Letter

Effective mass and interaction energy of heavy Bose polarons at unitarity

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We use the Gross-Pitaevskii equation (GPe) to study the motion of a heavy impurity immersed in a weakly interacting Bose-Einstein condensate and interacting with the bosons via an attractive boson-impurity potential. We construct a perturbative solution to the GPe in powers of impurity velocity in the case when the boson-impurity potential is tuned to unitarity, resulting in a unitary polaron, and calculate its effective mass. In addition, we calculate the interaction energy of two unitary polarons which are sufficiently far apart. Our formalism also reproduces the results for both the mass and interaction energy obtained at weak boson-impurity coupling.

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A Bose polaron is a quasiparticle that is formed when a quantum impurity is immersed into a gas of weakly interacting bosons below the condensation temperature. There has been a significant interest in the study of Bose polarons, especially in the regime when the impurity is allowed to interact with the bosons arbitrarily strongly [1–14]. We would like to consider the scenario where the boson-impurity two-body potential can be modeled by a short-ranged attractive potential. In the regime of weak boson-impurity interactions, all quasiparticle properties of the polaron depend only on the value of the boson-impurity scattering length a in a universal way. When the boson-impurity potential is made deeper, the value of the scattering length becomes more negative up until it becomes infinite. This happens when the potential is tuned to a threshold of supporting a bound state, the so-called unitary point. A polaron with this kind of a boson-impurity potential can be called a unitary polaron. In contrast, a polaron with a weak boson-impurity potential can be called a weak polaron. A unitary polaron's boson-impurity potential is strong and the properties of the polaron no longer depend on the boson-impurity scattering length which is formally infinite. Instead it could be characterized by other parameters that may depend on boson-impurity potential.

Recently, it has been shown that all static quasiparticle properties of a single unitary Bose polaron can be calculated analytically using the Gross-Pitaevskii equation (GPe), provided that the density of the Bose gas is sufficiently small and that the boson-impurity interactions are not too short ranged [equivalent to the condition (3) below] [15,16]. Furthermore, under the additional condition (4), all the properties of the unitary polaron depend on the boson-impurity potential via a single parameter R, which is generally of the order of the range of the potential r_c and formally defined below in Eq. (22). In this Letter we generalize these results and obtain analytic expressions for the effective mass and induced interaction energy between two unitary polarons. Our construction is based on the perturbative expansions of the energy which use the polaron's velocity in the former case and the inverse distance between the polarons in the latter case as small parameters.

First, we consider a slowly moving unitary polaron and present a derivation of the contribution to the energy of the Bose polaron which is quadratic in the impurity velocity. This leads to the following induced mass of the unitary polaron (that is, the mass of particles dragged by an impurity [17]):

$$m^* = \frac{4\sqrt{2}\pi\delta^{2/3}\xi^3 n_0 m}{3}. \tag{1}$$

Here m is the mass of the bosons forming the condensate, n_0 is the density of the Bose gas far away from the impurity, ξ is the coherence length of the condensate, and $\delta = R/\xi$. The calculation is done in the limit when the mass of the impurity $M \gg m$. The total effective mass of the polaron is clearly $m_{\rm polaron} = m^* + M$. Then we apply our technique to calculate the interaction energy of two polarons a distance d apart. We find that

$$E_{\rm ind}(d) = -\frac{4\pi n_0 \xi^2 \delta^{2/3}}{md} e^{-\sqrt{2}\frac{d}{\xi}} \tag{2}$$

if $d \gg \xi\delta^{1/3}$. The Yukawa form $\sim e^{-\sqrt{2}\frac{d}{\xi}}/d$ has been recently observed numerically in Ref. [18]. The method that we use demands that the following two inequalities are enforced [16]:

$$\left(na_B^3\right)^{1/4} \ll \frac{R}{a_B}, \tag{3}$$

$$\frac{R}{a_B} \ll \frac{1}{\sqrt{na_B^3}}. \tag{4}$$

Here a_B is the scattering length of the intraboson interactions. The inequality (3), if violated, signifies that the GPe is no longer a reliable approximation to the strong polaron problem. The inequality (4), equivalent to $\delta \ll 1$, represents the validity of a particular analytic solution to the GPe that we rely on here. Under these conditions, $m^* \gg m$.

