Infrared problem in quantum acoustodynamics

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Quantum electrodynamics (QED) provides a highly accurate description of phenomena involving the interaction of atoms with light. We argue that the quantum theory describing the interaction of cold atoms with a vibrating membrane—quantum acoustodynamics (QAD)—shares many issues and features with QED. Specifically, the adsorption of an atom on a vibrating membrane can be viewed as the counterpart to QED radiative electron capture. A calculation of the adsorption rate to lowest order in the atom-phonon coupling is finite; however, higher-order contributions suffer from an infrared problem mimicking the case of radiative capture in QED. Terms in the perturbation series for the adsorption rate diverge as a result of massless particles in the model (flexural phonons of the membrane in QAD and photons in QED). We treat this infrared problem in QAD explicitly to obtain finite results by regularizing with a low-frequency cutoff that corresponds to the inverse size of the membrane. Using a coherent-state basis for the soft-phonon final state, we then sum the dominant contributions to derive a new formula for the multiphonon adsorption rate of atoms on the membrane that gives results that are finite, nonperturbative in the atom-phonon coupling, and consistent with the Kinoshita-Lee-Nauenberg theorem. For micromembranes, we predict a reduction with increasing membrane size for the low-energy adsorption rate. We discuss the relevance of this to the adsorption of a cold gas of atomic hydrogen on suspended graphene.

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I. INTRODUCTION

The adsorption process, where a free atom or molecule adheres to the surface of a material, is central to a variety of phenomena in surface science [1]. Experimental study of adsorption relies on having clean surfaces and gases at low temperature. Recent experimental advances in the cooling and manipulation of ultracold atomic beams have opened up a new low-energy regime of adsorption where models of atom-surface interactions require a complete quantum mechanical treatment. Furthermore, newly discovered materials such as graphene provide truly two-dimensional solids where strong low-frequency fluctuations of the surface might dramatically alter the adsorption dynamics [2].

In addition to its centrality in surface science, it has been proposed that the dynamics of such a "quantum hybrid" system could be utilized for quantum information processing [3] or precision measurement [4]. It has been demonstrated that the interactions between a cold atom and a vibrating membrane can be engineered by placing the system in an optical cavity [5]. Laser light can be bounced off the membrane to form an optical lattice [6] that can strongly couple over large distances the motion of the atoms to the vibrational modes of the membrane. The dynamics of cold atoms with nanotubes and cantilevered beams has also been studied both experimentally [7,8] and theoretically [9–11].

Our focus here is the dynamics of a system consisting of a single atom interacting with an elastic membrane. Such a system can be realized with a cold atom coupled via the van der Waals (vdW) interaction to a suspended two-dimensional material such as graphene. While the vdW interaction between a cold neutral atom and graphene is weak, it is sufficiently strong for a hydrogen atom to bind to graphene at low temperatures. We examine the transition rate of a cold atom to a bound state on the clamped membrane at zero temperature.

It was previously recognized that there are similarities between the adsorption process and radiative capture [12,13]. Our work highlights the fact that quantum adsorption is a nonrelativistic, condensed matter analog of quantum electrodynamics (QED). We essentially study in this work the phonon analog to radiative corrections in scattering. It is interesting to note that another well-known analogous effect, the phononic Lamb shift, has been detected in a recent experiment [14] in a related system.

A straightforward perturbative expansion of the adsorption rate in the atom-phonon interaction has terms that become infrared divergent for macroscopic membrane size. In analogy to the well-known infrared problem in QED [15], we show explicitly that the infrared divergences in the perturbation expansion of the adsorption rate can be remedied by using an appropriate set of soft-phonon final states and summing over contributions corresponding to multiphonon emission. We subsequently obtain a closed-form expression for the multiphonon adsorption rate. The calculated rate is infrared finite, a result consistent with the Kinoshita-Lee-Nauenberg (KLN) theorem [16,17].

