Three terminal vibron coupled hybrid quantum dot thermoelectric refrigeration

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A three terminal nanoscale refrigeration concept based on a vibron coupled quantum dot hybrid system is proposed and analyzed in detail. In the regime of electrical driving, our investigation delves into the non-trivial role of electron-phonon interactions on the refrigeration performance. It is shown that, although such interactions are well known to be detrimental from a general refrigeration perspective, surprisingly, they can be engineered to favorably improve the trade-off between the cooling power and the coefficient of performance under practical operating conditions. Furthermore, our investigation manifests that an additional improvement in the trade-off can be facilitated by an electronic thermal bias along with the electron-phonon coupling. Next, we explore a number of viable design strategies such as tuning the on-site Coulomb repulsion and optimizing the coupling strength with the reservoirs to overcome the challenges posed by the electron-phonon interaction. Crucially, it is demonstrated from the principle of heat balance that, in a multi-terminal geometry, any change in the non-equilibrium phonon heat current at a fixed applied voltage, is counter-balanced by the heat currents flowing through the other terminals. Elucidating the physics of coupled charge and heat transport under non-equilibrium conditions, we demonstrate that a strong coupling with the thermal bath and the cold contact results in a substantial improvement in the peak cooling power and the coefficient of performance. Combining all these aspects, we believe that this study could offer important guidelines and paves the way for a possible experimental realization of molecular and quantum dot thermoelectric refrigeration.

I. INTRODUCTION

Exploring new vistas on nanoscale thermoelectric power generation, i.e., the conversion of waste heat into electrical energy, has in the past two and a half decades seen feverish activity both on the theoretical5–8 and experimental1–4 fronts. A major conceptual breakthrough on route was the proposal on the exploitation of sharp spectral features through nanostructuring1–4 to achieve a high figure-of-merit in the linear transport regime. Subsequently, studies in the non-linear transport regime9–12 have also gained precedence in order to address the power-efficiency trade-off13–23. Here, aspects that include lineshape engineering21–25 and energy filtering26–28 have been explored in great detail.

The complementary aspect, that is, nanoscale refrigeration using similar concepts29–30, namely sharp spectral features observed in quantum dot (QD) systems, was relatively less explored until recently with lot of attention31,32 due to the rising demand of on-chip cooling33. In general, the study of correlated charge and energy transport requires a deeper insight into the many-particle interactions of electrons with ancillary subsystems like phonons,34–36 photon cavity modes,37–40 magnons,41–47 and nuclear spins48–53 and as such can be categorized within the active research area of hybrid quantum systems.

In particular, there have been a lot of experimental advances on hybrid systems featuring the interplay of electronic modes with vibrational modes driven out of equilibrium with the vision of engineering these modes for various quantum technology applications54–57. Thermoelectric refrigeration involves, at a very basic level, the flow of an electronic charge current accompanied by energy exchange with bosons58–60 via electron-boson interaction, resulting in a heat current that cools one region while dumping heat into another. From a thermodynamic standpoint, in multi-terminal thermoelectric machines61–62, refrigeration can be triggered by two fundamentally different driving forces, namely, thermal58–59 and electrical bias63–64. In QD systems, it is shown that the latter proves to be much better in terms of efficient cooling due to strong on-dot charge fluctuations65.

In this paper, we propose and investigate in detail a three terminal nanoscale refrigeration concept66 based on a vibron coupled QD hybrid system67–69. The three terminal set up elucidated in Fig. 1 comprises a single vibron mode coupled quantum dot connected to two electronic contacts to facilitate electrical driving via a voltage gradient and a bulk phonon bath that acts as a heat leakage path.

It is important to understand the implications of two terminal10,11,17,18,22 and three terminal14,17,22 geometries, both of which have been proposed as viable set ups for thermoelectric energy harvesting and refrigeration. In a two-terminal thermoelectric setup, the temperature and the electrical bias are applied between the electronic contacts, due to which both the charge and heat currents flow along the same conducting channel. In a three-terminal geometry, energy is harvested from the environment whose effect can be captured via a third terminal, often modeled as a bath. In such a set up, the crossed flow of charge and heat currents allows the hot terminal to be electrically separated from the actual energy harvester.

Our study features a variant of the three terminal configuration, where the actual energy harvesting
Coupled by the electron-phonon interaction, the dot constitutes both electronic and phonon degrees-of-freedom which are coupled by the electron-phonon interaction ($\lambda$). A voltage bias applied between the contacts facilitates electrical driving of charge and heat currents from the cold to the hot terminal. Refrigeration performance is governed by the coupled transport of charge and heat currents through the entire setup.

The rest of this paper is organized as follows. In Sec. II we elaborate the model Hamiltonian of the device setup and explain its physics. Next, we present the transport formalism used in the simulation framework and discuss the key refrigeration parameters. The results are discussed in subsections of Sec. III. In Sec. III A we analyze the refrigeration performance via vibron assisted electronic transport. The trade-off characteristics and optimization study are presented in Secs. III B and III C respectively. We conclude in Sec. IV.

II. PHYSICS AND FORMULATION

A schematic of the three-terminal device studied here is presented in Fig. 1. It comprises the vibron-coupled QD as the central part coupled to three macroscopic reservoirs (or terminals), namely two electronic contacts ($H$ and $C$) and one thermal bath ($P$). A charge current $I$, is driven by the applied voltage ($V_{app}$) or thermal gradient $\Delta T = (T_H - T_C)$, or both. We will now describe the formulation and working principles of this set up and its refrigeration functionality, which is governed by the coupled transport of charge and heat currents through the entire setup.