We note that the above results in Eqs. (1) and (2) resemble the corresponding expressions for the polaron in the regime of weak interactions found previously and given here in Eqs. (9) and (28), if one makes the identification $\xi\delta^{1/3} \to |a|$. This is consistent with the weak polaron condition given in Ref. [16], as $|a| \ll \xi\delta^{1/3}$. We thus suggest that the properties of the polaron as $|a|$ increases past $\xi\delta^{1/3}$ quickly converge to the properties of the unitary polaron.

We show that in order to calculate the effective mass of the polaron it is sufficient to consider only the leading term in the velocity expansion of the solution to the GPe. Similarly, we argue that in order to compute the interaction energy between two polarons, it is sufficient to consider the solution to the GPe in the form (32), which is the sum of two independent polaronic solutions that satisfies the boundary condition at infinity.

Let us now present the derivation of these results. For the case of a moving polaron, we closely follow the method used by Astrakharchik and Pitaevskii, who solved the corresponding problem in the regime of weak boson-impurity interactions [17]. As they explained, a moving polaron satisfies the equation

$$i\frac{\partial\psi}{\partial t} = -\frac{\Delta\psi}{2m} + \lambda|\psi|^2\psi + [U(\mathbf{r} - \boldsymbol{v}t) - \mu]\psi. \qquad (5)$$

Here U is the interaction potential between the polaron and the bosons, $\lambda = 4\pi a_B/m$, and $\boldsymbol{v}$ is the velocity of the polaron. The solution to this equation is of the form $\psi(\mathbf{r} - \mathbf{v}t)$. Substituting and changing the variables $\mathbf{r} - \boldsymbol{v}t \to \mathbf{r}$, we find

$$-i\boldsymbol{v}\cdot\nabla\psi = -\frac{\Delta\psi}{2m} + \lambda|\psi|^2\psi + [U(\mathbf{r}) - \mu]\psi. \qquad (6)$$

Once the solution of Eq. (6) is found, the energy of the polaron can be computed by substituting the solution into the energy:

$$E = \int d^3x\left(\frac{|\nabla\psi|^2}{2m} + \frac{\lambda}{2}|\psi|^4 + [U(\boldsymbol{r}) - \mu]|\psi|^2\right) \qquad (7)$$

If the impurity energy potential U is weak, then Eq. (6) can be solved perturbatively in U. This approach was exploited by Astrakharchik and Pitaevskii [17], who obtained the following velocity dependence of the polaron energy:

$$E_{v^2} = \frac{2\sqrt{2}\pi n_0\xi m a^2 v^2}{3}, \qquad (8)$$

which obviously leads to the induced mass of the weak polaron:

$$m^*_{\text{weak}} = \frac{4\sqrt{2}\pi n_0\xi a^2}{3}m. \qquad (9)$$

Here a is the scattering length of the boson-impurity interactions.

As the interaction strength is increased and $|a|$ grows, Eq. (9) must break down. To calculate the induced mass of the unitary polaron whose scattering length a goes to infinity, we must solve Eq. (6) without assuming that U is small. While we have at our disposal a technique to solve it when U is tuned to unitary at $\boldsymbol{v} = 0$, solving it at nonzero $\boldsymbol{v}$ appears to be difficult. Instead we propose to solve it perturbatively, although as an expansion in powers of $\boldsymbol{v}$ instead of the potential U. After all, we are only interested in knowing the energy (7) up to terms quadratic in velocity $\boldsymbol{v}$.

To do this we can take advantage of the following mathematical observation. Suppose we have a function $f(x, \epsilon)$, where ϵ is small. We would like to minimize f with respect to x and find its minimum $x_m(\epsilon)$, and we would then like to compute the value of f at this minimum $f_m = f(x_m(\epsilon), \epsilon)$. We would like to calculate the expansion f_m in powers of ϵ up to terms quadratic powers of ϵ^2. We claim that to do that it is sufficient to compute $x_m(\epsilon)$ up to terms linear in ϵ.

