Monte Carlo (DQMC) methods [1–4], can determine correlations and using quantum Monte Carlo (QMC) techniques to study the physics of interacting electrons. Auxiliary field methods formulated in real space, like determinant quantum Monte Carlo (DQMC), can be severely limited by the sign problem [5,6], unless additional constraints are imposed [7]. The dynamic cluster approximation [8] and cluster dynamical mean-field theory [11–16] to finer momentum grids and generally have a more benign sign problem than DQMC, allowing them to access lower temperatures and/or more complex (e.g., multiband) models. Diagrammatic QMC is another relatively new technology which is currently being developed [17,18]. Despite the numerical challenges, QMC applied to models with electron-electron interactions, like the Hubbard model, has resulted in considerable qualitative insight into phenomena such as the Mott transition, magnetic order, and, to a somewhat lesser extent, exotic superconductivity (SC) [19], which arise from electron-electron interactions in real materials [20].

Analogous strong correlation effects can arise in solids due to electron-phonon coupling, including SC and charge density wave (CDW) formation; this is the type of interaction we examine in this paper. A simple model where such effects can be studied is the Holstein Hamiltonian [21]. Early QMC work in two dimensions near half-filling [22–27] examined CDW formation and its competition with SC. A second generation of simulations has considerably improved the quantitative accuracy of results, looking at both finite-temperature [28–30] and quantum-critical-point [31,32] physics in two spatial dimensions on square and honeycomb lattices. Much of this progress has been possible thanks to newer QMC methods, such as continuous-time [28] and self-learning Monte Carlo [29,33]. However, despite these improvements in effective update schemes, the cubic scaling with lattice size N of real-space QMC methods employed in existing work has precluded similar studies in three dimensions.

We report here QMC simulations of the half-filled Holstein model on cubic lattices as large as N = 143 sites. These studies are made possible by employing a linear-scaling QMC method based on a Langevin evolution of the phonon degrees of freedom [34–37]. The large linear sizes that are accessible allow us to perform the finite-size scaling needed to extract the CDW transition temperature TCdw from the scaling of the charge correlations, and also obtain the momentum dependence of the charge structure factor S(k) to reasonable resolution. We supplement the extraction of TCdw from Scdw ≡ S(π, π, π) with calculation of the specific heat and spectral function and show that while they provide a less precise determination of TCdw, their features are consistent with those obtained from Scdw.

Model and methods. The Holstein Hamiltonian,

\[ \hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma} + \text{H.c.}) - \mu \sum_{i, \sigma} \hat{n}_{i, \sigma} + \frac{X^2}{2} + \lambda \sum_{i, \sigma} \hat{n}_{i, \sigma} \hat{X}_i, \]
describes the coupling of electrons, with creation and destruction operators \( \hat{c}_{i\uparrow}, \hat{c}_{i\downarrow} \), to dispersionless phonon degrees of freedom \( \hat{\mu}, \hat{X}_i \), with the phonon mass normalized to \( M = 1 \). The parameter \( t \) multiplies a near-neighbor hopping (kinetic energy) term. We set \( t = 1 \) as our unit of energy, resulting in an electronic bandwidth for the cubic lattice equal to \( W = 12 \). The coupling between the phonon displacement and electron density on site \( i \) is controlled by \( \lambda \), while the chemical potential, \( \mu \), tunes the filling. In this study we focus on half-filling, obtained by setting \( \mu = -\lambda^2/\omega_0^2 \), and report results in terms of a dimensionless electron-phonon coupling constant \( \lambda_D = \lambda^2/\omega_0^2 W \). Despite its simplifications, the Holstein model captures many qualitative features of electron-phonon physics, including polaronic effects in the dilute limit \([38–40]\), SC and CDW formation, and their competition \([22,28,31,32,41–44]\).

The fermionic degrees of freedom appear only quadratically in the Holstein model, Eq. (1). Consequently, the fermions can be “integrated out,” resulting in the product of two identical matrix determinants which are nontrivial functions of the space and imaginary time dependent phonon field. The product of the two identical determinants is positive; thus there is no sign problem. Most prior numerical studies of the Holstein model employed DQMC, which explicitly calculates changes in the determinant as the phonon field is updated. At fixed temperature, DQMC scales cubically in the number of sites \( N \), and hence as \( L^3 \), where \( L \) is the linear system size in three dimensions. This limits DQMC simulations in three dimensions to relatively small \( L \).

