

Nonlinear transit of defects in quantum crystals

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The possibility of existence and motion of solitary plane-wave formation of defects in quantum crystals (in particular, vacancy soliton in solid ^4He) is proved. The parameters of solitons are calculated. It is shown that the solitons of defects could be observed experimentally under specific conditions obtained in the present paper. [S0163-1829(99)09017-7]

I. INTRODUCTION

Different types of motions in quantum crystals¹ caused by tunneling of admixture defects (such as vacancies in solid helium and hydrogen, ^3He atoms in solid ^4He or vice versa, etc.) have been the subject of intensive investigation for a long time (in particular, quantum diffusion phenomenon,² spin-lattice relaxation in solid ^3He ,^{3,4} and in solid hydrogen⁵ caused by vacancies, etc.).

We consider the case of a small concentration of defects $x \ll 10^{-3}$ ($x = n_d/N$, n_d is the number of defects and N is the number of lattice sites in a sample). Then the defects are free to move through the crystal even at zero temperature due to the quantum tunneling phenomenon. It was predicted that their mobilities can be characterized by linear wavelike excitations (defectons).^{1,6} This theoretical assumption was indirectly confirmed by experiments, namely, by measuring times of spin-lattice relaxation caused by vacancies in a solid ^3He crystal.^{3,4}

On the other hand, certain instability might cause the occurrence of nonlinear solitary waves of defects which can propagate within a sample with an amplitude enough to observe them experimentally. Such formation could be directly observed even in ^4He (with x-ray-diffraction technique) where the NMR measurements become useless. Therefore for simplicity and to be specific we consider vacancies in solid ^4He , i.e., we study nonlinear vacancy waves and investigate the properties of wave excitations (vacancions).

The method of inverse scattering problem⁷ is usually used to find exact soliton solutions of integrable nonlinear motion equations. Hence it could be applied to achieve our object—to describe the nonlinear transit of vacancies in solid ^4He . But as the amplitude of the solitary wave (the local relative concentration of vacancies) should be very small $x \ll 10^{-3}$ (otherwise the vacancies are localized at low temperatures²) we apply the reductive perturbation method developed in Ref. 8.

This method has been successfully used for the description of propagation of solitary waves in the plasma⁹ and magnetic materials.¹⁰ Moreover, the above method can be extended to the investigation of propagation of dynamical solitons consisting of short-wavelength excitations (of the order of lattice parameter), as was done in Ref. 11.

In this paper we will find a solution in the form of collective solitary motion of vacancies in solid ^4He and define the conditions under which the solution can be obtained.

II. NONLINEAR SOLUTION

Let us introduce the operators of creation S_f^+ and annihilation S_f^- of vacancy in the lattice site f . These operators should obey the Fermi commutation relations for the purpose of avoiding a double occupancy of the lattice sites. In the original papers⁶ these operators were considered to be the Bose operators. In the linear approximation over x these two approaches give the same results. But in order to consider nonlinear effects, a more strict approach¹ of Fermi operators must be used. These operators can be presented as the Pauli matrices, and the Hamiltonian describing vacancy mobilities could be written as follows:¹

$$\mathcal{H} = \omega_0 \sum_f^N (S_f^z + 1/2) - \sum_{f,g}^N A_{fg} S_f^+ S_g^-, \quad (1)$$

where ω_0 is an energy of the vacancy creation in frequency units ($\hbar = k_B = 1$); eigenvalues $S_f^z = -1/2$ and $S_f^z = 1/2$ correspond to the absence and presence of the vacancy in the lattice site f , respectively; A_{fg} is a constant characterizing tunneling of a defect from site f to the site g . It is supposed that $A_{fg} = A = \text{const}$ (the case of small concentration of vacancies,^{1,6}) for the nearest neighborhood, and $A_{fg} = 0$ for the other sites (tunneling takes place only in the nearest neighboring sites). Thus the Hamiltonian (1) has a strong resemblance with the Hamiltonian of Heisenberg ferromagnet with exchange interaction [except that the term proportional to $S_f^z S_g^z$ is absent in Eq. (1)]. Hence having written the motion equations for the fictitious spin system considered,