Indeed, suppose we compute x_m up to terms quadratic in ϵ. In other words,

$$x_m = x_0 + x_1\epsilon + x_2\epsilon^2 + \dots. \qquad (10)$$

Then it should be clear that the expansion in powers of ϵ of $f(x_0 + x_1\epsilon + x_2\epsilon^2, \epsilon)$ up to terms quadratic in ϵ will not contain x_2, as by construction

$$\left.\frac{\partial f(x,\epsilon)}{\partial x}\right|_{x=x_0,\,\epsilon=0} = 0. \qquad (11)$$

In fact, Astrakharchik and Pitaevskii implicitly used this observation in their paper [17].

This observation would allow us to find the energy E up to terms quadratic in velocity $\boldsymbol{v}$ by computing ψ only up to terms linear in $\boldsymbol{v}$ if Eq. (6) that we need to solve were obtained as a minimization of that energy E. However, it is not quite so, as minimizing E over $\bar\psi$ does not produce Eq. (6). Nevertheless we could write the energy (7) in the following convenient way:

$$E = E_1 + E_2, \qquad (12)$$

where

$$E_1 = \int d^3x\left(\frac{|\nabla\psi|^2}{2m} + \frac{\lambda}{2}|\psi|^4 + [U(\boldsymbol{r}) - \mu]|\psi|^2\right) + i\boldsymbol{v}\int d^3x\,\bar\psi\nabla\psi, \qquad (13)$$

and

$$E_2 = -i\boldsymbol{v}\int d^3x\,\bar\psi\nabla\psi. \qquad (14)$$

Minimizing E_1 with respect to $\bar\psi$ gives Eq. (6), therefore to calculate E_1 up to terms quadratic in $\boldsymbol{v}$ we only need to know ψ up to terms linear in $\boldsymbol{v}$ for reasons explained above. At the same time, E_2 is already proportional to $\boldsymbol{v}$, therefore to calculate it up to terms quadratic in $\boldsymbol{v}$ we again need to know ψ up to terms linear in $\boldsymbol{v}$. In other words, we can substitute ψ calculated up to terms linear in $\boldsymbol{v}$ directly into the energy (7) and find it up to terms quadratic in $\boldsymbol{v}$. This observation significantly simplifies the required algebra.

Let us now calculate the expansion of ψ in powers of $\boldsymbol{v}$. It is convenient to introduce dimensionless variable $\phi = \psi/\sqrt{n_0}$. It is normalized so that far away from the impurity $\phi = 1$. We then write

$$\phi = \phi_0 + \phi_1 + \dots, \qquad (15)$$

where ϕ_0 is independent of $\boldsymbol{v}$, ϕ_1 is linear in $\boldsymbol{v}$, and so on. Substituting into Eq. (6) and expanding in powers of $\boldsymbol{v}$ we find, first of all,

$$-\frac{\Delta\phi_0}{2m} + \mu(\phi_0^2 - 1)\phi_0 + U(\mathbf{r})\phi_0 = 0. \qquad (16)$$

Here we used that $\lambda n_0 = \mu$. We also used that ϕ_0 is real. This becomes clear if we note that Eq. (16) coincides with the GPe for the stationary polaron. Therefore, ϕ_0 coincides with the solution of the stationary unitary polaron problem found in Refs. [15,16], which was real.

At the same time, we find that

$$-i\boldsymbol{v}\nabla\phi_0 = -\frac{\Delta\phi_1}{2m} + \mu\big(\phi_0^2 - 1\big)\phi_1 + U(\mathbf{r})\phi_1. \tag{17}$$

Here we used that ϕ_1, as should be clear from this expression, is purely imaginary. If we find ϕ_1 by solving this equation, we will know ψ up to terms linear in $\boldsymbol{v}$. We can now substitute this into the expression for the energy (7) and expand in powers of $\boldsymbol{v}$ up to terms quadratic in it.

The zeroth-order term is the energy of the stationary polaron. The first-order term vanishes, as it turns out. This is not surprising as those terms if they were not zero would depend on the direction of $\boldsymbol{v}$, while we work with a rotationally invariant polaron. Finally, the terms quadratic in $\boldsymbol{v}$ can be brought to the form

$$E_{v^2} = -in_0\boldsymbol{v}\int d^3x\,\bar{\phi}_1\nabla\phi_0. \tag{18}$$

This remarkably simple expression tells us that to compute the energy we need to use ϕ_0 calculated in Refs. [15,16], determine ϕ_1 by solving Eq. (17), and substitute into the expression (18).