Instead, we use a method based on Langevin updates which exhibits nearly linear scaling in \( N \). Such methods were first formulated for lattice gauge theories \([45–47]\). Attempts to simulate the Hubbard Hamiltonian with Langevin updates were limited to relatively weak coupling and high temperature by the ill-conditioned nature of the matrices due to rapid fluctuations of the sampled Hubbard-Stratonovich fields in the imaginary time direction \([48]\). However, in the Holstein model the sampled phonon fields have an associated kinetic energy cost that moderates these fluctuations, giving rise to better conditioned matrices.

Here we briefly discuss the key steps in the algorithm and leave the details to Refs. \([34,35]\). The partition function for the Holstein model is first expressed as a path integral in momentum space, \( \int dx \exp \left( -\frac{1}{\beta} S(\hat{\mu}, \hat{X}_i, \hat{\sigma}, \hat{\tau}) \right) \), where \( S \) is the action. It is necessary to compute \( M^{-1} \) acting on vectors of length \( NL \), which is done using the conjugate gradient \( \text{CG} \) method. An essential refinement of the algorithm is the application of Fourier acceleration \([45–47]\) to reduce critical slowing down resulting from the slow phonon dynamics in imaginary time. See the Supplemental Material for more information on the simulations \([49]\).

Elements of the fermionic Green function are also obtained with a stochastic estimator. Once evaluated, one can measure all physical observables. We focus here on the charge structure factor,

\[
S(\mathbf{k}) = \sum_{\mathbf{r}} c(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}},
\]

where \( c(\mathbf{r}) = (\eta_{\mathbf{r}+\mathbf{k}} - \eta_{\mathbf{r}}) \), and the specific heat \( C = d\langle E \rangle/dT \). We also obtain the momentum integrated spectral function \( A(\omega) \), the analog of the density of states in the presence of interactions, by analytic continuation of the Green function via the classic maximum entropy method \([50,51]\). We use a flat default model, and, for simplicity, we employ only the “diagonal” statistical errors in \( G(\tau) \) rather than the full covariance matrix.

**Correlation length and charge structure factor.** At half-filling on a bipartite lattice the formation of a CDW phase is the fundamental ordering tendency of the Holstein model. At intermediate temperatures we observe the formation of local pairs due to the effective onsite attraction \( U_{\text{eff}} = -\lambda^2/\omega_0^2 \), between up and down electrons. At lower \( T \), the positions of the pairs become correlated, since the lowering of energy by virtual hopping is maximized by \(-4r^2/U_{\text{eff}} \) if each pair is surrounded by empty sites. A clear signature of this low-temperature physics is seen in the heat capacity \( C(T) \) as the temperature is lowered, which has a sharp peak at \( T \sim 0.28 \) corresponding to the CDW phase transition, as shown in Fig. 1.

It is also possible to detect the formation of this low-temperature CDW phase by studying the density-density correlation function and its Fourier transform, the charge structure factor, \( S(\mathbf{k}) \). In Fig. 2 we show \( S(\mathbf{k}) \), Eq. (2), versus \( \mathbf{k} \) for different \( T = \beta^{-1} \) and \( \lambda_D = 0.33 \) \( (\omega_0 = 0.5, \lambda = 1.0) \). We see that as \( T \) is lowered, the peak height at \( k = (\pi, \pi, \pi) \) increases by two orders of magnitude. The value of \( \beta \) for which the height increases most rapidly provides a rough value for the transition temperature, which can be more precisely determined via finite-size scaling (Fig. 4).

In real space, the density-density correlation function exhibits a pattern which oscillates in sign on the two sublattices, consistent with dominant ordering at \( k = (\pi, \pi, \pi) \) seen in Fig. 2. Above \( T_T \), the correlations die off exponentially, with a
Fig. 3. Correlation length obtained from Eq. (3) with $\omega_0 = 0.60$, $\lambda = 1.00$, $\lambda_D = 0.23$. Shaded gray bar shows the value of $T_c$ obtained from a finite-size scaling analysis of the CDW structure factor (Fig. 4).

Fig. 2. Charge structure factor as a function of momentum for different inverse temperature $\beta$ at fixed $\lambda_D = 0.33$ and $\omega_0 = 0.5$. As $T$ decreases, a peak develops at $\mathbf{k} = (\pi, \pi, \pi)$. The most rapid growth is for $T \sim 0.37 - 0.40$. Finite-size scaling analysis of the crossings of $S_{\text{cdw}}$ in Fig. 4 precisely identifies $T_c \sim 0.392 \pm 0.008$.

$\xi = \frac{L}{2\pi} \sqrt{\frac{S(q_1)/S(q_2) - 1}{4 - S(q_1)/S(q_2)}}$, \hspace{1cm} (3)

where $q_1 = (\pi, \pi, \pi - \frac{\pi}{L})$ and $q_2 = (\pi, \pi, \pi - \frac{2\pi}{L})$ are the two closest wave vectors to the ordering vector $\mathbf{k} = (\pi, \pi, \pi)$.