$$\begin{aligned} \frac{dS_f^\pm}{dt} &= \pm i \left(\omega_0 S_f^\pm + 2 \sum_g^N A_{fg} S_f^z S_g^\pm \right), \\ \frac{dS_f^z}{dt} &= -i \sum_g^N A_{fg} (S_f^- S_g^+ - S_f^+ S_g^-), \end{aligned} \quad (2)$$

we can use the Weiss field approximation¹ (neglecting quantum correlations, e.g., $\langle S_f^+ S_g^- \rangle \equiv \langle S_f^+ \rangle \langle S_g^- \rangle$, etc., where $f \neq g$) as in Ref. 12 where the nonlinear evolution of macroscopical quantities, particularly, components of the full spin was considered in the real spin systems (e.g., ferromagnets). Justification of this assumption for our case will be given below.

Denoting $M_f^\pm \equiv \langle S_f^\pm \rangle$, $M_f^z \equiv \langle S_f^z \rangle$ (brackets $\langle \dots \rangle$ express quantum statistical averaging) let us determine reduced dynamical part of \mathbf{M}_f as $\mathbf{m}_f \equiv (\mathbf{M}_f - \mathbf{M}_0)/M_0$, where $\mathbf{M}_0 = M_0 \mathbf{e}_z$, \mathbf{e}_z is a unit vector along z axis in the fictitious space, $M_0 \approx -1/2$, and \mathbf{M}_0 is a static value of \mathbf{M}_f . It should be noticed that using the above definitions the only physically measurable quantity—relative concentration of vacancies—can be presented by the averaged components of the fictitious spin as follows:

$$x = x_0 + \delta x, \quad x_0 = M_0 + 1/2, \quad \delta x = M_0 m_z \quad (3)$$

(x_0 is a static relative concentration of defects). Further, we get from Eq. (2) the equation

$$\frac{dm_f^\pm}{dt} = \mp i \left(\omega_0 m_f^\pm + 2M_0 \sum_g^N A_{fg} m_g^\pm \right) \mp 2iM_0 m_f^z \sum_g^N A_{fg} m_g^\pm \quad (4)$$

and relation

$$m_f^z = -\frac{1}{2} [m_f^+ m_f^- + (m_f^z)^2] \quad (5)$$

derived from the conservation law $|\mathbf{M}_f|^2 = M_0^2$, which can be easily obtained by averaging quantum statistically the set of Eqs. (2) in Weiss field approximation.

Following Ref. 8 and considering the weakly nonlinear fictitious spin excitations let us search for the solution of the set of Eqs. (4) and (5) in the form

$$m_g^\pm = \sum_{\alpha=1}^{\infty} \varepsilon^\alpha \sum_{l=-\infty}^{\infty} m_l^{\pm(\alpha)}(\xi_g, \tau) \cdot e^{i l(\mathbf{k} \mathbf{r}_g - \omega t)},$$

$$m_g^z = \sum_{\alpha=1}^{\infty} \varepsilon^\alpha \sum_{l=-\infty}^{\infty} m_l^{z(\alpha)}(\xi_g, \tau) \cdot e^{i l(\mathbf{k} \mathbf{r}_g - \omega t)}, \quad (6)$$

where $m_{-l}^{-\alpha} = (m_l^{+\alpha})^*$, $m_{-l}^{z(\alpha)} = (m_l^{z(\alpha)})^*$, and

$$\xi_g = \varepsilon(\mathbf{s} \mathbf{r}_g - \lambda t), \quad \tau = \varepsilon^2 t \quad (7)$$

are slowly varying space-time variables⁸ ($\mathbf{s} \equiv \mathbf{k}/k$, i.e., the modulation along \mathbf{k} is examined); λ is a propagation velocity of the modulated wave and ε is a formal small parameter. As we will see below, ε will enter in the combination with \mathbf{m} . This coupling will play the role of expansion parameter and in the final results we will set ε to unity. As components of $\mathbf{m}_l(\xi_g, \tau)$ depend only on slow variables (7) we can suppose that their inhomogeneous parameter Λ is much larger than a (a is a distance between the nearest-neighboring sites of lattice), so $\mathbf{m}_l(\xi_g, \tau)$ could be considered as a continuous function. Let us note that indices f and g numerate lattice sites while the index l specifies different harmonics of \mathbf{m}_f .