Let us now review the structure of the solutions ϕ_0 of the GPe both at weak coupling and at unitarity as described in Refs. [15,16]. For simplicity, we consider the potentials that vanish identically beyond some range r_c. The solution to Eq. (16) for the case of the weak potential $|a|^3 \ll \xi^2 r_c$, where $\xi^2 = 1/(2m\mu)$ is the square of the coherence length ξ, reads

$$\phi_0(r) \approx \begin{cases} \left(1 - \frac{a}{r_c}\right) r_c\Psi_0(r), & r < r_c, \\ 1 - \frac{a}{r}\exp(-\sqrt{2}r/\xi), & r > r_c. \end{cases} \tag{19}$$

Here $\Psi_0(r)$ is the solution to the zero energy Schrodinger equation

$$-\frac{1}{2m}\Delta\Psi_0 + U(\boldsymbol{r})\Psi_0 = 0 \tag{20}$$

in the potential U with the normalization that satisfies $\Psi_0(r_c) = 1/r_c$, and a is the corresponding scattering length.

When potential U is tuned to unitarity, the result becomes ($\delta = R/\xi \sim r_c/\xi \ll 1$)

$$\phi_0(r) \approx \begin{cases} \xi\delta^{1/3}\Psi_0(r), & r < r_c, \\ 1 + \frac{\xi\delta^{1/3}}{r}\exp(-\sqrt{2}r/\xi), & r > r_c. \end{cases} \tag{21}$$

Here R is defined as

$$R = \left[\int_0^\infty dr\, r^2\Psi_0^4\right]^{-1}. \tag{22}$$

One expects [16] $R \sim r_c$. Note that in the region where $r > r_c$ both solutions have the same structure, but differ only by a coefficient in front of the Yukawa tail.

Let us focus on the unitary case and solve Eq. (17) for $\phi_1(r)$. We seek solution in the form $\phi_1(\boldsymbol{r}) = ivP_1[\cos(\theta)]u_1(r)/r$, where $P_1[\cos(\theta)]$ is the first Legendre polynomial, θ is the angle between $\boldsymbol{v}$ and $\mathbf{r}$, while $u_1(r)$ is the radial part of the solution. Plugging this form into Eq. (17) we get

$$-rm\phi_0' = -\frac{u_1''}{2} + \frac{\phi_0^2 - 1}{2\xi^2}u_1 + \frac{u_1}{r^2} + mU(r)u. \tag{23}$$

If the potential U is unitary, we make the observation that $(\phi_0^2 - 1)/(2\xi^2) \ll 1/r^2$ for all r and can be neglected. To see that, we note that, for $r < r_c$, $\phi_0 \approx 1/\delta^{2/3} \gg 1$ and we find

$$\big(\phi_0^2 - 1\big)/(2\xi^2) \sim 1/(\xi^2\delta^{4/3}) \ll 1/r_c^2 < 1/r^2.$$

Next, for $r_c < r < \xi^{2/3}r_c^{1/3}$, $\phi_0 \sim \xi\delta^{1/3}/r \gg 1$ and we find

$$\big(\phi_0^2 - 1\big)/(2\xi^2) \sim \delta^{2/3}/r^2 \ll 1/r^2.$$

For $\xi^{2/3}r_c^{1/3} < r < \xi$, $\phi_0 - 1 \sim \xi\delta^{1/3}/r \ll 1$ and we find

$$\big(\phi_0^2 - 1\big)/(2\xi^2) \sim \delta^{1/3}/(\xi r) \ll 1/r^2.$$

Finally, for $r > \xi$, $\phi_0^2 - 1$ decays exponentially towards zero, so it is obviously much smaller than $1/r^2$.

Note that a potential weaker than unitary leads to even smaller $\phi_0^2 - 1$, therefore these arguments also apply at weak potential.

These observations allow us to significantly simplify Eq. 23, with the result

$$2mr\phi_0' = u_1'' - \frac{2}{r^2}u_1 - 2mUu_1. \tag{24}$$

Now for $r > r_c$, $U = 0$. While $U \neq 0$ at $r < r_c$, it turns out that the region $0 < r < r_c$ does not significantly contribute to the energy and therefore we can simplify this even further and solve

$$2mr\phi_0' = u_1'' - \frac{2}{r^2}u_1. \tag{25}$$

We will come back to this point below.