A. Model Hamiltonian

The composite Hamiltonian of the three terminal setup is expressed as $\hat{H} = \hat{H}_D + \hat{H}_R + \hat{H}_P + \hat{H}_{DR} + \hat{H}_{DP}$, where $\hat{H}_D$, $\hat{H}_R$ and $\hat{H}_P$ represent the Hamiltonians of the quantum dot, electronic reservoirs or contacts ($H$ and $C$) and external thermal bath ($P$), respectively. On the other hand, $\hat{H}_{DR}$ and $\hat{H}_{DP}$ describe the dot-to-contact electron tunnelings and dot-to-bath phonon relaxation processes, respectively. The dot Hamiltonian $\hat{H}_D$ is further subdivided as

$$\hat{H}_D = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph},$$  \hspace{1cm} (1)$$

where $\hat{H}_{el}$ and $\hat{H}_{ph}$ stand for the electronic and vibron degrees of freedom within the dot, and $\hat{H}_{el-ph}$ represents the electron-phonon coupling Hamiltonian between the
Figure 2. Truncated view of the state transition diagram in the electron-phonon Fock space following the polaron transformation. Each circle represents an electron-phonon product state $|n, q⟩ = |n⟩ ⊗ |q⟩$ designated by electron number $n$ and phonon number $q$ with energy $E_{n,q}$. Black solid arrows represent direct electron tunneling. Blue and brown dotted arrows signify phonon-assisted electron tunnelings causing phonon emissions ($|n, q⟩ → |n + 1, q'⟩$) and absorptions ($|n, q⟩ → |n - 1, q'⟩$), respectively. Red dotted arrows stand for bath-assisted phonon transitions ($|n, q⟩ → |n, q ± 1⟩$).

The electronic part $\hat{H}_{el}$ consists of a spin degenerate energy level with an on-site energy $\epsilon$ and a finite Coulomb interaction energy $U$ for double occupancy. The phonon part $\hat{H}_{ph}$ consists of a single vibron mode $\nu$ (vibron) with angular frequency $\omega_\nu$ and the interaction Hamiltonian $\hat{H}_{el-ph}$ is a function of dimensionless coupling strength of the electron-phonon interaction $\lambda_\nu$ within the dot. The Hamiltonians $\hat{H}_{el}$, $\hat{H}_{ph}$ and $\hat{H}_{el-ph}$ are written as

$$\hat{H}_{el} = \sum_{\sigma \in \uparrow, \downarrow} \epsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow,$$

$$\hat{H}_{ph} = \hbar \omega_\nu b_\nu^\dagger b_\nu,$$

$$\hat{H}_{el-ph} = \sum_\lambda \lambda_\nu \hbar \omega_\nu (b_\nu^\dagger + b_\nu) d_\sigma^\dagger d_\sigma, \quad (2)$$

where $d_\sigma^\dagger (d_\sigma)$ are the creation (annihilation) operators for the electrons with spin $\sigma$ and $b_\nu^\dagger (b_\nu)$ represent the phonon creation (annihilation) operators of the vibron mode $\omega_\nu$. The QD is weakly coupled with the macroscopic reservoirs. Among the reservoirs, the electronic contacts ($H$ and $C$) constitute non-interacting electrons with momentum states labeled by $k$ and spin $\sigma$. On the other hand, the thermal bath consists of numerous non-interacting phonon modes $r$. The Hamiltonians $\hat{H}_R$ and $\hat{H}_P$ read

$$\hat{H}_R = \sum_{R \in H,C,k,\sigma} \epsilon_{kR\sigma} \hat{c}_{kR\sigma}^\dagger \hat{c}_{kR\sigma},$$

$$\hat{H}_P = \sum_r \hbar \omega_r B_r^\dagger B_r. \quad (3)$$

Here, $\hat{c}_{kR\sigma}^\dagger (\hat{c}_{kR\sigma})$ creates (annihilates) an electron in contact $R \in H, C$ with momentum $k$ and spin $\sigma$ with energy $\epsilon_{kR\sigma}$. Similarly, $B_r^\dagger (B_r)$ creates (annihilates) a phonon of angular frequency $\omega_r$ in the thermal bath. If the electrons in the contacts are coupled to the electrons in the dot by an energy $\tau_{el}^{\nu,\sigma}$ and the phonons in the bath are coupled to the phonons in the dot by an energy $\tau_{ph}^{\nu,\nu}$, then the coupling Hamiltonians are put down as

$$\hat{H}_{DR} = \sum_{R \in H,C,k,\sigma} \left[ \tau_{el}^{\nu,\sigma} \epsilon_{kR\sigma} b_\nu^\dagger + h.c. \right],$$

$$\hat{H}_{DP} = \sum_r \left[ \tau_{ph}^{\nu,\nu} (B_r^\dagger B_r + B_r B_r^\dagger) \right], \quad (4)$$

where $h.c$ stands for the hermitian conjugate. Throughout our work, we assume that the electron tunneling processes conserve the momentum and spin and the phonon transitions are mode independent represented as $\tau^{el}$ and $\tau^{ph}$.

Next, we need to diagonalize the dot Hamiltonian $H_D$ to remove the linear term $H_{el-ph}$. To execute this, we employ polaron transformation on the dot Hamiltonian (such that, $\hat{H}_D \to e^{\hat{S}} \hat{H}_D e^{-\hat{S}}$, where $\hat{S} = \sum \lambda_\nu [b_\nu^\dagger b_\nu]$ is the transformation operator\cite{23}). Following this, the on-site energy and Coulomb interaction energy are renormalized as

$$\tilde{\epsilon} = \epsilon - \lambda_\nu^2 \hbar \omega_\nu,$$

$$\tilde{U} = U - 2\lambda_\nu^2 \hbar \omega_\nu. \quad (5)$$

After the diagonalization, the eigenstates of $\tilde{H}_D$ are expressed as the electron-phonon product states which are denoted by $|n, q⟩$, where $n$ and $q$ respectively, designate the electron and phonon numbers of that state. The corresponding eigen-energies are given by $E_{n,q} = \epsilon_n + q \hbar \omega_\nu$, where $\epsilon_0 = 0$, $\epsilon_1 = \tilde{\epsilon}$ and $\epsilon_2 = 2\tilde{\epsilon} + \tilde{U}$ for $n = 0, 1, 2$. One must note that the polaron transformation modifies the electronic coupling coefficient $\tau_{el}$ to $\tau_{el}' = \tau_{el} exp[\lambda_\nu (b_\nu^\dagger - b_\nu)]$ implying the dressing of electron tunneling energy by the electron-phonon interaction. However, the phonon coupling coefficient remains unaltered since the transformation operator $\hat{S}$ commutes with $b_\nu (b_\nu^\dagger)$.