For the calculation of combination $\sum_g^N A_{fg} m_g^\pm$ in Eq. (4) let us expand $m_l^{\pm(\alpha)}(\xi_g, \tau)$ in the vicinity of ξ_f [inhomoge-

neous scale of $m_l^{\pm(\alpha)}(\xi, \tau)$ is supposed much more than the tunneling distance which is of the order of a]. Thereby we get

$$\sum_g^N A_{fg} m_g^\pm = \sum_{l=-\infty}^{\infty} e^{i l(\mathbf{k} \mathbf{r}_f - \omega t)} \sum_{\alpha=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \varepsilon^{\alpha+n} \times \left\{ \left(\mathbf{s} \frac{\partial}{\partial \mathbf{q}} \frac{\partial}{\partial \xi_f} \right)^n [A(\mathbf{q}) m_l^{\pm(\alpha)}(\xi_f, \tau)] \right\}_{\mathbf{q}=\mathbf{l} \mathbf{k}}, \quad (8)$$

where

$$A(\mathbf{q}) \equiv \sum_g^N A_{fg} e^{i \mathbf{q}(\mathbf{r}_g - \mathbf{r}_f)}. \quad (9)$$

Substituting expressions (6) and (8) into Eqs. (4) and (5), and taking into consideration the operator relation

$$\frac{dm_f^\pm}{dt} \equiv \sum_{\alpha=1}^{\infty} \varepsilon^\alpha \sum_{l=-\infty}^{\infty} e^{i l(\mathbf{k} \mathbf{r}_f - \omega t)} \times \left(-i l \omega - \varepsilon \lambda \frac{\partial}{\partial \xi_f} + \varepsilon^2 \frac{\partial}{\partial \tau} \right) m_l^{\pm(\alpha)}(\xi_f, \tau) \quad (10)$$

[which follows from definitions (6) and (7)] and equating the coefficients of various powers of ε in the same harmonics to zero one can obtain the closed system of equations to calculate the values of $m_l^{\pm(\alpha)}(\xi, \tau)$ and $m_l^{z(\alpha)}(\xi, \tau)$.

Particularly in the first order of ε from Eq. (4) we get

$$[l \omega \mp \omega_0 \mp 2M_0 A(\mathbf{l} \mathbf{k})] m_l^{\pm(1)}(\xi, \tau) = 0. \quad (11)$$

If we assume that only the nonzero harmonic is $m_1^{+(1)}(\xi, \tau)$, then, from expression (15) we obtain the following dispersion law:

$$\omega = \omega_0 - 2|M_0|A(\mathbf{k}). \quad (12)$$

So, on the present stage Eq. (11) indicates that $m_1^{+(1)} = (m_{-1}^{-(1)})^*$ is an arbitrary function of the slow variables ξ , τ , and $m_1^{-(1)} = (m_{-1}^{+(1)})^* = 0$. Furthermore, from Eq. (5) we get

$$m_1^{z(1)}(\xi, \tau) = 0. \quad (13)$$

In the second order of ε we obtain from the motion Eq. (4) the relation

$$i[l \omega \mp \omega_0 \mp 2M_0 A(\mathbf{l} \mathbf{k})] m_l^{\pm(2)}(\xi, \tau) + \left(\lambda \mp 2M_0 \frac{\partial A(\mathbf{k})}{\partial \mathbf{k}} \mathbf{s} \right) \frac{\partial}{\partial \xi} m_l^{\pm(1)}(\xi, \tau) = 0.$$

Examining this equation for the main harmonic ($l=1$) and using Eq. (12) we get the expression for propagation velocity:

$$\lambda = \frac{\partial \omega}{\partial \mathbf{k}} \mathbf{s} = 2M_0 \frac{\partial A(\mathbf{k})}{\partial \mathbf{k}} \mathbf{s} \quad (14)$$

and conclude that $m_1^{+(2)}(\xi, \tau)$ is an arbitrary function of slow variables ξ , τ , and $m_1^{-(2)}(\xi, \tau) = 0$.