Equation (25) is simple enough where it can be solved explicitly, with the solution

$$u_1 = \frac{2m}{3}\left(r^2[\phi_0(r) - 1] - \frac{1}{r}\int_0^r ds\, s^3\phi_0'(s)\right). \tag{26}$$

Plugging this expression for u_1 together with the definition of $\phi_0(r)$, Eq. (21), into Eq. (18), we get

$$E_{v^2} = \frac{2\sqrt{2}\pi\delta^{2/3}\xi^3 n_0 m v^2}{3}. \tag{27}$$

The induced mass of the polaron at unitarity (1) follows immediately.

We still need to estimate the contribution of the region $0 < r < r_c$ to the energy. In that region, $\phi_0 \approx 1/\delta^{2/3}$, $u_1 \sim r_c^2/\delta^{2/3}$, so we can find that this region contributes $n_0 m v^2 \xi r_c^2$ to the energy. This is much smaller than (27) as $\xi r_c^2 \ll \xi^3\delta^{2/3}$.

As was discussed previously, both weak and unitary polaron solutions Eqs. (19) and (21) have the same r dependence in the region $r > r_c$. Therefore, an obvious substitution $\delta^{1/3}\xi \to |a|$ reduces our result for the energy of the unitary polaron to the energy obtained by Astrakharchik and Pitaevskii [Eq. (8)] for the weak polaron.

Just as with the result for the energy of the stationary polaron found earlier in Refs. [15,16], the result found here [Eq. (27)] is only valid when $\delta \ll 1$. In principle corrections to it proportional to higher powers of δ can also be calculated if needed.

We can also calculate the interaction energy of two stationary unitary polarons separated by a distance d. For the weak polaron, the real-space expression has been obtained before by Refs. [19–21], and it reads

$$E_{\rm int}(d) = -\frac{4\pi n_0 a^2}{md} e^{-\sqrt{2}\frac{d}{\xi}}. \quad (28)$$

To calculate this for the unitary heavy polarons, we need to solve the GPe with two potentials

$$-\frac{\Delta\psi}{2m} + \lambda|\psi|^2\psi + [U(\boldsymbol{r}) + U(\boldsymbol{r}-\boldsymbol{d}) - \mu]\psi = 0 \quad (29)$$

and calculate the energy of the solution:

$$E = \int d^3x \left(\frac{|\nabla\psi|^2}{2m} + \frac{\lambda}{2}|\psi|^4 + [U(\boldsymbol{r}) + U(\boldsymbol{r}-\boldsymbol{d}) - \mu]|\psi|^2\right). \quad (30)$$

We will not attempt to do this for a generic separation between the polarons d. Let us just compute this in the case when d is so large that the solution can be written as

$$\frac{\psi}{\sqrt{n_0}} \approx \phi_0(\boldsymbol{r}) + \phi_0(\boldsymbol{r}-\boldsymbol{d}) - 1 + f(\boldsymbol{r}), \quad (31)$$

where $|f| \ll 1$. Here $\phi_0(\boldsymbol{r})$ is the solution for a single stationary unitary polaron (21). Crucially, $|f|$ is indeed small if $|\phi_0(d) - 1| \ll 1$. This is because at very large separation between the polarons clearly $f = 0$ should solve the corresponding GPe (29). If d is large but finite, f will be nonzero but small. This is guaranteed by $\phi_0(d)$ approaching 1 at $d \gg \xi\delta^{1/3}$. All of this can be verified by a direct substitution of (31) into (29) with the help of (21).

The same theorem that earlier allowed us to compute energy for a moving polaron up to terms quadratic in velocity while calculating ψ up to terms linear in it allows us now to calculate the energy of two polarons by substituting the solution for two polarons at $f = 0$

$$\psi = \sqrt{n_0}[\phi_0(\boldsymbol{r}) + \phi_0(\boldsymbol{r}-\boldsymbol{d}) - 1] \quad (32)$$

into the expression (30). Subtracting the part of the energy independent of d, which is the energy of the condensate and the individual energies of the polarons, gives the interaction energy of the polarons.

This program gives the leading contribution to the interaction energy at large d. To compute corrections to that if needed, we would have to solve for f by substituting Eq. (31) in the GPe (29). We will not attempt to do it here.