Before delving into the transport formalism, it is customary to define the dot-to-contact electron tunneling rates and dot-to-bath phonon relaxation rates. To do this, we assume $\tilde{H}_D$ to be weakly perturbed by the reservoir Hamiltonians which allows us to compute electron and phonon transition rates via the Fermi’s golden rule.
The rates of electron tunneling $\gamma_R$ and phonon relaxation $\beta_P$ are thus derived as
\[
\gamma_R = \frac{2\pi}{\hbar} \sum_{R \in \{H,C\}} |\tilde{\rho}_{R,\sigma'}|^2 \rho_{R,\sigma'},
\]
\[
\beta_P = \frac{2\pi}{\hbar} \sum_{p} |\tilde{\epsilon}_p|^2 D_p,
\]
where $\rho_{R,\sigma'}$ and $D_p$ are the constant electron and phonon density of states associated with the contacts $R \in \{H,C\}$ and the thermal bath $P$, respectively. From now on, we shall simply denote $\beta_P$ as $\beta$. With the introduction of model Hamiltonians and the derivation of electron and phonon transition rates, we have set a perfect ground to formulate the transport methodology, which will be analyzed in the next subsection.

**B. Transport formalism**

We initiate our discussion on the transport methodology by elaborating the key approximations we made. First, the rate of dot-to-bath phonon relaxation processes is set much lower than the rate of dot-to-contact electron tunneling processes ($h\gamma_R \gg \hbar\beta$) to exclude the system damping\[^{[2]}\]. Additionally, in the absence of damping, the phonon currents emitting from different terminals remain uncorrelated and hence they can be computed separately. Next, we formulate all the transport calculations in the sequential tunneling limit\[^{[2]}\], where the energies associated with electron tunnelings and phonon relaxations are assumed to be much lesser than the thermal energy ($h\gamma_R, \hbar\beta << k_B T$)\[^{[2]}\]. In this limit, quantum transport through a spin degenerate energy level coupled to the macroscopic reservoirs is calculated via rate equations in the diagonal subspace of the reduced density matrix\[^{[2]}\],[^60]\]

Lastly, we ignore the overlap of two consecutive phonon sidebands by setting the energy gap between two sidebands much higher than the tunnel induced broadening of the energy levels ($\hbar\omega_\nu >> h\gamma_E$). With this assumption, transport equations can be formulated in the realm of Markov approximation and two consecutive electron tunnelings remain completely uncorrelated. This justifies the use of rate equations which discard the off-diagonal coherence terms of the reduced density matrix.

The rate of electron tunneling between the two states $|n, q\rangle$ and $|n \pm 1, q'\rangle$ (refer Fig.\[^{[2]}\]) depends on the contact Fermi-Dirac function of the energy difference between the two states and is given by
\[
P_{n,q}^{el}(n+1,q') = \sum_{n,q,R \in \{H,C\}} \gamma_R |\langle n, q|\tilde{d}_\sigma|n+1, q'\rangle|^2 \times f_R(E_{n+1,q'} - E_{n,q}),
\]
\[
P_{n,q}^{el}(n-1,q') = \sum_{n,q,R \in \{H,C\}} \gamma_R |\langle n, q|\tilde{d}_\sigma|n-1, q'\rangle|^2 \times [1 - f_R(E_{n+1,q'} - E_{n,q})],
\]
where $f_R(\zeta) = 1/[1 + \exp(-\zeta \mu_R / k_B T_R)]$ is the Fermi-Dirac distribution function associated with the contact $R \in \{H,C\}$ with chemical potential $\mu_R$ and temperature $T_R$. On the other hand, the rate of phonon absorption and emission between the the states $|n, q\rangle$ and $|n, q \pm 1\rangle$ obey the quasi-equilibrium Boltzmann’s ratio and is expressed as
\[
R_{n,q}^{ph}(n,q \pm 1) = \beta(q + 1) \exp\left[\frac{-\hbar\omega_{n,q}}{k_B T}\right],
\]
As we plug in the different electronic tunneling and phonon relaxation rates into the rate equation, it takes the following form in the electron-phonon Fock space (shown in Fig.\[^{[2]}\]):
\[
dP_{n,q}/dt = \sum_{q'q} \left[ R_{n,q}^{el}(n+1,q')P_{n,q'-1} - R_{n,q}^{el}(n,q')P_{n,q+1} \right]
\times \delta(n + 1, n') + \left[ R_{n,q}^{ph}(n,q')P_{n,q'-1} - R_{n,q}^{ph}(n,q')P_{n,q+1} \right]
\times \delta(q + 1, q').
\]
In the steady-state, the derivative in the left hand side of the equation becomes zero and can thus yield many-body electron-phonon probabilities $P_{n,q}$ by solving a set of algebraic equations through numerical computation. After evaluating $P_{n,q}$, we calculate the charge current ($I_R$), electronic heat current ($J_R^Q$) associated with the contacts $R \in \{H,C\}$, and the phonon current ($J_P^Q$) emanating from the thermal bath as follows
\[
I_R = \sum_{q=0}^{N_q} \sum_{q'=0}^{N_q} e \left[ R_{n+1,q'}^{el}(n,q)P_{n+1,q'} - R_{n,q}^{el}(n+1,q')P_{n+1,q} \right]
\times \delta(n+1, n') + \left[ R_{n,q}^{ph}(n,q')P_{n,q'-1} - R_{n,q}^{ph}(n,q')P_{n,q+1} \right]
\times \delta(q+1, q').
\]
where $e$ is the electronic charge unit and $N_q$ is the number of maximally allowed phonon sidebands. With the derived expressions of charge current and heat currents, we illustrate the performance metrics of our setup working as a thermoelectric refrigerator. From now on, we
will denote $\lambda_\nu$ and $\omega_\nu$ as $\lambda$ and $\omega$, respectively, due to the presence of a single vibron mode. Also, in the rest of our work we will denote $I_H = -I_C = I$ considering that charge is conserved inside the QD.