We should also determine overtones $\mathbf{m}_0^{(2)}(\xi, \tau)$ and $\mathbf{m}_2^{(2)}(\xi, \tau)$, which are necessary for our further calculations. Taking into consideration the conservation condition (5), we obtain that all components of the overtones are equal to zero except the following one:

$$m_0^{z(2)}(\xi, \tau) = -\frac{1}{2}|m_1^{+(1)}|^2. \quad (15)$$

Finally, in the third approximation, from Eq. (4) in view of Eqs. (8), (10), (12), (14), and (15) the nonlinear Schrödinger equation is obtained for the main harmonic ($l=1$):

$$2i \frac{\partial m_1^{+(1)}}{\partial \tau} + \omega'' \frac{\partial^2 m_1^{+(1)}}{\partial \xi^2} + \Delta m_1^{+(1)} |m_1^{+(1)}|^2 = 0, \quad (16)$$

where ($a, b=x, y, z$)

$$\omega'' = \sum_{a,b} \frac{\partial^2 \omega}{\partial k_a \partial k_b} s_a s_b = 2M_0 \sum_{a,b} \frac{\partial^2 A(\mathbf{k})}{\partial k_a \partial k_b} s_a s_b, \quad (17)$$

$$\Delta = 2M_0 A(\mathbf{k}).$$

Equation (16) has a trivial solution in a form of nonlinear plane wave with a constant amplitude $|m_1^{+(1)}|$:

$$m_1^{+(1)} = |m_1^{+(1)}| \cdot e^{-i\delta\omega_s t}, \quad \delta\omega_s = -\frac{1}{2}\Delta |m_1^{+(1)}|^2. \quad (18)$$

If Lighthill condition¹³ $\omega''\Delta > 0$ holds, the nonlinear plane waves become unstable under any modulation and Eq. (16) permits soliton solution in the following form:

$$m_1^{+(1)} = |m_1^{+(1)}|_{max} \cdot \text{sech} \left\{ \frac{1}{\Lambda} (\mathbf{sr} - \lambda t) \right\} e^{-i\delta\omega_s t}, \quad (19)$$

where the soliton width Λ and the shift of frequency $\delta\omega_s$ caused by the nonlinear "self-action" are given by the following expressions:

$$\Lambda = \frac{1}{|m_1^{+(1)}|_{max}} \sqrt{\frac{2\omega''}{\Delta}}, \quad \delta\omega_s = -\frac{1}{4}\Delta |m_1^{+(1)}|_{max}^2. \quad (20)$$

Now we will consider $|m_1^{+(1)}|_{max}$ instead of the small parameter ε (the weakly nonlinear excitations are examined), so $|m_1^{+(1)}|_{max} \ll 1$ and in view of Eqs. (3), (15), and (19) the relative concentration of defects can be expressed as

$$x = x_0 + \delta x, \quad \delta x = \delta x_m \cdot \text{sech}^2 \left\{ \sqrt{\frac{2\delta x_m \Delta}{\omega''}} (\mathbf{sr} - \lambda t) \right\} \quad (21)$$

if $\omega''\Delta > 0$,

$$\text{or } x = x_0 = \text{const if } \omega''\Delta < 0. \quad (22)$$

Here it is taken into account that $M_0 \approx -1/2$; δx_m is an amplitude of δx . So the width of the soliton of defects is

$$\Lambda = \sqrt{\frac{\omega''}{2\delta x_m \Delta}}. \quad (23)$$

It should be noted that the value of δx can be much more than static relative concentration x_0 (weak nonlinearity requires only the satisfaction of condition $\delta x_m \ll 1$).

Now let us consider the validity of Weiss field approximation (possibility of neglect of quantum correlations). This is easier to do using Dyson's transform¹⁴ of Fermi operators:

$$S_f^+ = b_f^+ - b_f^+ b_f^+ b_f, \quad S_f^- = b_f, \quad S_f^z = -1/2 + b_f^+ b_f$$

(b_f^+ and b_f are Bose operators) in momentum presentation

$$b_f^+ = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} b_{\mathbf{k}}^+ e^{i\mathbf{k}r_f}, \quad b_f = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} b_{\mathbf{k}} e^{-i\mathbf{k}r_f}.$$

