$

At $T \ll \Delta_i$ the condition for the applicability of the kinetic equation is $T\tau \gg 1$, where $\tau$ is the magnon mean free path. It is easy to verify, substituting in the estimate $\tau \sim \mu M$ the expression (3.7), that this condition is satisfied.

The temperature $T_0 \ll T \ll \varepsilon_F$ is the region of applicability of the results (3.6). For the spin diffusion coefficient we obtain from Einstein relation

$$D \sim (ax^{-2/3})^2 T. \tag{3.8}$$

The Fokker-Planck kinetic equation is applicable now under the condition $\Delta_i \tau \gg 1$. Taking into account the band character of the magnon-motion, we obtain the estimate $\tau \sim \mu T(\Delta_i)^{-2}$, from which we can easily conclude that the kinetic equation is applicable already on the lower limit of the region $T \sim T_0$.

## 4. CONCLUSION

We have considered the problem of vacancion diffusion for two- and three-dimensional lattices. In the one-dimensional case there is no scattering (actually, reflection) of the vacancion wave by the magnetic defect. In fact, for $d = 1$ the lattice breaks up into the regions $r_v < r_i$ and $r_v > r_i$. Writing down the Schrödinger equation in each of them with the conditions (2.3) and (2.6) we find that the general solution is the function

$$\Psi(R, r) = e^{\pm ik_0 R}(1-\delta_{r,0}),$$

in which the sign of the phase is determined by the condition at $R \to \infty$, and which does not contain a reflected wave. The meaning of this result becomes clear if it is recognized that in the one-dimensional case, in the considered Hubbard-model limit, the width of the vacancion band does not depend on the magnetic structure.[4]

The quantitative results obtained for the cross sections and for the diffusion should remain in force also for bcc, hcp, and planar triangular lattices, which are realized in quantum crystals. To obtain exact quantitative results it becomes necessary to solve the system (2.19), which contains a large number of equations. However, recognizing that the Green's function is numerically small, an exact solution of the system (2.19) can be replaced by the approximate solution obtained by iterating the difference equation (2.19). The zeroth approximation is of the form

$$\varphi_q(\rho) = \exp(i\mathbf{k}_0\rho).$$

For the case of an isotopic impurity in a quantum crystal ($He^4$ in an $He^3$ matrix), the amplitude of the vacancy-impurity exchange is generally speaking not equal to the amplitude of vacancy exchange with the matrix atoms. This fact is taken into account by replacing the second equation of (2.2) in the definition of the operator $H$ with

$$H\Psi(\mathbf{r}_v, \mathbf{r}_i) = -t'\Psi(\mathbf{r}_i, \mathbf{r}_v), \quad \mathbf{r}_v+\rho=\mathbf{r}_i, \tag{4.1}$$

where $t' = \gamma t$. The case $\gamma < 1$ corresponds to repulsion (at $\gamma = 0$ the repulsion is infinite), while $\gamma > 1$ corresponds to attraction. The answer now takes the following form (we write it in the limit as $k_0 a \to 0$):

$$[X(\mathbf{q}) - Y(\mathbf{q})]_{k_0 a \to 0} = \frac{\bar{F}_1 - \bar{F}_0}{1 + G_\perp \bar{F}_1 - G\bar{F}_0}, \tag{4.2}$$

where the following notation is introduced (cf. The corresponding Eq. (A4) of the Appendix):

$$\bar{F}_1(\mathbf{q}) = \gamma \sum_\rho F_q(\rho) e^{-i\mathbf{q}\rho}, \quad \bar{F}_0(\mathbf{q}) = \sum_\rho F_q(\rho), \tag{4.3}$$

$$F_q(\rho) = \frac{1 + (G_2 - G_0)\gamma e^{i\mathbf{q}\rho}}{1 + 2(G_2 - G_\perp)\gamma \cos \mathbf{q}\rho + \gamma^2[(G_\perp - G_2)^2 - (G_\perp - G_0)^2]}. \tag{4.4}$$

From expressions (4.2)–(4.4) we can conclude that at sufficiently large $\gamma$ the vacancion spectrum contains besides the considered scattering state also bound states.

The results can be verified in experiments on spin diffusion in strongly polarized quantum crystals. This polarization is produced in fact by the magnetic field, so that we are dealing with a check on the pre-exponential factor in Eqs.