II. MODEL

We take for our model the following Hamiltonian, $H = H_a + H_{\rm ph} + H_{bi} + H_{ki}$, where

$$H_a = E_k c_k^\dagger c_k - E_b b^\dagger b, \tag{1}$$

$$H_{\rm ph} = \sum_q \omega_q a_q^\dagger a_q, \tag{2}$$

$$H_{bi} = -g_{bb} b^\dagger b \sum_q (a_q + a_q^\dagger), \tag{3}$$

$$H_{ki} = -g_{kb}(c_k^\dagger b + b^\dagger c_k) \sum_q (a_q + a_q^\dagger). \tag{4}$$

The model was derived previously [2] by assuming that the atom moves slowly in the perpendicular direction toward an

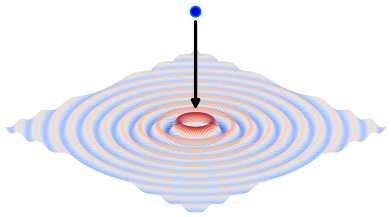

FIG. 1. Atom impinging on an elastic membrane. During adsorption, energy is transferred from the atom to the membrane and is radiated away by phonons.

elastic, clamped membrane under tension and can transfer energy through force-coupling to the membrane by exciting its circularly symmetric flexural modes (Fig. 1). The model has linear phonon dispersion with constant transverse speed of sound.

Here, c_k ($c_k^\dagger$) annihilates (creates) an atom in the continuum state with energy E_k; b ($b^\dagger$) annihilates (creates) an atom bound to the static membrane with energy $-E_b$; a_q ($a_q^\dagger$) annihilates (creates) a circularly symmetric flexural phonon in the membrane with energy ω_q; g_{kb} is the atom-phonon coupling for an atom in the continuum state; and g_{bb} is the atom-phonon coupling for an atom bound to the membrane.

If one regards the atom-phonon interactions as perturbations $H_i = H_{bi} + H_{ki}$, the adsorption rate can be estimated using Fermi's golden rule. The unperturbed Hamiltonian $H_0 = H_a + H_{\rm ph}$ has eigenstates $|n_k,n_b;\{n_q\}\rangle$ labeled by the number of atoms in the continuum n_k, the number of atoms bound n_b, and the number of phonons in each vibrational mode of the membrane $\{n_q\}$. The initial state has an atom in the continuum and the membrane in its ground state; the final state has a bound atom plus a phonon present. The adsorption rate Γ_0 for a micromembrane is then

$$\Gamma_0 = 2\pi \sum_q \delta(E_k + E_b - \omega_q)|\langle 0,1;1_q|H_i|1,0;0\rangle|^2 \quad (5)$$

$$= 2\pi g_{kb}^2 \rho, \quad (6)$$

where ρ is a partial phonon density of states for the circularly symmetric vibrational modes of the membrane. This result, finite in the limit of a large membrane, is of order g_{kb}^2 and is independent of g_{bb}. Higher-order contributions in g_{bb}, however, are divergent in the large-membrane limit where soft-phonon emission becomes possible. We use the inverse size of the membrane ϵ as an infrared regulator that provides a low-frequency cutoff to the vibrational spectrum; ω_D is the membrane's high-frequency limit.

The KLN theorem [16,17] informs us that infrared divergences are specious and are not contained in the true physical adsorption rate as $\epsilon \to 0$. Thus, approximations to the adsorption rate obtained by truncation of this (divergent) perturbation expansion must be carefully scrutinized for large membranes [18].