Then we can present Hamiltonian (1) in the following form:

$$\mathcal{H} = \sum_{\mathbf{k}} [\omega_0 - A(\mathbf{k})] b_{\mathbf{k}}^+ b_{\mathbf{k}} - \omega_1 \sqrt{N} (b_{\mathbf{q}} e^{i\omega t} + b_{\mathbf{q}}^+ e^{-i\omega t}) + \frac{1}{N} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} A(\mathbf{k}_1) b_{\mathbf{k}_1}^+ b_{\mathbf{k}_2}^+ b_{\mathbf{k}_3} b_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3}, \quad (24)$$

where the source field with amplitude ω_1 and wave number \mathbf{q} is added to get nonthermal concentration of vacancies with definite wave number (thermal concentration of vacancies at low temperatures is close to zero). Although we consider the nonlinear behavior after switching off this source field, the average value of vacancy concentration remains the same and we can use it for estimations.

Applying Eq. (24) one can examine the motion equations for operators $b_{\mathbf{q}}^+ b_{\mathbf{q}}$, $b_{\mathbf{q}} b_{\mathbf{q}}^+$, and $b_{\mathbf{q}}^+$, $b_{\mathbf{q}}$, e.g., the motion equation for $b_{\mathbf{q}}$ could be written in the following form:

$$\left\{ \frac{d}{dt} + \gamma_{\mathbf{q}} + i[\omega_0 - A(\mathbf{q})] \right\} b_{\mathbf{q}} + \frac{2i}{N} A(\mathbf{q}) b_{\mathbf{q}}^+ b_{\mathbf{q}} b_{\mathbf{q}} = i\omega_1 \sqrt{N} e^{-i\omega t}. \quad (25)$$

Here the damping constant $\gamma_{\mathbf{q}}$ is introduced. It appears from the four vacancy term of Hamiltonian and expresses the influence of thermal vacancies on the \mathbf{q} mode. $\gamma_{\mathbf{q}}$ is proportional to the concentration of thermal vacancies and, consequently, is close to zero.

Neglecting in Eq. (25) slow time evolution and nonlinear term expressing the self-action the stationary solutions are obtained for averaged values: $\langle b_{\mathbf{q}} \rangle = (\langle b_{\mathbf{q}}^+ \rangle)^* = \omega_1 \sqrt{N} e^{-i\omega t} / [\omega_0 - \omega + A(\mathbf{q}) - i\gamma_{\mathbf{q}}]$. Further, writing the motion equations for $b_{\mathbf{q}}^+ b_{\mathbf{q}}$ and $b_{\mathbf{q}} b_{\mathbf{q}}^+$ the following equalities can be easily derived: $\langle b_{\mathbf{q}}^+ b_{\mathbf{q}} \rangle = \langle b_{\mathbf{q}} b_{\mathbf{q}}^+ \rangle = \langle b_{\mathbf{q}}^+ \rangle \langle b_{\mathbf{q}} \rangle = n_d$, where n_d is a concentration of vacancies. But as far as $b_{\mathbf{q}}^+ b_{\mathbf{q}} = -1 + b_{\mathbf{q}} b_{\mathbf{q}}^+$ we see the possible error. However, it can be neglected in comparison with the macroscopical quantity $\langle b_{\mathbf{q}}^+ b_{\mathbf{q}} \rangle = n_d \gg 1$.

If the weakly nonlinear effects and slow time evolution are taken into account we obtain the following expressions: $\langle b_{\mathbf{q}}^+ b_{\mathbf{q}} \rangle = \langle b_{\mathbf{q}}^+ \rangle \langle b_{\mathbf{q}} \rangle [1 + \mathcal{O}(x)] = N[x + \mathcal{O}(x^2)]$ (let us remind that $x = n_d/N$ is relative concentration of vacancies). However, we consider approximation up to ε^3 , i.e., $x^{3/2}$, thus the corrections induced by the quantum correlations can be neglected.

III. DISCUSSION AND ESTIMATIONS

All parameters specifying the soliton depend upon the function $A(\mathbf{k})$ [see expressions (17) and (23)]. So we should determine it in the bcc and hcp phases of solid ^4He crystal.