(3.3) and (3.4). For the case of observation of a vacancion ferromagnet, we can use Eqs. (3.7) and (3.8) to study the spin diffusion in it. We note the possibility of obtaining a quasi-equilibrium state of "frozen-in vacancies" with controllable density in quantum two-dimensional crystals (such a state was observed[19] in the bcc phase of $He^3$). Of definite interest is also the observation of bound states of the vacancy and isotopic impurity, predicted by Eq. (4.4).

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## APPENDIX

1. The boundary conditions in the asymptotic form as $R \to \infty$ for the coordinate wave function $\Psi(\mathbf{R},\mathbf{r}_i)$ takes the following form.

a) Scattering by a localized flipped spin ($T \ll \varepsilon_F$):

$$\Psi(\mathbf{R},\mathbf{r}_i)|_{R\to\infty}=e^{i\mathbf{k}\mathbf{R}}\delta_{\mathbf{r},0}+f_{\mathbf{k}'}^{\mathbf{k}}(\mathbf{r})\frac{\exp(i\mathbf{k}'\mathbf{R})}{R^{(d-1)/2}}. \tag{A1}$$

Here $f_{\mathbf{k}'}^{\mathbf{k}}(\mathbf{r})$ is the scattering amplitude of a vacancion whose initial and final states are characterized by the quasimomenta $\mathbf{k}$ and $\mathbf{k}'$, while $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_0$ is the flip-spin shift vector.

b) Scattering of a vacancion by a magnon ($T \ll \varepsilon_F$):

$$\Psi(\mathbf{R},\mathbf{r}_i)|_{R\to\infty}=e^{i\mathbf{Q}\mathbf{r}_i}\left[e^{i\mathbf{k}\mathbf{R}}+f_{\mathbf{Q}}(\mathbf{k},\mathbf{k}')\frac{\exp(i\mathbf{k}'\mathbf{R})}{R^{(d-1)/2}}\right]. \tag{A2}$$

Here $\mathbf{Q}=\mathbf{k}+\mathbf{q}$, $\mathbf{q}$ is the magnon quasimomentum.

2. The asymptotic form of the function (2.15) $G(\mathbf{R})$ for a primitive cubic lattice (with a different sign of the spectrum) was obtained in Refs. 15 and 16 by the stationary-phase method. We write the result in a form that takes into account the singularity when the wave vector of the scattered wave $k_0'$ passes through the parabolic points of the equal-energy surface[20]:

$$G(\mathbf{R})=-i\frac{a}{16\pi}\frac{\exp(i\mathbf{k}_0'\mathbf{R})}{R}\times(1+i\,\mathrm{sign}\,B)\prod_{i=x,y,z}(1-i\,\mathrm{sign}\cos k_{0i}'a)\times\left|\sum_j\sin^2 k_{0j}'a/S(\mathbf{k}_0')\right|^{1/2}. \tag{A3}$$

Here

$$B=S(\mathbf{k}_0')/\cos k_{0x}'a\cos k_{0y}'a\cos k_{0z}'a,$$
$$S(\mathbf{k}_0')\equiv\sum\sin^2 k_{0x}'a\cos k_{0y}'a\cos k_{0z}'a. \tag{A4}$$

In the formula for $S$ the summation is over the cyclic permutation of $x$, $y$, and $z$. From (A3) and (A4) it can be seen that at $S(\mathbf{k}_0)>0$ expression (A3) is real and in the opposite case ($S(\mathbf{k}_0)<0$) it is pure imaginary. The singularity at $S(\mathbf{k}_0)=0$ is integrable. At small $k_0$ (near the bottom of the vacancion band) we obtain

$$G(R)=-\frac{a}{4\pi}\frac{\exp(i\mathbf{k}_0\mathbf{R})}{R}. \tag{A5}$$

Similar expressions can be written also in the case of a planar square lattice:

$$G(\mathbf{R})=-\frac{i}{8}\left(\frac{a}{\pi B}\right)^{1/2}e^{i\mathbf{k}_0'\mathbf{R}}(1+i\,\mathrm{sign}\,B_1)\times\prod_{i=x,y}(1-i\,\mathrm{sign}\cos k_{0i}a)\times|(\sin^2 k_{0x}'a+\sin^2 k_{0y}'a)^{1/2}/S_1(\mathbf{k}_0')|^{1/2}. \tag{A6}$$

here

$$B_1=S_1(\mathbf{k}_0')/\cos k_{0x}'a\cos k_{0y}'a,$$
$$S_1(\mathbf{k}_0')\equiv\sin^2 k_{0x}'a\cos k_{0y}'a+\sin^2 k_{0y}'a\cos k_{0x}'a. \tag{A7}$$