If one regroups the Hamiltonian so that H_{bi} is included in the unperturbed Hamiltonian, a quite different result follows for the lowest order adsorption rate. With H_{ki} as the only perturbation, the remaining terms of H form the unperturbed Hamiltonian which can be diagonalized with a canonical transformation (see the Appendix). We find that under the perturbation H_{ki}, the adsorption rate Γ_1 is given by

$$\Gamma_1 = 2\pi g_{kb}^2 \rho e^{-2F}\left(1 + \frac{\Delta}{E_s}\right)^{-2}, \quad (7)$$

where $F = \frac{g_{bb}^2}{2}\sum_q \frac{1}{\omega_q^2}$, $\Delta = g_{bb}^2 \sum_q \frac{1}{\omega_q}$, and $E_s = E_k + E_b$. Γ_1 is of order g_{kb}^2 and contains the effects of g_{bb} to all orders. Most importantly, in the large-membrane limit ($\epsilon \to 0$), we see that $F \sim \frac{\rho g_{bb}^2}{2}\int_\epsilon \frac{d\omega}{\omega^2}$, consequently growing as $1/\epsilon$. Thus, the lowest order adsorption rate becomes exponentially small for large membranes, a result in dramatic contrast to Eq. (6).

The rate of adsorption producing a multiphonon final state is found in a similar fashion (see the Appendix). In the large-membrane regime, the rate of adsorption via emission of n phonons is

$$\Gamma_n \approx 2\pi g_{kb}^2 \rho e^{-2F}\left(1 + \frac{\Delta}{E_s}\right)^{-2}\left(\frac{g_{bb}^2\rho}{\epsilon}\right)^{n-1}\frac{1}{(n-1)!}. \quad (8)$$

We conclude that the adsorption rate for *any* finite number of phonons emitted is vanishingly small in the large-membrane regime. The situation here is reminiscent of bremsstrahlung emission by a charged particle in QED [15]. We also note that, for large membranes where $\epsilon \ll \rho g_{bb}^2$, the multiphonon rate exceeds the one-phonon rate Γ_1, a familiar situation for soft-photon emission from a scattered electron in QED.

To obtain the total adsorption rate, we can sum over all n and obtain a finite result, namely,

$$\Gamma = \sum_{n=1}^{\infty}\Gamma_n \approx 2\pi g_{kb}^2 \rho\left(1 + \frac{\Delta}{E_s}\right)^{-2}. \quad (9)$$

We conclude that, as $\epsilon \to 0$, a nonvanishing adsorption rate results only with the emission of an infinite number of phonons. We further note that the multiphonon rate differs from the simplest golden rule estimate Γ_0 by a fractional factor $\mathcal{R} = (1 + \frac{\Delta}{E_s})^{-2}$ which depends logarithmically on the IR cutoff ϵ (see Fig. 2). Lastly, we observe that all adsorption rates Γ_n, as well as the total rate Γ, are finite (specifically, tending to zero) in the infrared limit $\epsilon \to 0$ in accord with the KLN theorem.

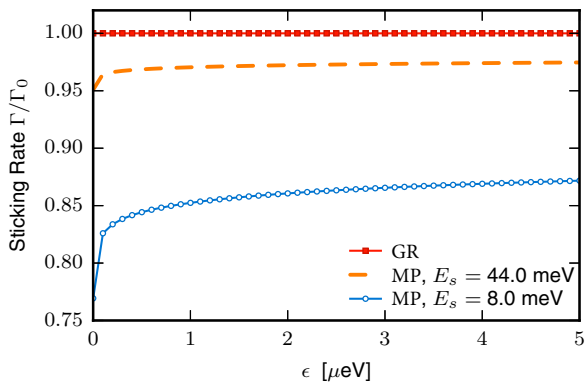

FIG. 2. Normalized sticking rate Γ/Γ_0 versus the IR cutoff ϵ for micromembranes with different binding energies. Multiphonon processes [MP, Eq. (9)] suppress the simple golden rule [GR, Eq. (6)] adsorption rate Γ_0. The suppression of the adsorption rate is stronger for shallow bound states. The GR can be a poor approximation for large membranes where soft-phonon processes are important.