C. Refrigeration Performance Parameters

A thermal bias ($\Delta T = T_H - T_C$) applied across the electronic contacts stimulates charge and heat currents. In a typical voltage controlled thermoelectric setup, the two contacts are connected by a variable load resistor which causes a potential drop across the contacts. This drop stimulates a back-flow of charge which opposes the flow due to the thermal bias, thereby reducing the net flow. At the open-circuit voltage ($V_{OC}$), these two opposite flows counter-balance each other resulting in a zero current. Therefore, the device works as a power generator in the regime $[0, V_{OC}]$. Beyond $V_{OC}$, the direction of charge flow reverses and the device enters into the power dissipation regime. However, in this regime, if the load is replaced by a voltage source ($V_{app}$) such that power is absorbed into the system, the device functions as a refrigerator as depicted in Fig. 1. In such a scenario, the electronic heat current flows from the cold to hot contact (positive direction as shown in Fig. 1 by blue arrows) which effectively cools the cold contact and heats up the hot one. Once $V_{app}$ is increased beyond the crossover voltage ($V_{TR}$), the heat current from the cold contact reverses its direction and the system enters into the dissipation regime as shown in Fig. 3(a). This restricts the refrigeration in the limit $[V_{OC}, V_{TR}]$ where the effective density-of-states (DOS) of the channel lies in between $E_0$ (reversible energy at which the Fermi-Dirac function of both the contacts are equal) and $\mu_C$ as displayed in Fig. 3(b). The system described above mimics a conventional two-terminal refrigerator setup where the key performance metrics are the cooling power ($J_C^Q$) and the coefficient-of-performance (COP). The cooling power is defined as the heat current extracted from the cold terminal which is ideally kept at ambient temperature and the COP is defined as

$$\eta = \frac{J_C^Q}{W},$$

(12)

where $W$ is power supplied by the voltage source. Following the principle of thermodynamics, $\eta$ is upper-bound by its reversible limit $\eta_{rev} = T_C/(T_H - T_C)$ and the energy balance equation holds $J_H^Q = J_C^Q + W$. In this study, we incorporate a third terminal (a thermal bath with temperature $T_P$) which acts as an ambient and enable phonon exchange with the dot. In our study, we consider $T_P = T_C$ to establish an isotherm between the ambient (thermal bath) and the heat sink (the cold contact) which justifies the refrigerator setup from the practical stand-point. This operating condition also ensures the leaking of dot phonons to the bath as shown in

![Figure 3](https://example.com/fig3.png)

**Figure 3.** Refrigeration window: (a) Heat extracted from the cold contact ($J_C^Q$), heat dumped into the hot contact ($J_H^Q$), and the power absorbed from the external source ($W$) are plotted as a function of the applied bias ($V_{app}$). All of them flip signs and become positive beyond the open-circuit voltage ($V_{OC}$) leading to a transition from generation to refrigeration regime. $J_H^Q$ further reverses its direction again at the crossover voltage ($V_{TR}$) and enters into the dissipation regime which restricts the refrigeration in the limit $[V_{OC}, V_{TR}]$. (b) Operational regimes and their boundaries are shown in an energy scale line plot. Refrigeration occurs only when the channel effective density-of-states lies in between $E_0$ (reversible energy) and $\mu_C$. Above $E_0$, the device operates in the power generation regime and below $\mu_C$, it enters the dissipation regime.

$$J_H^Q + J_C^Q = J_C^Q + W.$$  \hspace{1cm} (13)

However, considering the fact that the device is still driven solely by the electrical power, the expression for COP remains intact as in (12).

III. RESULTS AND DISCUSSION

A. Refrigeration via electron-phonon coupled transport

In the current section, we elaborate on the impact of vibron coupled electronic transport in controlling the refrigeration performance. Before going into the details, it is imperative to mention the values of several parameters used in our simulation framework. First, we as-
sume the QD system to be n-type ($\epsilon - \mu > 0$), with the dot on-site energy tuned at 0.1 eV above the equilibrium chemical potential ($\mu$) of the contacts. Second, the dot-to-contact electronic tunneling rates ($\gamma_{H,C}$) are varied in the range $0.015 k_B T^{-1}$ to $0.02 k_B T^{-1}$, so that the transport physics can be formulated in the realm of sequential tunneling limit. We also ignore the energy dependency of $\gamma_{H,C}$ considering the wideband approximation. Third, the dot-to-bath phonon relaxation rate ($\beta$) is assumed to be much smaller than $\gamma_{H,C}$ (typically $\beta \equiv 0.1 \gamma_{H,C}$) to exclude system damping. Next, the frequency ($\omega_v$) of the vibron mode is adjusted to be $10^{13}$ rad/sec in order to validate $\hbar \omega_v << \hbar \gamma_{H,C}$, which justifies Markov approximation and neglects the effect of bath memory. Typically, in the semiconducting quantum dots (GaAS or Ge), the dominant scattering event is the interaction of electrons with the acoustic phonons having frequency in the range of $1 \times 10^{13}$ to $5 \times 10^{13}$ rad/sec. 