Figure 3 shows the ratio $\xi/L$ as a function of temperature for three lattice sizes $L = 8, 10, 12$. $\xi/L$ exhibits a characteristic peak which sharpens with increasing lattice size. In the following section we will present data indicating $T_{\text{cdw}} \sim 0.31$, which is consistent with the peak in finite lattice sizes approaching $T_c$ from above in our data as well.

$T_{\text{cdw}} \sim 0.315 \pm 0.005$

$\omega_0 = 0.60$, $\lambda = 1.00$

$\lambda_D = 0.23$

CDW transition. Having seen the essential qualitative effects of the electron-phonon coupling, we now perform finite-size scaling to locate the transition precisely. The three panels of Fig. 4 exhibit the steps in this process. The upper-left panel (a) exhibits raw data for $S_{\text{cdw}}$ versus inverse temperature $\beta$. At high $T$ (small $\beta$) the values of $S_{\text{cdw}}$ for different system sizes coincide with each other, because the charge correlations are short ranged and the additional large distance values in the sum over $r$ in Eq. (2), present as $L$ increases, make no contribution. However, as $T$ decreases ($\beta$ increases) the correlation length reaches the lattice size, and values of $S_{\text{cdw}}$ now become sensitive to the cutoff $L$. As a consequence, a crude estimate of $T_{\text{cdw}}$ can already be made as the temperature at which the curves begin to separate, i.e., $T_{\text{cdw}} \sim 0.31$ ($\beta_c \sim 3.2$). A much more accurate determination of $T_{\text{cdw}}$ is provided by making a crossing plot [Fig. 4(c)] of $L^{\beta/\nu - D}$ versus $\beta$. Curves for different lattice sizes $L$ should cross at $\beta_c = 1/T_{\text{cdw}}$. In this analysis we make use of the expected universality class of the transition, the three-dimensional (3D) Ising model, to provide values for the exponents $\beta = 0.326$ and $\nu = 0.63$. We conclude $T_{\text{cdw}} = 0.315 \pm 0.005$. Finally, Fig. 4(c) gives the full scaling collapse, using $T_{\text{cdw}}$ from panel (b) and again employing 3D Ising exponents.

Combining plots like those of Fig. 4 for different values of $\lambda$ and $\omega_0$ allows us to obtain the finite-temperature phase diagram of the 3D Holstein model, Fig. 5, which is the central result of this paper. We see that $T_c$ is increased by roughly a factor of 2 in going from various two-dimensional (2D) geometries (square [28], Lieb [53], and honeycomb [31,32])
temperatures at fixed $\omega_d$ dynamical behavior. Figure 6 shows on a cubic lattice.

A suppression of $A(\omega) = 0$ develops a pronounced dip. This suppression continues to increase until, at $\beta = 8$, $A(\omega = 0)$ vanishes. This sequence, in which a dip first signals entry into the CDW phase, is consistent with the trends reported in [30].

Conclusions. We have used a Langevin QMC method to study the Holstein Hamiltonian on a three-dimensional cubic lattice. This approach allows us to access much larger lattice sizes, enabling us to perform a reliable finite-size scaling analysis to determine the CDW transition temperature. Using this method we obtained results that, in momentum space, were sufficient to resolve the width of the charge structure factor peak and the smearing of the Fermi surface by electron-phonon interactions. The specific heat and spectral function provide useful alternate means to examine the low-temperature properties. Their behavior is consistent with that seen by direct observation of charge correlations.

While a single band model of interacting electrons does seem to provide a reasonably accurate representation of cuprate physics [19] (although not that of the iron pnictides), realistic CDW materials generally have much richer band structures. Since, at a formal level, additional sites and additional orbitals are equivalent in real-space QMC simulations, an ability to simulate larger spatial lattices also opens the door to the study of more complex CDW systems. Of course, the accurate description of these materials requires not only several electronic bands but also a refinement of the description of the phonons and electron-phonon coupling, which are also treated at a very simple level in the Holstein Hamiltonian. Initial steps to include phonon dispersion have recently been made [55]. However, refinements to the electron-phonon coupling such as a momentum-dependent $\lambda(q)$ remain a challenge to simulations because of the phase separation that results in the absence of electron-electron repulsion [56].

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[49] See Supplemental Material at http://link.aps.org supplemental/10.1103/PhysRevB.102.161108 for additional information about (i) the energy components, (ii) real-space density correlation, (iii) the mean-field theory, and (iv) the parameters used in the Langevin simulations.