III. SUMMARY

We have studied a quantum model for low-energy atomic adsorption on a two-dimensional membrane. The strength of the atom-phonon interaction at low frequencies gives rise to an infrared divergence problem in the adsorption rate for large membranes. We use the inverse membrane size ϵ as a natural IR regulator. With a canonical transformation, we obtain the adsorption rate in each sector of the phonon Fock space, and we show that each rate vanishes exponentially in the limit of a vanishing cutoff, $\epsilon \to 0$. We sum the dominant terms in each sector of the phonon Fock space for small ϵ to obtain a new adsorption rate formula. We show that the simplest golden rule approximation to the adsorption rate lacks a factor that reduces the adsorption rate, vanishing slowly as $\ln^{-2}(\omega_D/\epsilon)$ as $\epsilon \to 0$. This prediction might be experimentally tested by comparing the cold-atom adsorption rates by samples with membranes that range up to macroscopic size.

This result provides the answer to the question raised previously [19] concerning the effect of the IR cutoff on the low-energy sticking of atomic hydrogen on suspended graphene [20]. It was anticipated [19] that changes in the low-frequency phonon spectrum will have "little impact" on the sticking process. This logic is used to justify an approximation of the phonon spectrum that ignores phonons with energies below 0.79 meV. Surprisingly, our result illustrates that the low-frequency phonon spectrum can have a substantial effect on the sticking, as the emission of an infinite number of soft phonons can dominate the sticking process for micromembranes. This differs from "quantum sticking" [12] where the emission of a finite number of quanta facilitates the adsorption. Lastly, we note that this result is in agreement with previous results based on a variational mean-field method [2,21,22] that find a suppression of the adsorption rate with respect to the simple golden rule rate for sticking via emission of a finite number of phonons.

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APPENDIX

We group the Hamiltonian in Eqs. (1)–(4) as $H = H_0 + H_1$, where

$$H_0 = E_k c_k^\dagger c_k - E_b b^\dagger b + \sum_q \omega_q a_q^\dagger a_q - g_{bb} b^\dagger b \sum_q (a_q + a_q^\dagger), \tag{A1}$$

$$H_1 = -g_{kb}(c_k^\dagger b + b^\dagger c_k) \sum_q (a_q + a_q^\dagger). \tag{A2}$$

H_0 contains the independent boson model [23] Hamiltonian and can be diagonalized with a canonical transformation,

$$\tilde{H}_0 = e^S H_0 e^{-S} \tag{A3}$$

$$= E_k c_k^\dagger c_k - (E_b + \Delta) b^\dagger b + \sum_q \omega_q a_q^\dagger a_q, \tag{A4}$$

where $S = -b^\dagger b \sum_q \frac{g_{bb}}{\omega_q}(a_q^\dagger - a_q)$ and $\Delta = g_{bb}^2 \sum_q \frac{1}{\omega_q}$. The unperturbed ground-state energy for one atom E_g is thus $E_g = -(E_b + \Delta)$.

Since the one-phonon eigenstate of $\tilde{H}_0$ is $|0,1;1_q\rangle$ with energy $E_q = -(E_b + \Delta) + \omega_q$, the corresponding unperturbed eigenstate of H_0 is $e^{-S}|0,1;1_q\rangle$, a product of phonon coherent states over the modes. (Technically, one state in the product is a "phonon-added" coherent state.) Thus, from the golden rule, the adsorption rate for first-order transitions under the perturbation H_1 is

$$\Gamma_1 = 2\pi \sum_q \delta(E_k + E_b + \Delta - \omega_q) |\langle 0,1;1_q|e^S H_1|1,0;0\rangle|^2 \tag{A5}$$

$$= 2\pi g_{kb}^2 \sum_q \delta(E_k + E_b + \Delta - \omega_q) |\langle 1_q|X^\dagger \sum_{q'} a_{q'}^\dagger|0\rangle|^2, \tag{A6}$$

where $X = \exp[\sum_q \frac{g_{bb}}{\omega_q}(a_q^\dagger - a_q)]$. We evaluate the phonon matrix element and find that

$$\sum_{q'} \langle 1_q|X^\dagger a_{q'}^\dagger|0\rangle = e^{-F}\left(1 - \frac{\Delta}{\omega_q}\right), \tag{A7}$$