Therefore, our assumption retains a strong analogy with experiments. Lastly, we assume a symmetric capacitive coupling between the dots and contacts so that for a given bias $V_{app}$, the Fermi level of the hot (cold) contact is shifted by $\epsilon \equiv \epsilon - \mu$ is tuned much larger than the thermal energy. However, $V_{TR}$ falls short as $\lambda$ goes up. Looking back to (11), we note that $J_{Q}^{\lambda}$ is derived by multiplying each component of $I_C$ by a weighing factor of $(E_{n+1,q} - E_{n,q})/e$, which is proportional to $\tilde{\epsilon} \equiv \epsilon - \lambda^2 \hbar \omega_v$. It is evident that as $\lambda$ goes up, the weighing factors decrease and leads to the fall of $J_{Q}^{\lambda}$. For the same reason, $J_{Q}^{\lambda}$ can be brought down to zero at lower $V_{TR}$ with the rise of $\lambda$. In parallel, we notice that the maxima of cooling power ($J_{Q,\max}^{\lambda}$) registers a sharp fall with $\lambda$ as shown in Fig. 4(a). Figure 4(b) shows the similar falling trend of peak COP ($\eta_{\max}^{\lambda}$) with $\lambda$.

Following the qualitative discussion, it is customary to elaborate the practical efficacy of our device. Our quantitative analysis estimates $J_{Q,\max}^{\lambda}$ and $\eta_{\max}^{\lambda}$ to be 0.76 nW and 0.97$\eta_C$, respectively when electron-phonon coupling vanishes ($\lambda = 0$). From the system-design viewpoint, this device when made of a self-assembled array of spherical quantum dots with an average diameter of 40 nm with a 50% fill factor, can produce a cooling power density of 0.3 $MW/m^2$. These figures are substantial and can be optimized further by modulating the dot size and filling factor. However, in a practical system, these numbers largely degrade due to the presence of electron-phonon coupling which calls for an investigation on the impact of $\lambda$ on CP and COP. From the discussion of the preceding section, we know that a finite $\lambda$ facilitates phonon-assisted-tunneling (PAT) over direct tunneling (DT). Therefore, our next objective is to perform a comparative study on the respective contributions of DT and PAT in $J_{Q,\max}^{\lambda}$.

A finite electron-phonon interaction shifts the potential profile of the dot and modifies the electron-tunneling rate between two Fock states $|n,q\rangle$ and $|n \pm 1,q\rangle$. The effective tunneling rate ($\gamma_{\text{eff}}$) is then defined as

$$\gamma_{\text{eff}} = \gamma \times |FC_{q_1,q_2}|^2 = \gamma \times \exp \left( -\frac{\lambda^2}{2} \right) \times \left( \frac{q!}{Q!} \right)^2 \times \lambda^{Q-q} \times L_q^{Q-q}(\lambda^2) \times \text{sgn}(q_1-q_2)^{|n_1-n_2|},$$

(14)

where $q = \min(q_1,q_2)$, $Q = \max(q_1,q_2)$ and $FC_{q_1,q_2}$ is the measure of the Frank-Condon overlap between the two electron-phonon states due to the finite $\lambda$. At $\lambda = 0$, the tunneling of electrons do not change the phonon count inside the dot since $\gamma_{\text{eff}}$ vanishes for $q_1 \neq q_2$ and the dot retains thermal equilibrium with the bath. As a consequence, the dot-to-bath phonon current freezes and the setup closely resembles to a conventional two-terminal architecture, where current flows only due to DT. This picture becomes more intriguing at non-zero $\lambda$ when the contribution of PAT to the charge and heat flux become notable as compared to DT. Figures 5(a) and 5(b) map the color variation of $\gamma_{\text{eff}}$ between two Fock states as a function of $\lambda$ and $q_2$ taking $q_1$ constant, at 0 and 1, respectively. In both the cases, $\gamma_{\text{eff}}$ vanishes for $q_1 \neq q_2$ at $\lambda = 0$. As $\lambda$ increases, $\gamma_{\text{eff}}$ corresponding to the tunnelings for $q_1 \neq q_2$ rises steadily indicating a strong signature of PAT.

Next, we describe the relative contributions of DT and PAT in $J_{Q,\max}^{\lambda}$. Referring to Fig. 5(c), we note that as $\lambda$
increases from 0, the DT component falls drastically and PAT rises steadily, leading to a gradual fall of $J_{C_{max}}^Q$. With further increase of $\lambda$, PAT component reaches its maxima and starts rolling down thereafter. Meanwhile, the fall of DT component becomes sluggish and tends to zero for large values of $\lambda$. Therefore, at large $\lambda$, $J_{C_{max}}^Q$ is solely driven by PAT. These interesting signatures of PAT are evident from Figs. 5(a) and 5(b). As we freeze $\lambda$, Fig. 5(a) shows that for $q_1 = 0$, $\gamma_{q_2}$ decreases gradually. In contrast, Fig. 5(b) shows that for $q_1 = 1$, $\gamma_{q_2}$ fluctuates for fixed $\lambda$ and these fluctuations increase as $q_1$ increases. The cumulative effect of all $\gamma_{q_1 q_2}$, multiplied with the probability of the respective states $|n, q\rangle$, leads to the signatures of PAT obtained in Figs. 5(a-b).

We now shift our attention towards discussing the optimum operational regime of the refrigerator. For a system with sharp energy levels, operating points corresponding to $J_{C_{max}}^Q$ and $\eta_{max}$ happen to be far from each other. An attempt to maximize one happens only at a huge cost of the other. Therefore, in pursuit of operating the system at a reasonable cooling power and COP, we first plot their product (II) as a function of $V_{app}$ for different $\lambda$. The peak value of II ($\Pi_{max}$) appears somewhere in between the peaks of $J_{C_{max}}^Q$ and $\eta_{max}$. To put things simple, Fig. 6(b) outlines the 2-D variation of $J_{C_{max}}^Q$ and $\eta_{max}$ at fixed $\lambda$ ($\lambda = 1$) and selectively highlights (red bullets) the three relevant operating points discussed earlier. Results suggest that by operating the system at $\Pi_{max}$, one can extract considerable amount of cooling power and simultaneously achieve high COP and maintain an excellent trade-off between them.