The real part of the asymptotic expression (A6) reverses sign when the denominator of the expression goes through zero. A divergence arises when the wave vector of the scattered wave is located on the open equal-energy surface. Near the bottom of the band we obtain

$$G(\mathbf{R})=-\frac{1}{2}\left(\frac{i}{2\pi k_0 R}\right)^{1/2}e^{ik_0R}. \tag{A8}$$

3. The exact amplitudes for the scattering of a vacancion by a localized flipped spin at $d=3$ are of the form

$$f_{\mathbf{k}_0'}^{\mathbf{k}_0}(r)=i\frac{a}{16\pi}(1+i\,\mathrm{sign}\,B)\prod_{i=x,y,z}(1-i\,\mathrm{sign}\cos k_{0i}'a)\times\left|\sum_{j=x,y,z}\sin^2 k_{0j}'a/S(\mathbf{k}_0')\right|^{1/2}I_3^{(\mathbf{k}_0)}(\mathbf{r}), \tag{A9}$$

and at $d=2$ we have

$$f_{\mathbf{k}_0'}^{\mathbf{k}_0}(\mathbf{r})=\frac{i}{8}\left(\frac{a}{\pi}\right)^{1/2}(1+i\,\mathrm{sign}\,B_1)\prod_{i=x,y}(1-i\,\mathrm{sign}\cos k_{0i}'a)\times|(\sin^2 k_{0x}'a+\sin^2 k_{0y}'a)^{1/2}/S_1(\mathbf{k}_0')|^{1/2}I_2^{(\mathbf{k}_0)}(\mathbf{r}). \tag{A10}$$

4. A solution of the system (2.19) can be obtained in relatively compact form only for a primitive cubic and planar quadratic lattice. In these cases the system (2.19) can be reduced to a system of two equations for $\varphi_{\mathbf{q}}(\pm\boldsymbol{\rho})$:

$$\varphi_{\mathbf{q}}(\boldsymbol{\rho})=e^{i\mathbf{k}_0\boldsymbol{\rho}}+(G_\perp-G_2)e^{-i\mathbf{q}\boldsymbol{\rho}}\varphi_{\mathbf{q}}(\boldsymbol{\rho})+(G_\perp-G_0)e^{i\mathbf{q}\boldsymbol{\rho}}\varphi_{\mathbf{q}}(-\boldsymbol{\rho})-G_\perp X(\mathbf{q})+GY(\mathbf{q}), \tag{A11}$$

where we have introduced the notation

$$X(\mathbf{q})=\sum_{\boldsymbol{\rho}}\varphi_{\mathbf{q}}(\boldsymbol{\rho})e^{-i\mathbf{q}\boldsymbol{\rho}},\quad Y(\mathbf{q})=\sum_{\boldsymbol{\rho}}\varphi_{\mathbf{q}}(\boldsymbol{\rho}); \tag{A12}$$

$$G(\pm\boldsymbol{\rho})=G,\quad G(\pm 2\boldsymbol{\rho})=G_2,$$
$$G(0)=G_0,\quad G(\boldsymbol{\rho}+\boldsymbol{\rho}_\perp)=G_\perp, \tag{A13}$$

with $\boldsymbol{\rho}\cdot\boldsymbol{\rho}_\perp=0$. The functions (A13) are expressed by means of an integral of a product of Bessel functions of integer index and of trigonometric functions[21,22] and are written out below. We note that to calculate the scattering amplitude we need the difference of the functions (A12), $X(\mathbf{q})-Y(\mathbf{q})$. The solution of the system (A11) is

$$\varphi_{\mathbf{q}}(\boldsymbol{\rho})=\Phi_{\mathbf{q}}^{\mathbf{k}_0}(\boldsymbol{\rho})+F_{\mathbf{q}}(\boldsymbol{\rho})[GY(\mathbf{q})-G_\perp X(\mathbf{q})], \tag{A14}$$

where

$$\Phi_q^{k_0}(\rho)=[e^{ik_0\rho}+(G_2-G_\perp)e^{i(q+k_0)\rho}+(G_\perp-G_0)e^{i(q-k_0)\rho}]D^{-1},$$

$$F_q(\rho)=[1+(G_2-G_0)e^{iq\rho}]D^{-1},$$

$$D\equiv 1+2(G_2-G_\perp)\cos q\rho+(G_\perp-G_2)^2+(G_\perp-G_0)^2.$$

Substituting (A14) in (A12), we obtain a system of equations for $X(\mathbf{q})$ and $Y(\mathbf{q})$:

$$\begin{aligned}&[1+G_\perp F_1(\mathbf{q})]X(\mathbf{q})-GF_1(\mathbf{q})Y(\mathbf{q})=\Phi_1^{k_0}(\mathbf{q}),\\&G_\perp F_0(\mathbf{q})X(\mathbf{q})+[1-GF_0(\mathbf{q})]Y(\mathbf{q})=\Phi_0^{k_0}(\mathbf{q}),\end{aligned}\tag{A15}$$

where

$$F_0(\mathbf{q})=\sum_\rho F_q(\rho),\quad F_1(\mathbf{q})=\sum_\rho F_q(\rho)e^{-iq\rho},$$

$$\Phi_0^{k_0}(\mathbf{q})=\sum_\rho \Phi_q^{k_0}(\rho),\quad \Phi_1^{k_0}(\mathbf{q})=\sum_\rho \Phi_q(\rho)e^{-iq\rho}.$$

Making up the sought difference from the solutions of the system (A15), we obtain

$$X_{k_0}(\mathbf{q})-Y_{k_0}(\mathbf{q})=\frac{\Phi_1^{k_0}-\Phi_0^{k_0}+(G_\perp-G)(\Phi_1^{k_0}F_0-F_1\Phi_0^{k_0})}{1+G_\perp F_1-GF_0}.\tag{A16}$$

The result becomes simpler for the case of the bottom of the band. As $k_0 a\to 0$ we have

$$X(\mathbf{q})-Y(\mathbf{q})=(F_1-F_0)/(1+G_\perp F_1-GF_0).\tag{A17}$$

5. When calculating the Green's functions (A13), the circuiting around the pole is governed by the required asymptotic form. Thus, in order that the asymptotic relation contain a diverging wave it is necessary, in the case of our spectrum, to add to the denominator of the integrand in (2.15) an infinitely small positive imaginary part. Using the integral representation of Bessel functions, we obtain for a primitive cubic lattice (cf. Refs. 21 and 22)

$$\begin{aligned}G&=\frac{1}{2}\int_0^\infty \exp(i\lambda t/2)J_1(t)J_0^2(t)\,dt,\\G_2&=\frac{i}{2}\int_0^\infty \exp(i\lambda t/2)J_2(t)J_0^2(t)\,dt,\\G_0&=-\frac{i}{2}\int_0^\infty \exp(i\lambda t/2)J_0^3(t)\,dt,\\G_\perp&=\frac{i}{2}\int_0^\infty \exp(i\lambda t/2)J_1^2(t)J_0(t)\,dt,\end{aligned}\tag{A18}$$

where $J_m(t)$ are Bessel functions of the first kind and of integer index. The functions (A18) can be expressed via the functions

$$\begin{aligned}C(k,m,n)&=\int_0^\infty J_k(t)J_m(t)J_n(t)\cos\lambda t/2dt,\\S(k,m,n)&=\int_0^\infty J_k(t)J_m(t)J_n(t)\sin\lambda t/2dt,\end{aligned}\tag{A19}$$

which are tabulated in Ref. 21. The Green's functions for a planar quadratic lattice are likewise written with the aid of the integrals in (A18), except that the integrand is divided by the function $J_0(t)$. They can be expressed in terms of the functions

$$\begin{aligned}C(m,n)&=\int_0^\infty J_m(t)J_n(t)\cos\lambda t/2dt,\\S(m,n)&=\int_0^\infty J_m(t)J_n(t)\sin\lambda t/2dt,\end{aligned}\tag{A20}$$

whose values are listed in the Table. We note that outside the band Im $G_i=0$ in both the three-dimensional and in the two-dimensional cases. However, whereas in the three-dimensional case Im $G_i$ goes to zero continuously (Im $G_i\sim k$), in the two-dimensional case Im $G_i$ has a jump, equal to 0.25, on the boundary of the band. This result can be easily understood by recalling that Im $G_i\propto\nu(\varepsilon)$, where $\nu(\varepsilon)$ is the state density.