where $F = \frac{g_{bb}^2}{2} \sum_q \frac{1}{\omega_q^2}$. Thus,

$$\Gamma_1 = 2\pi g_{kb}^2 e^{-2F} \sum_q \left(1 - \frac{\Delta}{\omega_q}\right)^2 \delta(E_k + E_b + \Delta - \omega_q) \tag{A8}$$

$$\approx 2\pi g_{kb}^2 e^{-2F} \int_\epsilon^{\omega_D} \rho d\omega \left(1 - \frac{\Delta}{\omega}\right)^2 \delta(E_k + E_b + \Delta - \omega) \tag{A9}$$

$$= 2\pi g_{kb}^2 e^{-2F} \rho \left(1 - \frac{\Delta}{E_s + \Delta}\right)^2, \tag{A10}$$

where the quasicontinuum approximation is used to evaluate the sum. As the IR cutoff ϵ approaches zero, Γ_1 exponentially vanishes.

For final states obtained from two-phonon eigenstates of $\tilde{H}_0$, the rate of adsorption is

$$\Gamma_2 = 2\pi \sum_{\{n_q\},\ \sum_q n_q = 2} \delta(E_k + E_b + \Delta - \textstyle\sum_p n_p \omega_p) |\langle 0,1;\{n_q\}|e^S H_1|1,0;0\rangle|^2 \tag{A11}$$

$$\approx 2\pi g_{kb}^2 e^{-2F} \rho^2 \frac{g_{bb}^2}{\epsilon}\left(1 - \frac{\Delta}{E_s + \Delta}\right)^2, \quad \epsilon \to 0, \tag{A12}$$

Other contributions to Γ_2 are subdominant as $\epsilon \to 0$. The use of a coherent-state phonon basis for the final state removes the IR divergence. This gives insight into the analogous method to remedy IR divergences in QED with coherent states [24]. In our case, the coherent states are a natural phonon basis, given our choice of H_0.

The dominant contribution to the adsorption rate from n-phonon eigenstates has $(n-1)$ soft phonons ($\omega \sim \epsilon$) and

a hard phonon ($\omega \sim E_s$) to satisfy energy conservation:

$$\Gamma_n = 2\pi \sum_{\{n_q\},\ \sum_q n_q = n} \delta(E_k + E_b + \Delta - \textstyle\sum_p n_p \omega_p) |\langle 0,1;\{n_q\}|e^S H_1|1,0;0\rangle|^2 \quad \text{(A13)}$$

$$\approx 2\pi g_{kb}^2 e^{-2F} \frac{\rho^n}{(n-1)!} \left(\frac{g_{bb}^2}{\epsilon}\right)^{n-1} \times \left(1 - \frac{\Delta}{E_s + \Delta}\right)^2, \quad \epsilon \to 0. \quad \text{(A14)}$$

Thus, the IR divergences have been successfully removed to all orders in g_{bb}.

The total adsorption rate for a micromembrane is obtained by summing over the n-phonon contributions,

$$\Gamma = \sum_{n=1}^{\infty} \Gamma_n \approx 2\pi g_{kb}^2 \rho e^{-2F} \left(1 + \frac{\Delta}{E_s}\right)^{-2} \sum_{n=0}^{\infty} \left(\frac{\rho g_{bb}^2}{\epsilon}\right)^n \frac{1}{n!} \quad \text{(A15)}$$

$$\approx 2\pi g_{kb}^2 \rho \left(1 + \frac{\Delta}{E_s}\right)^{-2}, \quad \text{(A16)}$$

since $2F = (\rho g_{bb}^2/\epsilon)$ in the quasicontinuum approximation for a dense phonon spectrum. Remarkably, the exponentially decaying factor e^{-2F} is canceled with the infinite summation, and the resulting rate is the product of the simple GR rate Γ_0 with a cutoff-dependent reduction factor of $\mathcal{R} = (1 + \Delta/E_s)^{-2}$.

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