From our discussion so far, one may apparently label $\lambda$ as a detrimental factor since it brings down $J_{C_{max}}^Q$ and shrinks the regime of refrigeration $[V_{OC}, V_{TR}]$. However, it must be noted that there is a clear improvement in terms of $J_{C_{max}}^Q - \eta_{max}$ trade-off as $\lambda$ increases. Turning back to Fig. 4, it is evident that the gap between the operating voltages corresponding to $\eta_{max}$ and $J_{C_{max}}^Q$ becomes narrower with $\lambda$ going up, signaling an improved trade-off between them. In the next subsection, we aim to elaborate this trade-off behavior with respect to different parameters.

B. Interaction and temperature regulated trade-off between CP and COP

We now elaborate on the impact of $\lambda$ in the relative trade-off between CP and COP. Referring to the preceding section (refer to Fig. 4), we note that in the absence of $\lambda$, COP maximizes at a voltage where CP is low. Likewise, CP reaches its peak when $\eta$ is minimal. Therefore, the optimization of thermoelectric refrigeration calls for...
the enhancement of two performance metrics, namely (i) the cooling power extracted at maximum COP denoted as $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and (ii) COP acquired at peak cooling power $(\eta_{C_{\text{max}}})$. Here, we test both the quantities by switching on a finite $\lambda$.

Earlier, we note from Fig. 4 that both $J_{C_{\text{max}}}$ and $\eta_{\text{max}}$ undergo monotonic decline as $\lambda$ increases. However, the $\lambda$ dependence of both $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ carry some interesting signatures. The double ordinate plot in Fig. 7(a) exhibits that primarily $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ increases with $\lambda$ as long as $\lambda$ is small or moderate. As $\lambda$ becomes large, $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ takes downturn and starts falling steadily. A similar trend is also obtained for $\eta_{C_{\text{max}}}$ as depicted in Fig. 7(b). This observation strongly indicates the significance of the electron-phonon coupling in improving the CP-COP trade-off. In the current existing technology, $\lambda$ can be experimentally tailored in the CNT-based quantum dots and hence, we believe that this study can lead to reality in terms of achieving excellent CP-COP trade-off.

So far, we have performed our simulations by keeping $\Delta T = T_H - T_C$ constant at 90 K. Now, we reexamine the CP-COP trade-off by varying $\Delta T$. Figures 8(a) and 8(b), respectively, note that $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ increase as $\Delta T$ rises. However, in both the cases we perceive that the maxima of $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ undergo a non-trivial shift towards the smaller value of $\lambda$ as $\Delta T$ increases. These results necessitate an in-depth analysis of the role of $\lambda$ and $\Delta T$ on the non-trivial characteristics of $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ which will be addressed now.

First, we inspect the contribution of $\Delta T$ in the CP-COP trade-off keeping $\lambda$ constant. Figures 9(a) and 9(b) plot the respective voltage dependence of $J_C^{\text{Q}}$ and $\eta$ for different values of $\Delta T$. Comparing Fig. 4(a-b) and Fig. 9(a-b), we note that both $\lambda$ and $\Delta T$ bring down $J_{C_{\text{max}}}$ and $\eta_{\text{max}}$ as they go up. However, the impact of $\lambda$ is stronger in reducing $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{\text{max}}$, while the effect of $\Delta T$ is relatively weak. In addition, there are some dissimilarities too. An increase in $\Delta T$ enhances $V_{OC}$, maintaining $V_{TR}$ fixed and drags the refrigeration regime $[V_{OC}, V_{TR}]$ towards the high input voltage. In contrast, $\lambda$ pulls the $[V_{OC}, V_{TR}]$ towards the low input voltage.

Finally, we are in a position to describe the non-trivial characteristics of $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ captured in Figs. 7 and 8. Until now, our simulations observe the following outcomes: (i) $J_C^{\text{Q}}$ maximizes at a voltage slightly greater than the $V_{mid} = [V_{OC} + V_{TR}] / 2$ (refer to Fig. 4 and 9), (ii) $\eta_{\text{max}}$ appears at a voltage marginally larger than $V_{OC}$ (refer to Fig. 4 and 9) and (iii) Both $J_{C_{\text{max}}}^{\text{Q}}$ and $\eta_{C_{\text{max}}}$ slump drastically with $\lambda$ and nominally with $\Delta T$. Now, we test the characteristics of the voltage $V_{C_{\text{max}}}^{\text{Q}}$ and $V_{\eta_{\text{max}}}$ at which $J_C^{\text{Q}}$ and $\eta$ maximize, respectively. Figures 9(c) and 9(d) depict that $V_{C_{\text{max}}}^{\text{Q}}$ moves closer to $V_{mid}$ and $V_{\eta_{\text{max}}}$ moves away from $V_{OC}$ as $\lambda$ and $\Delta T$ rises. From our earlier observation, we noted that close to $V_{OC}$, $J_C^{\text{Q}}$ increases and $\eta$ registers a monotonic fall around $V_{mid}$. Consequently, both $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ shoot up with $\lambda$ and $\Delta T$.

The discussion thus far elaborated on the uprise of $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ with $\lambda$ for low and medium values of $\lambda$. At large $\lambda$, we observe a fall in both quantities. This happens since both $J_C^{\text{Q}}$ and $\eta$ fall rapidly at larger $\lambda$. Simultaneously, $(J_C^{\text{Q}})_{\text{Q}_{\text{max}}}$ and $\eta_{C_{\text{max}}}$ undergo the respective falls. Next, to minimize the negative effects of $\lambda$, we focus on enhancing $J_{C_{\text{max}}}$ and $\eta_{\text{max}}$, incorporating different design parameters and many-particle interactions inherently present in the system.
C. Performance optimization

This section outlines the criteria for optimizing $J_{C_{\text{max}}}^Q$ and $\eta_{\text{max}}$ when Coulomb interaction ($U$) and other design parameters co-exist along with the electron-photon coupling. First, we discuss the effect of $U$, which being polaron shifted by the finite electron-photon interaction, regulates the variation of both CP and COP. We describe the effect of $U$ via Fig. 10.