At first let us examine bcc phase. Directing the axes of reference along lattice edges (crystallographic axes), supposing that quantum tunneling is restricted only to eight neighboring sites and denoting $A_{fg}=A$ we get from the definition (9)

$$A(\mathbf{k}) = 8A \cdot \cos \frac{ak_x}{\sqrt{3}} \cos \frac{ak_y}{\sqrt{3}} \cos \frac{ak_z}{\sqrt{3}}. \quad (26)$$

Considering the long-wavelength excitations $ka \ll 1$ we easily obtain

$$A(\mathbf{k}) = 8A \left(1 - \frac{1}{6}(ak)^2 + \dots \right) \quad (27)$$

and thereby, and in view of Eq. (12), we get the same dispersion law as in Refs. 4 and 6. It can be easily seen from Eqs. (17) and (27) that the Lighthill condition is not satisfied and, consequently, there is no possibility of existence of solitary formation of defects for the long-wavelength excitations. Further analysis of Eq. (27) shows that solitary solution does not exist if \mathbf{k} is directed along the crystallographic axes x , y , z . But it can be easily shown that soliton solution exists in the wide range of k_x , k_y , k_z space. Indeed, if we examine for simplicity the case when \mathbf{k} is in the xy plane, in view of Eqs. (23), (17), and (26) the following expression for the width of soliton can be obtained:

$$\Lambda = \frac{a}{3\sqrt{\delta x_m}} \sqrt{s_x s_y t g \frac{ak_x}{\sqrt{3}} t g \frac{ak_y}{\sqrt{3}} - 1/2}. \quad (28)$$

It is valid if $t g(ak_x/\sqrt{3}) t g(ak_y/\sqrt{3}) > (1/2)s_x s_y$. It follows from Eqs. (28) and (23) that generally $\Lambda \sim a/\sqrt{\delta x_m}$ (consequently $\Lambda \gg a$ as it should be) and we should exclude from consideration the points in \mathbf{k} space where the condition $\Lambda \gg a$ does not hold. Furthermore, as it can be easily seen from Eq. (28), the width of the soliton grows rapidly if $\cos(ak_x/\sqrt{3}) \rightarrow 0$, $k_y \neq 0$ or $\cos(ak_y/\sqrt{3}) \rightarrow 0$, $k_x \neq 0$.

Let us consider briefly another hcp phase of solid helium. We examine the axes of reference where xy plane coincides with a hexagon plane of lattice and x axis coincides with a

line connecting opposite sites of the hexagon. Restricting ourselves only to 12 neighboring sites and denoting again $A_{fg}=A$ we get

$$A(\mathbf{k}) = 2A \left\{ 2 \cos \frac{ak_x}{2} \left[\cos \frac{\sqrt{3}}{2} ak_y + \cos \frac{a}{2\sqrt{3}} (2\sqrt{2}k_z - k_y) \right] + \cos ak_x + \cos \frac{a}{\sqrt{3}} (\sqrt{2}k_z + k_y) \right\}.$$

As in the previous case we obtain that there is no solitary solution for the long-wavelength excitations ($ka \ll 1$). But regarding the propagation along z axis (i.e., $s_x = s_y = 0$) we can make a conclusion that the solitary solution exists (Lighthill condition is satisfied) in the range of $-1 \leq \cos(\sqrt{2/3}ak_z) < 0$. Moreover, if $\cos(\sqrt{2/3}ak_z/2) \rightarrow -1$ we obtain that $\Lambda \rightarrow \infty$ and $\lambda \rightarrow 0$.

In the case of propagation along x axis the solitary solution exists in the range of $0 \leq \cos(ak_x/2) < 1/2$. At the point $\cos(ak_x/2) \rightarrow 0$ we get that $\Lambda \rightarrow \infty$ and $|\lambda| \rightarrow 4aA \neq 0$.

IV. CONCLUSIONS

We have investigated the collective solitary motion of vacancies in solid ^4He . This motion is possible to observe using x-ray-diffraction technique⁴ in the range of the wave numbers of vacancy excitations where the soliton solution exists. Moreover, the above consideration can be extended to the case of motion of vacancies in solid ^3He , or to motion of admixture ^4He atoms in ^3He where the collective solitary motion can be observed by measuring times of spin-lattice relaxation. However, it should be mentioned that in the latter cases there exist real spins besides the fictitious spins. Thus considering the mobilities of defects in solid ^3He we cannot directly use the results of the above calculations and a separate consideration is required.

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