Carrying out this program produces the interaction energy (2) of two polarons distance d apart. Note that replacing $\xi\delta^{1/3} \to |a|$ gives the interaction energy of weak polarons (28), as we should have expected on general grounds discussed earlier. This result is in agreement with the recent numerical study by Ref. [18] who observed the Yukawa-type behavior consistent with Eq. (2) holding up to distances of the order of ξ. At smaller distances two polarons start to have a significant overlap and one cannot longer use Eq. (32) to compute the energy. As a starting point one needs to solve the GPe in the spherically nonsymmetric potential analytically. This goes beyond formalism described in Refs. [15,16].

As a side note, while for the unitary case we had to use the assumption that two polarons must be well separated in order to be able to use Eq. (32), for weak polarons this form is correct for arbitrary separation d. Indeed, for the weak polaron, one can linearize the GPe and the solution to the two polaron problem will be just a linear combination of the solutions to a single polaron problem. The contribution to the interaction energy reads

$$E_{\rm int}(d) = 2n_0 \int d^3x\, U(r)[\phi_0(\boldsymbol{r}-\boldsymbol{d}) - 1]. \quad (33)$$

For the short-ranged potentials $r_c \ll \xi$ and for distances $d \gg r_c$, $\phi_0(\boldsymbol{r}-\boldsymbol{d}) = 1 - \frac{a}{|\boldsymbol{r}-\boldsymbol{d}|} e^{-\sqrt{2}\frac{|\boldsymbol{r}-\boldsymbol{d}|}{\xi}} \approx 1 - \frac{a}{d} e^{-\sqrt{2}\frac{d}{\xi}}$ in the vicinity of $r = r_c$. Recalling the definition of the scattering length that is valid in the weak-coupling regime $\frac{2\pi a}{m} = \int d^3x\, U(r)$, one retrieves Eq. (28). The result in Eq. (33) is valid for arbitrary distances between two impurities and arbitrary potentials conforming to the second Born approximation. For example, when $d = 0$, one would retrieve physics of a single polaron sitting in the potential with the strength that is twice the strength of the original potential, provided one redefines the scattering length in an appropriate manner. In the general case, the form of the induced potential will be complicated and can resemble the form of the original potential like in the case of the exponential potential $U \sim e^{-\frac{r}{r_c}}$, or the polarization potential analyzed in Ref. [22] which was studied by the means of many-body perturbation theory.

Finally, we note that to the leading order both the effective mass and the two polaron interaction energy at unitarity are related to the weak-coupling limit by the identification $\xi\delta^{1/3} \to |a|$. The same identification also reproduces results for some other quasiparticle properties, such as Tan's contact and the quasiparticle residue that have been studied in the context of the bosonic orthogonality catastrophe in Ref. [23], but not the energy (to work for the energy, the substitution has to be modified to $\xi\delta^{1/3} \to 2|a|/3$) [15,16]. We leave the question of how robust this property is and what other quantities obey this identification to a future study.

The interaction energy (29) between two weak polarons is known to have corrections due to the effects of the fluctuations (phonons) in the Bose-Einstein condensate (BEC), as studied in Ref. [24]. We expect that the interactions between unitary polarons would also have similar corrections. Those have not yet been studied, except in one dimension where interactions between polarons, including due to fluctuations, were studied for polarons of arbitrary strength [25].

In summary, we derived a compact formula for the effective mass of the slowly moving impurity in the BEC which is valid both for weak and unitary potentials, generalizing the result by Astrakharchik and Pitaevskii. We used it to find an analytic expression for the effective mass of the Bose polaron at unitarity. We also derived the expression for the interaction energy between two unitary polarons separated by a large distance d. We observed that the qualitative difference between weak and unitary polarons in those scenarios can be captured by a trivial substitution of the amplitudes of the solution of the unitary polaron into the the corresponding expression at weak coupling similar to other quasiparticle properties. When applied to weak polarons, our method allows us to compute the interaction energy between two polarons at arbitrary distance between two impurities and it serves as a generalization of previous results at weak coupling. Because our method relies on a perturbative construction, we were unable to compute the drag force and the induced interactions at small impurity separations which requires full nonperturbative dependence on the impurity velocity and knowledge of the solution to the GPe in the noncentral potential. We leave those problems for a future study.

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