Figure 10(a) shows that at $\lambda = 0$, $J_{C_{\text{max}}}^Q$ becomes maximum at $U = 0$. As $U$ increases, $J_{C_{\text{max}}}^Q$ starts falling and settle to a constant value for large $U$. Turning on a nonzero $\lambda$, we notice some interesting patterns. Primarily, $J_{C_{\text{max}}}^Q$ slumps as $\lambda$ rises. Keeping $\lambda$ fixed, $J_{C_{\text{max}}}^Q$ increases when $U$ is increased from zero, reaches maximum at a non-zero $U$, drops down as $U$ increases further and finally saturates for large value of $U$. From the discussion of the preceding section, we know two things: first, in the presence of finite $\lambda$, $U$ gets polaron shifted to $\tilde{U} = U - 2\lambda^2\hbar\omega$ and second, $U$ splits up the channel into the energy modes tuned at $\tilde{\epsilon} + n\hbar\omega$ and $\tilde{\epsilon} + \tilde{U} + n\hbar\omega$, respectively (where $n=0,1,2,\ldots$). At $U = 0$, the levels at $\tilde{\epsilon} + n\hbar\omega$ and $\tilde{\epsilon} + \tilde{U} + n\hbar\omega$ overlap and maximizes charge current. As an outcome, cooling power as well as $J_{C_{\text{max}}}^Q$ maximizes at $U = 0$. When $\lambda$ is non-zero, the whole curve is right shifted owing to the polaron transformation, and $\tilde{U}$ becomes zero at some finite value of $U$. If $U$ is lowered beyond that maxima point, $\tilde{U}$ becomes negative and the levels at $\tilde{\epsilon} + \tilde{U} + n\hbar\omega$ fall below the levels at $\tilde{\epsilon} + n\hbar\omega$, leading to the fall of charge current. As a result, cooling power and $J_{C_{\text{max}}}^Q$ decrease as shown in Fig. 10(a).

Now we turn our attention to Fig. 10(b), which plots the variation of $\eta_{\text{max}}$ as a function of $U$. Here also, we observe the similar trend except a minute difference. Unlike $J_{C_{\text{max}}}^Q$, $\eta_{\text{max}}$ at $\tilde{U} \to \infty$ asymptotically approach the same value of $\eta_{\text{max}}$ at $\tilde{U} \to 0$. Putting things together, Fig. 10 concludes that as we keep electron-phonon coupling finite, we have to have a finite $U$ to optimize $J_{C_{\text{max}}}^Q$ and $\eta_{\text{max}}$.

Next, we look into the effect of dot-to-bath coupling $\beta$ in manipulating the cooling power and COP. Figures 11(a) and 11(b) exhibit that both $J_{C_{\text{max}}}^Q$ and $\eta_{\text{max}}$ remain unaltered when $\lambda = 0$ as we vary $\beta$. From Fig. 10, we have seen that the heat balance equation holds $J_Q^Q = W = J_P^Q + J_H^Q$. Here, the rule of thumb is that at $\lambda = 0$, the dot phonons equilibrate via the thermal bath and the dot-to-bath phonon flow ceases. When $\lambda \neq 0$, the dot phonons go out of equilibrium and kick-start $J_P^Q$. Throughout our work, we maintain $T_P = T_C$, so that the phonons always leak through the bath, giving rise to a parasitic heat flow from the dot to the ambient, i.e $J_Q^Q > 0$. As $\beta$ gets stronger, the magnitude of $J_P^Q$ rises proportionally. However, any change in $\beta$ should not modulate $I$ or $W$ as reported in our previous work. Therefore, to validate the heat balance, $J_Q^Q$ must increase with $J_P^Q$. The color maps shown in Figs. 11(c) and 11(d) depict the rise of $J_Q^Q$ with $\beta$ and the invariance of $W$.

Figure 9. Impact of electronic thermal bias in refrigeration: Variation of (a) $J_{C_{\text{max}}}^Q$ and (b) $\eta$ as a function of $V_{\text{app}}$ for different values of $\Delta T$ at $\lambda = 1$ and $T_C = 300K$. As $\Delta T$ increases, both $J_{C_{\text{max}}}^Q$ and $\eta$ fall slowly and $V_{\text{OC}}$ shifts towards $V_{TRK}$. Plot of (c) $[V_{OC_{C_{max}} - V_{\text{mid}}}]$ and (d) $[V_{\text{max}} - V_{OC}]$ as a function of $\lambda$ for different values of $\Delta T$ at $T_C = 300K$. Results show that the rise of both of $\Delta T$ and $\lambda$, drags $V_{OC_{C_{max}}}$ closer to $V_{\text{mid}}$ and takes $V_{\text{max}}$ away from $V_{OC}$. These signatures directly impact the CP-COP trade-off as depicted in Fig. 8.

Figure 10. Role of Coulomb coupling: Variation of (a) $J_{C_{\text{max}}}^Q$ and (b) $\eta_{\text{max}}$ as a function of Coulomb coupling energy ($U$) for different values of $\lambda$. At $\lambda = 0$, both of them maximize at $U = 0$ and start to fall as $U$ goes up. As $\lambda$ rises, the peaks of $J_{C_{\text{max}}}^Q$ and $\eta_{\text{max}}$ shift towards higher value of $U$. This suggests that for optimized refrigeration $U$ should be moderately high for higher values of $\lambda$. 