6. We present two relations between the functions (A20). These can be easily obtained by integrating by parts and were used by us to check on the Table:

$$G_0=\lambda^{-1}(1-4G),\quad G=-\lambda^{-1}(2G_\perp+G_0+G_2).\tag{A21}$$

7. We write down several formulas of the two-dimensional scattering theory. The scattering amplitude $f$ is defined as the coefficient of the diverging wave in the asymptotic form of the exact wave function

$$\begin{aligned}\Psi_m&=\exp(ik_m z)+r^{-1/2}f_{mm}(\theta)\exp(ik_m r),\\\Psi_t&=r^{-1/2}f_{mt}(\theta)\exp(ik_t r),\end{aligned}\tag{A22}$$

where $m$ is the index of the input channel and $t$ is the index of any inelastic channel. The cross section $d\delta\propto|f(\theta)|^2d\theta$ has the dimensionality of length. The unitary scattering matrix $S$ is connected with the amplitude $f$ in the following manner:

TABLE I. Values of the functions $C(m,n)$ and $S(m,n)$ for certain values of the parameter $\lambda$.

| $\lambda/2$ | $C(1,0)$ | $S(1,0)$ | $C(2,0)$ | $S(2,0)$ | $C(0,0)$ | $S(0,0)$ | $C(1,1)$ | $S(1,1)$ |
|---|---|---|---|---|---|---|---|---|
| 0.0 | 0.50 | 0.00 | −1.04 | 0.00 | 2.31 | 0.00 | 1.68 | 0.00 |
| 0.4 | 0.40 | 0.19 | 0.22 | −0.15 | 0.97 | 0.51 | 0.30 | 0.49 |
| 0.6 | 0.34 | 0.25 | 0.26 | −0.01 | 0.84 | 0.52 | 0.14 | 0.47 |
| 0.8 | 0.29 | 0.30 | 0.22 | 0.11 | 0.75 | 0.53 | 0.02 | 0.44 |
| 1.0 | 0.233 | 0.341 | 0.172 | 0.208 | 0.683 | 0.534 | −0.085 | 0.395 |
| 1.2 | 0.168 | 0.381 | 0.074 | 0.267 | 0.636 | 0.553 | −0.176 | 0.345 |
| 1.4 | 0.090 | 0.418 | −0.046 | 0.285 | 0.597 | 0.586 | −0.264 | 0.277 |
| 1.6 | −0.012 | 0.448 | −0.181 | 0.250 | 0.560 | 0.640 | −0.347 | 0.177 |
| 1.8 | −0.161 | 0.470 | −0.327 | 0.126 | 0.522 | 0.734 | −0.422 | 0.014 |
| 2.0 | −0.766 | 0.500 | −0.500 | −0.539 | 0.500 | 1.266 | −0.500 | −0.631 |
| 2.2 | −0.246 | 0.00 | 0.00 | −0.103 | 0.00 | 0.678 | 0.00 | −0.150 |
| 2.4 | −0.160 | 0.00 | 0.00 | −0.053 | 0.00 | 0.551 | 0.00 | −0.083 |
| 2.8 | −0.091 | 0.00 | 0.00 | −0.021 | 0.00 | 0.422 | 0.00 | −0.034 |
| 3.0 | −0.075 | 0.00 | 0.00 | −0.015 | 0.00 | 0.383 | 0.00 | −0.027 |
| 3.6 | −0.047 | 0.00 | 0.00 | −0.008 | 0.00 | 0.304 | 0.00 | −0.014 |
| 4.0 | −0.036 | 0.00 | 0.00 | −0.005 | 0.00 | 0.268 | 0.00 | −0.009 |

$$\hat{S}_{mt}=\delta_{mt}+(2ik)^{1/2}\hat{f}_{mt}, \tag{A23}$$

where $\hat{f}_{mt}$ is an integral operator:

$$\hat{f}_{mt}F(\mathbf{n})=-(4\pi)^{-1/2}\int f_{mt}(\mathbf{n},\ \mathbf{n}')F(\mathbf{n}')d\theta. \tag{A24}$$

In the case of isotropic scattering the only nonzero element in the $S$ matrix is the one corresponding to scattering with zero angular momentum. Denoting it by $S$, we obtain:

a) the elastic-scattering cross section

$$\sigma_e=\pi^{1/2}|1-S_{mm}|^2/k; \tag{A25}$$

b) the total inelastic-scattering cross section

$$\sigma_i=\pi^{1/2}(1-|S_{mm}|^2)/k. \tag{A26}$$

The optical theorem in the two-dimensional case takes the form

$$\operatorname{Im} f_{mm}(0)-\operatorname{Re} f_{mm}(0)=(k/4\pi)^{1/2}(\sigma_e+\sigma_i). \tag{A27}$$


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