[Image 55x483 to 169x597]

[Image 64x292]
for a given $\beta/\gamma$ which results in improved $\beta$ to flow. As is proportional to the conductance between the contact depth analysis. contrast between these two trends which needs an in-

Figure 11. Role of $\beta$ in thermoelectric refrigeration: Variation of (a) $J_{C_{\text{max}}}^Q$ and (b) $\eta_{\text{max}}$ plotted as a function of $\beta$ (normalized by $\gamma$) for different values of $\lambda$ in semi-log graphs. When $\lambda \neq 0$, the dot goes out of equilibrium and $J_{C_{\text{max}}}^Q$ starts to flow. As $\beta$ goes up, the rise of $J_{C_{\text{max}}}^Q$ is compensated by $J_{C}^Q$ which results in improved $J_{C_{\text{max}}}^Q$ and $\eta_{\text{max}}$ at large $\beta$. Color map of (c) $J_{C}^Q$ and (d) $W$ displayed as a function of $V_{\text{app}}$ and $\beta/\gamma$ for a given $\lambda$. $J_{C}^Q$ increases with $\beta$ but $W$ remains constant which signifies that $J_{C}^Q$ increases as a counter-balancing effect of rise in $J_{C_{\text{max}}}^Q$ aided by higher values of $\beta$.

with $\beta$, respectively. Therefore, the COP being the ratio of $J_{C_{\text{max}}}^Q$ and $W$, should shoot up for large $\beta$ as shown in Fig. 11(b). From this discussion, we infer that to improve the refrigeration performance in the three terminal setup, one should enhance the coupling strength between the dot and bath.

Finally, we study the effect of dot-to-contact couplings ($\gamma_{H(C)}$) in optimizing thermoelectric refrigeration. In due course, we introduce a multiplying factor $a$ to scale $\gamma_H$ to $\gamma_H/a$ and $\gamma_C$ to $a\gamma_C$ such that their product remains constant. From the system design outlook, an asymmetry between the dot-to-contact coupling is very common and hence it is imperative to examine the effect of it in the peak refrigeration performance. Figures 12(a) and 12(b), respectively, capture that both $J_{C_{\text{max}}}^Q$ and $\eta_{\text{max}}$ maximize around $a = 1$ and decline as $a$ is increased or decreased further. However, there is a clear contrast between these two trends which needs an in-depth analysis.

From elementary network theory, we know that $\gamma_{H(C)}$ is proportional to the conductance between the contact $H(C)$ and the channel. As these conductances add in parallel, the current flowing through the channel becomes proportional to an effective $\gamma$ which is even lesser than the weaker $\gamma$. Hence, the charge current, cooling power as well as $J_{C_{\text{max}}}^Q$ should maximize at $a = 1$ and fall down as $a$ is increased or decreased further. However, a close observation of Fig. 12(a) reveals that $J_{C_{\text{max}}}^Q$ is slightly asymmetric around its peak and a marginal improvement in cooling power is obtained when the dot is strongly coupled to the hot contact ($a < 1$). This effect arises due to the inherent Coulomb interaction present in the system. From our previous observation, it is evident that for an $n$-type system, refrigeration happens at $V_{\text{app}} > 0$. In this case, due to the finite Coulomb interaction, both $I$ and $J_{C_{\text{max}}}^Q$ become relatively higher for $a < 1$ as compared to the limit $a > 1$. This can be established by simple analytics described in standard quantum transport literature. However, since the margin of improvement in $J_{C_{\text{max}}}^Q$ is very tiny, the result shown in Fig. 12(a) does not hold much significance in the present context of the study.
This gives rise to two obvious questions: (i) Does the asymmetry in contact coupling make any notable difference?, (ii) If yes, how should one design the system to achieve better refrigeration? To answer these questions, we inspect the variation of $\eta_{\text{max}}$ with respect to $a$ for different values of $\lambda$ as depicted in Fig. 12(b). It is noted that $\eta_{\text{max}}$ is invariant for $\lambda = 0$, but exhibits a non-trivial trend for nonzero $\lambda$. Results show that the fall of $\eta_{\text{max}}$ around $a = 1$ is purely asymmetric in nature and is less affected when $a > 1$.

To justify this trend, we recall that $\eta \propto |J_H^0 + J_D^0|/W$, referring (12) and (13). At $\lambda = 0$, $J_D^0$ vanishes and the ratio $J_H^0/W$ remains invariant with respect to $a$ which results in a constant $\eta_{\text{max}}$ as shown in Fig. 12(b). However at nonzero $\lambda$, Figs. 12(c) and 12(d) collectively depict some interesting patterns. Figure 12(c) shows that at $\eta_{\text{max}}$, ratio $|J_H^0/W|$ is high at $a > 1$, moderate at $a = 1$ and low at $a < 1$. On the other hand, Fig. 12(d) registers an opposite trend of $|J_D^0/W|$ with $a$ at maximum COP. The net effect of both of them leads to the variation of $\eta_{\text{max}}$ shown in Fig. 12(b), which suggests that to achieve better COP, the dot should be strongly coupled with the colder contact. This study establishes that in the presence of on-site Coulomb interaction and inherent asymmetry of the dot-to-contact coupling in the system level, one achieves slightly higher cooling power for $\gamma_H > \gamma_C$ and better COP in the opposite limit.

IV. CONCLUSION

This paper presented a three terminal nanoscale refrigeration concept based on a vibron coupled quantum dot hybrid system. In setting up the simulation framework, we ensured the device to be singly driven by electronic bias and the transport physics was elucidated in the sequential tunneling limit. Our key results evidenced that the electron-phonon coupling, although being apparently detrimental from a general refrigeration perspective, can be engineered to favorably improve the trade-off between the cooling power and the COP under practical operating conditions. Furthermore, it was manifested that an additional improvement in the trade-off could be facilitated by the electronic thermal bias along with the electron-phonon coupling. Next, we explored a number of viable design strategies such as tuning the on-site Coulomb repulsion and optimizing the coupling strength with the reservoirs to overcome the challenges posed by the electron-phonon interaction. Specifically, it was shown that an enhanced phonon coupling between the dot and thermal bath and a strong electronic coupling between the dot and cold contact could boost up the cooling efficiency significantly. To put things together, our work specified the regime of optimizing thermoelectric refrigeration and proposed key design guidelines for a possible experimental realization of molecular and quantum dot thermoelectric refrigeration. We believe that some of the key aspects developed in this work might merit a separate study of thermoelectric refrigeration with double-driving.

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